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CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
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ENGINEERING CHANGE NOTICE

Page 1 of 2

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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-U-111 Headspace Gas and Vapor Characterization Results for Samples Collected in February 1995

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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 and Carbon Dioxide	4
3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium	5
3.4 Discussion of Inorganic Gases and Vapors	5
4.0 ORGANIC VAPORS	7
4.1 Positively Identified Organic Compounds	7
4.2 Tentatively Identified Organic Compounds	8
4.3 Discussion of Organic Compounds	9
5.0 SUMMARY	11
6.0 REFERENCES	12

Acronyms and Abbreviations

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

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Tank 241-U-111 Headspace Gas and Vapor Characterization Results
for Samples Collected in February 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank U-111 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 U-111 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 1994). However, current governing operating specifications for single shell waste tanks, such as tank U-111 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 tank U-111 headspace when the tank was sampled (Meacham et al. 1995), and samples analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents. No assessment of how the tank U-111 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 U-111 is the second tank in a 3-tank cascade with tanks U-110 and U-112. It is connected to tanks U-110 and U-112 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade lines. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank U-110 or tank U-112 may be transferred to tank U-111 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for either tanks U-110 or U-112 to assess their potential transfer of gases and vapors to tank U-111.

The cascade of tanks U-110, U-111, and U-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 U-111 using the vapor sampling system (VSS) on February 28, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-U-111 Tank Characterization Plan* (Carpenter 1995). The tank headspace temperature was determined to be 20 °C. Air from the U-111 headspace was withdrawn from a single elevation via a 6.1-m long heated sampling probe mounted in riser 4, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 60 °C. All tank air samples were collected between 10:45 a.m. and 2:07 p.m., with no anomalies noted.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), and Pacific Northwest Laboratories (PNL). The 40 tank air samples and 2 ambient air control samples collected are listed in Table 2-1 by analytical laboratory. Table 2-1 also lists the 14 trip blanks and 2 field blanks provided by the laboratories.

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

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{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 reported 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).

Analyses of inorganic analytes in sorbent traps and SUMMATM canisters were performed within 16 and 30 days, respectively, after sample collection (Ligotke 1995). This was within the allowed 60-day holding time of the WHC quality assurance project plan (Keller 1994). It should be noted that the 60-day holding time was administratively chosen, and that analytical holding times have not been established by an appropriate study of analyte stabilities in the sampling devices and in the chemical matrix of the tank air samples.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 676 ppmv, is relatively high compared to other waste tanks sampled to date. Ammonia has been observed in virtually all of the passively ventilated waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), to 1040 ppmv in BY-108 (McVeety et al. 1995). Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 676 ppmv corresponds to about 0.45 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank U-111 was determined to be 247 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, 247 ppmv hydrogen concentration in tank U-111 corresponds to about 0.6 % of its LFL. At this level, hydrogen is not a flammability concern in tank U-111.

The nitrous oxide concentration in tank U-111, 327 ppmv, is also relatively high compared to other waste tanks sampled to date. Nitrous oxide has been detected in other passively ventilated waste tanks at average concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as 868 ppmv in tank U-103 (Ligotke et al. 1995). 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 U-111 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank U-111 headspace was measured as < 12 ppmv. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. Carbon monoxide has not been

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

measured at very high levels in any of the waste tanks, the highest level measured to date was [26.7 ppmv] in tank C-103² (Huckaby and Story 1994).

The carbon dioxide concentration in the tank U-111 headspace, reported as < 64 ppmv, is significantly lower than it is in ambient air. Carbon dioxide is normally present in the ambient air at a concentration of 350 to 400 ppmv, and is typically lower than ambient in the waste tank headspaces. The 2 ambient air samples collected at the start of the tank U-111 gas and vapor sampling event, for example, were measured to have an average 368 ppmv of carbon dioxide.

Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids in the waste tanks, and converted to carbonate in solution. Like the carbon monoxide measurements, because different analytical methods have been used to measure carbon dioxide in the waste tank samples, the information on waste tank carbon dioxide varies. The < 64 ppmv of carbon dioxide characterization of the tank U-111 headspace is consistent with typical values for the waste tanks sampled to date.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank U-111 headspace were determined to be ≤ 0.04 and ≤ 0.01 ppmv, respectively. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank U-111. The measurable presence of nitric oxide is not uncommon in the waste tank headspaces, and may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. These constituents could potentially serve as oxidizers to support combustion, but at the measured concentrations would have a negligible effect on the flammability of the tank U-111 headspace.

The water vapor concentration of tank U-111 was determined to be about 11.3 mg/L, at the measured tank headspace temperature of 20 °C and pressure of 1004 mbar (753.0 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 15.2 mbar (11.4 torr), to a dew point of 13.2 °C, and to a relative humidity of 65 %.

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, the most abundant waste constituents in the tank U-111 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. The concentrations of these are higher in tank U-111 than in most passively ventilated tanks that have been sampled, but within the typical range of values.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are excellent for the methods used. Relative standard deviations range from less than 1 % for ammonia

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.

WHC-SD-WM-ER-452 REV. 1

vapor to about 3 % for nitrous oxide and water vapor results. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

4.0 ORGANIC VAPORS

Organic vapors in the tank U-111 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Gas chromatographs (GCs) equipped with mass spectrometer (MS) detectors were used by PNL and ORNL to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Clauss et al. (1995) and Jenkins et al. (1995a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank U-111. These results were produced at PNL quality assurance impact level 2. All PNL analyses of SUMMA™ canisters for organic compounds were completed within 31 days after sample collection, well below the specified 60-day allowed holding time (Keller 1994).

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 et al. 1995a).

4.1 Positively Identified Organic Compounds

Positive identification of organic analytes using the methods employed by PNL and ORNL involves matching the GC retention times and MS data from a sample with that obtained 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 derived from a review of the tank C-103 headspace constituents by a panel of toxicology experts (Mahlum et al. 1994). The PNL target analyte list included 39 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of tank C-103 vapor data.

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ samples, and the methane analysis result. SUMMA™ analyses were performed according to the TO-14 methodology, and methane was analyzed with the inorganic gases (Clauss et al. 1995). Only 2 of the 39 TO-14 target analytes and 7 of the 14 additional target analytes were measured to be above the 0.005 ppmv quantitation limit of the analyses. Averages reported are from analyses of 3 SUMMA™ canister samples.

ORNL positively identified 24 of 27 target analytes selected by WHC. 1,1-Dichloroethene, dichloromethane, and dibutyl butylphosphonate were the only TST target analytes not detected. Despite

calibration of the instrument over about a 20-fold concentration range, 18 of the 24 positively identified compounds were measured to be outside of the calibration range in at least 1 of the TST samples. Table 4-2 lists 5 of the quantitated analytes, with their reported 4-TST average concentrations. The measured concentrations of 16 positively identified analytes, which were not quantitated in all of the TST samples, are given in Table 4-3. One quantitated analyte (butanal) and 2 non-quantitated analytes (1-butanol and 2-pentanone) are listed in Table 4-4, because the ORNL practical holding time for these analytes was exceeded. Data in Tables 4-3 and 4-4 may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

The ORNL practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. Jenkins et al. (1995b) describe the practical holding time study and its results. TST samples were not analyzed until 48 days after being collected (Jenkins 1995), which was longer than the practical holding times established for the 3 compounds in Table 4-4. It should be noted that the analyses were performed before the holding time study, and that the contractual holding time for the TST samples was 60 days.

Both PNL and ORNL report target analyte concentrations in ppmv of analyte in dry air. To correct for the measured water vapor content of tank U-111 and obtain concentration in ppmv of analyte in moist tank air, multiply the dry-air ppmv concentrations by 0.985.

Table 4-5 lists the 11 target analytes common to both TST and SUMMA™ analyses. Results from these 2 sampling and analytical methods, also summarized in Table 4-5, are in fairly good agreement for propanone and toluene. The reported concentrations of propanenitrile, n-butanenitrile, benzene, n-hexane, n-heptane, and n-decane in TST samples are moderately higher than the SUMMA™ sample analytical quantitation limit, yet were not reported as being present in the SUMMA™ samples.

The largest discrepancy between the target analyte results from the 2 methods is for ethanenitrile, which was determined to be present at 0.20 ppmv in TST samples, and 0.023 ppmv in SUMMA™ samples. None of these compounds, however, even assuming the higher concentrations to be correct, are at or above levels of concern.

The most abundant analytes in Tables 4-1 through 4-4 are 1-butanol, ethanenitrile, and propanone, each of which was measured to have an average concentration of between 0.1 and 1 ppmv in TST samples. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

4.2 Tentatively Identified Organic Compounds

In addition to the target analytes, the ORNL and PNL analytical procedures allow the tentative identification of other organic compounds. Tentative identification of analytes was performed by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and may also determine its molecular weight. The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Using this method, many analytes can be tentatively identified with reasonable confidence without having to inject 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 list of tentatively identified compounds recovered from SUMMA™ samples, with estimated concentrations, is given in Table 4-6. Compounds are listed in Table 4-4 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table 4-7. Compounds are listed in Table 4-7 according to the order by which they eluted chromatographically. The averages reported by ORNL in Table 4-7 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Clauss et al. (1995), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-6 and 4-7 should be considered rough estimates.

4.3 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-5 is to separate them into 2 categories: 1) Organic compounds added to tank U-111 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes the semivolatile straight-chain alkanes, which were used as diluents of tributyl phosphate in various plutonium extraction processes. These alkanes (i.e., n-undecane, n-dodecane, n-tridecane, n-tetradecane, and n-pentadecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs). Though NPHs are positively identified in tank U-111, their concentrations are very low compared to other NPH-rich tanks.

Tributyl phosphate was also added to the tank as waste. The measured concentration of tributyl phosphate in the tank U-111 samples may not be representative of its headspace concentration. Informal tests by ORNL indicate that tributyl phosphate is adsorbed by the glass fiber filters used during sampling to protect the samples from radiolytic particulate contamination. This would result in loss of tributyl phosphate from the sampled air, and an underestimation of its actual concentration in the tank headspace.

The tentatively identified cyclosiloxanes (i.e., Cmpd # 11 and 16 in Table 4-5) are also in this category. Small quantities of siloxanes may have been introduced to the waste tank through their use as defoaming agents, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables 4-1 through 4-5 fall into this category, including the alcohols, aldehydes, ketones, nitriles, and volatile alkanes, all of which have been associated with the degradation of the NPHs. 1-Butanol is known to be a product of the hydrolysis of tributyl phosphate.

Though not present in high concentrations, 6 straight-chain alkyl nitriles were identified in TST samples. Nitrogen-containing cyclic compounds were also detected in both SUMMA™ and TST samples, including pyridine, pyrazine, and 2 oxazoles.

On the basis of concentrations, alcohols are the dominate type of organic compounds in the tank U-111 headspace. Methanol, ethanol, 1-propanol, 2-propanol, and 1-butanol account for about 79 % of the total estimated concentration of organic compounds in TST samples. Similarly, about 76 % of the total estimated organic compound concentration in SUMMA™ samples is due to methanol, 1-propanol, 2-propanol, and 1-butanol. Ethanol was not detected in the SUMMA™ samples from tank U-111. The abundance of volatile alcohols is common to tanks U-106, U-107, and U-111. Also similar to tanks U-106 and U-107, and in contrast to tanks having higher NPH concentrations, tank U-111 has relatively few ketones.

The total organic vapor concentration of tank U-111 was estimated by Jenkins et al. (1995a) to be about 9.1 mg/m³ from the analysis of 3 TST samples by GC/MS. A similar summation of organic compounds measured in SUMMA™ samples from tank U-111 provides an estimated total organic vapor concentration of 4.3 mg/m³. This disagreement is largely due to the different estimated concentrations of the dominant alcohols in the 2 sample types.

Ambient air SUMMA™ samples collected during the tank U-111 sampling event suggest the VSS manifold may have been contaminated with trace amounts of propanone. Specifically, analysis of an ambient air sample collect upwind of the VSS (not through the VSS manifold) indicated propanone to be present at < 0.005 ppmv, while an ambient air sample collected through the VSS (to check system cleanliness) was determined to have about 0.0077 ppmv of propanone. Residual amounts of propanone, used as a cleaning solvent, may have been present in the VSS transfer tubing.

In summary, the organic vapor concentrations in tank U-111 are relatively low. The organic vapors in tank U-111 clearly indicate the presence of tributyl phosphate, the semivolatile NPHs and their degradation products in the tank waste. As with the other 241-U farm tanks that have been sampled, the concentrations of short-chain alcohols are higher in tank U-111 than in waste tanks with higher NPH vapor concentrations. Conversely, ketones and aldehydes are less abundant in tank U-111 than in NPH-rich waste tanks.

5.0 SUMMARY

The tank U-111 headspace was sampled in February 1995 for gases and vapors to address flammability and industrial hygiene concerns. Results of sample collection and analysis have been reported. It was determined that no headspace constituents exceeded the flammability notification limit, but that ammonia, measured to be an average 676 ppmv, did exceed its 150 ppmv industrial hygiene notification limit specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank U-111 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device ¹	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.2	Organic vapors	4 tank air samples
		1.0	Organic vapors	4 tank air samples
		4.0	Organic vapors	4 tank air samples
				+ 2 trip blanks + 2 field blanks
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blank
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blank
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blank
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Carbon Dioxide, Carbon Monoxide, Hydrogen, Methane, Nitrous Oxide, Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

¹ Sampling Temperature ~ 60°C

Table 3-1
Tank U-111 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	676	6	0.9
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	< 64	--	--
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 12	--	--
Hydrogen, H ₂	1333-74-0	SUMMA™	3	247	3	1.2
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.04	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.01	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	327	10	2.9
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	15,100 (11.3 mg/L)	440 (0.3 mg/L)	2.9

1 CAS = Chemical Abstracts Service.

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

Table 4-1
Tank U-111 Quantitatively Measured Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.023	0.003	13
2	Propanone (acetone)	67-64-1	0.076	0.007	10
3	Trichlorofluoromethane	75-69-4	0.014	0.001	10
4	Propanol	71-23-8	0.020	0.005	27
5	2-Butanone	78-93-3	0.019	0.0002	1.5
6	Tetrahydrofuran	109-99-9	0.020	0.0003	1.5
7	Cyclohexane	110-82-7	0.020	0.0003	1.5
8	Pyridine	110-86-1	0.0069	0.0008	11
9	Toluene	108-88-3	0.030	0.0004	1.3
10	Methane	74-82-8	< 12	—	—
Sum of positively identified compounds:			0.71	mg/m ³	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples.

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

Table 4-2
Tank U-111 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	0.20	0.03	17
2	Propanone (acetone)	67-64-1	0.11	0.03	25
3	Toluene	108-88-3	0.026	0.002	8
4	n-Dodecane	112-40-3	0.0042	0.0001	3
5	n-Tridecane	629-50-5	0.0086	0.0005	6

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

Table 4-3
Tank U-111 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	0.0073	0.0008	11
2	n-Hexane	110-54-3	0.004	0.0001	3
3	Benzene	71-43-2	0.0057	0.0017	29
4	n-Butanenitrile	109-74-0	0.0093	0.0006	7
5	n-Heptane	142-82-5	0.0040	0.0001	3
6	n-Pentanenitrile	110-59-8	0.00083	0.00011	14
7	2-Hexanone	591-78-6	0.0014	0.0001	8
8	n-Octane	111-65-9	0.0018	0.0001	6
9	n-Hexanenitrile	628-73-9	0.00070	0.00013	20
10	2-Heptanone	110-43-0	0.0013	0.0002	11
11	n-Nonane	111-84-2	0.0010	0.00004	4
12	n-Heptanenitrile	629-08-3	0.00038	0.00006	15
13	2-Octanone	111-13-7	0.00057	0.00005	8
14	n-Decane	124-18-5	0.0012	0.00001	1
15	n-Undecane	1120-21-4	0.0013	0.0001	5
16	Tributyl phosphate	126-73-8	0.00040	0.00060	151

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

Table 4-4
Tank U-111 Positively Identified Organic Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Butanal ⁵	123-72-8	0.016	0.0004	3
2	1-Butanol ⁶	71-36-3	0.26	0.01	4
3	2-Pentanone ⁶	107-87-9	0.0022	0.0004	16

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

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

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

Table 4-5
Tank U-111 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Oak Ridge National Laboratory
and Pacific Northwest Laboratory

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	RPD ⁴ (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.0023	< 0.005	—
Dichloromethane (methylene chloride)	75-09-2	< 0.0053	< 0.005	—
Propanone (acetone)	67-64-1	0.11	0.076	36
Ethanenitrile (acetonitrile)	75-05-8	0.20	0.023	159
Propanenitrile	107-12-0	0.0073	< 0.005	> 37
n-Butanenitrile	109-74-0	0.0094	< 0.005	> 61
Benzene	71-43-2	0.0057	< 0.005	> 13
Toluene	108-88-3	0.026	0.030	14
n-Hexane	110-54-3	0.0042	< 0.005	—
n-Heptane	142-82-5	0.0040	< 0.005	—
n-Decane	124-18-5	0.0013	< 0.005	—

1 CAS = Chemical Abstract Service.

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

3 Average of 3 samples by PNL.

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

Table 4-6
Tank U-111 Tentatively Identified Organic Compounds in SUMMA™ Samples--
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Propane	74-98-6	0.20	0.01
2	Methanol (methyl alcohol)	67-56-1	2.98	0.20
3	n-Butane	106-97-8	0.070	0.007
4	2-Propanol (isopropyl alcohol)	67-63-0	0.19	0.01
5	2-Butanol	78-92-2	0.072	0.002
6	N-Nitrosodimethylamine	62-75-9	0.042	0.007
7	Pyrazine	290-37-9	0.035	0.004
Sum of tentatively identified compounds:			3.59	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples. The values given are estimates.

Table 4-7
Tank U-111 Tentatively Identified Organic Compounds in TST Samples
in Order of Chromatographic Elution –
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1.	Methanol (methyl alcohol)	67-56-1	2.49	0.49
2	Ethanol	64-17-5	3.55	0.34
3	2-Propanol (isopropyl alcohol)	67-63-0	0.17	0.02
4	1-Propanol	71-23-8	0.072	0.002
5	Furan, tetrahydro-	109-99-9	0.043	0.046
6	1,4-Dioxane	123-91-1	0.048	0.011
7	Pyrazine	290-37-9	0.15	0.06
8	N-Nitrosodimethylamine	62-75-9	0.14	0.03
9	Propylene Glycol	57-55-6	0.020	0.034
10	Pentanal, 3-methyl-	15877-57-3	0.19	0.05
11	Cyclotrisiloxane, hexamethyl-	541-05-9	0.044	0.019
12	Oxazole, 4,5-dihydro-2-methyl- & C2 Benzene		0.011	0.019
13	Ethylbenzene	100-41-4	0.011	0.018
14	p-Xylene	106-42-3	0.0079	0.0137
15	Octanal	124-13-0	0.0095	0.0165
16	Cyclotetrasiloxane, octamethyl-	556-67-2	0.036	0.010
17	1-Hexanol, 2-ethyl-	104-76-7	0.031	0.002
18	Oxazole, 4,5-dimethyl-2-propyl-	53833-32-2	0.019	0.016
19	Benzyl Alcohol	100-51-6	0.016	0.014
20	n-Tetradecane	629-59-4	0.052	0.005
21	Benzenesulfonamide, n-butyl-	3622-84-2	0.094	0.019
22	Isopropyl Palmitate	142-91-6	0.012	0.021
Sum of tentatively identified compounds:			7.21	

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples by ORNL. The values given are estimates.