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TANK 241U105 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
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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.

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Tank 241-U-105 Headspace Gas and Vapor Characterization Results for Samples Collected in February 1995

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**Tank 241-U-105 Headspace Gas and Vapor Characterization Results
for Samples Collected in February 1995**

September 17, 1995

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Multimedia Exposure Assessment
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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%
TNMOC	Total Nonmethane Organic Compounds
TST	triple sorbent trap
vol%	percent by volume, 1 vol% = 10,000 ppmv
VSS	vapor sampling system
WHC	Westinghouse Hanford Company
wt%	percent by weight

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**Tank 241-U-105 Headspace Gas and Vapor Characterization Results
for Samples Collected in February 1995**

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank U-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 U-105 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 was collected to help in the evaluation of 1) headspace flammability, and 2) identification and quantification of compounds of toxicological concern.

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1994). However, current governing operating specifications for single shell waste listed waste tanks, such as tank U-107 specify that combustible constituents be maintained at or below 20 % of the LFL (WHC 1995a).

Headspace characterization data are used by Westinghouse Hanford Company (WHC) Tank Waste Remediation Systems Industrial Hygiene as source term data in the industrial hygiene strategy to protect workers from tank fugitive emissions. Because selection of worker protective equipment must be based on industrial hygiene monitoring of the work place and not on source term data (29 CFR 1910.120), tank headspace characterization data can not be used for this purpose. Furthermore, because there are mechanisms by which headspace constituents can be either diluted or concentrated as they are released to the atmosphere, the headspace characterization data should not be considered to be representative of emissions at the point of emission.

These statements notwithstanding, the data quality objectives document specifies that the industrial hygiene group be advised if constituents with toxicological properties exceed 50 % of the appropriate consensus exposure standard (CES) for non-carcinogens, or 10 % of the appropriate CES for carcinogens. A CES is defined as the most stringent of known regulatory or recommended toxicological values for the workplace (Osborne et al. 1994).

1.3 Sampling Overview

Tank headspace characterization data presented here are from a single sampling event. Samples collected are thought to have been representative of the tank U-105 headspace when the tank was sampled, and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents (Meacham et al. 1995). No assessment has been made of how the tank U-105 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-105 is the second tank in a 3-tank cascade with tanks U-104 and U-106. It is connected to tanks U-104 and U-106 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-104 or tank U-106 may be transferred to tank U-105 (unless the cascade lines are obstructed). Section 3.4 briefly compares the headspace constituents of tanks U-105 and U-106 and discusses the potential transfer of gases and vapors to tank U-105. At this time there are no comparable headspace characterization data for tank U-104.

The cascade of tanks U-104, U-105, and U-106 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-105 using the vapor sampling system (VSS) on February 24, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-U-105 Tank Characterization Plan* (Horn 1995). The tank headspace temperature was determined to be 42.6 °C. Air from the U-105 headspace was withdrawn from a single elevation via a 6.1-m long heated sampling probe mounted in riser 9, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. All tank air samples were collected between 11:27 a.m. and 2:56 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 and Babad (1995). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody information, and a discussion of the sampling event itself are given in WHC 1995b.

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions and are given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were prepared and analyzed by PNL at quality assurance impact level 2 (Pool et al. 1995).

Inorganic sorbent trap analyses were performed within 13 days of sample collection, but analyses of SUMMATM canisters for inorganic compounds were completed until 75 days after sample collection (Ligotke 1995). The latter exceeded the administratively chosen holding time specified in the WHC quality assurance project plan (Keller 1994). However, it should be noted that the inorganic compounds sampled by SUMMATM canisters (i.e., the permanent gases) would be expected to be very stable in the SUMMATM canisters, and the results may not have been affected even though the 60-day holding time requirement was exceeded.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Analysis of 6 ammonia sorbent trap samples from tank U-105 indicated the ammonia concentration to be 325 ppmv. This is a moderately high ammonia concentration compared to other waste tanks that have been vapor sampled. 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. 1995a). Given the LFL of ammonia in air is about 15 by volume (vol%), the measured 325 ppmv corresponds to about 0.2 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank U-105 was determined to be < 49 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the lower flammability limit (LFL) for hydrogen in air is about 4 % by volume, < 49 ppmv hydrogen concentration in tank U-105 corresponds to less than about 0.1 % of its LFL. At this level, hydrogen is not a flammability concern in tank U-105.

The average nitrous oxide concentration in 3 SUMMATM samples from tank U-105 was determined to be 154 ppmv. Nitrous oxide is commonly detected in other waste tanks. The 154 ppmv of nitrous oxide measured in tank U-105 is typical of other passively ventilated waste tanks that have been sampled. In the passively ventilated tanks, nitrous oxide has been measured at concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995a), and as high as 878 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-105 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank U-105 headspace was measured to be < 23 ppmv in each of the 3 SUMMATM samples. 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

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

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 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-105 headspace, reported by PNL as < 23 ppmv in each of the 3 SUMMA™ samples, 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-105 gas and vapor sampling event, for example, were measured to have an average 367 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 < 23 ppmv of carbon dioxide characterization of the tank U-105 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-105 headspace were determined to be ≤ 0.03 and ≤ 0.002 ppmv, respectively. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank U-105. 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-105 headspace.

The water vapor concentration of tank U-105 was determined to be about 11.9 mg/L, at the measured tank headspace temperature of 42.6 °C and pressure of 992 mbar (744.2 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 17.2 mbar (12.9 torr), to a dew point of 15.2 °C, and to a relative humidity of about 20 %. In terms of relative humidity, presuming there is no error in water vapor measurement, tank U-105 is unusually dry compared to other tanks that have been sampled.

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-105 headspace are nitrous oxide, ammonia, and hydrogen. These have been detected in most tank headspaces sampled to date, and are usually the dominant gaseous species. Though the 325 ppmv of ammonia in tank U-105 is high compared to most other waste tanks, tank U-105 has the lowest ammonia concentration of the 5 tanks in

² The carbon monoxide measurement in tank C-103 was made by Oregon Graduate Institute of Science and Technology, and have been placed in brackets to indicate it should be considered secondary data.

241-U farm that have been sampled. Tanks U-103, U-106, U-107, and U-111 had measured ammonia concentrations of 730, 988, 453, and 676 ppmv, respectively (Ligotke et al. 1995, Klinger et al. 1995b, McVeety et al. 1995b, Clauss et al. 1995). Similarly, tank U-105 has the lowest concentrations of nitrous oxide and hydrogen of the 5 sampled 241-U farm tanks.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are good for the methods used. Relative standard deviations range from about 1.1 % for water vapor to about 9 % for ammonia. 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.

As discussed in Section 1.4, the headspaces of tanks U-104 and U-106 are both connected to the tank U-105 headspace by underground cascade lines. No headspace characterization data for tank U-104 are available at this time to assess possible transport of constituents from tank U-104 to tank U-105, however, the tank U-106 headspace has been sampled. Selected data for tanks U-105 and U-106 are presented in Table 3-2 for comparison. Consideration of the data in Table 3-2 indicates that while tank U-105 does not breathe solely via tank U-106, the possibility that the much of the waste vapors are coming from tank U-106 can not be excluded.

4.0 ORGANIC VAPORS

Organic vapors in the tank U-105 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both laboratories used a gas chromatograph (GC) equipped with a mass spectrometer (MS) detector to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995) and Pool et al. (1995).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank U-105. These results were produced at PNL quality assurance impact level 2. PNL analyses of organic compounds in SUMMA™ were not complete until 76 days after sample collection, and exceeded the administratively chosen 60-day holding time (Keller 1994). No holding time study has been performed to address the stability of organic compounds in SUMMA™ canisters in the chemical matrix of the waste tank samples. Ambient air SUMMA™ samples collected during the tank U-105 sampling event suggest that neither the VSS manifold nor the ambient air itself contained organic contaminants at detectable levels.

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 analyzed 4 of the 12 TST tank samples, 1 of the 2 TST field blanks, and 1 of the 2 TST trip blanks. ORNL used a single 1.0 L TST tank sample to estimate the concentration of organic vapors sampled. Because the measured organic vapor concentrations were relatively low, the 4.0 L TST tank samples were analyzed in triplicate for analyte identification and quantification.

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 surrogate recovery standard deviation values were within the 95 % confidence interval for variance, indicating that no bias was introduced in the measurement of analyte quantities (Jenkins 1995a).

4.1 Positively Identified Organic Compounds

Positive identification of organic analytes using the methods employed by PNL and ORNL involves matching the GC retention times and MS data from a sample with that obtained 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.

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ samples by PNL. SUMMA™ analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Pool et al. 1995). Only 2 of the 39 TO-14 target analytes and 5 of the 14 additional target analytes were measured to be above the 0.005 ppmv detection limit of the analyses. Averages reported are from analyses of 3 SUMMA™ canister samples.

Jenkins et al. (1995) report the positive identification of 23 of 27 target analytes in TST samples. 1,1-Dichloroethene, dichloromethane, butanal, and hexanenitrile were the only TST target analytes not detected. ORNL reported the positive identification of tributyl phosphate and dibutyl butylphosphonate, but their concentrations of these were not quantitatively measured. Both tributyl phosphate and dibutyl butylphosphonate were estimated to be present at less than 0.0001 ppmv.

Despite calibration of the instrument over about a 20-fold concentration range, only 2 analytes (ethanenitrile and propanone) were measured to be within the instrument calibration range in all 4 TST samples. The average concentrations for positively identified analytes in TSTs are given in Tables 4-2, 4-3, and 4-4. Table 4-2 lists the 2 quantitated analytes, Table 4-3 lists the positively identified analytes for which at least 1 sample result was outside the instrument calibration range (i.e., not quantitated), and Table 4-4 lists the 2 analytes determined to have exceeded their ORNL practical holding times. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables.

The ORNL practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. As indicated in Table 4-4, butanal and 1-butanol exceeded their practical holding times, and may have been affected by the 46 day period between sample collection and analysis (Jenkins 1995b). Jenkins et al. (1995b) describe the ORNL practical holding time study, and report the practical holding times of butanal, 1-butanol, and 2-pentanone are 1, 17, and 34 days, respectively. It is possible that 2-pentanone was not identified in the tank U-105 TST samples because the practical holding time for this compound was exceeded. It should be noted that the contractual holding time for the TST samples was 60 days.

Analysis of the trip and field blanks indicated 7 of the TST target analytes and 3 other compounds to be present as contaminants of the TST samples. ORNL identified the probable source of contamination as being improperly cleaned equipment used to spike the TSTs with surrogate compounds. Contaminants were estimated to account for 4 to 22 % of the observed sample levels of propanone, benzene, toluene, n-nonane, n-undecane, n-dodecane, and n-tridecane. No correction of the results in Tables 4-2, 4-3, or 4-4 has been attempted. Jenkins et al. (1995a) provide details of the trip and field blank results.

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-105 and obtain concentration in ppmv of analyte in moist tank air, multiply the dry-air ppmv concentrations by 0.985.

Eleven target analytes were common to both TST and SUMMA™ analyses. Table 4-5 lists these, and their reported average concentrations in TST and SUMMA™ samples. Only 2 of these analytes were detected in either type of sample above the 0.005 ppmv analytical detection limit of the SUMMA™ analyses. Results from the TST and SUMMA™ sample analyses for these 2 analytes, propanone and ethanenitrile, are in reasonably good agreement.

The most abundant analytes listed 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 0.03 and 0.1 ppmv. 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 SUMMATM samples. Analyses of the samples are designed to recover, separate, and identify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (e.g., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (e.g., butanal) from SUMMATM samples has been problematic.

The list of tentatively identified compounds recovered from SUMMATM samples, with estimated concentrations, is given in Table 4-6. Compounds are listed in Table 4-6 in order of decreasing estimated concentration, 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 in the order by which they eluted chromatographically. The averages reported by ORNL in Table 4-7 are all 4-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/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. (1995) and Pool et al. (1995), respectively, and should be reviewed before this data is 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-105 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

Organic vapors in the first category (those that were placed into the tank as waste) include the semivolatile straight-chain alkanes, which were used as diluents of tributyl phosphate in various plutonium extraction processes. These alkanes (i.e., n-undecane, n-dodecane, n-tridecane, and n-tetradecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs). Though NPHs are positively identified in tank U-105, their concentrations are very low compared to other NPH-rich tanks.

Tributyl phosphate and dibutyl butylphosphonate are also in the category of compounds added as waste. Tributyl phosphate was used as an extractant in several processes, and dibutyl butylphosphonate was a known contaminant of the tributyl phosphate. Their estimated < 0.0001 ppmv concentrations in TST samples by ORNL may not be representative of their headspace concentrations. 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 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 4-7 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, 5 straight-chain alkyl nitriles were identified in TST samples. Several nitrogen-containing heterocyclic compounds were also detected TST samples, namely pyrazine, 2-ethyl aziridine, 2-pyrrolidinone, and 4,5-dihydro-2-methyl oxazole.

On the basis of concentrations, alcohols are the dominant type of organic compounds in the tank U-105 headspace. Methanol and ethanol account for about 77 weight percent (wt%) of the total estimated concentration of organic compounds in TST samples. Similarly, about 72 wt% of the total estimated organic compound concentration in SUMMATM samples is due to methanol. Ethanol was not detected in the SUMMATM samples from tank U-105. The abundance of volatile alcohols is common to tanks U-103, U-106, U-107, and U-111 (Huckaby 1995a, 1995b, 1995c, 1995d). Also like these other 241-U farm tanks, and in contrast to tanks having higher NPH concentrations, tank U-105 has very low concentrations of aldehydes.

The total organic vapor concentration of tank U-105 was estimated by Jenkins et al. (1995) to be about 4.4 mg/m³ from the analysis of 4 TST samples by GC/MS. A similar summation of organic compounds measured in SUMMATM samples from tank U-105 provides an estimated total organic vapor concentration of 3.0 mg/m³. This disagreement is largely due to the different estimated concentrations of the dominant alcohols in the 2 sample types.

In summary, the organic vapor concentrations in tank U-105 are relatively low. The organic vapors in tank U-105 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 sampled to date, the concentrations of short-chain alcohols are higher in tank U-105 than in waste tanks with higher NPH vapor concentrations. Conversely, aldehydes are less abundant in tank U-105 than in NPH-rich waste tanks.

5.0 SUMMARY

The tank U-105 space was sampled in February 1995 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the sampling event and essentially all results have been reported. It was determined that no headspace constituents exceeded the flammability notification limits, but that ammonia, measured to be 325 ppmv, exceeded the 150 ppmv industrial hygiene notification limit specified in the current *Vapor Sampling and Analysis Plan* (Horn 1995).

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Table 2-1
Tank U-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	0.2	Organic vapors	4 tank air samples
		1.0	Organic vapors	4 tank air samples
		4.0	Organic vapors	4 tank air samples
				+ 2 trip blanks + 2 field blanks
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blank
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blank
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blank
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Carbon Dioxide, Carbon Monoxide, Hydrogen, Methane, Nitrous Oxide, Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank U-105 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	325	28	9
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	< 23	--	--
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	< 23	--	--
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	< 49	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.03	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.002	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	154	2.5	2
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	17,400 (11.9 mg/L)	200 (0.1 mg/L)	1.1

¹ CAS = Chemical Abstracts Service.

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

Table 3-2
Comparison of Tank U-105 and U-106 Headspace Constituents --
Inorganic Analyses by Pacific Northwest Laboratory
and Organic Analyses by Oak Ridge National Laboratory¹

Tank:	U-105	U-106 ²
Date sampled, (mo/day/yr)	2/24/95	3/7/95
Headspace temperature, (°C)	42.6	21.9
Ammonia, (ppmv)	325	988
Hydrogen, (ppmv)	< 49	210
Carbon dioxide, (ppmv)	< 23	46.5
Carbon monoxide, (ppmv)	< 23	< 12
Nitric oxide, (ppmv)	≤ 0.03	≤ 0.04
Nitrogen dioxide, (ppmv)	≤ 0.002	≤ 0.04
Nitrous oxide, (ppmv)	154	559
Water vapor, (mg/m ³)	11.9	12.9
Water vapor, (% relative humidity)	20	67
Ethanenitrile (acetonitrile), (ppmv)	0.037	(0.10)
Propanone (acetone), (ppmv)	0.033	0.064
1-Butanol, (ppmv)	(0.096)	(0.51)
n-Dodecane, (ppmv)	(0.0012)	0.0022
n-Tridecane, (ppmv)	(0.0046)	0.0046
Total estimated organic vapor ³ (mg/m ³)	(4.4)	(10.1)

1 Organic vapor results are from ORNL, with non-quantitated values in parentheses and quantitative values not in parentheses.

2 Data are from Huckaby 1995b.

3 This value is the summation of quantitated and estimated organic vapor concentrations in ORNL TST samples.

Table 4-1
Tank U-105 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	75-05-8	0.017	0.001	8
2	Propanone	67-64-1	0.037	0.003	9
3	Trichlorofluoromethane	75-69-4	0.032	0.001	4
4	Propanol	71-23-8	0.010	0.004	43
5	2-Butanone ⁴	78-93-3	0.0065	—	—
6	Tetrahydrofuran	109-99-9	0.012	0.0004	3
7	Toluene	108-88-3	0.006	0.0001	2
8	Methane	74-82-8	< 23	—	—
Sum of positively identified compounds:			0.43	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 %.

4 Detected in only 1 sample.

Table 4-2
Tank U-105 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	0.037	0.007	20
2	Propanone (acetone)	67-64-1	0.033	0.015	45

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

2 CAS = Chemical Abstract Service.

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

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

Table 4-3
Tank U-105 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	0.0029	0.0008	27
2	n-Hexane	110-54-3	0.0022	0.0002	11
3	Benzene	71-43-2	0.0017	0.0005	28
4	n-Butanenitrile	109-74-0	0.0032	0.0009	29
5	n-Heptane	142-82-5	0.0018	0.0008	46
6	Toluene	108-88-3	0.0047	0.0020	43
7	n-Pentanenitrile	110-59-8	0.00031	0.00010	33
8	2-Hexanone	591-78-6	0.00063	0.00012	19
9	n-Octane	111-65-9	0.00038	0.00008	20
10	2-Heptanone	110-43-0	0.00051	0.00027	54
11	n-Nonane	111-84-2	0.00051	0.00027	53
12	n-Heptanenitrile	629-08-3	0.00028	0.00018	64
13	2-Octanone	111-13-7	0.00040	0.00024	62
14	n-Decane	124-18-5	0.00029	0.00002	67
15	n-Undecane	1120-21-4	0.00064	0.00038	60
16	n-Dodecane	112-40-3	0.0012	0.0007	61
17	n-Tridecane	629-50-5	0.0046	0.0031	68

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples: 3 were 2-L and 1 was 6-L.

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

Table 4-4
Tank U-105 Positively Identified 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	1-Butanol ⁵	71-36-3	0.096	0.028	29
2	2-Pentanone ⁵	107-87-9	0.00085	0.00042	49

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples: 3 were 2-L and 1 was 6-L.

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.

Table 4-5
Tank U-105 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)	PRD ⁴ (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.00058	< 0.005	--
Dichloromethane (methylene chloride)	75-09-2	< 0.0013	< 0.005	--
Propanone (acetone)	67-64-1	0.033	0.037	11
Ethanenitrile (acetonitrile)	75-05-8	0.037	0.017	74
Propanenitrile	107-12-0	0.0029	< 0.005	--
n-Butanenitrile	109-74-0	0.0032	< 0.005	--
Benzene	71-43-2	0.0017	< 0.005	--
Toluene	108-88-3	0.0047	0.006	24
n-Hexane	110-54-3	0.0022	< 0.005	--
n-Heptane	142-82-5	0.0018	< 0.005	--
n-Decane	124-18-5	0.00029	< 0.005	--

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples; 3 were 2-L and 1 was 6-L.

3 Average of 3 samples analyses.

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

Table 4-6
Tank U-105 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Methanol (methyl alcohol)	67-56-1	2.19	0.19
2	Propane	74-98-6	0.25	0.01
3	1-Butanol	71-36-3	0.11	0.01
4	1-Propene, 2-methyl- ³	115-11-7	0.05	—
Sum of tentatively identified compounds:			2.6	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples by PNL, presented values are estimates.

3 Detected in only 1 sample.

Table 4-7
 Tank U-105 Tentatively Identified Organic Compounds in TST Samples
 in Order of Chromatographic Elution --
 Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-Propene, 2-methyl-	115-11-7	0.0048	0.0095
2	Methyl Alcohol	67-56-1	0.69	0.49
3	Hydrazine, 1,1-dimethyl and nitric oxide		0.012	0.023
4	Ethanol	64-17-5	2.71	0.72
5	Trichloromonofluoromethane	75-69-4	0.042	0.084
6	Pyrazine	290-37-9	0.12	0.03
7	N-Nitrosodimethylamine	62-75-9	0.069	0.050
8	Propylene Glycol	57-55-6	0.0083	0.0166
9	Aziridine, 2-ethyl	2549-67-9	0.055	0.042
10	Cyclotrisiloxane, hexamethyl	541-05-9	0.026	0.044
11	Oxazole, 4,5-dihydro-2-methyl-	1120-64-5	0.0057	0.0115
12	Propane, 1-chloro-2,2-dimethyl-	753-89-9	0.0044	0.0089
13	Cyclotetrasiloxane, octamethyl	556-67-2	0.012	0.024
14	2-Pyrrolidinone and others		0.0083	0.0097
15	trans-Undec-4-enal and others		0.014	0.009
16	Tetradecane and others		0.0051	0.0101
17	Benzenesulfonamide, N-butyl	3622-84-2	0.013	0.009
Sum of tentatively identified compounds:			3.80	

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 2-L and 1 was 6-L, presented values are estimates.