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Title/Desc:

TANK 241C105 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
2/1994

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 21. ECN 626279Proj.
ECN

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13a. Justification (mark one) Criteria Change ☒ Design Improvement ☐ Environmental ☐ Facility Deactivation ☐ As-Found ☐ Facilitate Const ☐ Const. Error/Omission ☐ Design Error/Omission ☐			
13b. Justification Details Complete rewrite which includes all vapor sampling events to date and data qualification.			
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ENGINEERING CHANGE NOTICE				Page 2 of 2	1. ECN (use no. from pg. 1) 626279
15. Design Verification Required	16. Cost Impact			17. Schedule Impact (days)	
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☐ Yes ☒ No	Additional	☐ \$	Additional	☐ \$	Improvement ☐
	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	☐
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Vendor Information	☐	Operating Procedure	☐	Electric Circuit Schedule	☐
OM Manual	☐	Operational Safety Requirement	☐	ICRS Procedure	☐
FSAR/SAR	☐	IEFD Drawing	☐	Process Control Manual/Plan	☐
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Environmental Impact Statement	☐	Fac. Proc. Samp. Schedule	☐	Tickler File	☐
Environmental Report	☐	Inspection Plan	☐		☐
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20. Approvals																																																																				
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**This document was reviewed following the
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APPROVED FOR PUBLIC RELEASE

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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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Tank 241-C-105 Headspace Gas and Vapor Characterization Results for Samples Collected in February 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 Monoxide	5
3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium	5
3.4 Discussion of Inorganic Gases and Vapors	6
4.0 ORGANIC VAPORS	7
4.1 Positively Identified Organic Analytes	7
4.2 Tentatively Identified Organic Analytes	9
4.3 Total Nonmethane Organic Carbon	10
4.4 Discussion of Organic Analytes	10
5.0 SUMMARY	13
6.0 REFERENCES	14

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
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
TST	triple sorbent trap
vol%	percent by volume, 1 vol% = 10,000 ppmv
VSS	vapor sampling system
WHC	Westinghouse Hanford Company

Acknowledgements

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**Tank 241-C-105 Headspace Gas and Vapor Characterization Results
for Samples Collected in February 1994**

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank C-105 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). Tank C-105 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994). Results presented here represent the best available data on the headspace constituents of tank C-105.

1.2 Characterization Data Criteria

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

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). However, current governing operating specifications for single shell waste tanks, such as tank C-105, specify that combustible constituents be maintained at or below 20 % of the LFL (Boyles 1994).

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 C-105 headspace characterization data presented here are from a single sampling event. Samples were collected from the exhaust piping of tank C-105, and are thought to have been representative of the tank headspace exhaust when the tank was sampled. 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 C-105 headspace composition changes with time.

1.4 Tank Headspace Dynamics

Gas and vapor concentrations in tank C-105 are very strongly affected by the active ventilation of the headspace. Unlike the passively ventilated waste tanks, it can not be assumed that the headspace is well-mixed by thermally-induced convection and diffusion. Though mixing is generally more vigorous in an actively ventilated tank headspace (other factors being equal), discrete sources of fresh air and the single outlet would result in concentration gradients within the headspace. Therefore, while a strong argument can be made that samples collected from any central region of a passively ventilated headspace are representative of nearly the entire headspace, sample collection in tank C-105 is probably location-dependent.

Consequently, samples from tank C-105 were collected from a port on the exhaust header, and while the exhauster was operating. Though concentrations in the headspace are higher in some places (and lower in others), the exhaust header was deemed the best place to sample to address the exposure risks to tank farm workers.

The active ventilation of tank C-105 affects its headspace gas and vapor concentrations in yet another way. Because tank C-105 is connected via a cascade line to tank C-104, gases and vapors from waste stored in tank C-104 are thought to be drawn into the tank C-105 headspace. Thus, when considering the relationship between the waste in tank C-105 and the gases and vapors in the exhaust from that tank, it should be kept in mind that some, if not most, may actually be coming from tank C-104. Results of gas and vapor samples from tank C-104 provide evidence that tank C-104 is venting through its cascade line to tank C-105 (Huckaby and Bratzel 1995a).

Tank C-105 is also connected via a similar cascade line to tank C-106, however, the effect of this on the tank C-105 headspace constituents is probably negligible. This appraisal stems from the fact that tank C-106 is itself actively ventilated (indeed, typically at higher flowrates than tank C-105), and samples from the exhaust of tank C-106 have very low concentrations of compounds of interest (Huckaby and Bratzel 1995b). Thus, assuming no extraordinary conditions exist and that the headspace of tank C-106 is similar to its exhaust, the introduction of air from tank C-106 is comparable to the introduction of ambient air.

2.0 SAMPLING EVENT

Gas and vapor samples were collected from tank C-105 using the vapor sampling system (VSS) on February 16, 1994 by WHC Sampling & Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by the sample and analysis plan¹ (WHC 1995, Appendix A). Air from the tank C-105 headspace was withdrawn from a port on the exhaust header on riser 11, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C.

Tank C-105 was the third tank to be sampled using the VSS, and was sampled only about 3 weeks after the first use of the VSS on a tank. Because the methods and equipment were relatively new, problems with sample handling (e.g., chain-of-custody and shipping) were encountered (WHC 1995, Clauss et al. 1995). The precision of the sampling results, however, is generally good. Sorbent trap collection problems noted in a subsequent sampling event² do not appear to have occurred when tank C-105 was sampled.

Flowrate and temperature measurements of the tank C-105 exhaust were made on February 4 and March 2, 1994 (Minter 1995). On those dates, the flowrate and temperature of the exhaust was determined to be 37.7 m³/min (1,330 ft³/min), 15.5 °C, and 39.1 m³/min (1,380 ft³/min), 16.1 °C, respectively. Given a calculated headspace volume of 2,470 m³ (87,000 ft³) these flowrates correspond to 1 turn-over of the headspace every 63 to 66 min. By contrast, the average exchange of air between a passively ventilated waste tank and the atmosphere due to barometric pressure fluctuations is less than 0.5 % of the headspace volume per day, which corresponds to 1 turn-over of the headspace every 200 days.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), Pacific Northwest Laboratories (PNL), and Oregon Graduate Institute of Science and Technology (OGIST) through a contract with Sandia National Laboratories. The 40 tank air samples and 6 ambient air control samples collected are listed in Table 2-1 by analytical laboratory. Table 2-1 also lists the 5 trip blanks provided by the laboratories.

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

¹ The current requirement that sampling and analysis parameters be specified by a tank characterization plan was not in effect for gas and vapor sampling until October 1, 1994.

² Because of a valve-sequencing error, sample air volumes through specific sampling ports were not properly measured during sample job 7A of tank C-103. The error resulted in obvious and significant differences in sorbent trap results, but had no effect on SUMMATM samples.

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,3} 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 were prepared and analyzed by PNL. SUMMATM canisters were analyzed for inorganic analytes by OGIST. Reports by PNL (Clauss et al. 1995) and OGIST (Rasmussen 1994) describe sample preparation and analyses.

PNL analyses of sorbent traps for inorganic compounds were performed 39 days after sample collection (Ligothke 1995). Analysis of SUMMATM canisters by OGIST were begun 7 days after the sample collection. It should be noted that the inorganic compounds from SUMMATM canister analyses (i.e., the permanent gases) would be expected to be very stable in the SUMMATM canisters, and the results would not have been affected even if the 60-day holding time requirement (Keller 1994) had been exceeded. The 60-day holding time was administratively chosen, and no holding time study has been performed to address the stability of inorganic compounds in SUMMATM canisters in the chemical matrix of the waste tank samples.

PNL results were produced at PNL quality assurance impact level 3. OGIST did not have a WHC-approved quality assurance project plan in place when performing analyses, so OGIST data have been placed in square brackets both in Table 3-1 and elsewhere in the text of this report to indicate that they represent secondary results.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The ammonia concentration in headspace of tank C-105 was reported to be 2.4 ppmv. Ammonia has been observed in virtually all of the passively ventilated waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), to 1040 ppmv in tank BY-108 (McVeety et al. 1995). Active ventilation of the tank C-105 headspace accounts for the relatively low ammonia concentration in the tank C-105 exhaust. Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 2.4 ppmv corresponds to about 0.002 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in the exhaust from tank C-105 was determined to be [22 ppmv]. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, the measured 22 ppmv of hydrogen corresponds to about 0.05 % of its LFL, and indicates hydrogen is not a flammability concern.

The nitrous oxide concentration in the tank C-105 exhaust was [5.3 ppmv]. Nitrous oxide has been detected in the passively ventilated waste tanks at concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as about 868 ppmv in tank U-103 (Ligothke et al. 1995). Under the proper conditions, nitrous oxide can serve as an oxidizer to support combustion. However, Cashdollar et al. (1992) found that nitrous oxide had no significant effect on the flammability of hydrogen and air mixtures for hydrogen concentrations less than 20 vol%, and that "small amounts of nitrous oxide (relative to air) do not appear to have much effect on the flammability". Their results suggest the measured nitrous oxide concentration is much too low to have a significant effect on the flammability of the tank C-105 headspace.

³ SUMMA is a trademark of Molectrics, Inc., Cleveland, Ohio.

Neither hydrogen nor nitrous oxide is highly soluble in the aqueous wastes of the tanks, so except for situations where bubbles are trapped within the waste and released episodically, the gases are released as they are generated. The concentration of these gases in the tank headspaces is consequently determined by a simple balance between their overall generation rate and the rate at which they are vented to the atmosphere. If the ventilation rate of tank C-105 when samples were collected (February 16, 1994) is estimated to be the average of its measured rates on February 4 and March 2, 1994 (i.e., 38.4 m³/min), then the 22 ppmv of hydrogen and 5.3 ppmv of nitrous oxide equates to about 100 g of hydrogen and 540 g of nitrous oxide being exhausted each day. Given the configuration of tank C-105, this should probably be considered the combined generation rates of tanks C-104 and C-105.

3.2 Carbon Monoxide

Carbon monoxide in the exhaust of tank C-105 headspace, measured to be [0.29 ppmv] in SUMMA™ samples, is above its concentration in ambient air, where it typically ranges from 0.05 to 0.15 ppmv. Ambient air samples collected at the beginning of the tank C-105 vapor sampling event were measured to have < 0.1 ppmv. Elevated waste tank headspace carbon monoxide concentrations are common (e.g., carbon monoxide concentration in tank C-103 was [26.7 ppmv], Huckaby and Story 1994), and are thought to be due to the decomposition of organic waste in the tanks. The elevated carbon monoxide in the exhaust of tank C-105 may be due to in-leakage from tank C-104, which is thought to have residual amounts of organic solvent wastes, and which was determined to have about [2 ppmv] of carbon monoxide in its headspace (Huckaby and Bratzel 1995a).

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank C-105 exhaust were both determined to be ≤ 0.1 ppmv. These are acid gases that would have very low equilibrium concentrations above the high pH supernatant liquid in tank C-105. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. These constituents could potentially serve as oxidizers to support combustion, but at the measured concentrations would have a negligible effect on the flammability of the tank C-105 headspace.

The water vapor concentration of tank C-105 exhaust was determined to be about 6.8 mg/L, using a tank headspace temperature of 17 °C and the ambient pressure of 980 mbar (735 torr). This corresponds to a water vapor partial pressure of 9.1 mbar (6.8 torr), to a dew point of 5.5 °C, and to a relative humidity of 47 %. Psychrometric measurements of the exhaust from tank C-105 were made on February 4 and March 2, 1994 (when flowrates were measured), that indicated the relative humidity of the exhaust on those dates to be about 44 % and 85 %, respectively (Minter 1995).

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. Analysis of the silica gel, which would have trapped approximately 22 mg of water vapor⁴, indicated the total activity of the sample to be below the method detection limit of 50 pCi (WHC 1995).

⁴ The water vapor trapped by tritium traps was not directly measured.

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor, the most abundant waste constituents in the tank C-105 headspace are ammonia, nitrous oxide, and hydrogen. These have been detected in most tank headspaces sampled to date, and are usually the dominate waste species. Because tank C-105 is actively ventilated, these constituents are lower in tank C-105 than in most passively ventilated tanks.

The relative standard deviations of the inorganic gas and vapor results are given in the last column in Table 3-1. The precision of reported results is generally good for the methods used. Relative standard deviations range from about 4 % for carbon monoxide results to 13 % 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 small relative standard deviations suggest adequate controls were maintained both in the field and in the laboratories.

Table 3-2 lists selected average gas and vapor concentrations for tanks C-104, C-105, and C-106. Tank C-104 is believed to be ventilated via its cascade line to tank C-105, and virtually all constituents in the tank C-104 headspace would be introduced to tank C-105 by this process. Make-up air for the ventilation of tank C-105 comes primarily from a filtered air inlet riser on the tank, to a lesser extent from tank C-104, and possibly to a small extent from tank C-106. The air, gases, and vapors drawn in from tank C-104 are consequently diluted by ambient air, as indicated in Table 3-2.

4.0 ORGANIC VAPORS

Organic vapors in the tank C-105 exhaust were sampled using SUMMA™ canisters, which were analyzed by PNL and OGIST, and triple sorbent traps (TSTs), which were analyzed by ORNL. PNL, OGIST, and ORNL each used gas chromatographs (GCs) equipped with mass spectrometer (MS) detectors to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Clauss et al. (1995), Rasmussen (1994), and Jenkins et al. (1994). A quantitative measurement of the total nonmethane organic carbon (TNMOC) by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method was also performed by OGIST (EPA 1988, Rasmussen 1994).

PNL SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-105. PNL results were produced at PNL quality assurance impact level 3. However, because of laboratory instrumentation problems and a low WHC priority assignment, PNL SUMMA™ canister analyses were not completed until 296 days after sample collection. This greatly exceeded the administratively chosen 60-day holding time of the WHC quality assurance project plan (Keller 1994). Though many of the organic analytes would be expected to be very stable, no holding time study has been performed to address organic compound stability in SUMMA™ canisters in the typical chemical matrix of the tank headspace samples.

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

ORNL 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. In an attempt to provide ORNL with additional samples for scoping purposes, 7 of the TSTs were collected simultaneously, in parallel, with a single flow controller. Because flow through these 7 TSTs was very non-uniform, analytical results from these samples are not discussed here.

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. 1994). 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 from the analysis of standards. The concentration of an analyte in the sample is said to be quantitatively measured if the response of the GC/MS has been established at several known concentrations of that analyte (i.e., the GC/MS has been calibrated for that analyte), and the MS response to the analyte in the sample is

between the lowest and highest responses to the known concentrations (i.e., the analyte is within the calibration range).

ORNL and PNL were assigned different lists of organic compounds, or target analytes, to positively identify and measure quantitatively. The ORNL target analyte list was based on advice from a panel of toxicology experts (Goheen 1994). The PNL target analyte list included 40 compounds of the EPA task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988).

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ samples by OGIST. Because OGIST did not have a WHC-approved quality assurance project plan in place, these results should be considered secondary (Burnum 1995). SUMMA™ analyses were performed according to the EPA TO-14 methodology (EPA 1988, Rasmussen 1994), and all are considered quantitative. Averages reported are from analyses of 3 SUMMA™ samples. Three of the compounds listed, 1,1,2-trichloro-1,2,2-trifluoroethane, 1,1,1-trichloroethane, and tetrachloromethane, were detected in ambient air samples at virtually the same levels as in the tank C-105 exhaust samples. This probably indicates that either the compounds were not associated with the waste, or they were contaminants introduced during sample preparation, collection, or analysis. Trace quantities of several other analytes listed in Table 4-1 were also detected in the ambient air samples, complete analytical results are given by Rasmussen (1994).

Analysis of SUMMA™ samples by PNL according the same EPA TO-14 method indicated none of the 40 TO-14 analytes to be above the 0.002 ppmv quantitation limit. Data in Table 4-1, which are strictly from OGIST, agree with the PNL analyses except for 1,3-butadiene, which is not an EPA TO-14 analyte and consequently was not on the PNL target analyte list, and trichlorofluoromethane, which OGIST measured to be slightly above the PNL detection limit.

Jenkins et al. (1994) report the positive identification of 25 of 26 target analytes in TST samples. The only target analyte not detected in the tank C-105 samples was trans-1,2-dichloroethene. Despite calibration of the instrument over about a 20-fold concentration range, only 9 of the positively identified compounds were measured to be within the calibration range in all 3 TST samples. The average concentrations of 23 positively identified compounds are given in Tables 4-3 and 4-4. The 3 compounds in Table 4-4 are segregated because the ORNL practical holding time for these had been exceeded. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so no compounds appears in more than 1 table. Results in Tables 4-3 and 4-4 may not be accurate to within the $\pm 30\%$ specified by Burnum.

Two other target analytes, dibutyl butylphosphonate and tributyl phosphate, were positively identified but not quantitatively measured. Tributyl phosphate was estimated to be present at 0.02 ppmv (0.2 mg/m³) and dibutyl butylphosphonate was estimated to be present at 0.004 ppmv (0.05 mg/m³). These 2 compounds were found at very similar levels in tank C-104.

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, propanone, 1-butanol, and 2-pentanone, exceeded their practical holding times, and may have been affected by the 19 day period between sample collection and analysis (Jenkins 1995b). Jenkins et al. (1995) describe the ORNL practical holding time study, and report the practical holding times of these compounds. It should be noted that the contractual holding time for the TST samples was 60 days.

Dichloromethane, benzene, and toluene were common to both the TST and SUMMA™ analyses. The OGIST SUMMA™ sample and ORNL TST sample results for benzene and toluene were very similar. Benzene and toluene were measured to be 0.0005 ppmv and 0.0004 ppmv, respectively, in SUMMA™

samples by OGIST, and 0.00059 ppmv and 0.00052 ppmv, respectively, in TST samples by ORNL. This agreement is important because of concerns about the TST sample volume measurements made with the VSS (see Section 2.0); unlike the TST samples, SUMMA™ samples would not be affected by sample volume errors.

Analyses of TSTs for dichloromethane have a high relative standard deviation, and do not agree with analyses of SUMMA™ samples by either OGIST or PNL. It was noted that dichloromethane had been used to clean sections of the VSS transport tubing and valves, and it is likely that its appearance in the TST samples was the result of residual contamination of valves in the sorbent trap sampling station of the VSS. TST trip blanks were analyzed and not found to contain detectable levels of dichloromethane.

The most abundant positively identified organic analyte in the tank C-105 exhaust was 1-butanol, measured to be present at about 0.17 ppmv from TST samples. Excluding the questionable dichloromethane result, the next most abundant were ethanenitrile (acetonitrile), n-tridecane, n-dodecane, propanone (acetone), and n-butanenitrile. None of these are at or above their industrial hygiene action levels, nor do they individually or cumulatively represent a flammability hazard.

4.2 Tentatively Identified Organic Analytes

In addition to the target analytes, the ORNL, OGIST, and PNL analytical procedures allow the tentative identification of other organic compounds. Tentative identification of analytes was performed by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and may also determine its molecular weight. The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Using this method, many analytes can be tentatively identified with reasonable confidence without having to inject standards of each into the GC/MS to determine their GC retention times or specific MS patterns.

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and 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 tentatively identified compounds recovered from PNL SUMMA™ samples, in the order by which the eluted chromatographically, are given in Table 4-5 with estimated concentrations. 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 4-6. Compounds are listed in Table 4-6 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-6 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. 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 4-7. Table 4-7 gives the same list, sorted in order of decreasing estimated concentration. Numbers in the first columns of Tables 4-7 and 4-8 (Cmpd #) identify the location of the compound in Table 4-6. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

OGIST provided total-ion chromatograms for each of the tank C-105 SUMMA™ samples and assigned tentative identities to the significant peaks, but did not estimate their concentrations. Table 4-9 lists the analytes tentatively identified by OGIST, and designates which analytes were detected in each of the 3 SUMMA™ samples. As a rough guide, the analytes listed in Table 4-9 were probably detected at greater than 0.001 ppmv. It should also be noted that some peaks in the total-ion chromatograms were not labeled, despite being relatively high, because confidence in assigning a chemical identity was very low.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Clauss et al. (1995), respectively, and should be reviewed before this data are used for decision making. Results in Tables 4-6 through 4-8 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 1, 2, and 3 in Table 4-6) or the assignment of the same identity to different peaks (e.g., Cmpd # 69 and 83 in Table 4-6). 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 4-5 through 4-8 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.

4.3 Total Nonmethane Organic Carbon

OGIST measured the TNMOC concentration in 3 SUMMA™ canister samples using the EPA TO-12 method. The sample mean was [1.5 mg/m³], with a standard deviation of [0.1 mg/m³]. This value is low compared to most passively ventilated tanks that have been sampled. TO-12 method TNMOC measurements for tanks C-104 and C-106 are given in Table 3-2 for comparison; tank C-104 is thought to be actively ventilated, but its ventilation rate is much smaller than that of tanks C-105 and C-106.

4.4 Discussion of Organic Analytes

It is assumed here that the in-leakage of air, gases, and vapors from tank C-104 has a significant effect on the concentrations of the organic constituents in tank C-105 and in its exhaust. While assessing the extent of that effect is not within the scope of this report, comparison of sample results presented here with tank C-104 headspace sample results does provide evidence that tank C-104 is venting through tank C-105.

Specifically, comparison of TST sample results in Tables 4-2 through 4-4 with the analogous Tables 4-3 through 4-5 of *Tank 241-C-104 Headspace Gas and Vapor Characterization Results for Samples Collected in March 1994* (Huckaby and Bratzel 1995a) indicates that each positively identified TST analyte in tank C-104 is present, albeit at a lower concentration, in the tank C-105 exhaust. These 22 analytes in tank C-104 are, with the exception of toluene which appears unexpectedly high, between 3- and 17-times more concentrated than in tank C-105. Given that these organic vapors are not directly associated with any historically documented waste in tank C-105 (Anderson 1990), it is possible that virtually all of the organic vapors detected in the tank C-105 exhaust samples had actually originated in tank C-104 (which is believed to have contained about 30,000 L of organic liquid, Hall 1972).

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-5 is to separate them into 2 categories: 1) Organic compounds added as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes tributyl phosphate, dibutyl butylphosphonate, and the semivolatile branched alkanes and normal paraffinic hydrocarbons (NPHs), which ostensibly came from various chemical separation processes at the Hanford site.

One type of semivolatile compound commonly detected in the NPH-rich waste tanks, but not in the tank C-105 exhaust, is a group of semivolatile bicyclic alkanes. Decahydronaphthalene and several methyl-substituted decahydronaphthalenes have been tentatively identified in many of the 241-BY and 241-C farm tanks, but were not identified in the tank C-105 exhaust. Several such compounds were noted in the tank C-104 samples, but their concentrations relative to other semivolatiles are much lower than in other NPH-rich tanks. This may be an indication that the organic vapors in the tank C-105 exhaust are remnants of waste from a period when the PUREX process was using a relatively pure NPH diluent.

The second category includes all organic compounds that were not placed into the tank as waste, but instead have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables 4-1 through 4-10 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, nitrates, nitrites, and volatile alkanes. By far the most abundant of these in the headspace are the short-chain volatile compounds, however, some long-chain low volatility compounds may also be waste reaction products.

Samples from the tank C-105 exhaust, like tank C-104 samples, were found to have several alkyl nitrates. Though it is reasonable to expect alkyl nitrates to be produced via chemical and radiolytic processes of the NPH with other waste, the solubility of alkyl nitrates in the aqueous waste supernates would also be expected to significantly reduce their vapor-phase concentrations. Indeed, their presence in other NPH-rich tanks has been minimal. That several alkyl nitrates are at detectable levels in tank C-104 and in the tank C-105 exhaust may indicate dry conditions where they are formed.

The tank C-105 exhaust was tentatively determined to contain the homologous series of:

- 1) straight-chain nitriles from ethanenitrile (acetonitrile) through n-nonanenitrile;
- 2) straight-chain alkyl nitrates from methyl to hexyl nitrate;
- 3) normal alkanes from propane through n-nonane⁵;
- 4) straight-chain 2-ketones from propanone (acetone) through 2-octanone;
- 5) straight-chain aldehydes from ethanal (acetaldehyde) through decanal;

as well as several partially complete series of other functionally related organic compounds such as alkenes and alcohols. As has been noted in other NPH-rich waste tanks, many of the volatile species

⁵ n-Decane through n-pentadecane were also detected, however, these are principally constituents of the original waste and not waste reaction products.

(presumed to be degradation products of the NPHs) have functional groups on the molecule's first or second carbon atom.

1-Butanol is prominent amongst the alcohols detected. It is known to be a degradation product of tributyl phosphate, and has been found in virtually all of the waste tanks sampled to date.

In summary, there is evidence that concentrations of compounds in the tank C-105 headspace and exhaust are strongly affected by in-leakage of air from the tank C-104 headspace. The constituents of the tank C-105 exhaust are typical of most NPH-rich tank headspaces, except that the alkyl nitrate signature, like tank C-104, is stronger than typical.

5.0 SUMMARY

The tank C-105 headspace exhaust was sampled in February 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 or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank C-105 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	0.5	Organic vapors	7 tank air samples
		10	Organic vapors	3 tank air samples + 1 trip blank
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous Oxide, Carbon Monoxide, Organic vapors	3 tank air samples, 6 ambient air samples
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 1 trip blank
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 1 trip blank
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 1 trip blank
	Silica Gel Sorbent Trap	3.0	Water vapor	5 tank air samples + 1 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	3.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
 Tank C-105 Inorganic Gas and Vapor Concentrations
 Analyses by Oregon Graduate Institute of Science and Technology and by Pacific Northwest Laboratory

Compound	CAS ¹ Number	Sample Type	Number of Samples	Average ² (ppmv)	Standard Deviation ² (ppmv)	RSD ^{2,3} (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	2.4	0.3	12
Carbon Monoxide, CO	630-08-0	SUMMA™	3	[0.29]	[0.01]	[4]
Hydrogen, H ₂	1333-74-0	SUMMA™	3	[22]	[2]	[9]
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.1	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.1	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	[5.3]	[0.26]	[5]
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	5	9,200 (6.8 mg/L)	1,200 (0.9 mg/L)	13

¹ CAS = Chemical Abstracts Service.

² Bracketed values are from OGIST and should be considered secondary results, non-bracketed values are from PNL and should be considered primary results.

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

Table 3-2
Comparison of Tank C-104, C-105, and C-106 Headspace Constituents --
Inorganic Analyses by Pacific Northwest Laboratory and
Oregon Graduate Institute of Science and Technology,
and Organic Analyses by Oak Ridge National Laboratory¹

Tank:	C-104 ²	C-105	C-106 ³
Date sampled, (mo/day/yr)	3/3/94	2/16/94	2/15/94
Headspace temperature, (°C)	28	17	19
Ammonia, (ppmv)	44	2.4	≤ 9
Hydrogen, (ppmv)	[68]	[22]	[9.7]
Carbon monoxide, (ppmv)	[2]	[0.29]	[0.25]
Nitric oxide, (ppmv)	0.37	≤ 0.1	≤ 0.1
Nitrogen dioxide, (ppmv)	≤ 0.02	≤ 0.1	≤ 0.1
Nitrous oxide, (ppmv)	[64]	[5.3]	[3.7]
Water vapor, (mg/m ³)	12.9	6.8	17.8
Water vapor, (% relative humidity)	47	47	100
Ethanenitrile (acetonitrile), (ppmv)	(0.13)	(0.026)	(0.0023)
Propanone (acetone), (ppmv)	(0.15)	(0.014)	(0.00018)
1-Butanol, (ppmv)	(2.90)	(0.17)	(0.011)
n-Dodecane, (ppmv)	(0.072)	(0.016)	(0.0036)
n-Tridecane, (ppmv)	(0.079)	(0.019)	(0.0087)
Total nonmethane organic carbon, (mg/m ³)	[28.1]	[1.5]	[0.41]

¹ OGIST results are given in brackets to indicate the data should be considered secondary results. Organic vapor results are from ORNL, with non-quantitative 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.

Table 4-1
Tank C-105 Quantitatively Measured Organic Analytes in OGIST SUMMA™ Samples¹

Cmpd #	Compound	CAS ² Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Dichlorodifluoromethane	75-71-8	[0.00033]	[0.00006]	[17]
2	Chloromethane	74-87-3	[0.00027]	[0.00006]	[22]
3	1,3-Butadiene	106-99-0	[0.0022]	[0.0015]	[69]
4	Trichlorofluoromethane	75-69-4	[0.0037]	[0.0006]	[15]
5	1,1-Dichloroethene (vinylidene chloride)	75-35-4	[0.0002]	[0.0002]	[87]
6	Dichloromethane (methylene chloride)	75-09-2	[0.00011]	[0.00014]	[133]
7	1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	[0.0001]	[< 0.00005]	--
8	Trichloromethane (chloroform)	67-66-3	[0.00017]	[0.00006]	[35]
9	1,1,1-Trichloroethane	71-55-6	[0.00013]	[0.00006]	[43]
10	Benzene	71-43-2	[0.0005]	[0.0001]	[20]
11	Tetrachloromethane (carbon tetrachloride)	56-23-5	[0.0001]	[< 0.00005]	--
12	Toluene	108-88-3	[0.0004]	[0.0001]	[25]
13	Tetrachloroethene	127-18-4	[0.0001]	[< 0.00005]	--
14	Ethyl benzene ⁴	100-41-4	[0.0001]	--	--
15 & 16	1,3-Dimethylbenzene (m-xylene) + 1,4-Dimethylbenzene (p-xylene) ⁵	108-38-3 106-42-3	[0.00013]	[0.00006]	[43]
17	o-Xylene ³	95-47-6	[0.0001]	--	--
18	4-Ethyltoluene ⁶ (p-ethyl toluene)	622-96-8	[0.0001]	--	--
19	1,3,5-Trimethylbenzene ⁵	108-67-8	[0.0001]	--	--
20	1,2,4-Trimethylbenzene ³	95-63-6	[0.00025]	--	--

¹ Because OGIST did not have a WHC-approved quality assurance project plan in place when analyses were conducted, these results should be considered secondary (Burnum 1995).

² CAS = Chemical Abstracts Service.

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

⁴ Detected in only 2 samples.

⁵ m-xylene and p-xylene coelute and the reported value represents the sum of their concentrations.

⁶ Detected in only 1 sample.

Table 4-2
Tank C-105 Quantitatively Measured Organic Analytes 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	0.0079	0.0022	27
2	n-Hexane	110-54-3	0.0049	0.0010	20
3	n-Pentanenitrile	110-59-8	0.0022	0.0004	19
4	2-Hexanone	591-78-6	0.0011	0.0002	15
5	n-Octane	111-65-9	0.0016	0.0001	5
6	n-Hexanenitrile	628-73-9	0.0021	0.0013	59
7	n-Nonane	111-84-2	0.00092	0.00007	8
8	n-Heptanenitrile	629-08-3	0.0012	0.00001	9

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 10-L TST samples.

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

Table 4-3
Tank C-105 Positively Identified Organic Analytes 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	0.026	0.006	22
2	Dichlorormethane (methylene chloride)	75-09-2	0.041	0.071	173
3	Benzene	71-43-2	0.00059	0.00014	24
4	n-Butanenitrile	109-74-0	0.014	0.003	23
5	n-Heptane	142-82-5	0.0009	0.0001	13
6	Toluene	108-88-3	0.00052	0.00006	12
7	2-Heptanone	110-43-0	0.00092	0.00015	16
8	2-Octanone	111-13-7	0.00062	0.00001	19
9	n-Octanenitrile	124-12-9	0.0010	0.00003	34
10	n-Nonanenitrile	2243-27-8	0.00054	0.00003	57
11	n-Dodecane	112-40-3	0.016	0.002	16
12	n-Tridecane	629-50-5	0.019	0.003	15

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, 10-L TST samples.

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

Table 4-4
Tank C-105 Positively Identified Organic Analytes 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 ⁵ (acetone)	67-64-1	0.014	0.003	21
2	1-Butanol ⁵	71-36-3	0.17	0.03	16
3	2-Pentanone ⁶	107-87-9	0.0024	0.0006	26

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 10-L TST samples.

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

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

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

Table 4-5
Tank C-105 Tentatively Identified Compounds in PNL SUMMA™ Samples

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Propene	115-07-1	0.05	0.00
2	1-Butanol	71-36-3	0.18	0.05
3	n-Undecane	1120-21-4	0.22	0.01
4	n-Dodecane	112-40-3	0.29	0.00
5	n-Tridecane	629-50-5	0.27	0.04
Sum of tentatively identified compounds:			1.01	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples; presented values are estimates.

Table 4-6
Tank C-105 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/m ³)	Standard Deviation (mg/m ³)
1	Carbon Dioxide	124-38-9	0.14	0.05
2	Carbon Dioxide	124-38-9	1.1	1.6
3	Carbon Dioxide	124-38-9	1.7	1.4
4	1-Propene	115-07-1	0.22	0.03
5	1-Propene, 2-methyl-	115-11-7	0.49	0.19
6	Butane	106-97-8	0.20	0.03
7	1-Propene, 2-methyl-	115-11-7	0.10	0.09
8	1-Propene, 2-fluoro-	1184-60-7	0.023	0.04
9	1-Propene, 2-methyl-	115-11-7	0.062	0.11
10	3-Buten-2-one	78-94-4	0.19	0.05
11	2-Butanone	78-93-3	0.39	0.03
12	Acetic acid, ethyl ester	141-78-6	0.093	0.161
13	Acetic acid	64-19-7	0.19	0.07
14	Furan, tetrahydro-	109-99-9	0.074	0.074
15	2-Butenal	4170-30-3	0.024	0.042
16	Nitric acid, propyl ester	627-13-4	0.066	0.059
17	Acetic acid	64-19-7	0.27	0.25
18	Hexanal	66-25-1	0.024	0.020
19	Acetic acid, butyl ester	123-86-4	0.022	0.019
20	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0078	0.0135
21	Nitric acid, butyl ester	928-45-0	0.040	0.006
22	Formic acid, butyl ester	592-84-7	0.0067	0.0115
23	Alkanone		0.0068	0.0118
24	2,2-Dimethyl-1-propanethiol	1679-08-9	0.31	0.07
25	Pyridine, 4-methyl-	108-89-4	0.025	0.028
26	Alkene and C2-Benzene		0.0038	0.0067

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	Alkyne		0.0054	0.0094
28	3-Heptanone	106-35-4	0.040	0.007
29	Acetamide, N,N-dimethyl-	127-19-5	0.033	0.032
30	alkyl-dihydrofuran		0.015	0.0005
31	2(3H)-Furanone, dihydro-	96-48-0	0.0042	0.0073
32	1,5-Pentanediol, dinitrate	3457-92-9	0.0036	0.0063
33	2(3H)-Furanone, dihydro-	96-48-0	0.10	0.15
34	C2-cyclohexane		0.0021	0.0036
35	2-Hexene, 2,4-dimethyl-		0.0031	0.0053
36	C8-Alkanone		0.022	0.0041
37	Butanamide	541-35-5	0.035	0.004
38	Alkyl Acetate		0.0060	0.0052
39	4-Octanone	589-63-9	0.0060	0.0105
40	Cyclotetrasiloxane, octamethyl-	556-67-2	0.059	0.084
41	Phenol	108-95-2	0.0035	0.0061
42	Butanoic acid, butyl ester	109-21-7	0.0095	0.0012
43	Decane	124-18-5	0.095	0.011
44	Octanal	124-13-0	0.021	0.001
45	Alkene		0.0028	0.005
46	2-Propanone, 1-fluoro- and others		0.0034	0.0059
47	Mixture		0.0018	0.0031
48	Octanone		0.013	0.011
49	Alkanone		0.0046	0.0041
50	Ethanone, 1-phenyl-	98-86-2	0.0022	0.0039
51	Alkene		0.0088	0.0082
52	2-Undecanone	112-12-9	0.0059	0.0103
53	Undecane	1120-21-4	0.43	0.07
54	Nonanal	124-19-6	0.033	0.009

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	Octane, 3-ethyl,2,7-dimethyl and others		0.0031	0.0054
56	4,4-Dimethyl dioxane	766-15-4	0.0029	0.0051
57	Trimethylsilylester of methoxy benzoic acid		0.010	0.009
58	6-Methylundecane	17302-33-9	0.0079	0.0093
59	Decane, 2,4,6-trimethyl-	62108-27-4	0.0079	0.0138
60	Alkanone		0.0022	0.0038
61	Undecane, 3-methyl-	1002-43-3	0.0033	0.0058
62	4-Decanone	624-16-8	0.018	0.002
63	Alkane		0.0035	0.0031
64	C12-Alkane		0.0051	0.0046
65	2-Decanone	693-54-9	0.0064	0.0056
66	Alkanol and others		0.0028	0.0048
67	Decanal	112-31-2	0.0045	0.0041
68	C13-Alkane		0.028	0.022
69	Undecane, 2,7-dimethyl-	17301-24-5	0.0031	0.0054
70	1-Butanamine, N-pentylidene and others		0.0028	0.0026
71	C13-Alkene		0.0053	0.0051
72	Alkene		0.0011	0.0019
73	Benzene, 1-butoxy-4-methoxy-	20743-95-7	0.0012	0.0021
74	Cyclohexane, hexyl-	4292-75-5	0.0096	0.0167
75	Alkene		0.0011	0.0020
76	C11-Ketone		0.0030	0.0027
77	Dodecane, 4-methyl-	6117-97-1	0.0033	0.0058
78	Alkane		0.0057	0.0052
79	C14-Alkane		0.044	0.020
80	Cyclobutane, 3-hexyl-1,1,2-trimethyl-, other		0.0022	0.0038
81	2-Tridecanol	1653-31-2	0.0018	0.0031

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
82	Trimethylsilylester of methoxy benzoic, other		0.0018	0.0032
83	Undecane, 2,7-dimethyl-	17301-24-5	0.0014	0.0025
84	5-Undecanone	33083-83-9	0.027	0.024
85	Alkenol		0.0049	0.0043
86	Butyl Heptanoate	5454-28-4	0.0059	0.0052
87	3-Undecanone	2216-87-7	0.017	0.015
88	6-Tridecane	24949-38-0	0.0014	0.0024
89	1,12-Tridecadiene	21964-48-7	0.0018	0.0032
90	C13-alkene		0.00086	0.00149
91	Alkane		0.0076	0.0081
92	Tridecane, 6-methyl-	13287-21-3	0.010	0.018
93	Alkane		0.0053	0.0064
94	1,3-Benzenediol, 4-hexyl-	136-77-6	0.0035	0.0031
95	Alkene		0.0032	0.0030
96	Tridecane, 4-methyl-	26730-12-1	0.0038	0.0034
97	C12 or C13 Alkane		0.017	0.018
98	2-Heptanone, 6-(2-furanyl)-6-methyl-	51595-87-0	0.0029	0.0026
99	Alkane		0.016	0.009
100	Dodecane, 2,7,10-trimethyl-	74645-98-0	0.081	0.012
101	Alkenol		0.0048	0.0044
102	C1-hydroxy-quinoline		0.0087	0.0081
103	3-Dodecanone	1534-27-6	0.026	0.023
104	Tetradecane	629-59-4	0.14	0.02
105	Alkenol		0.016	0.015
106	Oxygenated Compound		0.0028	0.0026
107	C14-Alkane		0.0025	0.0026
108	Pentadecane	629-62-9	0.0044	0.0076
9	C14-Alkane		0.0011	0.0019

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
110	C15-Alkane		0.044	0.040
111	C15-Alkane		0.0065	0.0112
112	Tridecanone		0.051	0.028
113	C2-hydroxy-quinoline		0.0098	0.0087
114	3-Tridecanone	1534-26-5	0.031	0.029
115	Pentadecane	629-62-9	0.076	0.072
116	Alkanone		0.012	0.011
117	Alkane		0.017	0.015
118	Alkanol		0.0011	0.0019
119	Alkanol		0.0015	0.0027
120	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	128-37-0	0.011	0.012
121	Phosphonate, homolog of dibutyl butylphosphonate		0.0033	0.0029
122	C17-Alkane		0.0039	0.0068
123	Dodecane, 2-methyl-8-propyl-	55045-07-3	0.0046	0.0080
124	Phosphate, homolog of tributyl phosphate		0.0047	0.0041
125	Alkane		0.0042	0.0072
126	Alkane		0.0033	0.0057
127	Tetradecanone		0.029	0.020
128	Tetradecanone		0.012	0.011
129	Octadecanoic acid, butyl ester	123-95-5	0.029	0.006
130	Phosphate, homolog of tributyl phosphate		0.0059	0.0052
131	3-Undecanone	2216-87-7	0.013	0.012
132	Hexadecane	544-76-3	0.019	0.033
133	Tetradecanone		0.014	0.012
134	Tetradecane	629-59-4	0.013	0.022
135	Pentadecane	629-62-9	0.025	0.022

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
136	Phthalate		0.0032	0.0055
137	Dibutyl Butyl Phosphonate	78-46-6	0.051	0.004
138	Benzene, (1-butylheptyl)-	4537-15-9	0.0032	0.0036
139	Pentadecane, 2,6,10-trimethyl-	3892-00-0	0.0053	0.0092
140	Tributyl Phosphate	126-73-8	0.24	0.22
141	Benzene, (1-ethylnonyl)-	4536-87-2	0.0027	0.0047
142	alkyl benzene		0.0037	0.0043
143	Butyl Myristate	110-36-1	0.033	0.005
144	Heptadecane	629-78-7	0.0092	0.0070
145	Phosphate, isomer of tributyl phosphate		0.014	0.007
146	Mixture		0.0013	0.0022
147	Benzene, (1-methyldecyl)-	4536-88-3	0.0039	0.0034
148	Benzene, (1-pentylheptyl)-	2719-62-2	0.0040	0.0011
149	Benzene, (1-butylloctyl)-	2719-63-3	0.0039	0.0035
150	Benzene, (1-propylnonyl)-	2719-64-4	0.0012	0.0021
151	Butyl Myristate	110-36-1	0.023	0.003
152	Pentadecane, 2,6,10-trimethyl-	3892-00-0	0.00076	0.00132
153	alkyl benzene		0.0066	0.0027
154	alkyl benzene		0.00079	0.00136
155	Butyl Myristate	110-36-1	0.0078	0.0008
Sum of tentatively identified compounds:			8.20	

1 CAS = Chemical Abstract Service

2 Average of 3, 10-L TST samples; presented values are estimates.

Table 4-7
Tank C-105 Tentatively Identified Organic Compounds in TST Samples
in Alphanumerical Order --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
9	1-Propene, 2-methyl-	115-11-7	0.062	0.11
8	1-Propene, 2-fluoro-	1184-60-7	0.023	0.04
70	1-Butanamine, N-pentylidene and others		0.0028	0.0026
4	1-Propene	115-07-1	0.22	0.03
5	1-Propene, 2-methyl-	115-11-7	0.49	0.19
7	1-Propene, 2-methyl-	115-11-7	0.10	0.09
94	1,3-Benzenediol, 4-hexyl-	136-77-6	0.0035	0.0031
32	1,5-Pentanediol, dinitrate	3457-92-9	0.0036	0.0063
89	1,12-Tridecadiene	21964-48-7	0.0018	0.0032
98	2-Heptanone, 6-(2-furanyl)-6-methyl-	51595-87-0	0.0029	0.0026
11	2-Butanone	78-93-3	0.39	0.03
46	2-Propanone, 1-fluoro- and others		0.0034	0.0059
81	2-Tridecanol	1653-31-2	0.0018	0.0031
65	2-Decanone	693-64-9	0.0064	0.0056
15	2-Butenal	4170-30-3	0.024	0.042
52	2-Undecanone	112-12-9	0.0059	0.0103
35	2-Hexene, 2,4-dimethyl-		0.0031	0.0053
24	2,2-Dimethyl-1-propanethiol	1679-08-9	0.31	0.07
31	2(3H)-Furanone, dihydro-	96-48-0	0.0042	0.0073
33	2(3H)-Furanone, dihydro-	96-48-0	0.10	0.15
87	3-Undecanone	2216-87-7	0.017	0.015
114	3-Tridecanone	1534-26-5	0.031	0.029
103	3-Dodecanone	1534-27-6	0.026	0.023
131	3-Undecanone	2216-87-7	0.013	0.012
28	3-Heptanone	106-35-4	0.040	0.007

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
10	3-Buten-2-one	78-94-4	0.19	0.05
39	4-Octanone	589-63-9	0.0060	0.0105
62	4-Decanone	624-16-8	0.018	0.002
56	4,4-Dimethyl dioxane	766-15-4	0.0029	0.0051
84	5-Undecanone	33083-83-9	0.027	0.024
58	6-Methylundecane	17302-33-9	0.0079	0.0093
88	6-Tridecane	24949-38-0	0.0014	0.0024
29	Acetamide, N,N-dimethyl-	127-19-5	0.033	0.032
12	Acetic acid, ethyl ester	141-78-6	0.093	0.161
13	Acetic acid	64-19-7	0.19	0.07
17	Acetic acid	64-19-7	0.27	0.25
19	Acetic acid, butyl ester	123-86-4	0.022	0.019
63	Alkane		0.0035	0.0031
78	Alkane		0.0057	0.0052
91	Alkane		0.0076	0.0081
93	Alkane		0.0053	0.0064
99	Alkane		0.016	0.009
117	Alkane		0.017	0.015
125	Alkane		0.0042	0.0072
126	Alkane		0.0033	0.0057
66	Alkanol and others		0.0028	0.0048
118	Alkanol		0.0011	0.0019
119	Alkanol		0.0015	0.0027
23	Alkanone		0.0068	0.0118
49	Alkanone		0.0046	0.0041
60	Alkanone		0.0022	0.0038
116	Alkanone		0.012	0.011
26	Alkene and C2-Benzene		0.0038	0.0067

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
45	Alkene		0.0028	0.005
51	Alkene		0.0088	0.0082
72	Alkene		0.0011	0.0019
75	Alkene		0.0011	0.0020
95	Alkene		0.0032	0.0030
85	Alkenol		0.0049	0.0043
101	Alkenol		0.0048	0.0044
105	Alkenol		0.016	0.015
30	alkyl-dihydrofuran		0.015	0.0005
142	alkyl benzene		0.0037	0.0043
153	alkyl benzene		0.0066	0.0027
154	alkyl benzene		0.00079	0.00136
38	Alkyl Acetate		0.0060	0.0052
27	Alkyne		0.0054	0.0094
73	Benzene, 1-butoxy-4-methoxy-	20743-95-7	0.0012	0.0021
138	Benzene, (1-butylheptyl)-	4537-15-9	0.0032	0.0036
141	Benzene, (1-ethylnonyl)-	4536-87-2	0.0027	0.0047
147	Benzene, (1-methyldecyl)-	4536-88-3	0.0039	0.0034
148	Benzene, (1-pentylheptyl)-	2719-62-2	0.0040	0.0011
149	Benzene, (1-butylloctyl)-	2719-63-3	0.0039	0.0035
150	Benzene, (1-propylnonyl)-	2719-64-4	0.0012	0.0021
37	Butanamide	541-35-5	0.035	0.004
6	Butane	106-97-8	0.20	0.03
42	Butanoic acid, butyl ester	109-21-7	0.0095	0.0012
86	Butyl Heptanoate	5454-28-4	0.0059	0.0052
143	Butyl Myristate	110-36-1	0.033	0.005
151	Butyl Myristate	110-36-1	0.023	0.003
155	Butyl Myristate	110-36-1	0.0078	0.0008

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
102	C1-hydroxy-quinoline		0.0087	0.0081
76	C11-Ketone		0.0030	0.0027
64	C12-Alkane		0.0051	0.0046
97	C12 or C13 Alkane		0.017	0.018
68	C13-Alkane		0.028	0.022
71	C13-Alkene		0.0053	0.0051
90	C13-alkene		0.00086	0.00149
79	C14-Alkane		0.044	0.020
109	C14-Alkane		0.0011	0.0019
107	C14-Alkane		0.0025	0.0026
111	C15-Alkane		0.0065	0.0112
110	C15-Alkane		0.044	0.040
122	C17-Alkane		0.0039	0.0068
113	C2-hydroxy-quinoline		0.0098	0.0087
34	C2-cyclohexane		0.0021	0.0036
36	C8-Alkanone		0.022	0.0041
1	Carbon Dioxide	124-38-9	0.14	0.05
2	Carbon Dioxide	124-38-9	1.1	1.6
3	Carbon Dioxide	124-38-9	1.7	1.4
80	Cyclobutane, 3-hexyl-1, 1,2-trimethyl-, other		0.0022	0.0038
74	Cyclohexane, hexyl-	4292-75-5	0.0096	0.0167
40	Cyclotetrasiloxane, octamethyl-	556-67-2	0.059	0.084
20	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0078	0.0135
67	Decanal	112-31-2	0.0045	0.0041
43	Decane	124-18-5	0.095	0.011
59	Decane, 2,4,6-trimethyl-	62108-27-4	0.0079	0.0138
137	Dibutyl Butyl Phosphonate	78-46-6	0.051	0.004
77	Dodecane, 4-methyl-	6117-97-1	0.0033	0.0058

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
100	Dodecane, 2,7,10-trimethyl-	74645-98-0	0.081	0.012
123	Dodecane, 2-methyl-8-propyl-	55045-07-3	0.0046	0.0080
50	Ethanone, 1-phenyl-	98-86-2	0.0022	0.0039
22	Formic acid, butyl ester	592-84-7	0.0067	0.0115
14	Furan, tetrahydro-	109-99-9	0.074	0.074
144	Heptadecane	629-78-7	0.0092	0.0070
132	Hexadecane	544-76-3	0.019	0.033
18	Hexanal	66-25-1	0.024	0.020
47	Mixture		0.0018	0.0031
146	Mixture		0.0013	0.0022
16	Nitric acid, propyl ester	627-13-4	0.066	0.059
21	Nitric acid, butyl ester	928-45-0	0.040	0.006
54	Nonanal	124-19-6	0.033	0.009
129	Octadecanoic acid, butyl ester	123-95-5	0.029	0.006
44	Octanal	124-13-0	0.021	0.001
55	Octane, 3-ethyl,2,7-dimethyl and others		0.0031	0.0054
48	Octanone		0.013	0.011
106	Oxygenated Compound		0.0028	0.0026
108	Pentadecane	629-62-9	0.0044	0.0076
115	Pentadecane	629-62-9	0.076	0.072
135	Pentadecane	629-62-9	0.025	0.022
139	Pentadecane, 2,6,10-trimethyl-	3892-00-0	0.0053	0.0092
152	Pentadecane, 2,6,10-trimethyl-	3892-00-0	0.00076	0.00132
41	Phenol	108-95-2	0.0035	0.0061
120	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	128-37-0	0.011	0.012
124	Phosphate, homolog of tributyl phosphate		0.0047	0.0041

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
130	Phosphate, homolog of tributyl phosphate		0.0059	0.0052
145	Phosphate, isomer of tributyl phosphate		0.014	0.007
121	Phosphonate, homolog of dibutyl butylphosphonate		0.0033	0.0029
136	Phthalate		0.0032	0.0055
25	Pyridine, 4-methyl-	108-89-4	0.025	0.028
104	Tetradecane	629-59-4	0.14	0.02
134	Tetradecane	629-59-4	0.013	0.022
127	Tetradecanone		0.029	0.020
128	Tetradecanone		0.012	0.011
133	Tetradecanone		0.014	0.012
140	Tributyl Phosphate	126-73-8	0.24	0.22
92	Tridecane, 6-methyl-	13287-21-3	0.010	0.018
96	Tridecane, 4-methyl-	26730-12-1	0.0038	0.0034
112	Tridecanone		0.051	0.028
57	Trimethylsilylester of methoxy benzoic acid		0.010	0.009
82	Trimethylsilylester of methoxy benzoic, other		0.0018	0.0032
53	Undecane	1120-21-4	0.43	0.07
61	Undecane, 3-methyl-	1002-43-3	0.0033	0.0058
69	Undecane, 2,7-dimethyl-	17301-24-5	0.0031	0.0054
83	Undecane, 2,7-dimethyl-	17301-24-5	0.0014	0.0025

1 CAS = Chemical Abstract Service

2 Average of 3, 10-L TST samples; presented values are estimates.

Table 4-8
Tank C-105 Tentatively Identified Organic Compounds in TST Samples
in Order of Estimated Concentration --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
3	Carbon Dioxide	124-38-9	1.7	1.4
2	Carbon Dioxide	124-38-9	1.1	1.6
5	1-Propene, 2-methyl-	115-11-7	0.49	0.19
53	Undecane	1120-21-4	0.43	0.07
11	2-Butanone	78-93-3	0.39	0.03
24	2,2-Dimethyl-1-propanethiol	1679-08-9	0.31	0.07
17	Acetic acid	64-19-7	0.27	0.25
140	Tributyl Phosphate	126-73-8	0.24	0.22
4	1-Propene	115-07-1	0.22	0.03
6	Butane	106-97-8	0.20	0.03
10	3-Buten-2-one	78-94-4	0.19	0.05
13	Acetic acid	64-19-7	0.19	0.07
1	Carbon Dioxide	124-38-9	0.14	0.05
104	Tetradecane	629-59-4	0.14	0.02
7	1-Propene, 2-methyl-	115-11-7	0.10	0.09
33	2(3H)-Furanone, dihydro-	96-48-0	0.10	0.15
43	Decane	124-18-5	0.095	0.011
12	Acetic acid, ethyl ester	141-78-6	0.093	0.161
100	Dodecane, 2,7,10-trimethyl-	74645-98-0	0.081	0.012
115	Pentadecane	629-62-9	0.076	0.072
14	Furan, tetrahydro-	109-99-9	0.074	0.074
16	Nitric acid, propyl ester	627-13-4	0.066	0.059
9	1-Propene, 2-methyl-	115-11-7	0.062	0.11
40	Cyclotetrasiloxane, octamethyl-	556-67-2	0.059	0.084
137	Dibutyl Butyl Phosphonate	78-46-6	0.051	0.004
112	Tridecanone		0.051	0.028

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
110	C15-Alkane		0.044	0.040
79	C14-Alkane		0.044	0.020
28	3-Heptanone	106-35-4	0.040	0.007
21	Nitric acid, butyl ester	928-45-0	0.040	0.006
37	Butanamide	541-35-5	0.035	0.004
54	Nonanal	124-19-6	0.033	0.009
29	Acetamide, N,N-dimethyl-	127-19-5	0.033	0.032
143	Butyl Myristate	110-36-1	0.033	0.005
114	3-Tridecanone	1534-26-5	0.031	0.029
129	Octadecanoic acid, butyl ester	123-95-5	0.029	0.006
127	Tetradecanone		0.029	0.020
68	C13-Alkane		0.028	0.022
84	5-Undecanone	33083-83-9	0.027	0.024
103	3-Dodecanone	1534-27-6	0.026	0.023
135	Pentadecane	629-62-9	0.025	0.022
25	Pyridine, 4-methyl-	108-89-4	0.025	0.028
18	Hexanal	66-25-1	0.024	0.020
15	2-Butenal	4170-30-3	0.024	0.042
151	Butyl Myristate	110-36-1	0.023	0.003
8	1-Propene, 2-fluoro-	1184-60-7	0.023	0.04
19	Acetic acid, butyl ester	123-86-4	0.022	0.019
36	C8-Alkanone		0.022	0.0041
44	Octanal	124-13-0	0.021	0.001
132	Hexadecane	544-76-3	0.019	0.033
62	4-Decanone	624-16-8	0.018	0.002
87	3-Undecanone	2216-87-7	0.017	0.015
117	Alkane		0.017	0.015
97	C12 or C13 Alkane		0.017	0.018

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
105	Alkenol		0.016	0.015
99	Alkane		0.016	0.009
30	alkyl-dihydrofuran		0.015	0.0005
133	Tetradecanone		0.014	0.012
145	Phosphate, isomer of tributyl phosphate		0.014	0.007
134	Tetradecane	629-59-4	0.013	0.022
48	Octanone		0.013	0.011
131	3-Undecanone	2216-87-7	0.013	0.012
116	Alkanone		0.012	0.011
128	Tetradecanone		0.012	0.011
120	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	128-37-0	0.011	0.012
92	Tridecane, 6-methyl-	13287-21-3	0.010	0.018
113	C2-hydroxy-quinoline		0.0098	0.0087
74	Cyclohexane, hexyl-	4292-75-5	0.0096	0.0167
42	Butanoic acid, butyl ester	109-21-7	0.0095	0.0012
144	Heptadecane	629-78-7	0.0092	0.0070
57	Trimethylsilylester of methoxy benzoic acid		0.010	0.009
51	Alkene		0.0088	0.0082
102	C1-hydroxy-quinoline		0.0087	0.0081
59	Decane, 2,4,6-trimethyl-	62108-27-4	0.0079	0.0138
58	6-Methylundecane	17302-33-9	0.0079	0.0093
155	Butyl Myristate	110-36-1	0.0078	0.0008
20	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0078	0.0135
91	Alkane		0.0076	0.0081
23	Alkanone		0.0068	0.0118
22	Formic acid, butyl ester	592-84-7	0.0067	0.0115

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
153	alkyl benzene		0.0066	0.0027
111	C15-Alkane		0.0065	0.0112
65	2-Decanone	693-54-9	0.0064	0.0056
38	Alkyl Acetate		0.0060	0.0052
39	4-Octanone	589-63-9	0.0060	0.0105
86	Butyl Heptanoate	5454-28-4	0.0059	0.0052
130	Phosphate, homolog of tributyl phosphate		0.0059	0.0052
52	2-Undecanone	112-12-9	0.0059	0.0103
78	Alkane		0.0057	0.0052
27	Alkyne		0.0054	0.0094
55	Octane, 3-ethyl,2, 7-dimethyl and others		0.0031	0.0054
139	Pentadecane, 2,6,10-trimethyl-	3892-00-0	0.0053	0.0092
93	Alkane		0.0053	0.0064
71	C13-Alkene		0.0053	0.0051
64	C12-Alkane		0.0051	0.0046
85	Alkenol		0.0049	0.0043
101	Alkenol		0.0048	0.0044
124	Phosphate, homolog of tributyl phosphate		0.0047	0.0041
49	Alkanone		0.0046	0.0041
123	Dodecane, 2-methyl-8-propyl-	55045-07-3	0.0046	0.0080
67	Decanal	112-31-2	0.0045	0.0041
108	Pentadecane	629-62-9	0.0044	0.0076
31	2(3H)-Furanone, dihydro-	96-48-0	0.0042	0.0073
125	Alkane		0.0042	0.0072
148	Benzene, (1-pentylheptyl)-	2719-62-2	0.0040	0.0011
122	C17-Alkane		0.0039	0.0068

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
149	Benzene, (1-butyloctyl)-	2719-63-3	0.0039	0.0035
147	Benzene, (1-methyldecyl)-	4536-88-3	0.0039	0.0034
96	Tridecane, 4-methyl-	26730-12-1	0.0038	0.0034
26	Alkene and C2-Benzene		0.0038	0.0067
80	Cyclobutane, 3-hexyl-1, 1,2-trimethyl-, other		0.0022	0.0038
142	alkyl benzene		0.0037	0.0043
32	1,5-Pentanediol, dinitrate	3457-92-9	0.0036	0.0063
63	Alkane		0.0035	0.0031
41	Phenol	108-95-2	0.0035	0.0061
94	1,3-Benzenediol, 4-hexyl-	136-77-6	0.0035	0.0031
46	2-Propanone, 1-fluoro- and others		0.0034	0.0059
77	Dodecane, 4-methyl-	6117-97-1	0.0033	0.0058
126	Alkane		0.0033	0.0057
61	Undecane, 3-methyl-	1002-43-3	0.0033	0.0058
121	Phosphonate, homolog of dibutyl butylphosphonate		0.0033	0.0029
138	Benzene, (1-butylheptyl)-	4537-15-9	0.0032	0.0036
82	Trimethylsilylester of methoxy benzoic, other		0.0018	0.0032
136	Phthalate		0.0032	0.0055
95	Alkene		0.0032	0.0030
69	Undecane, 2,7-dimethyl-	17301-24-5	0.0031	0.0054
35	2-Hexene, 2,4-dimethyl-		0.0031	0.0053
76	C11-Ketone		0.0030	0.0027
98	2-Heptanone, 6-(2-furanyl)-6-methyl-	51595-87-0	0.0029	0.0026
56	4,4-Dimethyl dioxane	766-15-4	0.0029	0.0051
106	Oxygenated Compound		0.0028	0.0026
66	Alkanol and others		0.0028	0.0048

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
45	Alkene		0.0028	0.005
141	Benzene, (1-ethylnonyl)-	4536-87-2	0.0027	0.0047
70	1-Butanamine, N-pentylidene and others		0.0028	0.0026
107	C14-Alkane		0.0025	0.0026
50	Ethanone, 1-phenyl-	98-86-2	0.0022	0.0039
60	Alkanone		0.0022	0.0038
34	C2-cyclohexane		0.0021	0.0036
89	1,12-Tridecadiene	21964-48-7	0.0018	0.0032
47	Mixture		0.0018	0.0031
81	2-Tridecanol	1653-31-2	0.0018	0.0031
119	Alkanol		0.0015	0.0027
88	6-Tridecane	24949-38-0	0.0014	0.0024
83	Undecane, 2,7-dimethyl-	17301-24-5	0.0014	0.0025
146	Mixture		0.0013	0.0022
150	Benzene, (1-propylnonyl)-	2719-64-4	0.0012	0.0021
73	Benzene, 1-butoxy-4-methoxy-	20743-95-7	0.0012	0.0021
75	Alkene		0.0011	0.0020
72	Alkene		0.0011	0.0019
109	C14-Alkane		0.0011	0.0019
118	Alkanol		0.0011	0.0019
90	C13-alkene		0.00086	0.00149
154	alkyl benzene		0.00079	0.00136
152	Pentadecane, 2,6,10-trimethyl-	3892-00-0	0.00076	0.00132

1 CAS = Chemical Abstract Service

2 Average of 3, 10-L TST samples; presented values are estimates.

Table 4-9
Tank C-105 Tentatively Identified Compounds in OGIST SUMMA™ Samples

Cmpd #	Compound	CAS ¹ Number	Sample Number ²		
			1	2	3
1	Carbonyl Sulfide (OCS)	463-58-1			x
2	Propene	115-07-1	x	x	x
3	Propane	74-98-6	x	x	x
4	Methyl nitrite	624-91-9	x	x	x
5	Cyclopropane	75-19-4	x	x	
6	2-Methylpropane	75-28-5	x	x	x
7	Ethanal (acetaldehyde)	75-07-0	x	x	x
8	2-Methylpropene	115-11-7	x	x	x
9	n-Butane	106-97-8	x	x	x
10	trans-2-butene	624-64-6	x	x	x
11	cyclobutane	287-23-0	x	x	x
12	cis-2-butene	590-18-1	x	x	x
13	ethanol	64-17-5	x	x	x
14	Ethanenitrile (acetonitrile)	75-05-8	x	x	x
15	2-Propenal (acrolein)	107-02-8	x	x	x
16	2-Methylbutane	78-78-4	x	x	x
17	Propanone (acetone)	67-64-1	x	x	x
18	Propanal (propionaldehyde)	123-38-6	x	x	x
19	1-Pentene	109-67-1	x	x	x
20	2-Propanol	67-63-0	x	x	x
21	n-Pentane	109-66-0	x	x	x
22	Methyl Nitrate	598-58-3	x	x	x
23	Ethylcyclopropane	1191-96-4	x	x	x
24	Carbon disulfide	75-15-0	x	x	x
25	2-Methyl-2-propanol	75-65-0	x		
26	Nitromethane	75-52-5	x	x	x
27	2-Methylpropanal	78-84-2	x		

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Sample Number ²		
			1	2	3
28	Propanenitrile	107-12-0	x	x	x
29	2-Methyl-2-propenal (methacrolein)	78-85-3	x		
30	1-Propanol	71-23-8	x	x	x
31	3-Buten-2-one (methylvinyl ketone)	78-94-4	x	x	x
32	2-Methylpentane	107-83-5	x	x	x
33	Butanal	123-72-8	x	x	x
34	2-Butanone	78-93-3	x	x	x
35	1-Hexene	592-41-6	x	x	x
36	2-Butanol	78-92-2	x	x	x
37	n-Hexane	110-54-3	x	x	x
38	Ethyl Nitrate	625-58-1	x	x	x
39	Tetrahydrofuran	109-99-9	x	x	x
40	2-Butenal (crotonaldehyde)	4170-30-3	x	x	x
41	Butanenitrile	109-74-0	x	x	x
42	1-Butanol	71-36-3	x	x	x
43	2-Pentanone	107-87-9	x	x	x
44	Pentanal	110-62-3	x	x	x
45	1-Heptene	592-76-7	x	x	x
46	Propyl Nitrate	627-13-4	x	x	x
47	n-Heptane	142-82-5	x	x	
48	2,4,4-Trimethyl-1-pentene	107-39-1	x	x	x
49	Pentanenitrile	110-59-8	x	x	x
50	1-Pentanol	71-41-0	x	x	
51	3-Hexanone	589-38-8	x	x	x
52	2-Hexanone	591-78-6	x	x	x
53	3-Methylheptane	589-81-1	x	x	x
54	Hexanal	66-25-1	x	x	x
55	1-Octene	111-66-0	x	x	x

WHC-SD-WM-ER-443 REV. 1

Cmpd #	Compound	CAS ¹ Number	Sample Number ²		
			1	2	3
56	n-Octane	111-65-9	x	x	x
57	Butyl Nitrate	928-45-0	x	x	x
58	Hexanenitrile	628-73-9	x	x	x
59	4-Heptanone	123-19-3	x	x	x
60	3-Heptanone	106-35-4	x	x	x
61	2-Heptanone	110-43-0	x	x	x
62	1-Nonene	124-11-8	x	x	
63	n-Nonane	111-84-2	x	x	x
64	Pentyl Nitrate	1002-16-0	x	x	x
65	Heptanenitrile	629-08-3	x		
66	2-Octanone	111-13-7	x	x	
67	n-Decane	124-18-5	x	x	x
68	Hexyl Nitrate	20633-11-8		x	
69	1-Undecene	821-95-4	x		
70	n-Undecane	1120-21-4	x	x	x
71	1-Dodecene	112-41-4	x	x	x
72	n-Dodecane	112-40-3	x	x	x
73	2,6-Dimethylundecane	17301-23-4	x	x	x
74	n-Tridecane	629-50-5	x	x	x
75	n-Tetradecane	629-59-4	x	x	x

1 CAS = Chemical Abstract Service.

2 An x is placed in the column if the analyte was tentatively identified in the sample. Here 1 = sample S4005-01.B16; 2 = sample S4005-02.B16; and 3 = sample S4005-03.B16 (Rasmussen 1994, WHC 1995).

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