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7. Abstract

Tank 241-C-105 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-105 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-105 Vapor Sampling and Analysis Tank Characterization Report**X.0 INTRODUCTION**

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

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

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

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

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

exhaust, the introduction of air from tank C-106 is comparable to the introduction of ambient air.

X.1 SAMPLING EVENT

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

Tank C-105 was the third tank to be sampled using the VSS, and was sampled only about 3 weeks after the first use of the VSS on a tank. Because the methods and equipment were relatively new, problems with sample handling (e.g., chain-of-custody and shipping) were encountered (WHC 1995, Clauss et al. 1995). The precision of the sampling results, however, is generally good. Sorbent trap collection problems noted in a subsequent sampling event¹ do not appear to have occurred when tank C-105 was sampled.

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

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

A general description of vapor sampling and sample analysis methods is given by Huckaby (1995c). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody

¹ Because of a valve-sequencing error, sample air volumes through specific sampling ports were not properly measured during sample job 7A of tank C-103. The error resulted in obvious and significant differences in sorbent trap results, but had no effect on SUMMATM samples.

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 OGIST. Reports by PNL (Clauss et al. 1995) and OGIST (Rasmussen 1994a) describe sample preparation and analyses.

The relative standard deviations of the inorganic gas and vapor results are given in the last column in Table X-2. The precision of reported results is generally good for the methods used. Relative standard deviations range from about 4 % for carbon monoxide results to 13 % for water vapor results. The precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), and the small relative standard deviations suggest adequate controls were maintained both in the field and in the laboratories.

X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia, hydrogen, and nitrous oxide are commonly detected in the waste tanks. Thought to be products of radiolysis and oxidation-reduction reactions of the waste, they appear ubiquitously with the high-level waste. These headspace constituents have been the most abundant waste artifacts in virtually every tank headspace sampled to date.

The reported ammonia concentration, 2.4 ppmv, is well below 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 tank BY-108 (McVeety et al. 1995). Active ventilation of the tank C-105 headspace accounts for the relatively low ammonia concentration in the tank C-105 exhaust.

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

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

The nitrous oxide concentration in the tank C-105 exhaust, 5.3 ppmv, is well below the NIOSH 8-hr REL of 25 ppmv for nitrous oxide (NIOSH 1995). Nitrous oxide, also known as laughing gas, has been detected in the 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).

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

X.2.2 Carbon Monoxide, Nitric Oxide, Nitrogen Dioxide, Water and Tritium

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

Nitric oxide and nitrogen dioxide concentrations in the tank C-105 exhaust were both determined to be \leq 0.1 ppmv. These are acid gases that would have very low equilibrium concentrations above the high pH supernatant liquid in tank C-105. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. 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-105 exhaust was determined to be about 6.8 mg/L, using a tank headspace temperature of 17 °C and the ambient pressure of 980 mbar (735 torr). This corresponds to a water vapor partial pressure of 9.1 mbar (6.8 torr), to a dew point of 5.5 °C, and to a relative humidity of 47 %. Psychrometric measurements of the exhaust from tank C-105 were made on February 4 and March 2, 1994 (when flowrates were measured), that indicated

the relative humidity of the exhaust on those dates to be about 44 % and 85 %, respectively (Minter 1995).

Silica gel sorbent traps were used to test for tritium. It is assumed that tritium produced by the waste combines with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Analysis of the silica gel, which would have trapped approximately 22 mg of water vapor, indicated the total activity of the sample to be below the method detection limit of 50 pCi (WHC 1995).

X.3 ORGANIC VAPORS

Organic vapors in the tank C-105 exhaust were sampled using SUMMA™ canisters, which were analyzed by PNL and OGIIST, and triple sorbent traps (TSTs), which were analyzed by ORNL. All laboratories used gas chromatography (GC) and mass spectroscopy (MS) to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994), Rasmussen (1994a), and Clauss et al. (1995). In an attempt to provide ORNL with additional samples for scoping purposes, 7 of the TSTs were collected simultaneously, in parallel, with a single flow controller. Because flow through these 7 TSTs was very non-uniform, analytical results from these samples are not discussed here. A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method was also performed by OGIIST (EPA 1988, Rasmussen 1994a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-105. 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 Analytes

Table X-3 lists the organic compounds positively identified and quantitated in SUMMA™ samples by OGIIST. SUMMA™ analyses were performed according to the EPA TO-14 methodology (EPA 1988, Rasmussen 1994a). Averages reported are from analyses of 3 SUMMA™ samples. Three of the compounds listed, 1,1,2-trichloro-1,2,2-trifluoroethane, 1,1,1-trichloroethane, and tetrachloromethane, were detected in ambient air samples at virtually the same levels as in the tank C-105 exhaust samples. This probably indicates that either the compounds were not associated with the waste, or they were contaminants introduced during sample preparation, collection, or analysis. Trace quantities of several other analytes listed in Table X-3 were also

detected in the ambient air samples, complete analytical results are given by Rasmussen (1994a).

Analysis of SUMMA™ samples by PNL according the same EPA TO-14 method indicated none of the 40 TO-14 analytes to be above the 0.002 ppmv quantitation limit (Clauss et al. 1995 provide the complete TO-14 analyte list). Data in Table X-3, which are strictly from OGIST, agree with the PNL analyses except for 1,3-butadiene, which is not technically an EPA TO-14 analyte and consequently was not on the PNL target analyte list, and trichlorofluoromethane, which OGIST measured to be slightly above the PNL detection limit.

Jenkins et al. (1994) report the positive identification of 25 of 26 target analytes in TST samples. The target analyte list was based on advice from a panel of toxicology experts (Goheen 1994). The average concentrations of the 23 quantitatively measured target analytes, from the analysis of 3 TSTs, are given in Table X-4. One target analyte, 1,2-dichloroethene, was below the method detection limit. Two other target analytes, dibutylbutyl phosphonate and tributyl phosphate, were positively identified but not quantitatively measured. Tributyl phosphate was estimated to be present at 0.02 ppmv (0.2 mg/m³) and dibutyl butylphosphonate was estimated to be present at 0.004 ppmv (0.05 mg/m³). These 2 compounds were found at very similar levels in tank C-104.

Dichloromethane, benzene, and toluene were common to both the TST and SUMMA™ analyses. The SUMMA™ and TST sample results for benzene and toluene were in excellent agreement. Benzene and toluene were measured to be 0.0005 ppmv and 0.0004 ppmv, respectively, in SUMMA™ samples by OGIST, and 0.00059 ppmv and 0.00052 ppmv, respectively, in TST samples by ORNL. This agreement is important because of concerns about the TST sample volume measurements made with the VSS (see Section X.1); unlike the TST samples, SUMMA™ samples would not be affected by sample volume errors.

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

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

X.3.2 Tentatively Identified Organic Analytes

In addition to targeted analytes, OGIST, ORNL, and PNL analytical procedures allow the tentative identification of other organic vapors. By the nature of the samples and their analysis, virtually all 3- to 15-carbon organic compounds present in the tank headspace above analytical detection limits are observable. The PNL list of tentatively identified compounds, with estimated concentrations, is given in Table X-5, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table X-6. Estimated concentrations given in Tables X-5 and X-6 are in mg/m^3 , based on dry air at 0 °C and 1.01 bar.

OGIST provided total-ion chromatograms for each of the tank C-105 exhaust SUMMA™ samples and assigned tentative identities to the significant peaks, but did not estimate their concentrations. Table X-7 lists the analytes tentatively identified by OGIST, and designates which analytes were detected in each of the 3 SUMMA™ samples. As a rough guide, the analytes listed in Table X-7 were probably detected at greater than 0.001 ppmv. It should also be noted that some peaks in the total-ion chromatograms were not labeled, despite being relatively high, because confidence in assigning a chemical identity was very low.

Tentative identification of organic 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. Entries in Table X-6 illustrate this, particularly near the bottom of the table where the analytes have higher molecular weights.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Clauss et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables X-5 and X-6 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 1, 2, and 3 in Table X-6) or the assignment of the same identity to different peaks (e.g., Cmpd # 69 and 83 in Table X-6). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

Concentrations given in Tables X-5 and X-6 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

X.3.3 Total Nonmethane Organic Compounds

OGIST measured the total nonmethane organic compound (TNMOC) concentration in 3 SUMMA™ canister samples using the EPA TO-12 method (Rasmussen 1994a). The sample mean was 1.5 mg/m³, with a standard deviation of 0.1 mg/m³. This value is low compared to most passively ventilated waste tanks sampled to date. 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 Analytes

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

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

A convenient way to consider the organic compounds listed in Tables X-3 through X-7 is to separate them into 2 categories: 1) Organic compounds added as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes tributyl phosphate, dibutyl butylphosphonate, and the semivolatile branched alkanes and normal paraffinic hydrocarbons (NPHs), all of which ostensibly came from the Plutonium-Uranium Extraction (PUREX) process. It also includes the volatile halogenated compounds present at trace levels, such as chloromethane, dichlorodifluoromethane, and trichlorofluoromethane, which may have been used as cleaning solvents, and may have been sent to the waste tanks when contaminated.

One type of semivolatile compound commonly detected in the NPH-rich waste tanks, but not in the tank C-105 exhaust, is a group of semivolatile bicyclic alkanes. Decahydronaphthalene and several methyl-substituted decahydronaphthalenes have been tentatively identified in many of the 241-BY

and 241-C farm tanks, but were not identified in the tank C-105 exhaust. Several such compounds were noted in the tank C-104 samples, but their concentrations relative to other semivolatiles are much lower than in other NPH-rich tanks. This may be an indication that the organic vapors in the tank C-105 exhaust are remnants of waste from a period when the PUREX process was using a relatively pure NPH diluent.

The second category includes all organic compounds that were not placed into the tank as waste, but instead have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables X-3 through X-7 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, nitrates, nitrites, and volatile alkanes. By far the most abundant of these in the headspace are the short-chain volatile compounds, however, some long-chain low volatility compounds may also be waste reaction products.

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

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

- 1) straight-chain nitriles from ethanenitrile (acetonitrile) through nonanenitrile;
- 2) straight-chain alkyl nitrates from methyl to hexyl nitrate;
- 3) normal alkanes from propane through n-nonane³;
- 4) straight-chain 2-ketones from propanone (acetone) through 2-octanone;
- 5) straight-chain aldehydes from ethanal (acetaldehyde) through decanal;

as well as several partially complete series of other functionally related organic compounds such as alkenes and alcohols. As has been noted in other NPH-rich waste tanks, many of the volatile species (presumed to be degradation products of the NPHs) have functional groups on the molecule's first or second carbon atom.

³ n-Decane through n-pentadecane were also detected, however, these are principally constituents of the original waste and not waste reaction products.

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

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

Table X-1
 Tank C-105 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.5 and 10	Organic vapors	10 tank air samples, + 1 trip blank
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous Oxide, Carbon Monoxide, Organic vapors	3 tank air samples, 6 ambient air samples
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 1 trip blank
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 1 trip blank
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 1 trip blank
	Silica Gel Sorbent Trap	3.0	Water vapor	5 tank air samples + 1 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	3.0	Tritium-Substituted Water Vapor	1 tank air sample

Table X-2
Tank C-105 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	2.4	0.3	12
Carbon Monoxide, CO	630-08-0	SUMMA™	3	0.29	0.01	4
Hydrogen, H ₂	1333-74-0	SUMMA™	3	22	2	9
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.1	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.1	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	5.3	0.26	5
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	5	9,200 (6.8 mg/L)	1,200 (0.9 mg/L)	13

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

Table X-3
Tank C-105 Positively Identified Organic Analytes in OGIST SUMMA™ Samples

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

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

3. Detected in only 2 samples.

4. These analytes co-elute, so the given concentration is their sum.
5. Detected in only 1 sample.

Table X-4
Tank C-105 Positively Identified Organic Analytes in TST Samples

Cmpd #	Compound	CAS ¹ Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
1	Ethanenitrile ³ (Acetonitrile)	75-05-8	0.026	0.006	22
2	Propanone (acetone)	67-64-1	0.014	0.003	21
3	Dichlorormethane ³ (methylene chloride)	75-09-2	0.041	0.071	173
4	Propanenitrile	107-12-0	0.0079	0.0022	27
5	n-Hexane	110-54-3	0.0049	0.0010	20
6	Benzene	71-43-2	0.00059	0.00014	24
7	1-Butanol ³	71-36-3	0.17	0.03	16
8	Butanenitrile ³	109-74-0	0.014	0.003	23
9	2-Pentanone	107-87-9	0.0024	0.0006	26
10	n-Heptane	142-82-5	0.0009	0.0001	13
11	Toluene	108-88-3	0.00052	0.00006	12
12	Pentanenitrile	110-59-8	0.0022	0.0004	19
13	2-Hexanone	591-78-6	0.0011	0.0002	15
14	n-Octane	111-65-9	0.0016	0.0001	5
15	Hexanenitrile	628-73-9	0.0021	0.0013	59
16	2-Heptanone	110-43-0	0.00092	0.00015	16
17	n-Nonane	111-84-2	0.00092	0.00007	8
18	Heptanenitrile	629-08-3	0.0012	0.00001	9
19	2-Octanone	111-13-7	0.00062	0.00001	19
20	Octanenitrile	124-12-9	0.0010	0.00003	34
21	Nonanenitrile	2243-27-8	0.00054	0.00003	57
22	n-Dodecane ³	112-40-3	0.016	0.002	16
23	n-Tridecane ³	629-50-5	0.019	0.003	15
Sum of positively identified compounds:			1.24 mg/m ³		

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.
3. Two or more samples were outside calibration range.

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

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

1. CAS = Chemical Abstract Service.

Table X-6
Tank C-105 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
1	Carbon Dioxide	124-38-9	0.14	0.05
2	Carbon Dioxide	124-38-9	1.1	1.6
3	Carbon Dioxide	124-38-9	1.7	1.4
4	1-Propene	115-07-1	0.22	0.03
5	1-Propene, 2-methyl-	115-11-7	0.49	0.19
6	Butane	106-97-8	0.20	0.03
7	1-Propene, 2-methyl	115-11-7	0.10	0.09
8	1-Propene, 2-fluoro	1184-60-7	0.023	0.04
9	1-Propene, 2-methyl	115-11-7	0.062	0.11
10	3-Buten-2-one	78-94-4	0.19	0.05
11	2-Butanone	78-93-3	0.39	0.03
12	Acetic acid, ethyl ester	141-78-6	0.093	0.161
13	Acetic acid	64-19-7	0.19	0.07
14	Furan, tetrahydro	109-99-9	0.074	0.074
15	2-Butenal	4170-30-3	0.024	0.042
16	Nitric acid, propyl ester	627-13-4	0.066	0.059
17	Acetic acid	64-19-7	0.27	0.25
18	Hexanal	66-25-1	0.024	0.020
19	Acetic acid, butyl ester	123-86-4	0.022	0.019
20	Cyclotrisiloxane, hexamethyl	541-05-9	0.0078	0.0135
21	Nitric acid, butyl ester	928-45-0	0.040	0.006
22	Formic acid, butyl ester	592-84-7	0.0067	0.0115
23	Alkanone		0.0068	0.0118
24	2,2-Dimethyl-1-propanethiol		0.31	0.07
25	Pyridine, 4-methyl	108-89-4	0.025	0.028
26	Alkene and C2-Benzene		0.0038	0.0067
27	Alkyne		0.0054	0.0094

WHC-SD-WM-ER-443 REV. 0

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
28	3-Heptanone	106-35-4	0.040	0.007
29	Acetamide, N,N-dimethyl	127-19-5	0.033	0.032
30	alkyl-dihydrofuran		0.015	0.0005
31	2(3H)-Furanone, dihydro	96-48-0	0.0042	0.0073
32	1,5-Pentanediol, dinitrate	3457-92-9	0.0036	0.0063
33	2(3H)-Furanone, dihydro	96-48-0	0.10	0.15
34	C2-cyclohexane		0.0021	0.0036
35	2-Hexene, 2,4-dimethyl		0.0031	0.0053
36	C8-Alkanone		0.022	0.0041
37	Butanamide	541-35-5	0.035	0.004
38	Alkyl Acetate	112-06-1	0.0060	0.0052
39	4-Octanone	589-63-9	0.0060	0.0105
40	Cyclotetrasiloxane, octamethyl	556-67-2	0.059	0.084
41	Phenol	108-95-2	0.0035	0.0061
42	Butanoic acid, butyl ester	109-21-7	0.0095	0.0012
43	Decane	124-18-5	0.095	0.011
44	Octanal	124-13-0	0.021	0.001
45	Alkene		0.0028	0.005
46	2-Propanone, 1-fluoro and others		0.0034	0.0059
47	Mixture		0.0018	0.0031
48	Octanone		0.013	0.011
49	Alkanone		0.0046	0.0041
50	Ethanone, 1-phenyl	98-86-2	0.0022	0.0039
51	Alkene		0.0088	0.0082
52	2-Undecanone	112-12-9	0.0059	0.0103
53	Undecane	1120-21-4	0.43	0.07
54	Nonanal	124-19-6	0.033	0.009

WHC-SD-WM-ER-443 REV. 0

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

WHC-SD-WM-ER-443 REV. 0

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
81	2-Tridecanol	1653-31-2	0.0018	0.0031
82	Trimethylsilylester of methoxy benzoic, other		0.0018	0.0032
83	Undecane, 2,7-dimethyl	17301-24-5	0.0014	0.0025
84	5-Undecanone	33083-83-9	0.027	0.024
85	Alkenol		0.0049	0.0043
86	Butyl Heptanoate		0.0059	0.0052
87	3-Undecanone	2216-87-7	0.017	0.015
88	6-Tridecane	24949-38-0	0.0014	0.0024
89	1,12-Tridecadiene	21964-48-7	0.0018	0.0032
90	C13-alkene		0.00086	0.00149
91	Alkane		0.0076	0.0081
92	Tridecane, 6-methyl	13287-21-3	0.010	0.018
93	Alkane		0.0053	0.0064
94	1,3-Benzenediol, 4-hexyl	136-77-6	0.0035	0.0031
95	Alkene		0.0032	0.0030
96	Tridecane, 4-methyl	26730-12-1	0.0038	0.0034
97	C12 or C13 Alkane		0.017	0.018
98	2-Heptanone, 6-(2-furanyl)-6-methyl	51595-87-0	0.0029	0.0026
99	Alkane		0.016	0.009
100	Dodecane, 2,7,10-trimethyl		0.081	0.012
101	Alkenol		0.0048	0.0044
102	C1-hydroxy-quinoline		0.0087	0.0081
103	3-Dodecanone	1534-27-6	0.026	0.023
104	Tetradecane	629-59-4	0.14	0.02
105	Alkenol		0.016	0.015
106	Oxygenated Compound		0.0028	0.0026
107	C14-Alkane		0.0025	0.0026

WHC-SD-WM-ER-443 REV. 0

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
108	Pentadecane	629-62-9	0.0044	0.0076
109	C14-Alkane		0.0011	0.0019
110	C15-Alkane		0.044	0.040
111	C15-Alkane		0.0065	0.0112
112	Tridecanone		0.051	0.028
113	C2-hydroxy-quinoline		0.0098	0.0087
114	3-Tridecanone	1534-26-5	0.031	0.029
115	Pentadecane	629-62-9	0.076	0.072
116	Alkanone		0.012	0.011
117	Alkane		0.017	0.015
118	Alkanol		0.0011	0.0019
119	Alkanol		0.0015	0.0027
120	Phenol, 2,6-bis(1,1-dimethylethyl)-4-meth	128-37-0	0.011	0.012
121	Phosphonate, homolog of dibutyl butylphosphonate		0.0033	0.0029
122	C17-Alkane		0.0039	0.0068
123	Dodecane, 2-methyl-8-propyl	55045-07-3	0.0046	0.0080
124	Phosphate, homolog of tributyl phosphate		0.0047	0.0041
125	Alkane		0.0042	0.0072
126	Alkane		0.0033	0.0057
127	Tetradecanone		0.029	0.020
128	Tetradecanone		0.012	0.011
129	Octadecanoic acid, butyl ester		0.029	0.006
130	Phosphate, homolog of tributyl phosphate		0.0059	0.0052
131	3-Undecanone	2216-87-7	0.013	0.012
132	Hexadecane	544-76-3	0.019	0.033

WHC-SD-WM-ER-443 REV. 0

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
133	Tetradecanone		0.014	0.012
134	Tetradecane	629-59-4	0.013	0.022
135	Pentadecane		0.025	0.022
136	Phthalate		0.0032	0.0055
137	Dibutyl Butyl Phosphonate	78-46-6	0.051	0.004
138	Benzene, (1-butylheptyl)-	4537-15-9	0.0032	0.0036
139	Pentadecane, 2,6,10-trimethyl		0.0053	0.0092
140	Tributyl Phosphate	126-73-8	0.24	0.22
141	Benzene, (1-ethylnonyl)-	4536-87-2	0.0027	0.0047
142	alkyl benzene		0.0037	0.0043
143	Butyl Myristate		0.033	0.005
144	Heptadecane	629-78-7	0.0092	0.0070
145	Phosphate, isomer of tributyl phosphate		0.014	0.007
146	Mixture		0.0013	0.0022
147	Benzene, (1-methyldecyl)-	4536-88-3	0.0039	0.0034
148	Benzene, (1-pentylheptyl)-	2719-62-2	0.0040	0.0011
149	Benzene, (1-butylloctyl)-	2719-63-3	0.0039	0.0035
150	Benzene, (1-propylnonyl)-	2719-64-4	0.0012	0.0021
151	Butyl Myristate		0.023	0.003
152	Pentadecane, 2,6,10-trimethyl		0.00076	0.00132
153	alkyl benzene		0.0066	0.0027
154	alkyl benzene		0.00079	0.00136
155	Butyl Myristate		0.0078	0.0008
Sum of tentatively identified compounds:			8.20	

1. CAS = Chemical Abstract Service

Table X-7
Tank C-105 Tentatively Identified Compounds in OGIST SUMMA™ Samples

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

WHC-SD-WM-ER-443 REV. 0

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

WHC-SD-WM-ER-443 REV. 0

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

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

2. CAS = Chemical Abstract Service.

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