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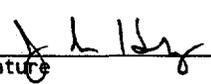
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7. Abstract Tank 241-C-107 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. The drivers and objectives of waste tank headspace sampling and analysis are discussed in "Program Plan for the Resolution of Tank Vapor Issues" (Osborne and Huckaby 1994). Tank 241-C-107 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-C-107 Vapor Sampling and Analysis Tank Characterization Report**X.0 INTRODUCTION**

Tank C-107 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). Tank C-107 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 from the tank C-107 headspace were collected on June 16, 1994 using the *in situ* sampling (ISS) method (Pingel 1994), and again on September 29, 1994 using the more robust vapor sampling system (VSS), (WHC 1995). Because sorbent trap samples from the June 16, 1994 event were contaminated, only the SUMMA^{TM,1} canister samples from this event were analyzed. Results presented here represent the best available data on the headspace constituents of tank C-107.

X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank C-107 using VSS on September 29, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by the sample and analysis plan (WHC 1995, Appendix A). The tank headspace temperature was determined to be 45.9 °C. Air from the C-107 headspace was withdrawn from a single elevation via a 7.9-m long heated sampling probe mounted in riser 8, and transferred via heated tubing to the VSS sampling manifold.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 7:22 a.m. and 10:45 a.m., with no anomalies noted.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), Pacific Northwest Laboratories (PNL), and Oregon Graduate Institute of Science and Technology (OGIST) through a contract with Sandia National Laboratories. The 39 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 (1995a). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody

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

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^{TM,2} 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 were prepared and analyzed by PNL. SUMMATM canisters were analyzed for inorganic analytes by OGIIST. Reports by Pool et al. (1995) and Rasmussen (1994a) describe sample preparation and analyses.

X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 84 ppmv, is over 3 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 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 C-107 was determined to be 230 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, the 230 ppmv hydrogen concentration in tank C-107 corresponds to about 0.6 % of its LFL. At this level, hydrogen is not a flammability concern in tank C-107.

The nitrous oxide concentration in tank C-107, 78 ppmv, is about 3 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 concentrations as low as about 12 ppmv in tank TX-105 (Klinger 1995), and as high as about 800 ppmv in tank C-103 (Huckaby and Story 1994).

X.2.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank C-107 headspace, measured to be 1.7 ppmv in SUMMATM samples (Rasmussen 1994a), is much higher than in ambient air, where it typically ranges from 0.05 to 0.15 ppmv. 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 1.7 ppmv of carbon monoxide in tank C-107 is much less than the NIOSH 8-hr REL of 35 ppmv.

² SUMMA is a trademark of Molectrics, Inc., Cleveland, Ohio.

The average carbon dioxide concentration in the tank C-107 headspace, 725 ppmv, is higher 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. In principle, above-ambient concentrations of carbon dioxide could result from the oxidation of organic material in the waste, but its solubility in the aqueous waste would be expected to prevent it from evolving into the gas phase. Carbon dioxide concentrations in tanks C-108 and C-109, given in Table X-3, indicate that the source of carbon dioxide is within tank C-107.

A SUMMATM sample collected on June 16, 1994 (Pingel 1994), archived by PNL, was analyzed in March 1995 for comparison with the 725 ppmv of carbon dioxide reported by OGIST. PNL found the carbon dioxide concentration in the archived SUMMATM to be 554 ppmv³. While this is not as high a concentration as reported by OGIST, it is significantly above the normal level in ambient air.

It should be noted that SUMMATM samples collected in June 1994 were not intended to be used for analysis of carbon dioxide, because the sample collection method used could affect the carbon dioxide observed in the samples. Specifically, SUMMATM canisters were filled with tank air on June 16, 1994 by drawing air from the headspace through about 15 m (50 ft) of unheated tubing. Because tank C-107 is warm and moist (see Section X.2.3), it is likely that water vapor condensed in the unheated tubing, and that some carbon dioxide was absorbed by the condensate, potentially reducing its concentration in the sample.

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

Nitric oxide and nitrogen dioxide concentrations in the tank C-107 headspace were determined to be 0.20 ppmv and ≤ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank C-107. The measurable presence of nitric oxide 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 C-107 was determined to be about 58.8 mg/L, at the measured tank headspace temperature of 45.9 °C and pressure of 984 mbar (737.7 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 86.4 mbar (64.8 torr), to a dew point of 43.0 °C, and to a relative humidity of 86 %. The relative humidity in tank C-107 is similar to that in other 241-C farm tanks that contain primarily sludge waste.

³ Pertinent analysis records are kept in PNL file 550405.s. Archived sample was SUMMATM canister "PNL 033". WHC Sampling and Mobile Laboratories maintain sampling event records in the file for sampling job S4056.

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 and carbon dioxide, the most abundant waste constituents in the tank C-107 headspace are ammonia, hydrogen, and nitrous oxide. These have been detected in most tank headspaces sampled to date, and are usually the dominate waste species. For comparison and perspective, Table X-3 presents selected inorganic gas and vapor concentrations for tanks C-107, C-108, and C-109.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table X-2 are very good. Relative standard deviations range from about 1 % for carbon dioxide and nitrous oxide, to 7 % for 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.), the small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

As discussed in Section X-X, the headspaces of tanks C-107 and C-108 are connected by an underground cascade line. Similarly, the headspaces of tanks C-108 and C-109 are connected by a cascade line. To examine the possibility that constituents of the tank C-107 headspace are actually generated in tank C-108 or C-109 and introduced to tank C-107 via the cascade line, the inorganic gas and vapor results from the headspace characterization of tanks C-107, C-108, and C-109 are given in Table X-3. From Table X-3 it can be concluded (assuming all results presented are valid) that the primary source of ammonia, hydrogen, carbon dioxide, carbon monoxide, and water vapor in the tank C-107 headspace is the waste in tank C-107.

The elevated level of carbon dioxide in tank C-107 is not understood. Tank C-101 has also been observed to have a carbon dioxide concentration higher than that of ambient air. The tank C-101 carbon dioxide concentration in samples collected on September 1, 1994 was measured to be an average 1425 ppmv in 3 SUMMA™ samples by OGIST, and 1401 ppmv in a single SUMMA™ sample by PNL (Huckaby 1995b).

X.3 ORGANIC VAPORS

Organic vapors in the tank C-107 headspace were sampled using SUMMA™ canisters, which were analyzed by OGIST and 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. Methane and total nonmethane organic compound (TNMOC) concentrations were measured by OGIST using GC and flame ionization detection (FID). Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994), Rasmussen (1994a), and Pool et al. (1995).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-107. 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 when known compounds were analyzed. 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 the 40 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 15 analytes selected from the toxicology panel's review of tank C-103.

Table X-4 lists the organic compounds positively identified and quantitated in SUMMA™ samples. Analysis for methane was performed by OGIST (Rasmussen 1994a), other SUMMA™ analyses were performed according to the TO-14 methodology by PNL (EPA 1988, Pool et al. 1995). None of the 40 TO-14 target analytes and only 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. (1994) report the positive identification of 25 of 27 target analytes in TST samples. 1,1-Dichloroethene and dibutyl butylphosphonate were the only TST target analytes not detected in the TST samples. Tributyl phosphate was positively identified, but its concentration was too low to be quantitatively measured. The average concentrations of the remaining 24

target analytes, from the analysis of 3 TSTs, are given in Table X-4. Despite calibration of the instrument over about a 20-fold concentration range, 12 of the compounds listed in Table X-5 were outside of the calibration range in at least 2 of the TST samples.

Eleven target analytes were common to both TST and SUMMA™ analyses. Table X-6 lists these, and their reported average concentrations in TST and SUMMA™ samples. The reported TST sample concentrations of 1,1-dichloroethene and nonpolar compounds (i.e., benzene, toluene, n-hexane, n-heptane, and n-decane) in Table X-6 are all < 0.003 ppmv, and below the SUMMA™ analysis method detection limit.

The acetone concentration in the SUMMA™ samples was reported to be 8.8 times as high as in TST samples. Comparison of SUMMA™ and TST analyses of acetone in other waste tank samples indicates a similar relationship in 7 of the 8 waste tanks reported to date⁴, for which acetone has been quantitatively measured in SUMMA™ samples. When compared to the 250 ppmv NIOSH 8-hr REL for acetone, even the more conservative value of 0.83 ppmv appears to be insignificant.

Differences between the TST and SUMMA™ results for dichloromethane were significant, but may be due to problems with the TST preparation, handling, or analysis. Specifically, the reported dichloromethane results from the 3 TST samples are very inconsistent, being 0.0096, < 0.0011, and 0.41 ppmv. Disagreement between TST and SUMMA™ results for dichloromethane have been noted in other waste tank samples (e.g., in tank C-105, Huckaby 1995c). Though the average concentration reported for TSTs is only 0.14 ppmv, dichloromethane is considered by NIOSH to be a potential carcinogen, and NIOSH "recommends that occupational exposures to carcinogens be limited to the lowest feasible concentration" (NIOSH 1995).

There is also disagreement regarding nitrile concentrations in SUMMA™ and TST samples from tank C-107. Acetonitrile was measured in SUMMA™ samples to be 0.64 ppmv, and only 0.25 ppmv in TST samples. Also, as shown in Table X-6, the average concentrations of propanenitrile, and butanenitrile in TST samples were well above the 0.005 ppmv SUMMA™ method detection limit, yet these analytes were not found in the SUMMA™ samples. In lieu of reasons to discount either sampling and analysis method, the higher results should be used as the best measurement of these nitriles.

The most abundant analytes in Tables X-3 and X-4 are methane, acetone, n-dodecane, acetonitrile, n-tridecane, 1-butanol, and n-undecane. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

⁴ The acetone concentrations in tanks BY-103, BY-107, BY-110, BY-111, C-103, TX-105, and TX-118 in SUMMA™ samples were reported to be 1.7 to 4.5 times higher than in TST samples. In the tank BY-108 samples the same factor was about 0.5.

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 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 (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-7. Compounds are listed in Table X-7 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-8. Compounds are listed in Table X-8 according to the order by which they eluted chromatographically. The averages reported by ORNL in Table X-8 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. (1994) and Pool et al. (1995), 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-7 and X-8 should be considered rough estimates. Results in Tables X-7 and X-8 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 13 and 14 in Table X-8) or the assignment of the same identity to different peaks (e.g., Cmpd # 120, 131, 138, and 141 in Table X-8). In

these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

X.3.3 Total Nonmethane Organic Compounds

OGIST measured the total nonmethane organic compound (TNMOC) concentration in 3 SUMMA™ canister samples using the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method (Rasmussen 1994a, EPA 1988). The sample mean was 3.6 mg/m³, with a standard deviation of 0.1 mg/m³. Though data on other tanks is limited, this value is relatively low compared to other waste tanks sampled to date.

The sum of quantitatively measured and estimated TST organic analyte concentrations, by GC/MS analyses, is 3.7 mg/m³ (Jenkins et al. 1994). This is in excellent agreement with the EPA TO-12 result. EPA TO-12 method TNMOC measurements of other waste tanks have ranged from as high as 5,000 mg/m³ in tank C-103 (Rasmussen and Einfeld 1994), to as low as 0.18 mg/m³ in tank C-111 (Rasmussen 1994b), while the TNMOC concentration of clean ambient air ranges from about 0.03 to 0.1 mg/m³.

X.3.4 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables X-4 through X-8 is to separate them into 2 categories: 1) Organic compounds added to tank C-107 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes tributyl phosphate and the semivolatile branched alkanes and NPHs, all of which ostensibly came from the Plutonium-Uranium Extraction (PUREX) process. It also includes any volatile halogenated compounds, such as trichlorofluoromethane, which may have been used as cleaning solvents, and which may have been sent to the waste tanks when contaminated. The tentatively identified cyclosiloxanes (i.e., Cmpd # 25 and 46 in Table X-8) are also in this category. Small quantities of siloxanes may have been introduced to the waste tank through their use as process surfactants, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

Decahydronaphthalene and methyl-substituted decahydronaphthalenes have been tentatively identified in many of the NPH-rich waste tanks, but were not found in tank C-107. This may be an indication that the organic waste in tank C-107 originated during a period when the PUREX process was using a relatively pure NPH diluent.

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-4 through X-8 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, alkyl nitrates, and volatile alkanes, all of which have been associated with the degradation of the NPHs.

The hydrolysis of tributyl phosphate, for example, is thought to be the principal source of 1-butanol. By far the most abundant of these in the headspace are the short-chain volatile compounds, however, Table X-8 lists many long-chain low volatility compounds that are also probably waste reaction products.

Samples from tank C-107 were found to have several alkyl nitrates and organic acids. Though it is reasonable to expect alkyl nitrates and organic acids to be produced via chemical and radiolytic processes of the NPH with other waste, their solubility in the aqueous waste supernates would also be expected to significantly reduce their vapor-phase concentrations. That these constituents are at detectible levels in tank C-107 may indicate dry conditions where they are formed.

Selected organic vapor concentrations in tanks C-107, C-108, and C-109 are given in Table X-3 for comparison. Because the listed organic vapors are at higher concentrations in tank C-107 than in tank C-108, it can be concluded that their presence in the tank C-107 headspace is due principally to their presence in the waste of that tank.

In summary, the organic vapor concentrations in tank C-107 are relatively low. While not completely typical of NPH-rich tanks, the organic vapors in tank C-107 clearly indicate the presence of trace amounts of the semivolatile NPHs and their degradation products. Consideration of data given in Table X-3 and the cascade line between the headspaces of tanks C-107 and C-108 suggests that most organic vapors in the headspace of tank C-107 are generated by evaporation or chemical reaction within tank C-107, and are not from tank C-108.

Table X-1
Tank C-107 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.5 and 2.0	Organic vapors	8 tank air samples, + 2 trip blanks + 2 field blanks
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous Oxide, Carbon Dioxide, Carbon Monoxide, Methane, TNMOC	3 tank air samples
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	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. TNMOC = total nonmethane organic compound[s].

**Table X-2
Tank C-107 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	84	2	2
Carbon dioxide, CO ₂	124-38-9	SUMMA TM	3	725	0.6	1
Carbon monoxide, CO	630-08-0	SUMMA TM	3	1.7	0.05	3
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	230	15	6
Nitric oxide, NO	10102-43-9	Sorbent Trap	5	0.20	0.01	--
Nitrogen dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous oxide, N ₂ O	10024-97-2	SUMMA TM	3	78	0.2	1
Water vapor, H ₂ O	7732-18-5	Sorbent Trap	5	87,800 (58.8 mg/L)	6,200 (4.2 mg/L)	7

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

Table X-3
Comparison of Tank C-107, C-108, and C-109 Headspace Constituents

Tank:	C-107	C-108 ¹	C-109 ²
Date sampled, (mo/day/yr)	9/9/94	8/5/94	8/10/94
Headspace temperature, (°C)	45.9	25	27
Ammonia, (ppmv)	84	2.7	10.1
Hydrogen, (ppmv)	230	15.3	125
Carbon dioxide, (ppmv)	725	16.3	3
Carbon monoxide, (ppmv)	1.7	0.10	0.41
Nitric oxide, (ppmv)	0.20	0.24	0.51
Nitrogen dioxide, (ppmv)	≤ 0.02	≤ 0.04	≤ 0.06
Nitrous oxide, (ppmv)	78	344	369
Water vapor, (mg/m ³)	70.7	17.5	20.4
Water vapor, (% relative humidity)	86	76	79
Ethanenitrile (acetonitrile), (ppmv)	0.25	0.0052	0.26
Propanone (acetone), (ppmv)	0.094	0.018	0.012
1-Butanol, (ppmv)	0.0025	0.00049	0.0032
n-Dodecane, (ppmv)	0.0073	0.00053	0.00026
n-Tridecane, (ppmv)	0.0092	0.0011	0.00047
Total nonmethane organic compounds, (mg/m ³)	3.6	0.35	0.65

1. Data are from Huckaby 1995d; results for organic vapors are from TST samples.

2. Data are from Huckaby 1994e; results for organic vapors are from TST samples.

Table X-4
Tank C-107 Positively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS ¹ Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
1	Methane ³	74-82-8	3.4	< 0.06	< 2
2	2-Butanone	78-93-3	0.011	0.003	27
3	Propanone (acetone)	67-64-1	0.83	0.07	8
4	Ethanimitrile (acetonitrile)	75-05-8	0.64	0.03	5

1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. Methane results are from Rasmussen 1994a.

Table X-5
Tank C-107 Positively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS ¹ Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
1	Ethanenitrile ³ (acetonitrile)	75-05-8	0.25	0.10	39
2	Propanone (acetone)	67-64-1	0.094	0.090	96
3	Dichloromethane ³ (methylene chloride)	75-09-2	0.14	0.24	167
4	Propanenitrile	107-12-0	0.064	0.020	32
5	Butanal ³	123-72-8	< 0.0016	--	--
6	n-Hexane ³	110-54-3	< 0.0013	--	--
7	Benzene ³	71-43-2	< 0.00086	--	--
8	1-Butanol	71-36-3	0.0025	0.0009	36
9	Butanenitrile	109-74-0	0.012	0.003	28
10	2-Pentanone ³	107-87-9	0.0022	0.0022	100
11	n-Heptane	142-82-5	0.0012	0.0014	113
12	Toluene ³	108-88-3	0.00066	0.00030	45
13	Pentanenitrile ³	110-59-8	0.0085	0.0020	24
14	2-Hexanone	591-78-6	0.0013	0.0003	26
15	n-Octane	111-65-9	0.0012	0.0005	41
16	Hexanenitrile	628-73-9	0.0051	0.0009	17
17	2-Heptanone	110-43-0	0.0011	0.0005	45
18	n-Nonane	111-84-2	< 0.0011	--	--
19	Heptanenitrile	629-08-3	0.0028	0.0010	36
20	2-Octanone ³	111-13-7	< 0.00079	--	--
21	n-Decane ³	124-18-5	< 0.0027	--	--
22	n-Undecane ³	1120-21-4	0.0056	0.0006	10
23	n-Dodecane ³	112-40-3	0.0073	0.0005	6
24	n-Tridecane ³	629-50-5	0.0092	0.0012	13
Sum of positively identified compounds:			1.7 mg/m ³		

WHC-SD-WM-ER-445 REV. 0

1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. Two or more samples were outside calibration range.

Table X-6
Tank C-107 Comparison of Positively Identified 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	< 0.00058	< 0.005
Dichloromethane (methylene chloride)	75-09-2	0.14	< 0.005
Propanone (acetone)	67-64-1	0.094	0.83
Ethanenitrile (acetonitrile)	75-05-8	0.25	0.64
Propanenitrile	107-12-0	0.064	< 0.005
Butanenitrile	109-74-0	0.012	< 0.005
Benzene	71-43-2	< 0.00086	< 0.005
Toluene	108-88-3	0.00066	< 0.005
n-Hexane	110-54-3	< 0.0013	< 0.005
n-Heptane	142-82-5	0.0012	< 0.005
n-Decane	124-18-5	< 0.0027	< 0.005

1. CAS = Chemical Abstract Service.

Table X-7
Tank C-107 Tentatively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
1	Cyclopropane ²	75-19-4	0.15	0.01
2	Acetaldehyde	75-07-0	0.09	0.01
3	Methyl Nitrate	598-58-3	0.19	0.01
4	Unknown Alkane		0.13	0.01
5	Unknown Alkane		0.18	0.02
6	Nitric Acid, Ethyl Ester	625-58-1	0.23	0.01
7	Unknown Alkane		0.12	0.01
8	n-Dodecane	112-40-3	0.24	0.23
9	n-Tridecane	629-50-5	1.18	1.26
10	n-Tetradecane	629-59-4	0.46	0.64

1. CAS = Chemical Abstract Service.
2. Detected in only 2 samples.

Table X-8
Tank C-107 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
1	Methane, oxybis	115-10-6	0.044	0.012
2	Methane, trichlorofluoro	75-69-4	0.049	0.039
3	nitro compound		0.021	0.020
4	1-Propene, 2-fluoro and others		0.0080	0.0140
5	2-Butanone	78-93-3	0.0089	0.0154
6	Nitric acid, ethyl ester	625-58-1	0.051	0.010
7	Butane, 1-chloro	109-69-3	0.030	0.006
8	Cyclopropanecarbonitrile	5500-21-0	0.0072	0.0124
9	2-Butanenitrile and others		0.0025	0.0044
10	Hexane, 2,3-dimethyl	584-94-1	0.0048	0.0083
11	Nitric acid, propyl ester	627-13-4	0.0057	0.0099
12	Mixture		0.0063	0.0056
13	Acetic acid	64-19-7	0.16	0.17
14	Acetic acid	64-19-7	0.067	0.115
15	1-Pentene	109-67-1	0.011	0.019
16	Propane, 2-methyl-2-nitro	594-70-7	0.034	0.030
17	Acetic acid	64-19-7	0.031	0.053
18	Cyclopropane, 1,2-dimethyl, cis	930-18-7	0.011	0.010
19	1H-Pyrrolle	109-97-7	0.0040	0.0070
20	Ethene, 1,1'-oxybis	109-93-3	0.0056	0.0097
21	Ethene, 1,1'-oxybis	109-93-3	0.027	0.047
22	Oxirane, ethenyl	930-22-3	0.019	0.002
23	Hexanal	66-25-1	0.0045	0.0078
24	Propane, 2-methyl-2-nitro	594-70-7	0.015	0.003
25	Cyclotrisiloxane, hexamethyl	541-05-9	0.27	0.23
26	Nitric acid, propyl ester	627-13-4	0.019	0.017
27	Nitric acid, butyl ester	928-45-0	0.0039	0.0067

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Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
28	Methylamine, N-(1-methylbutylidene)-	22431-09-0	0.0061	0.0106
29	Pyrazine, methyl	109-08-0	0.0033	0.0057
30	Benzene, ethyl	100-41-4	0.0013	0.0022
31	Benzene, 1,2-dimethyl	95-47-6	0.0036	0.0031
32	3-Heptanone	106-35-4	0.0022	0.0038
33	Butane, 2-bromo	78-76-2	0.0034	0.0059
34	Heptanal	111-71-7	0.0048	0.0005
35	1,5-Pentanediol, dinitrate	3457-92-9	0.0040	0.0003
36	2(3H)-furanone, dihydro and C3-benzene		0.0013	0.0022
37	Mixture		0.0016	0.0027
38	2-Heptanone, 6-methyl	928-68-7	0.0027	0.0024
39	Hexane 3,4-dimethyl and others		0.0032	0.0029
40	2(3H)-Furanone, dihydro-5-methyl	108-29-2	0.0012	0.0020
41	Alkenol		0.0050	0.0087
42	4-Octanone	589-63-9	0.0017	0.0030
43	Phenol and 1-propenyl benzene		0.0034	0.0059
44	Mixture		0.0019	0.0033
45	5-Hepten-2-one, 6-methyl	110-93-0	0.0023	0.0040
46	Cyclotetrasiloxane, octamethyl	556-67-2	0.060	0.037
47	Octanal	124-13-0	0.0082	0.0016
48	Nitric acid, butyl ester	928-45-0	0.010	0.003
49	1-Hexanol, 2-ethyl	104-76-7	0.0015	0.0026
50	3-Hexene-2-one and others		0.0034	0.0029
51	2(3H)-Furanone, 5-ethyl dihydro	695-06-7	0.0034	0.0030
52	2H-pyran-3(4H)-one, dihydro	23462-75-1	0.0032	0.0028
53	4-Nonanone	4485-09-0	0.0015	0.0026

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Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
54	Cyclopropane, pentyl	2511-91-3	0.0015	0.0026
55	Ethanone, 1-phenyl	98-86-2	0.0049	0.0045
56	Octanenitrile	124-12-9	0.021	0.006
57	4-Undecene, (E)-	693-62-9	0.0014	0.0023
58	2-Nonanone	821-55-6	0.0060	0.0053
59	Nonanal	124-19-6	0.011	0.001
60	1,3-Benzenediol, 2-methyl	608-25-3	0.0037	0.0033
61	Nitric acid, hexyl ester	20633-11-8	0.0081	0.0007
62	Benzeneacetic acid, a-4-bis[(trimethylsilyl)]	37148-64-4	0.0047	0.0042
63	Cyclohexanone,2,5-dimethyl-2-(1-methyl)et	6711-26-8	0.0011	0.0020
64	2(3H)-Furanone, dihydro-5-propyl	105-21-5	0.0082	0.0018
65	Decane, 2-methyl	6975-98-0	0.0078	0.0067
66	5-Undecanone, 2-methyl	50639-02-6	0.0041	0.0071
67	Nonanenitrile	2243-27-8	0.017	0.009
68	4-Dodecene	7206-15-7	0.0068	0.0023
69	1-Dodecene	112-41-4	0.0016	0.0029
70	2-Decanone	693-54-9	0.0059	0.0008
71	Naphthalene	91-20-3	0.0010	0.0017
72	4-Dodecene, cis=trans		0.0029	0.0031
73	Decanal	112-31-2	0.0089	0.0010
74	1,3-Benzodioxal-2-one, hexahydro	20192-66-9	0.0025	0.0004
75	Benzene, 1-chloro-4-nitro	100-00-5	0.0052	0.0011
76	2(3H)-furanone, 5-butylidihydro	104-50-7	0.0028	0.0027
77	1,3,5,7-Tetraazatricyclo[3.3.1.13.7]decane	100-97-0	0.0023	0.0040
78	5-Undecanone	33083-83-9	0.012	0.003

WHC-SD-WM-ER-445 REV. 0

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
79	alkyl-cyclopentane		0.0017	0.0029
80	alkyl nitrile		0.019	0.004
81	2-Undecanone	112-12-9	0.0076	0.0025
82	1-Tridecene	2437-56-1	0.00080	0.00139
83	1-Tridecene	2437-56-1	0.00070	0.00122
84	Tridecanal	10486-19-8	0.00066	0.00114
85	6-Dodecanone	6064-27-3	0.0072	0.0024
86	Decane, 5-propyl- and others		0.013	0.003
87	1H-Inden-1-one, 2,3-dihydro-3,3-dimethyl	26465-81-6	0.00098	0.0017
88	3-Octanone	106-68-3	0.0010	0.0018
89	3-Dodecanone	1534-27-6	0.013	0.0026
90	Tetradecane	629-59-4	0.025	0.005
91	3-Octen-2-ol, 2-methyl, cis	18521-07-8	0.0024	0.0021
92	Cyclohexanone, 4-hydroxy-4-methyl	17429-02-6	0.00082	0.00142
93	5,9-Undecadien-2-one,6,10-dimethyl (Z)	3879-26-3	0.0069	0.0029
94	5-Undecanone, 2-methyl	50639-02-6	0.012	0.002
95	2,5-Cyclohexadiene, 1,4-dione, 2,6-bis(1,1	719-22-2	0.0077	0.0025
96	3-Tridecanone	1534-26-5	0.011	0.002
97	2-Tridecanone	593-08-8	0.0084	0.0065
98	2-Pentene, 5-(pentyloxy)- (E)-	56052-85-8	0.0013	0.0023
99	Cyclohexadecane	295-65-8	0.0019	0.0019
100	Dodecanoic acid	143-07-7	0.014	0.002
101	5-Undecanone, 2-methyl	50639-02-6	0.0033	0.0008
102	Mixture		0.0022	0.0020
103	3-Dodecanone	1534-27-6	0.00064	0.00110
104	Undecane, 3,8-dimethyl	17301-30-3	0.00065	0.00112

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Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
105	Alkanone		0.0015	0.0013
106	Mixture		0.00095	0.00164
107	Butyric acid, ester w/ p-hydroxybenzotrile	29052-10-6	0.00094	0.00162
108	Phthalate		0.0055	0.0056
109	Tributyl phosphate and benzamine, N-phenyl		0.0068	0.0028
110	3-Phenoxybenzaldehyde	39515-51-0	0.0014	0.0012
111	Hexanedioic acid, bis-(1-methylpropyl)-est	38447-22-2	0.00064	0.00111
112	1-Dodecanol	112-53-8	0.00073	0.00127
113	Heptadecane, 8-methyl	13287-23-5	0.00069	0.00119
114	9-Octadecenoic acid, (Z)-	112-80-1	0.00064	0.00112
115	9-Octadecenoic acid, (Z)-	112-80-1	0.0036	0.0063
116	Tetradecanoic acid	544-63-8	0.031	0.051
117	Benzamide, N-methyl	613-93-4	0.00079	0.0014
118	9-Octadecenoic acid, methyl ester (E)	1937-62-8	0.0055	0.0050
119	Tetradecanoic acid	544-63-0	0.057	0.049
120	1-Hexadecanol	36653-82-4	0.0083	0.014
121	Alkane and Alkanoic acid		0.0011	0.0019
122	Hexadecanoic acid, 2,3-dihydroxypropyles	542-44-9	0.0027	0.0023
123	Benzenesulfonamide, N-butyl	3622-84-2	0.091	0.015
124	Eicosane	112-95-8	0.0042	0.0074
125	Tetradecanoic acid, 12-methyl, cis	5746-58-7	0.0063	0.0054
126	9-Octadecenoic acid, (Z)-	112-80-1	0.0023	0.0041
127	Alkane		0.0054	0.0093
128	Hexanedioic acid, dioctyl ester	123-79-5	0.047	0.081

WHC-SD-WM-ER-445 REV. 0

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
129	14-Pentadecenoic acid	17351-34-7	0.0067	0.0069
130	Pentadecanoic acid	1002-84-2	0.029	0.026
131	1-Hexadecanol	36653-82-4	0.0068	0.0061
132	1-Hexadecene	629-73-2	0.0043	0.0075
133	1-Octadecanol	112-92-5	0.0089	0.015
134	Nonadecane	629-92-5	0.00087	0.00152
135	9-Hexadecenoic acid	2091-29-4	0.090	0.009
136	Hexadecanoic acid	57-10-3	0.12	0.06
137	Eicosane	112-95-8	0.0014	0.0025
138	1-Hexadecanol	36653-82-4	0.0025	0.0044
139	1-Hexadecanol, acetate	629-70-9	0.0030	0.0028
140	Hexadecanoic acid	57-10-3	0.024	0.006
141	1-Hexadecanol	36653-82-4	0.043	0.038
142	1-Octadecanol	112-92-5	0.027	0.046
143	Heptadecane, 2,6,10,15-tetramethyl	54833-48-6	0.0025	0.0044
144	Heneicosane	629-94-7	0.0043	0.0075
145	Pentadecane, 8-hexyl	13475-75-7	0.0035	0.0061
Sum of tentatively identified compounds:			2.04	

1. CAS = Chemical Abstract Service.

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