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7. Abstract

Tank 241-U-106 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. The drivers and objectives of waste tank headspace sampling and analysis are discussed in "Program Plan for the Resolution of Tank Vapor Issues" (Osborne and Huckaby 1994). Tank 241-U-106 was vapor sampled in accordance with "Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution (Osborne et al., 1994).


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# Tank 241-U-106 Vapor Sampling and Analysis Tank Characterization Report

## X.0 INTRODUCTION

Tank U-106 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-106 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

Gas and vapor samples were collected from tank U-106 on August 25, 1994 using the *in situ* sampling (ISS) method (Pingel 1994), and again on March 7, 1995 using the more robust vapor sampling system (VSS) method (WHC 1995). Analytical results from the 2 sampling events are similar but not identical. Differences in the results may be attributed to the less accurate sample air flow measurement of the ISS equipment, and various differences in the sampling methods. Because the VSS method has been more thoroughly tested and its limitations are better understood, nearly all of results presented here are from the March 7, 1995 VSS sampling event.

One of the organic vapor samples from the August 25, 1994 ISS event was determined to have trace levels of methyl isocyanate. This compound would not be expected to be stable in the high-ammonia, high-humidity headspace of tank U-106, and may actually have been an artifact of the analytical method. Nevertheless, extra samples were collected on March 7, 1995 to address the possible existence of methyl isocyanate in tank U-106. No discussion of methyl isocyanate is presented in this report, pending a review of all data by WHC.

## X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank U-106 using the VSS on March 7, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-U-106 Tank Characterization Plan* (the TCP), (Homi 1995). The tank headspace temperature was determined to be 21.9 °C. Air from the U-106 headspace was withdrawn from a single elevation via a 7.3-m long heated sampling probe mounted in riser 2, 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 10:27 a.m. and 3:47 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 46 tank air samples and 2 ambient air control samples collected are listed in Table X-

1 by analytical laboratory. Table X-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 (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 and references therein.

## X.2 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA™,[1] canister tank air samples for selected inorganic gases and vapors are given in Table X-2 in parts per million by volume (ppmv). Inorganic analyte sorbent traps and SUMMA™ canisters were prepared and analyzed by PNL (Klinger et al. 1995a).

### X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 988 ppmv, is the second highest measured in any waste tank to date. It is nearly 40 times the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv for ammonia (NIOSH 1995). 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).

The concentration of hydrogen in tank U-106 was determined to be 210 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, 210 ppmv hydrogen concentration in tank U-106 corresponds to less than 0.6 % of its LFL. At this level, hydrogen is not a flammability concern in tank U-106.

The nitrous oxide concentration in tank U-106, 559 ppmv, is the among highest measured in any waste tank to date. It is more than 22 times the NIOSH 8-hr REL of 25 ppmv for nitrous oxide (NIOSH 1995). Nitrous oxide, also known as laughing gas, has been detected in other passively ventilated waste tanks at average concentrations as low as about 12 ppmv in tank TX-105 (Klinger 1995b), and as high as 763 ppmv in tank C-103 (Huckaby and Story 1994).

### X.2.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank U-106 headspace, characterized as < 12 ppmv, is below the NIOSH 8-hr REL of 35 ppmv for carbon monoxide. 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,

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

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-103 (Huckaby and Story 1994).

The average carbon dioxide concentration in the tank U-106 headspace, 46.5 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. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. The 46.5 ppmv of carbon dioxide measured in tank U-106 is within the range of typical values for the waste tanks sampled to date.

### X.2.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank U-106 headspace were both determined to be $\leq$ 0.04 ppmv. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank U-106. 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. The NIOSH 8-hr REL is 25 ppmv for nitric oxide, and the 15-minute short term exposure limit (STEL) for nitrogen dioxide is 1 ppmv.

The water vapor concentration of tank U-106 was determined to be about 12.9 mg/L, at the measured tank headspace temperature of 21.9 °C and pressure of 995.5 mbar (746.8 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 17.5 mbar (13.2 torr), to a dew point of 15.4 °C, and to a relative humidity of 67 %.

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 1995).

### X.2.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor, the most abundant waste constituents in the tank U-106 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. Ammonia in tank U-106 is particularly high compared to other waste tanks.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table X-2 are excellent for the methods used. Relative standard deviations range from about 1.1 % for water vapor to 3 % for ammonia and hydrogen 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.

## X.3 ORGANIC VAPORS

Organic vapors in the tank U-106 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Gas chromatography (GC) and mass spectroscopy (MS) 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 Jenkins et al. (1995) and Klinger et al. (1995a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank U-106. 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.

### X.3.1 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 from 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. In addition to these customary target analytes, positive identification of methyl isocyanate in both SUMMA™ and TST samples was sought.

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-106 and obtain concentration in ppmv of analyte in moist tank air, multiply by 0.983.

Table X-3 lists the organic compounds positively identified and quantitated in SUMMA™ samples. SUMMA™ analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Klinger et al. 1995a). Only 2 of the 39 TO-14 target analytes and 3 of the 15 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 22 of 27 target analytes in TST samples. 1,1-Dichloroethene, dichloromethane, butanal, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected. The average concentrations of the detected target analytes, from the analysis of 4 TSTs, are given in Table X-4. Despite calibration of the instrument over about a 20-fold concentration range, 1-butanol in the TST samples was above the upper calibration limit, and 6 other compounds listed in Table X-4 were below the lower calibration range in at least 2 of the TST samples.

Eleven target analytes were common to both TST and SUMMA™ analyses. Table X-5 lists these, and their reported average concentrations in TST and SUMMA™ samples. Results from these 2 sampling and analytical methods are in fairly good agreement for acetone, and in very good agreement for toluene. As indicated in Table X-5, the reported concentrations of propanenitrile, benzene, n-hexane, and n-heptane in TST samples are moderately higher than the SUMMA™ sample analytical detection 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 acetonitrile, which was determined to be present at 0.10 ppmv in TST samples, and < 0.005 ppmv in SUMMA™ samples. None of these compounds, however, even assuming the higher concentrations to be correct, are at or above levels of concern. Benzene and acetonitrile have the lowest NIOSH RELs of the identified compounds in Table X-5, being 0.1 and 20 ppmv, respectively.

The most abundant analytes in Tables X-3 and X-4 are 1-butanol, n-tridecane, acetone, and n-dodecane, each of which was measured to be above 1 ppmv. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

### X.3.2 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. 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, identify, and quantify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (i.e., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (i.e., butanal) from SUMMA™ samples has been problematic.

The list of tentatively identified compounds recovered from SUMMA™ samples, with estimated concentrations, is given in Table X-6. Compounds are listed in Table X-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table X-7. Compounds are listed in Table X-7 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table X-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 $mg/m^3$, 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 Klinger et al. (1995a), respectively, and should be reviewed before this data is used for decision making. The quantitative measurement 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.

Concentrations given in Tables X-6 and X-7 should be considered rough estimates. Results in Tables X-6 and X-7 are presented in terms of observed chromatographic peaks, and are not adjusted for the occurrence of split peaks or the assignment of the same identity to different peaks (e.g., Cmpd # 25 and 26 in Table X-7). In these instances, the estimated concentration of a compound appearing in more than 1 peak is simply the sum of the individual peak estimates.

### X.3.4 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables X-3 through X-7 is to separate them into 2 categories: 1) Organic compounds added

to tank U-106 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-106, their concentrations are very low compared to other NPH-rich tanks.

The tentatively identified cyclosiloxanes (i.e., Cmpd # 21 and 33 in Table X-7) 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. Silcon-containing compounds are frequently detected in blanks, and their appearance in TST tank samples may be due to column bleed in the gas chromatograph.

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 X-3 through X-7 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, and volatile alkanes, all of which have been associated with the degradation of the NPHs. While both larger and smaller molecules are generated from the waste, the most abundant of these in the headspace are the smaller, short-chain volatile compounds.

The absence of tributyl phosphate in the tank U-106 samples does not necessarily indicate it is not present in the waste. The identification of the tributyl phosphate diluents and their degradation products is reason to expect tributyl phosphate may be present in the tank waste. 1-Butanol, which is one of the more abundant compounds in tank U-106 samples, is known to be a product of the hydrolysis of tributyl phosphate. Furthermore, 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. Based on these considerations, the lack of tributyl phosphate in the tank U-106 headspace samples should not be taken as proof it is not present in the headspace.

On the basis of concentrations, alcohols are the dominate type of organic compound in the tank U-106 headspace. Methanol, ethanol, 1-propanol, and 1-butanol account for about 89 % of the total estimated concentration of organic compounds in SUMMA™ samples. Similarly, about 64 % of the total estimated organic compound concentration in TST samples is due to the 12 alcohols identified. In contrast to tanks having higher NPH concentrations, tank U-106 has relatively few aldehydes and ketones.

Though not present in high concentrations, 8 straight-chain alkyl nitriles were identified in TST samples. A relatively large number of nitrogen-

containing cyclic compounds were also detected in TST samples from tank U-106, including pyridines, pyrazines, pyrazoles, oxazoles, and a piperidine.

The total organic vapor concentration of tank U-106 was estimated by Jenkins et al. to be about 10.1 $mg/m^3$ from the analysis of the 3 TST samples by GC/MS. A similar summation of positively and tentatively identified organic compounds measured in SUMMA™ samples gives a total organic vapor concentration of 12.4 $mg/m^3$. While these estimated total organic vapor concentrations are not completely equivalent to the total nonmethane organic compound (TNMOC) concentration obtained using the EPA task order 12 (TO-12) method, they are comparable. TNMOC measurements of other waste tanks have ranged from as high as about 5,000 $mg/m^3$ in tank C-103 (Rasmussen and Einfeld 1994), to as low as 0.18 $mg/m^3$ in tank C-111 (Rasmussen 1994), while the TNMOC concentration of clean ambient air ranges from about 0.03 to 0.1 $mg/m^3$.

Ambient air SUMMA™ samples collected during the tank U-106 sampling event suggest the VSS manifold may have been contaminated with trace amounts of acetone. Specifically, analysis of an ambient air sample collect upwind of the VSS (not through the VSS manifold) indicated acetone 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 0.012 ppmv of acetone. Residual amounts of acetone, used as a cleaning solvent, may have been present in the VSS transfer tubing.

In summary, the organic vapor concentrations in tank U-106 are moderately low compared to other waste tanks. The organic vapors in tank U-106 clearly indicate the presence of the semivolatile NPHs and their degradation products in the tank waste. Short-chain alcohols are more prominent in tank U-106 and there are fewer ketones and aldehydes than in NPH-rich waste tanks. Though tributyl phosphate was not detected in any of the headspace samples, there is strong evidence that it is also present in the waste.

**Table X-1**
**Tank U-106 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 | 2.0 and 6.0 | Organic vapors | 12 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 | 9 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 X-2**
**Tank U-106 Inorganic Gas and Vapor Concentrations**

| Compound | CAS[1] Number | Sample Type | Number of samples | Average (ppmv) | Standard Deviation (ppmv) | RSD[2] (%) |
|---|---|---|---|---|---|---|
| Ammonia, $NH_3$ | 7664-41-7 | Sorbent Trap | 6 | 988 | 29 | 3 |
| Carbon Dioxide, $CO_2$ | 124-38-9 | SUMMA™ | 3 | 46.5 | 1.2 | 2 |
| Carbon Monoxide, CO | 630-08-0 | SUMMA™ | 3 | < 12 | -- | -- |
| Hydrogen, $H_2$ | 1333-74-0 | SUMMA™ | 3 | 210 | 6 | 3 |
| Nitric Oxide, NO | 10102-43-9 | Sorbent Trap | 6 | ≤ 0.04 | -- | -- |
| Nitrogen Dioxide, $NO_2$ | 10102-44-0 | Sorbent Trap | 6 | ≤ 0.04 | -- | -- |
| Nitrous Oxide, $N_2O$ | 10024-97-2 | SUMMA™ | 3 | 559 | 8 | 1.4 |
| Water Vapor, $H_2O$ | 7732-18-5 | Sorbent Trap | 6 | 17,600 (12.9 mg/L) | 200 (0.15 mg/L) | 1.1 |

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

**Table X-3**
**Tank U-106 Positively Identified Organic Compounds in SUMMA™ Samples**

| Cmpd # | Compound | CAS[1] Number | Average (ppmv) | Standard Deviation (ppmv) | RSD[2] (%) |
|---|---|---|---|---|---|
| 1 | Trichlorofluoromethane | 75-69-4 | 0.040 | 0.002 | 4 |
| 2 | Toluene | 108-88-3 | 0.039 | 0.002 | 6 |
| 3 | Propanone (acetone) | 67-64-1 | 0.044 | 0.004 | 10 |
| 4 | Tetrahydrofuran | 109-99-9 | 0.024 | 0.002 | 10 |
| 5 | 1-Propanol | 71-23-8 | 0.34 | 0.002 | 1 |
| 6 | Pyridine[3] | 110-86-1 | 0.068 | -- | -- |
| 7 | Methane | 74-82-8 | < 61 | -- | -- |
| Sum of positively identified compounds: | | | 1.75 | $mg/m^3$ | |

1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. Detected in only 1 sample.

**Table X-4**
**Tank U-106 Positively Identified Organic Compounds in TST Samples**

| Cmpd # | Compound | CAS[1] Number | Average (ppmv) | Standard Deviation (ppmv) | RSD[2] (%) |
|---|---|---|---|---|---|
| 1 | Ethanenitrile (acetonitrile) | 75-05-8 | 0.10 | 0.03 | 27 |
| 2 | Propanone (acetone) | 67-64-1 | 0.064 | 0.021 | 33 |
| 3 | Propanenitrile | 107-12-0 | 0.012 | 0.002 | 14 |
| 4 | n-Hexane | 110-54-3 | 0.0075 | 0.0020 | 26 |
| 5 | Benzene | 71-43-2 | 0.0076 | 0.0006 | 8 |
| 6 | 1-Butanol[3] | 71-36-3 | 0.51 | 0.13 | 26 |
| 7 | Butanenitrile | 109-74-0 | 0.0036 | 0.0003 | 9 |
| 8 | 2-Pentanone | 107-87-9 | 0.0031 | 0.0002 | 8 |
| 9 | n-Heptane | 142-82-5 | 0.011 | 0.002 | 19 |
| 10 | Toluene | 108-88-3 | 0.036 | 0.008 | 22 |
| 11 | Pentanenitrile[4] | 110-59-8 | 0.0015 | 0.0002 | 12 |
| 12 | 2-Hexanone | 591-78-6 | 0.0028 | 0.0001 | 4 |
| 13 | n-Octane | 111-65-9 | 0.0026 | 0.0002 | 8 |
| 14 | Hexanenitrile[4] | 628-73-9 | 0.00047 | 0.00009 | 19 |
| 15 | 2-Heptanone | 110-43-0 | 0.0024 | 0.0002 | 9 |
| 16 | n-Nonane[4] | 111-84-2 | 0.0016 | 0.0002 | 10 |
| 17 | Heptanenitrile[4] | 629-08-3 | 0.00061 | 0.00006 | 10 |
| 18 | 2-Octanone[4] | 111-13-7 | 0.00065 | 0.00008 | 12 |
| 19 | n-Decane[4] | 124-18-5 | 0.00093 | 0.00005 | 5 |
| 20 | n-Undecane | 1120-21-4 | 0.0016 | 0.00005 | 3 |
| 21 | n-Dodecane | 112-40-3 | 0.0022 | 0.0001 | 6 |
| 22 | n-Tridecane | 629-50-5 | 0.0046 | 0.0002 | 5 |
| Sum of positively identified compounds: | | | 2.47 $mg/m^3$ | | |

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. Two or more samples were above upper calibration limit.

4. Two or more samples were below lower calibration limit.

**Table X-5**
**Tank U-106 Comparison of Organic Compounds in TST and SUMMA™ Samples**

| Compound | CAS[1] Number | TST Average (ppmv) | SUMMA™ Average (ppmv) |
|---|---|---|---|
| 1,1-Dichloroethene (vinylidene chloride) | 75-35-4 | < 0.00039 | < 0.005 |
| Dichloromethane (methylene chloride) | 75-09-2 | < 0.00089 | < 0.005 |
| Propanone (acetone) | 67-64-1 | 0.064 | 0.044 |
| Ethanenitrile (acetonitrile) | 75-05-8 | 0.10 | < 0.005 |
| Propanenitrile | 107-12-0 | 0.012 | < 0.005 |
| Butanenitrile | 109-74-0 | 0.0036 | < 0.005 |
| Benzene | 71-43-2 | 0.0076 | < 0.005 |
| Toluene | 108-88-3 | 0.036 | 0.039 |
| n-Hexane | 110-54-3 | 0.0075 | < 0.005 |
| n-Heptane | 142-82-5 | 0.011 | < 0.005 |
| n-Decane | 124-18-5 | 0.000933 | < 0.005 |

1. CAS = Chemical Abstract Service.

**Table X-6**
**Tank U-106 Tentatively Identified Organic Compounds in SUMMA™ Samples**

| Cmpd # | Compound | CAS[1] Number | Average ($mg/m^3$) | Standard Deviation[2] ($mg/m^3$) |
|---|---|---|---|---|
| 1 | Propene | 115-07-1 | 0.11 | 0.02 |
| 2 | Unknown[3] | | 0.067 | -- |
| 3 | Dimethyl ether | 115-10-6 | 0.085 | 0.008 |
| 4 | Cyclopropane[3] | 75-19-4 | 0.064 | -- |
| 5 | Methanol | 67-56-1 | 4.67 | 0.63 |
| 6 | 1-Propene, 2-methyl- | 115-11-7 | 0.38 | 0.04 |
| 7 | n-Butane | 106-97-8 | 0.18 | 0.02 |
| 8 | Propane, 2-methyl-2-nitro- | 594-70-7 | 0.062 | 0.007 |
| 9 | Ethanol | 64-17-5 | 3.75 | 0.59 |
| 10 | Propanone[3] (acetone) | 67-64-1 | 0.33 | -- |
| 11 | n-Pentane[3] | 109-66-0 | 0.076 | -- |
| 12 | 2-Propanol, 2-Methyl | 75-65-0 | < 0.03 | -- |
| 13 | 2-Propanal, 2-Methyl | 78-85-3 | < 0.03 | -- |
| 14 | 1-Butanol | 71-36-3 | 1.16 | 0.17 |
| 15 | Unknown C7 Alkane | | 0.10 | 0.01 |
| 16 | N-Nitrosodimethylamine | 62-75-9 | 0.059 | 0.003 |
| 17 | Pyrazine[4] | 290-37-9 | 0.055 | 0.005 |
| Sum of tentatively identified compounds: | | | 10.62 | |

1. CAS = Chemical Abstract Service.

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

3. Detected in only one sample.

4. Detected in only two samples.

**Table X-7**
**Tank U-106 Tentatively Identified Organic Compounds in TST Samples**

| Cmpd # | Compound | CAS[1] Number | Average ($mg/m^3$) | Standard Deviation ($mg/m^3$) |
|---|---|---|---|---|
| 1 | Methanol | 67-56-1 | 2.24 | 0.24 |
| 2 | Ethanol | 64-17-5 | 3.25 | 0.77 |
| 3 | 2-Propanol | 67-63-0 | 0.15 | 0.05 |
| 4 | 2-Propanol, 2-methyl- | 75-65-0 | 0.010 | 0.017 |
| 5 | 1-Propanol | 71-23-8 | 0.15 | 0.04 |
| 6 | Ethanal (acetaldehyde) | 75-07-0 | 0.018 | 0.031 |
| 7 | Furan, tetrahydro- | 109-99-9 | 0.13 | 0.04 |
| 8 | 1-Propanol, 2-methyl- | 78-83-1 | 0.0094 | 0.0162 |
| 9 | 3-Hexanol | 623-37-0 | 0.037 | 0.006 |
| 10 | 1,2,3,6-Tetrahydro-pyridine | 694-05-3 | 0.075 | 0.089 |
| 11 | Pyrazine | 290-37-9 | 0.10 | 0.09 |
| 12 | 1-Butanol, 2-methyl-, (S)- | 1565-80-6 | 0.0089 | 0.0154 |
| 13 | N-Nitrosodimethylamine | 62-75-9 | 0.13 | 0.01 |
| 14 | Pyridine | 110-86-1 | 0.023 | 0.026 |
| 15 | Heptane, 3-methyl- | 589-81-1 | 0.020 | 0.017 |
| 16 | Cyanamide, dimethyl- | 1467-79-4 | 0.13 | 0.11 |
| 17 | 1-Butene, 3,3-dimethyl- | 558-37-2 | 0.021 | 0.019 |
| 18 | 1H-Pyrazole, 4,5-dihydro-5-methyl- | 1568-20-3 | 0.040 | 0.012 |
| 19 | 1-Butanamine, N-ethylidene- | 6898-74-4 | 0.012 | 0.020 |
| 20 | 1H-Pyrazole, 4,5-dihydro-4, 5-dimethyl- | 28019-94-5 | 0.016 | 0.014 |
| 21 | Cyclotrisiloxane, hexamethyl | 541-05-9 | 0.081 | 0.038 |
| 22 | Pyrazine, methyl- | 109-08-0 | 0.0064 | 0.0111 |
| 23 | 1H-Pyrazole, 4,5-dihydro-5-methyl- | 1568-20-3 | 0.027 | 0.010 |

| Cmpd # | Compound | CAS[1] Number | Average ($mg/m^3$) | Standard Deviation ($mg/m^3$) |
|---|---|---|---|---|
| 24 | 1H-Pyrazole, 4,5-dihydro-5-methyl & others | | 0.031 | 0.010 |
| 25 | Oxazole, 4,5-dihydro-2-methyl- | 1120-64-5 | 0.053 | 0.009 |
| 26 | Oxazole, 4,5-dihydro-2-methyl- | 1120-64-5 | 0.0091 | 0.0158 |
| 27 | Benzene, 1,3-dimethyl- | 108-38-3 | 0.079 | 0.013 |
| 28 | 3-Heptanone | 106-35-4 | 0.046 | 0.010 |
| 29 | p-Xylene | 106-42-3 | 0.019 | 0.017 |
| 30 | 2-Hexene, 4,4,5-trimethyl- | 55702-61-9 | 0.034 | 0.004 |
| 31 | 2-Heptanone, 6-methyl- | 928-68-7 | 0.017 | 0.015 |
| 32 | 2-Nonen-4-one | 32064-72-5 | 0.063 | 0.008 |
| 33 | Cyclotetrasiloxane, octamethyl- | 556-67-2 | 0.038 | 0.008 |
| 34 | 1-Nonanol | 143-08-8 | 0.0037 | 0.0064 |
| 35 | 2-Undecene, 4,5-dimethyl-[R*,R*-(E)]- | 55170-92-8 | 0.0037 | 0.0064 |
| 36 | 1-Hexanol, 2-ethyl- | 104-76-7 | 0.029 | 0.003 |
| 37 | Benzyl Alcohol | 100-51-6 | 0.049 | 0.002 |
| 38 | Aniline, N-methyl- & others | | 0.0056 | 0.0097 |
| 39 | Nonanenitrile | | 0.011 | 0.010 |
| 40 | Decanenitrile | | 0.0037 | 0.0064 |
| 41 | 2(3H)-Furanone, 5-ethyldihydro- | 695-06-7 | 0.089 | 0.009 |
| 42 | 2-Oxazolidinone, 5-methyl-3-(2-propenyl)- | 55956-20-2 | 0.067 | 0.006 |
| 43 | 1,4-Cyclohexanedione | 637-88-7 | 0.017 | 0.002 |
| 44 | Mixture | | 0.022 | 0.021 |
| 45 | 4-Piperidinemethanol, 1-methyl- | 20691-89-8 | 0.014 | 0.025 |
| 46 | n-Tetradecane | 629-59-4 | 0.029 | 0.004 |

| Cmpd # | Compound | CAS[1] Number | Average ($mg/m^3$) | Standard Deviation ($mg/m^3$) |
|---|---|---|---|---|
| 47 | Tetradecanoic acid | 544-63-8 | 0.023 | 0.008 |
| 48 | Benzenesulfonamide, N-butyl- | 3622-84-2 | 0.043 | 0.011 |
| 49 | Pentadecanoic acid | 1002-84-2 | 0.0053 | 0.0091 |
| 50 | 9-Hexadecenoic acid | 2091-29-4 | 0.016 | 0.027 |
| 51 | Hexadecanoic acid | 57-10-3 | 0.059 | 0.024 |
| 52 | Isopropyl Palmitate | 142-91-6 | 0.0056 | 0.0097 |
| Sum of Tentatively Identified Compounds: | | | 7.6 | |

1. CAS = Chemical Abstract Service.

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