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BY-110 Headspace Sampling Comparison Test

Volume 1

June 2019

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Richland, Washington 99352

Executive Summary

The Hanford Tank Operations Contractor, Washington River Protection Solutions, conducted comparison tests of two Hanford waste tank vapor-sampling systems to determine the relative differences in quantifying Chemicals of Potential Concern (COPC) while sampling the same waste tank. The systems are the traditional in situ, inline headspace sampling (HS) method and the recently developed slipstream sampling unit for testing respirator chemical cartridges known as the cartridge test (CT) rig. The comparison test was performed to determine if results obtained using the CT rig are similar to results obtained using the traditional HS method. Using the CT rig would provide efficiencies in headspace vapors sampling such as applying ALARA principles, minimizing worker entries to the tank farms, and eliminating the physical strain of manually lowering the headspace sampling bundles into the waste tanks. Six sampling events were conducted during January and February 2018 to collect headspace vapor samples from Hanford tank BY-110 with the two systems. Pacific Northwest National Laboratory was tasked with conducting an analysis of the analytical results to assess the comparability of the sampling methods and make recommendations on future testing or deployment of the CT method.

Comparison testing included sampling and analysis of 59 of the 61 tank vapor COPCs that are compatible with the two sorbent tube sampling systems. Ten of the COPCs were detected at sufficient concentration in the headspace of BY-110 to enable comparative evaluation of the two sampling methods. Measured concentrations of these COPCs spanned a wide range, from 1 ppb to 300 ppm, and from <1% of their respective occupational exposure limit (OEL) to nearly 1300% of their OEL. Five of the COPCs were measured with median concentrations exceeding 10% of their OEL while the remaining five COPCs were measured with median concentrations below 2% of their OEL.

For benzene, acetaldehyde, and propanenitrile, the median HS and CT concentrations were found to be statistically equivalent. The median HS concentration of ammonia was statistically greater than the median CT concentration. However, the difference was within analytical uncertainty and statistical variance of the replicate samples; therefore, the two sets of concentrations were determined to be quantitatively equivalent. The HS median concentrations of the remaining six COPCs—2-hexanone, furan, formaldehyde, acetonitrile, NDEA, and NMEA—were statistically higher than their corresponding CT concentrations.

Analytical data for 53 non-COPC organic vapor analytes also were available from the comparison test sampling results. Ten analytes were detected at sufficient concentration in the headspace of BY-110 to enable quantitative comparative evaluation as a complement to the COPC analysis. These analytes were all present at concentrations below 1% of their respective OEL. Six analytes—1-propanol, 2-butanone, cyclohexane, ethanol, hexane, and trichlorofluoromethane—were found to have statistically equivalent median HS and CT concentrations. The HS median concentrations of the remaining four analytes studied—3-heptanone, 4-methyl-2-pentanone, n-heptane, and toluene—were statistically higher than their corresponding CT concentrations.

Of the 20 COPC and non-COPC analytes evaluated, half exhibited an apparent bias between the mean CT and HS measurements that warranted further analysis to understand the significance and potential mechanisms contributing to the bias. The mean CT/HS ratios of two analytes—furan and 4-methyl-2-pentanone—were within parity when measurement uncertainty was considered. Six of the analytes exhibiting significant bias represented higher boiling point (≥209°F) compounds, indicating a general trend of increasing bias with increasing boiling points. Two COPCs—formaldehyde and acetonitrile—also exhibited significant bias but with lower boiling points (≤179°F). These results indicate that boiling point as well as potentially other factors may be contributors to the observed sampling bias.

Several mechanisms were evaluated as potential contributors to sampling and analytical bias. Based on this evaluation, the leading mechanism suspected of driving the observed bias in higher boiling point analytes was the lower temperature in the sample gas stream due to the 125+ ft extension hose required for the CT rig. Temperature data from the comparison test suggest that the hose heat tracing/insulation is not adequate for maintaining the inside gas temperatures, thus increasing the potential for higher boiling point compounds to adsorb or condense on the extension hose and other CT surfaces. Based on the apparent biases identified between the CT and HS systems, it is recommended that future CT testing be performed with improved temperature conditioning on the slip stream hose between the tank riser and CT rig, and on the CT rig components and enclosure to maintain temperatures within a degree or two of tank headspace temperatures. Such improvement will likely require a combination of improved heat tracing and insulation. Once improved temperature controls are achieved on the CT system, additional CT and HS comparisons are recommended to assure that biases are minimized, especially for compounds with boiling points greater than 200°F.

Several sampling, analysis, and data challenges impacted the ability to fully benefit from the substantial data collected during the comparison test. These challenges included large sample variances, elevated reporting limits, and data quality flags that limited the viable use of specific analytical data. Improvements in several areas could potentially enhance the value of future headspace data collection. Additional effort to assess and understand the potential cause and implications of sample variance observed with HS sampling is recommended, especially for analytes where variance greatly exceeded analytical laboratory control limits. Optimization of sampling flow rates and durations is also recommended to help assure quantitative results that fully support sampling objectives. Finally, the variance observed in this study reinforces the need for sample replicates in the future to assure statistically relevant results. Based on the data in this study replicate samples are recommended going forward. For the key COPCs four or more replicates on both the HS and CT systems are recommended to assure that the mean concentration is within 50% of the mean of the 12-replicate mean, and eight or more to be within 30%.

Acronyms and Abbreviations

ALARA	as low as reasonable achievable exposure to hazards
ALS	ALS Environmental Salt Lake City
APR	air-purifying respirator
CAS	Chemical Abstract Service
CBAL	Columbia Basin Analytical Laboratory, part of the RJ Lee Group
CFR	Code of Federal Regulations
COPC	Chemicals of Potential Concern
CT	cartridge test
CVAA	Cold Vapor Atomic Absorption
CV	coefficient of variation
DL	detection level/limit
DL | RL	reporting limit | detection limits
EPDM	ethylene propylene diene monomer rubber
EPA	U.S. Environmental Protection Agency
FEP	fluorinated ethylene propylene
GC–FID	gas chromatography–flame ionization detector
GC/MS	gas chromatography/mass spectrometry
GC–TEA	gas chromatography–thermal energy analyzer
HEPA	high-efficiency particulate air (filter)
HPLC	high performance liquid chromatography
HPLC–UV	high performance liquid chromatography–ultraviolet
HS	headspace sampling
$_{\text{HTF}}$OEL	Hanford Tank Farms Occupation Exposure Limit (
IC	ion chromatography
LCS	laboratory control sample
LCSD	laboratory control sample duplicates
MDL	method detection limit
MS	mass spectrometry
NDEA	N-Nitrosodiethylamine
NDMA	N-Nitrosodimethylamine
NIOSH	National Institute of Occupational Safety and Health
NMEA	N-Nitrosomethylethylamine
NPT	National Pipe Thread
NRTL	non-random two-liquid (method)
OEL	Occupational Exposure Limit
OSHA	Occupational Safety and Health Administration
SCBA	self-contained breathing apparatus
PAPR	powered air-purifying respirator
ppm	parts per million
PNNL	Pacific Northwest National Laboratory
PTFE	polytetrafluoroethylene

RPD	relative percent differences
RSE	relative standard error
RL	reporting limit
SVOA	semi-volatile organic analyte
SWIHD	Site-Wide Industrial Hygiene Database
TIC	Tentatively Identified Compound
TST	triple-sorbent tube
TWINS	Tank Waste Information Network System
UNIFAC	UNIQUAC functional-group activity coefficients (method)
VOA	volatile organic analyte
VOC	volatile organic compound
WC	water column
WHL	Wastren Hanford Laboratory (222S)
WRPS	Washington River Protection Solutions

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1.0 Introduction/Project Description

As the Tank Operations Contractor for U.S. Department of Energy operations at the Hanford site in Washington State, Washington River Protection Solutions (WRPS) is responsible for managing highly radioactive wastes stored in tanks at Hanford. WRPS conducted comparison tests of two Hanford waste tank vapor-sampling systems to determine the relative differences in collecting vapors for Chemicals of Potential Concern (COPC) while sampling the same waste tank. The systems are the traditional in situ, inline headspace sampling (HS) method and the recently developed slipstream sampling unit for testing powered air-purifying respirator (PAPR) chemical cartridges.

1.1 Project Description

The comparison of the different methods was performed to determine if the slipstream sampling unit (also referred to as the cartridge test [CT] rig) provides similar results to the traditional in situ, inline sampling. Using the slipstream sampling unit would provide efficiencies in headspace vapors sampling such as applying ALARA principles, minimizing worker entries to the tank farms, and eliminating the physical strain of manually lowering the HS bundles into the waste tanks.

Six sampling events were conducted during January and February 2018 to collect vapor samples from Hanford BY-110 waste tank using the two systems. Table 1 lists the sampling events (also referred to as dives) and the tank vapor COPC (and non-COPC) compound classes evaluated during each dive.[1,2]

While the in situ HS method has been used for decades at the Hanford tank farms, the CT rig was first deployed in 2017 to test the performance of cartridges commonly used in PAPRs at Hanford tank farms. The CT rig pulls headspace vapors from the tank to a location outside the tank farm fence where it can be sampled and used as a challenge gas for cartridge testing.

This report summarizes analysis of data that was that was obtained from samples collected by both the traditional HS method and the PAPR respirator CT rig. Relative differences in the analytical results from the vapors collected from BY-110 by the two methods are presented.

1.2 Background on Tank BY-110

Hanford waste tank 241-BY-110 (BY-110) is located in the 200 East area of the Hanford site north of Richland, Washington. It is a single-shell nuclear waste storage tank located in the BY tank farm.

The 241-BY tank farm is a second generation tank farm constructed at the Hanford site to store high-level radioactive waste generated from chemical processing of irradiated uranium fuel. The tanks were constructed in 1948 and 1949 by General Electric Company. The farm consists of 12 carbon steel underground waste tanks each with a total capacity of 758,000 gal.

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[1] Industrial Hygiene Sample Plan: Headspace Sampling Methodology Comparison, IHSP-VPRD-005R1, January 2018, Washington River Protection Solutions, Richland, Washington. (unpublished)

[2] The TDU Tenex TA, Carbotrap 150 TDU, and Carbotrap 300 TDU tubes were purchased new and prepared at the 222-S Laboratory at Hanford using cleaning procedures. All other tubes were purchased new and used directly from the manufacturer’s packaging.

Table 1. Summary of Comparison Sampling Events

		Target		Headspace		PAPR Cartridge Sampling Unit	
Test	**Sampling Tubes**	**Flow Rate Per Tube**	**Date**	**On**	**Off**	**On**	**Off**
Dive 1	Methanol and Nitrosamines		January 16, 2018	9:44	10:44	10:22	11:22
	SKC 226-51	50 mL/min					
	Thermosorb/N	800 mL/min					
Dive 2	Pyridine and Ethylamine		January 25, 2018	8:56	9:57	8:58	9:59
	SKC 226-01	800 mL/min					
	SKC 226-96	200 mL/min					
Dive 3	SVOC and Aldehyde		February 1, 2018	9:22	10:22	9:26-9:29	10:33
	Carbotrap 150 TDU	50 mL/min					
	SKC 226-119	400 mL/min					
Dive 4	Acetonitrile and 1,3 - Butadiene		February 6, 2018	8:40	9:40	9:06	10:06
	SKC 226-09	200 mL/min					
	SKC 226-37 (part A & B)	400 mL/min					
Dive 5	VOC and Ammonia		February 8, 2018	8:55	9:55	8:48	9:49
	Carbotrap 300 TDU	50 mL/min					
	Anasorb 747, SKC 226-29	350 mL/min					
Dive 6	Mercury and Furan		February 9, 2018	9:47	10:48	9:36	10:36
	Anasorb C300, SKC 226-17-1A	250 mL/min					
	TDU Tenex TA	50 mL/min					

Tank 241-BY-110 is 75 ft in diameter. The vessel height is nominally 37 ft including the concrete in the tank bottom and dome. Figure 1 shows the top center of the concrete dome is nominally covered by 8 ft of earth (Field et. al. 2011). The 2015 image of BY-110 shows most of the waste has been removed from the tank (see Figure 2). On January 31, 2018, the Tank Farm Dashboard[3] listed the BY-110 waste surface level as 131.46 in.

BY-110 is the fourth tank in a six-tank cascade consisting of tanks BX-110, BX-111, BX-112, BY-110, BY-111, and BY-112. A 3-in.-diameter overflow line connects tank 241-BY-110 to tanks 241-BY-111 and 241-BY-112 (WHC 1994). The elevation of each tank in the cascade is 1 ft lower than that of the preceding tank, with the cascade overflow height being ~23.7 ft from the tank center bottom and 1.2 ft below the top of the steel liner. An overflow line also connects 241-BY-110 and 241-BX-112; however, transfer records do not indicate any waste transfers between the two tanks (Agnew et al. 1997).

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[3] https://phoenix.pnnl.gov/apps/tankfarm/farm.html?farm=BY

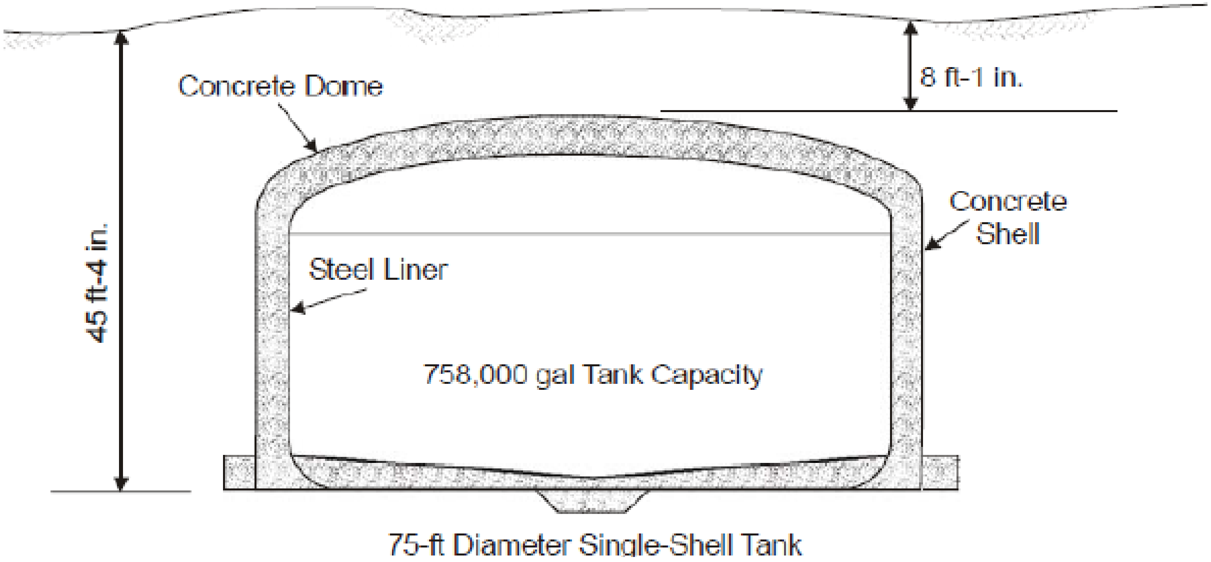

Figure 1. Tank Diagram of BY Waste Tanks

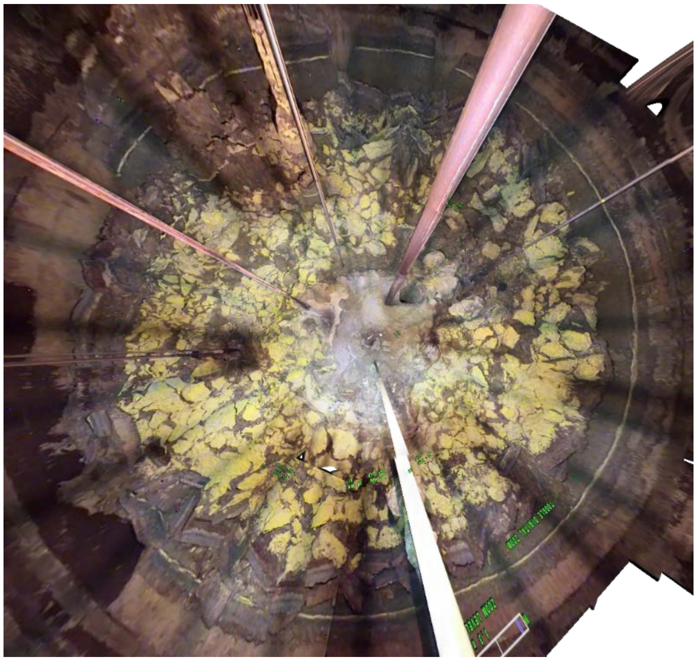

Figure 2. Image from Inside Tank BY-110

As of 2006, the headspace volume of BY-110 was 90,020 ft^3 (Hu 2009), and there have been no waste-changing operations since that time (Diedesch 2017). The passive ventilation rates of 15 and 21 ft^3/min were measured for tank BY-105 in April/May 1997 (Huckaby et.al. 2004). It should be noted that tank BY-105 is in a different cascade from BY-110, so it is not known if BY-110 has a different ventilation rate because of factors such as tank isolation, cascade line plugging, or differences in the extent of penetrations sealing. The accessible risers on the BY-110 tank are located near the top center of the tank as shown in Figure 3

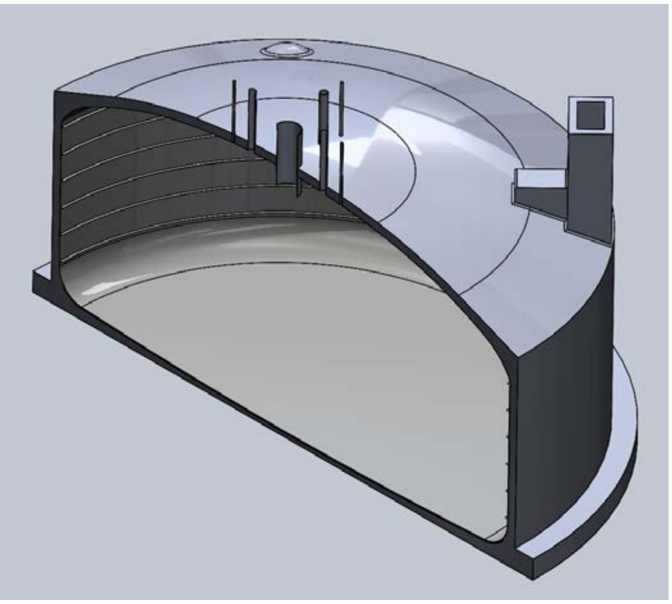

Figure 3. Model Rendering of the BY-110 Type 3 100 Series Capacity Waste Tank

The COPCs listed below have been measured[4] in BY-110 at concentrations that are above their Hanford Tank Farms Occupation Exposure Limit ($_{\text{HTF}}$OEL).

- N-Nitrosodimethylamine (NDMA) at 1874% of the $_{\text{HTF}}$OEL (2018)[5]
- N-Nitrosodiethylamine at 252% of the $_{\text{HTF}}$OEL (2018)
- N-Nitrosomethylethylamine at 150% of the $_{\text{HTF}}$OEL (2018)
- Ammonia at 1704% of the $_{\text{HTF}}$OEL (1994)
- 2,3-dihydrofuran at 309% of the $_{\text{HTF}}$OEL (2015)
- 2,5-dihydrofuran at 457% of the $_{\text{HTF}}$OEL (2015)
- Furan at 295% of the $_{\text{HTF}}$OEL (2015).

The results of analyses to determine the concentrations of these COPCs are summarized in the report entitled *Analysis of Air-Purifying Respirator (APR) and Powered Air-Purifying Respirator (PAPR) Cartridge Performance Testing on Hanford Tanks BY-108 and BY-110* report.[6]

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[4] Historic vapor measurements and measurements from the most recent 2018 cartridge sampling events are included. The measurements do not include the sampling results from the vapor comparison sampling documented in this report.

[5] This NDMA maximum concentration, measured during APR cartridge testing, had multiple quality issues and is considered dubious.

[6] Nune SK, CK Clayton, CJ Freeman, TM Brouns, J Liu, and LA Mahoney. 2018 (draft). *Analysis of Air-Purifying Respirator (APR) and Powered Air-Purifying Respirator (PAPR) Cartridge Performance Testing on Hanford Tanks BY-108 and BY-110*. Pacific Northwest National Laboratory, Richland, Washington. Unpublished.

2.0 Description of Testing

The testing compared results obtained using the CT rig to results from the HS methodology traditionally used to collect Hanford waste tank vapors. The two systems/methods are described below.

2.1 PAPR Respirator Cartridge Test Rig

The respirator cartridge testing system was developed by Washington River Protection Solutions and HiLine Engineering (Richland, Washington) as a means to comprehensively test respirator cartridge performance with actual Hanford tank headspace or exhauster gases. Tank headspace or exhauster vapors are pulled directly from the source through a flexible hose that connects the tank or exhauster sampling port within the tank farm/exhauster fence line to the respirator cartridge-testing outside the farm (Nune et al. 2016a, b; Nune et al. 2017a, b, c, d, e, f, g; Freeman et al. 2017).[7,8]

The CT rig has been termed a slipstream sampler, as it is connected to the waste tank via a hose that runs from the tank vapor space up through the riser, across the tank farm, and out of the tank farm to the sampling system. Multiple inline high efficiency particulate filters are attached to the hose near the top of the tank riser to remove potential radioactive particulates. The FSLW 14200 Millipore (Millipore Sigma, Billerica, Massachusetts) filters are hydrophobic Fluoropore™ polytetrafluoroethylene 3.0 micron 142 mm diameter (by 150 microns thick) filters. The filters are also described as a moderately High Efficiency Borosilicate glass fiber filter. This filter medium is the same material used for routine tank vapor monitoring and for sampling and analysis of sources (headspaces and exhausters). The filter was selected because of its broad chemical compatibility that minimizes sorption of, or reactions with, chemical compounds. Polytetrafluoroethylene as the filter medium was not expected to adversely impact the test objectives because this type of filter medium is used for all tank farm vapor sampling. The hose was wrapped in heat tape to maintain in-tank vapor temperatures as near as possible as vapors were transferred to the testing system.[9] Other benefits of maintaining the vapor temperature during transfer were reducing condensation of water, which can act as a sink for chemicals, and preventing potential condensation of other chemicals, including COPCs. There were two connection hoses:

1. The hose from the riser to the inlet of the CT testing system was a Centurion Process, LLC 1-in. RFRTP polytetrafluoroethylene (PTFE) Teflon-lined hose with an ethylene propylene diene monomer rubber (EPDM) cover with 1-in. 316 stainless steel male national pipe thread (NPT) ends, and
2. The return hose which is a Centurion Process, LLC 1-in. RT smoothbore fluorinated ethylene propylene (FEP) lined hose with an EPDM cover with 1-in. 316 stainless steel male NPT ends.

During actual cartridge testing, the test equipment allows for sampling a vapor stream both before and after the cartridge so its effectiveness in removing a given COPC can be quantified. During the comparison testing, no cartridge was mounted so the “cartridge influent” and “cartridge effluent” streams were nominally equivalent. Twelve tubes (six of each sorbent medium) were collected from the “influent” side, which is located before the cartridge mount, and twelve tubes (six of each sorbent medium) were

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[7] Industrial Hygiene Sampling and Analysis Plan for Respirator Cartridge Testing, TFC-PLN-168, REV A, June 16, 2016, Washington River Protection Solutions, Richland, Washington. (unpublished).

[8] Air Purifying Respirator Cartridge Test Apparatus Special Tool and Equipment Evaluation, RPP-STE-59226, Rev 0, June 22, 2016, Washington River Protection Solutions, Richland, Washington. (unpublished).

[9] Across all six dives, the measured in-tank thermocouple temperatures ranged between 59.7 and 69.8ºF during the sampling. The tent surrounding the CT rig was kept as near the in-tank temperatures as possible.

collected from the “effluent” side, which is located after the cartridge mount. Each dive employed two types of media (see Table 1); in total, 24 samples were collected per dive.

The sorbent media tubes captured the COPCs and other non-COPC vapor compounds. After testing, sorbent tubes were removed and analyzed. Sampling of the exhaust gas was performed for 1 hour, nominally.

Figure 4 and Figure 5 show a general schematic diagram for and photographs of the CT rig. The CT rig is a modified version of a system used previously to test air-purifying (APR) respirator cartridges. The modifications included:

- An enlarged cartridge housing and a mounting compatible with the larger PAPR cartridge.
- An additional sampling line and control valve to accommodate 12 simultaneous inlet and outlet sorbent tubes versus the 11 sorbent tubes used in the original APR test stand. The inlet and effluent portion of the test stand were used during the comparison testing.
- Additional instruments to directly measure pressure, temperature, and relative humidity immediately after the cartridge filter.

The test system uses vacuum to draw tank gases/vapors into the unit so the potential for leakage to atmosphere is minimized until the gases/vapors are under positive pressure downstream of the vacuum pumps (Nune et al. 2017b, c, d, e, f, g; Freeman et al. 2017).

Flows through each sorbent tube are set and controlled/maintained using manual flow control valves on the outlet of each rotameter. DryCal flow meters also are used downstream of the sorbent tubes to measure the flow through each sorbent tube (see Figure 6). All equipment connections were leak tested before the test began. Temperature, relative humidity, and pressure of the inlet gas/vapor stream are monitored by calibrated instrumentation.

The CT rig was constructed using Industrial Hygiene-approved materials to prevent influence or interference with vapor analysis. Stainless steel or Teflon™ tubing and fittings are used where possible because of their relatively inert nature to the vapors being analyzed. Limited portions of the assembly used acrylic, Viton™, glass, and Masterflex® C-flex tubing, which are commonly used materials for various vapor-sampling applications.

The vacuum sources for the CT rig are two large vacuum pumps set to a slipstream flow rate of 30 to 50 L/min. Recorded testing operations start at 29.6 to 30.8 L/min, and flows are monitored throughout testing to be sure they stayed in the range of 30 to 50 L/min. Rotameters control flow rates for each tube. The flow rates were checked nominally every 15 minutes during testing. Information about the flow rates, tubing used, and paired gases targeted for each dive is provided in Table 1.

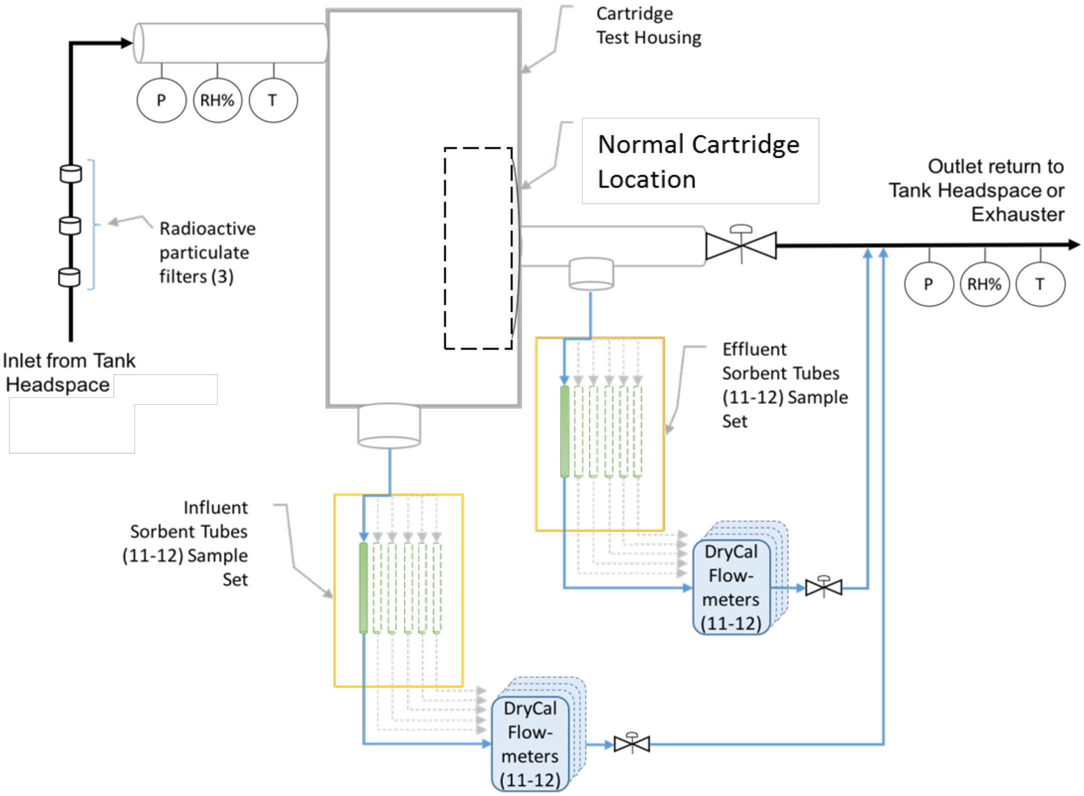

Figure 4. General Schematic of the CT Rig. (Note: the tubing that runs from the cartridge test housing and the post-cartridge sample collection to the sampling tubes is approximately 10 ft long with a ⅜-in. outer diameter and a ¼-in. inner diameter. Tygon®[10] PTFE (Teflon) tubing.[11]) During comparison tests, the cartridge was not installed.

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[10] Tygon is a registered trademark of Saint-Gobain Corporation, and Masterflex is a registered trademark of Cole-Parmer Instrument Company, LLC.

[11] Note: where there were bends in the tubing run, Masterflex® tubing was used in 6- to 12-in. long sections. The length of the total tubing assembly was ~10 ft.

Figure 5. Photograph of the CT Rig

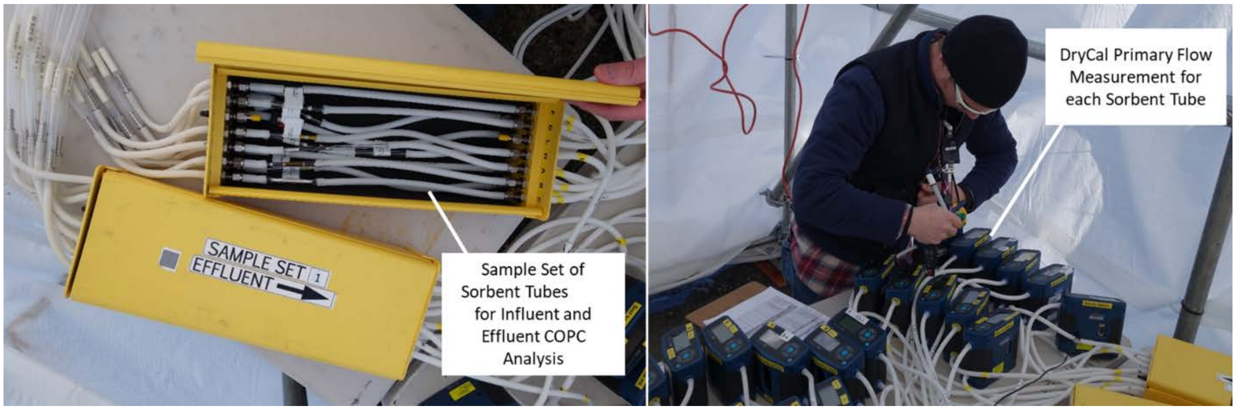

Figure 6. Photographs of the Sorbent Tube Sampling Test Equipment. Twelve sorbent tubes installed, six from each tube media being tested, were collected from the influent side and an additional 12 sorbent tubes were installed, six from each tube media being tested, were collected from the effluent side.[12]

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[12] It should be noted that the sorbent tubes are mounted horizontally in the cartridge sampling system and vertically in the headspace sampling system.

2.2 Headspace Sampling

During in situ headspace sampling, the tubes are lowered into the vapor headspace inside the tank with vacuum pumps (with DryCal meters for flow control) mounted outside of the tank. The test system uses vacuum pumps (one pump for each sample tube line) to draw tank gases/vapors though the sorption tubes. The flow through each sorbent tube is set and controlled/maintained using manual valves. DryCal flow meters are used downstream of the sorbent tubes to measure the flow through each sorbent tube. All equipment connections are leak tested before a test begins.

Temperature from the tank headspace thermocouple was recorded at the start and end of sampling.

The sorbent tubes are assembled into a tube bundle (see Figure 7) that is lowered into the waste tank through a riser on the top of the vessel. Two particulate filters are installed before each tube set. For the comparison testing, each sample line had a primary sampling tube that was directly exposed to the tank vapors. The primary tube was followed by a “breakthrough” sorption tube of the sample model and lot.[13] The primary tube is later referred to as Series A and the breakthrough tube as Series B. This setup allows the analysis to determine if the primary tube had become saturated and if excess COPC vapor had passed by the primary tube.

Figure 7. Photograph of a Routine HS Tube Bundle

During the comparison testing, a single set of 12 sorbent tubes followed by a set of 12 breakthrough sorbent tubes were placed into a single bundle (see Figure 8). Two bundles (each with a different type of sorbent tube as listed in Table 1) were lowered into the waste tank vapor space. The result was the collection of 12 replicate samples[14] for one type of gas collection tube (and 12 breakthrough tubes). Each tube and breakthrough tube set had its own sampling pump and rotameter (with a DryCal flow meter) that was checked nominally every 15 min during testing (see Figure 9). The flow rates, tubing used, and paired gases targeted for each dive are shown in Table 1.

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[13] In the exceptional case of butadiene, there were four tubes in series, two for Series A and two for Series B.

[14] Multiple samples representing the same population characteristic, time, and place which are independently carried through all steps of the sampling and measurement process in an identical manner (EPA, QA Glossary. https://archive.epa.gov/emap/archive-emap/web/html/qa_terms.html#dd). Replicate samples are used to assess total sampling and analysis method variance. Replicate samples are not the same as experimental replication, which would include repeating the sampling campaign under varying tank headspace conditions over time to evaluate performance over a range of operating conditions.

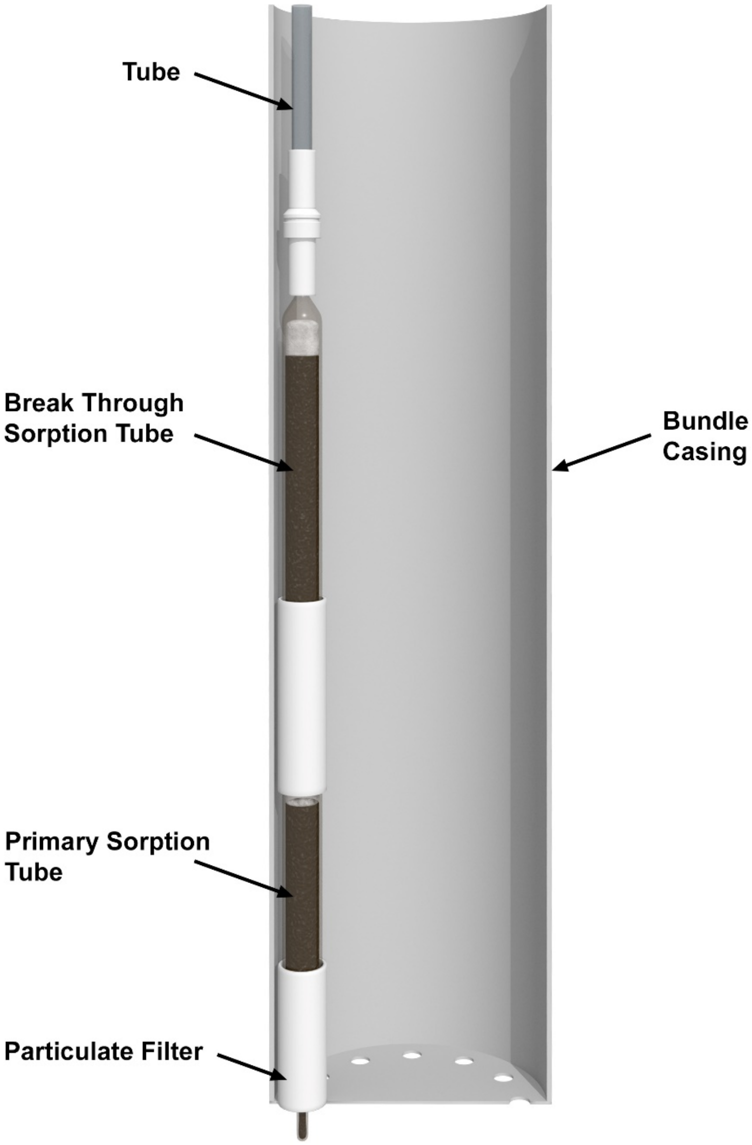

Figure 8. A Single Bundle Assembly Cut-away Diagram. Twelve primary and breakthrough tubes were mounted in a bundle. The bottom is open to the tank vapor headspace**.**

At the bottom of each tube set in a bundle assembly were two 13mm polytetrafluoroethylene (PTFE) membrane filters (0.2 micron) in two part housings.

During each dive, two bundles were lowered into the vapor space, with each bundle collecting samples using different types of tubes (see Table 1 and Figure 10).

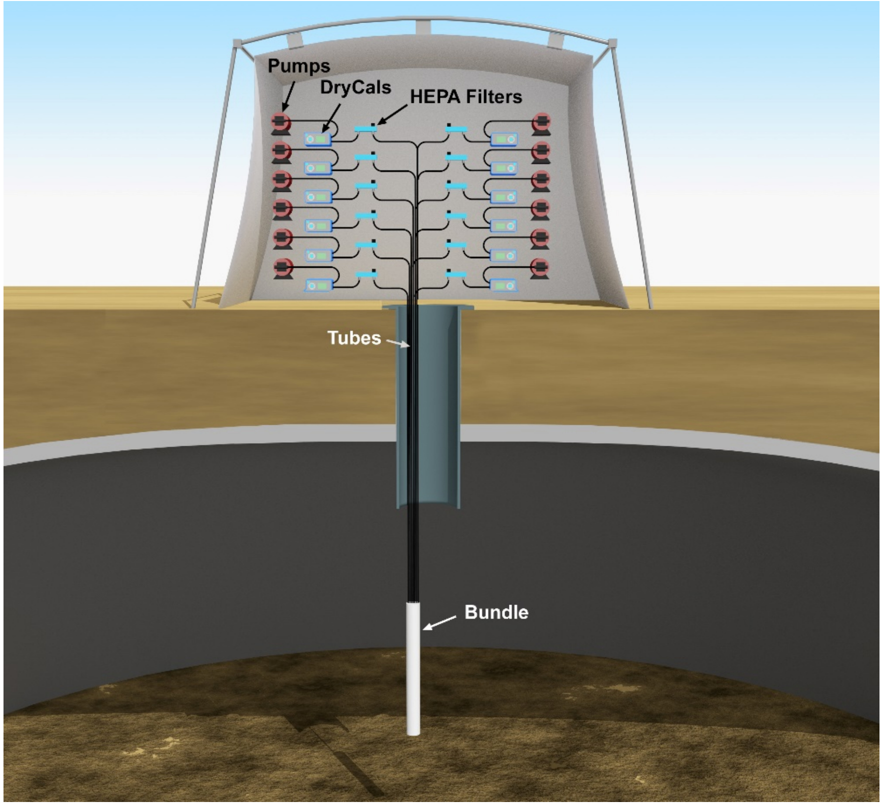

Figure 9. Diagram of the Tubing and Instrumentation for a Single Gas Bundle. Note, the headspace instrumentation is located within the tank farm directly on top of the waste tank.

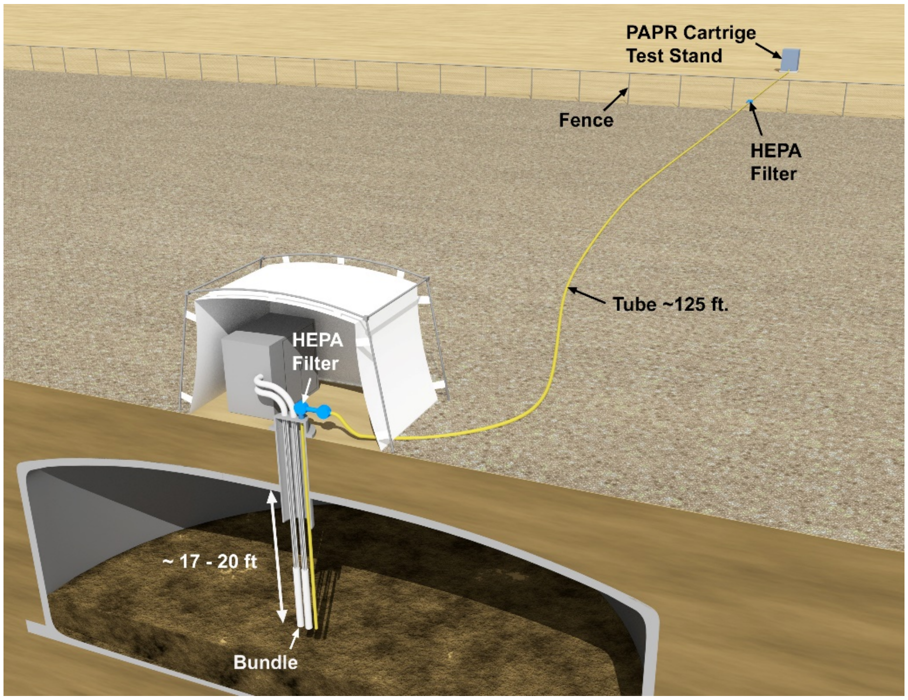

Figure 10. Two Bundles and the CT Rig Sample Collection Hose Lowered into the Waste Tank (cut-away diagram)

2.3 Vapor Collection Position

The HS bundles were placed inside the tank by lowering them 27 ft into the tank from the top of the riser (241-BY-110 riser 12B[15]). This was projected to place the bundles into the tank headspace at the targeted depth of 17 to 20 ft below the bottom of the riser. The sample collection tube for the CT rig was run down inside the same riser such that its inlet was at the same depth as the HS bundle (see Figure 10 and Figure 11). The hoses and tubing on the CT rig were flushed with air both before and after sampling.

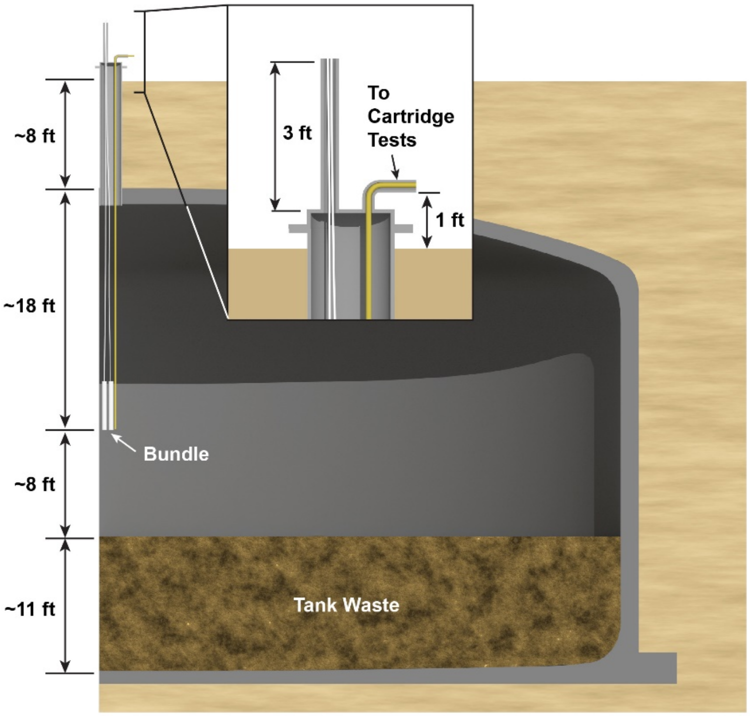

Figure 11. Relative elevations of the Two Bundles and the CT Rig Sample Collection Hose inside the Waste Tank Vapor Space (cut-away diagram)

2.4 Vapor Return Lines

Vapors that were collected from the tank for both the HS system and the CT rig are returned to the tank headspace through the riser. On both systems, after the sorbent tube sampling the remaining vapor and gas go through vacuum pumps that pump the gas through hoses and tubes back to connections on the top of the tank riser above ground level. The gas then flows down the riser pipe into the top of the tank headspace. The flow of gas from the two systems could range from 36 L/min to ~65 L/min depending on the dive.

The gas returns into the headspace through the same riser used for the collection units, entering 17 to 20 ft above the collection points for the sampling (see Figure 11).

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[15] Riser 12B is a 12” diameter sub-riser on the top of Riser 12 which is 42” in diameter. It is located along the north south axis of the tank ~ 20’ from the north wall of the tank. Riser 12B is ~20’ from the overflow nozzle N6 on the north wall of the tank.

3.0 Analysis Approach

The intention of the BY-110 Comparison Test was to determine if results from use of the HS method are comparable to results from use of the CT rig. Raw data providing quantitative results of laboratory analysis of both CT and HS sorbent tubes for each of the six sampling dives were provided to PNNL, along with sample volumes, copies of field logs, and sample chain-of-custody records. PNNL scientists and engineers performed data calculations, data reduction, and statistical analysis of the raw data to draw conclusions regarding the comparability of the two sampling methods.

3.1 Data Reduction and Concentration Calculations

Raw test data, including mass of chemicals captured on each CT or HS sorbent tube from analytical laboratory results and volumes of gas sampled, were converted into vapor concentrations for each COPC and selected non-COPC analytes that were detected. Calculated concentrations for each of the 12 CT and 12 HS sorbent tube samples[16] for each COPC and non-COPC analyte of interest[17] were documented, along with information regarding measured concentrations below analytical reporting limits or measurements with analytical laboratory quality flags indicating potential limitations of the quantitative results. The raw data input received by PNNL is included in Appendix A. Appendix B provides additional details of the data reduction process and presents the calculated sample concentration data that was generated from the raw data.

3.2 Statistical Analysis

To adequately compare the quantitative results of two distinct sampling methods (i.e., CT and HS), statistical analysis methods must be employed. Statistical analysis enables higher confidence in conclusions regarding comparability of the data, including determinations of no significant difference, significant difference, or inconclusive result due to limitations of the data. When significant differences are observed, it is useful to apply statistical methods to determine whether correction factors can be applied with confidence to make results of one method (e.g., CT) equivalent to measurements from the other method. In this case, the limitations of these correction factors also may be assessed through use of statistical analysis.

Evaluation of the new sampling method requires statistical comparisons of the following types:

- Field precision (the variability of CT measurements) as compared to the traditional method that, for the present purpose, will be regarded as the standard
- Bias (additive or multiplicative) of the mean CT concentration data in relation to the mean HS concentration

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[16] Each of the 12 HS samples included a series A and series B, for a total of 24 sorbent tube samples.

[17] Numerous tank vapor non-COPC analytes are routinely detected in headspace samples. The majority of these analytes are either volatile or semi-volatile organic compounds (VOCs or SVOCs) that are sorbed on the Carbotrap 150 or 300 thermal desorption unit (TDU) tubes, respectively (see Table 1, dives 5 and 3). Those non-COPC VOC or SVOC analytes consistently detected at concentrations above their analytical reporting limit were considered analytes of interest in this study. COPCs are a subset of all analytes detected in tank vapors, specifically those analytes that exceed 10% of their respective occupational exposure limit (OEL) or other similar criterion. Therefore, there was interest in assessing the comparability of the CT and HS sampling methods for quantitation of VOCs and SVOCs, from which new COPCs, if present, are likely to emerge.

- Detection sensitivity (probability of detection when the chemical is present, compared to the standard) and specificity (probability of a lack of detection when the chemical is not present, compared to the standard)
- Accuracy (the overall difference between CT concentrations and mean HS concentrations (e.g., the mean squared error, a combination of bias and precision).

Mean additive bias is usually expressed as the average of the difference between each observed CT concentration and the true value as determined by the mean or median (the latter is used in this analysis to reduce the influence of extreme values) of the standard measurements. However, in Table 2 we calculate the reverse difference so that the bias can be added to the CT results to estimate the median headspace concentration. Similarly, the mean multiplicative bias is generally expressed as the average of the ratio of each CT observation and the mean HS concentration. However, in Table 2 we calculate the inverse so that the CT result can be multiplied by the multiplicative bias to estimate the headspace concentration. The choice between using either a multiplicative or additive bias correction is based on physical mechanisms discussed further in Section 5.

We calculated the additive and multiplicative bias and the associated uncertainty assuming the HS median or mean was known with and without error. The estimate of uncertainty with the mean HS estimated with error and assuming multiplicative bias was calculated based on the concentration data distributed as a lognormal so that $Y = \ln(CT)$ and $X = \ln(HS)$ were normally distributed. Details of these calculations are presented in Appendix C.

As a first step, descriptive statistics were calculated for each chemical and sampling method. These statistics included the number of concentrations detected, mean concentration, standard deviation, minimum and maximum concentration, and the first, second (median), and third quartiles of the data. The coefficient of variation (CV%), which is the standard deviation divided by the mean times 100, also was calculated and provided a standardized measure of variability that can be compared across chemicals.

The data description also included data visualization. Appendix C and Section 4.0 contain box plots for individual chemicals and sampling methods based on the detected observations and the unique detection limits. Each box plot was overlaid on a plot of the individual values in sample order (1-12). Detected/reported values were indicated as a solid symbol (●) and values less than the detection/reporting limit were indicated as an open symbol (∇). Single flags associated with the quality of the concentration estimate were indicated by the flag value (e.g., "E," "a," "L," etc.) overlaid on the solid or open symbol. For the sake of comprehensive visualization, concentration values associated with multiple flags were indicated with an "X," although they were eliminated from statistical analysis. The box plot was only generated for those chemicals with at least four detected values and plots were produced if there was at least one detected value.

Assessment of the new CT method, by comparison with the traditional HS method, involved a number of statistical comparison tests, all of which are presented in Appendix C. Tests chosen for this analysis are appropriate when the methods being compared do not have equal numbers of samples, sample sizes are small (<20), and data are skewed and not normally distributed. Minitab (Version 18.1, Minitab, Inc., 2017), Sigmaplot (Version 13.0, Systat Software, Inc. 2014), and Microsoft Excel spreadsheets (Microsoft Office 365 ProPlus) were used for this analysis.

Table 2. Data Quality Attributes, Estimators, and Methods used to Compare the CT and HS Methods

Attribute	Estimates		Method of Comparison
Detection **Sensitivity** and **Specificity**	**Sensitivity** = the probability that CT will detect a chemical when HS detects it (concentration greater than the detection limit) p_{HS} = number detected/sample size in headspace (the standard) p_{CT} = number detected/sample size in CT **Specificity** = the probability that CT will not detect/report a chemical when HS does not detect/report it. If CT detects a chemical that HS does not, it is considered conservative and is not tested.		**Section 3.2.1** Binomial Test of One Proportion H_0: $p_{CT} = p_{HS}$ versus H_1: $p_{CT} < p_{HS}$ where p is the proportion of observations greater than the detection/reporting limit.
Bias in Sample Concentration and Sample Volume	Median Additive Bias (B_a) based on medians: $B_a = (m_{HS} - x_i)$ where x_i equals the ith CT measurement for i = 1 to n the number of samples and m_{HS} is the median headspace measurement assumed known without error.	Mean Multiplicative Bias (B_m) based on the median of HS assumed known without error and the average of the ratios $B_m = \frac{1}{n}\sum_i (m_{HS}/x_i)$ where x_i equals the ith CT measurement for i = 1 to n.	**Section 3.2.2** Mann-Whitney Test H_0: $\eta_{CT} - \eta_{HS} = 0$ versus H_1: $\eta_{CT} - \eta_{HS} < 0$ where the medians of sets of measurements, mCT and mHS, are used as estimates of their respective true medians (η).
Precision of Sample Concentrations and Sample Volumes	Standard Deviation (s) $s = \sqrt{\frac{\sum_i (x_i - \bar{x})^2}{n-1}}$ where x_i equals the ith measurement for i = 1 to n the number of samples and $\bar{x}$ equal to the mean of the n measurements.	CV or relative standard deviation $CV = \frac{s}{\bar{x}}\ 100\%$	**Section 3.2.3** Modified Levene's Test H_0: $\sigma_{CT} / \sigma_{HS} = 1$ versus H_1: $\sigma_{CT} / \sigma_{HS} > 1$ where s is an unbiased estimate of σ and CT and HS denote CT rig and headspace sampling.
Accuracy of Concentration	A function of **Bias** and **Precision** $A_{CT} = B_a^2 + s_{CT}^2$	Relative Accuracy (RA_{CT}) $RA_{CT} = A_{CT}/m_{HS}^2$	Compare Relative Accuracy to other sampling methods if available or across chemicals

3.2.1 Number of Samples Detected

Rates of chemical detection can be regarded as an unfair coin flip where the coin has a point known probability of resulting in a head (value detected) or a tail (value censored). The proportion of detected values from HS provides the known probabilities against which to compare the results from CT. The proportion of detected values using CT were compared using a binomial test for one proportion assuming the HS proportion of detects (p_{HS}) is the true value. The binomial calculation tests the null hypothesis H_0: proportion of samples detected using the CT = p_{HS} versus H_1: proportion of samples detected using the CT <p_{HS}. When HS detected all available samples, p_{HS} was set to 0.99 to allow for a small probability of a censored observation. The rationale for the one-sided test was that detecting fewer observations for a given analyte than the standard HS method was of concern (low sensitivity) whereas detecting more observations than the standard (low specificity) was desired.

3.2.2 Sample Concentration

Sample concentration is calculated from the sample volume and the observed mass of a given chemical. Thus, the CT sampling method can introduce bias by having different sample volumes compared to the headspace sampling or low mass sorbed in the tubes. Under independent and normally distributed assumptions, a two-sample t-test could be used to compare the mean sample volumes or concentrations between sampling methods. However, the sample sizes are small (12 or less), and the data are skewed. Thus, a nonparametric approach was taken. Both the median volume and median concentration of samples obtained were compared using a nonparametric Mann-Whitney test of H_0: median result obtained for each method was equal versus H_1: median result for CT less than the median volume obtained for HS. The rationale for the one-sided test was that obtaining less sample volume (especially when concentrations are near the detection limit) or lower concentrations with the CT method for a given analyte than the standard HS method was of concern whereas obtaining a greater sample volume or concentration than the standard was desired and conservative (protective). Further, one-sided statistical tests have greater power to detect a significant result than two-sided tests with the same number of observations.

Sample volumes are unique by analytical method (i.e., by type of sorbent tube, not by individual chemical, except where there is only one chemical per analytical method). There were 10 unique | sets (10 each for the CT and HS methods) of sample volumes compared using the Mann-Whitney test. All but the 1,3-butadiene and the aldehydes methods had 12 observations for CT and 12 for HS for each analytical method. Tables associated with this comparison test show the median values and percentage difference between medians.

For comparison of the median sample concentrations, the variability between censored observations can affect the value of the test statistic and, hence, the probability of rejecting the null hypothesis. For this comparison and for a given chemical, censored values were set to the minimum of the set of unique reporting limits|detection limits (DL|RL) if the minimum value was less than all detected values for both methods. Otherwise, censored values were set to 90% of the minimum detected value for both methods. The nonparametric (rank-based) Mann-Whitney test of equal medians adjusts the p-value for ties (e.g., censored values). Thus, several censored values set to a constant value for a given method and chemical will not affect the decision to reject the null hypothesis. The constant DL/RL was only used for the statistical analysis and not the tabulated median values and percentage difference between medians. Medians and percentage differences presented in tables were calculated using the unique detection limits for censored values. A minimum of six detected values from each method was required to conduct this statistical comparison test.

3.2.3 Sample Variance

The variability among sample concentrations and sample volumes was compared using a modified Levene's test of H_0: $\sigma CT / \sigma HS = 1$ versus H_1: $\sigma CT / \sigma HS > 1$ where σ is the actual standard deviation of either the CT or HS concentrations or volumes. Only those chemicals with a ratio of sCT to sHS greater than 1 were tested with the modified Levene's test where s is the observed standard deviation. The modified one-sided Levene's test is based on a F-statistic calculated from the absolute deviations of the sample result from the group median. The rationale for the one-sided test was that obtaining greater variability for a given analyte than the standard HS method was of concern whereas obtaining less variability in concentration and sample volume than the standard was desired. In this case, the variability of the sample concentrations would be artificially reduced if a constant RL/DL was used for those values that were censored. Thus, the unique detection limits were used for this analysis. A minimum of six detected values from each method was required to conduct the Levene's test.

A rule-of-thumb two-sided comparison of the equality of the standard deviations (Moore et al. 2009; an application of the Hartley test with a "rule-of-thumb" critical value) also was conducted; that is, if the maximum standard deviation was greater than 1.5-times the minimum standard deviation, the variances are not equal. A lack of equality of variance based on the rule-of-thumb comparison provides a rationale for nonparametric analyses or demonstrates the need for a data transformation for parametric analyses.

4.0 Results

This section is organized to describe those COPCs and non-COPC analytes detected at sufficient concentration in the headspace and CT rig sampling comparison testing to enable a quantitative evaluation of the comparability of the sampling methods, including statistical analysis of the data.

In total 10 COPCs, listed in Table 3, were detected at sufficient concentrations in the BY-110 headspace to enable comparative evaluation of the two sampling methods. Measured concentrations of these COPCs spanned a wide range from 1 ppb to 300 ppm, and from <1% of their respective occupational exposure limit (OEL), to almost 1300% of their OEL. Five of the COPCs were measured with median concentrations exceeding 10% of their OEL while the remaining five COPCs were measured with median concentrations below 2% of their OEL. For three COPCs—benzene, acetaldehyde, and propanenitrile—the HS and CT concentrations were found to be statistically equivalent. The median HS concentration of one additional COPC—ammonia—was statistically greater than the median CT concentration. However, the difference was within analytical uncertainty and statistical variance of the replicate samples, and the two sets of concentrations were therefore quantitatively equivalent. The HS concentrations of six of the COPCs were higher than their corresponding CT concentrations to a statistically significant degree.

The results of the process to screen those chemical compounds that lacked sufficient quantitative test data is described first (Section 4.1), followed by detailed assessment of each COPC that had sufficient test data (Section 4.2). Finally, non-COPCs that were detected at sufficient concentration for analysis are described in Section 4.3. Appendix C provides further information on all of the COPCs and other analytes.

Table 3. COPCs Detected in HS and CT Samples at Sufficient Number and Data Quality to Support Comparative Statistical Analysis

COPC Name	**CAS No.**	**HS** # Detect.	**HS** Median Concentration (ppm)	**HS** Median Concentration (%OEL)	**CT** # Detect.	**CT** Median Concentration (ppm)	**CT** Median Concentration (%OEL)	**Statistical Test Result - Medians**	**Mult. Bias** (CT*Bias =HS)[a]	**K = 2 Uncert. of Bias** (±)
Ammonia	7664-41-7	12	318	1273%	12	306	1223%	HS>CT	1.04	0.31
Benzene	71-43-2	12	0.0024	0.48%	12	0.0024	0.48%	HS=CT	0.95	0.26
2-Hexanone	591-78-6	12	0.0077	0.15%	12	0.0041	0.083%	HS>CT	1.75	1.01
Formaldehyde	50-00-0	7	0.0042	1.4%	7	0.0018	0.59%	HS>CT	1.95	0.82
Acetaldehyde	75-07-0	10	0.0784	0.31%	12	0.0928	0.37%	HS=CT	0.85	1.89
Furan	110-00-9	11	0.0018	180%	6	0.0014	142%	HS>CT	1.15	0.23
Acetonitrile	75-05-8	12	0.0905	0.45%	12	0.0616	0.31%	HS>CT	1.38	0.37
Propanenitrile	107-12-0	12	0.0043	0.07%	11	0.0044	0.07%	HS=CT	0.98	0.46
NDEA	55-18-5	11	0.0002	223%	12	0.0001	62%	HS>CT	3.96	3.78
NMEA	10595-95-6	12	0.0011	357%	12	0.0001	34%	HS>CT	12.0	8.66

[a] Assuming mean CT and HS concentrations with error

4.1 Data Review and Screening

The measured concentrations and analytical quality flags associated with each HS and CT sample were evaluated to assess whether the data available were acceptable for subsequent statistical analysis. This process included evaluating the significance of quality flags associated with analytical results and other considerations described in subsections 4.1.1 through 4.1.3 below. Out of 61 COPCs, acceptable analytical data were available for 10 COPCs to conduct detailed statistical analysis (Table 3). Analytical data for 14 additional tank vapor non-COPC analytes allowed for quantitative and qualitative analysis of other organic compounds commonly found in tank HS samples (Table 4). Detailed analysis and discussion of the analytes in Table 3 and Table 4 are discussed in Sections 4.2, and 4.3, respectively.

Table 4. Non-COPC Organic Compounds Detected in the Tank Headspace Selected for Comparative Quantitative or Qualitative Analysis

Non-COPC Name	CAS No.	Non-COPC Name	CAS No.
1-Propanol	71-23-8	Dodecane	112-40-3
2-Butanone	78-93-3	Ethanol	64-17-5
2-Heptanone	110-43-0	Hexane	110-54-3
3-Heptanone	106-35-4	n-Heptane	142-82-5
4-Methyl-2-Pentanone	108-10-1	Toluene	108-88-3
Cyclohexane	110-82-7	Trichlorofluoromethane	75-69-4
Decane	124-18-5	Tridecane	629-50-5

4.1.1 Quality Flags

A number of vapor chemicals were removed from consideration for statistical analysis because of measurement quality issues that were identified in the analytical laboratory reports or in subsequent data interrogation. Data quality issues were principally identified with quality flags in the analysis reports, which were carried forward into the documentation of data reduction calculations. Quality flags associated with comparison test data are described in Appendix B and identified for each COPC in Table B.1. Analytes observed with potentially significant quality issues that warranted evaluation and disposition are summarized in Table 5.

Data for several other vapor chemicals were also flagged with potentially significant quality issues. However, further examination from 222-S analytical management indicated that the data was acceptable for use (see Appendix D).

4.1.2 Breakthrough on Headspace Samples

Headspace sampling was conducted with two sorbent tubes in series, Part A and Part B, as a test of whether the Part A tubes had sufficient capacity to capture the entire mass of chemical analyte. Significant mass detected on the Part B tube is an indication that the Part A HS tube may have become CT test sorbent tube could be quantitatively inaccurate. Two COPCs had at least six detected values in the Series B tubes (acetonitrile and NDMA) and one other COPC, n-nitrosomethylethylamine (NMEA), had one detected value in the Series B tubes. NDMA data was rejected due to quality flags as indicated in Section 4.1.1. For acetonitrile, the mass collected in the Series A tube ranged from 67% to 91% of the total analyte mass collected on both tubes, with a median of 88%. For NMEA, 96% of the total analyte mass was present on the Series A tube. The HS and CT data for acetonitrile and NMEA were retained for comparative analysis given the relatively low fraction of total mass observed on the Part B tubes, but with greater analytical uncertainty resulting from this observed breakthrough.

Table 5. Analytes with Data Quality Issues Determined to be Unusable

Analyte	CAS No.	Quality Concern	Disposition
3-Buten-2-one	78-94-4	Concentration data with odd bimodal distribution. No quality flags.	The 222-S Laboratory analytical management confirmed that the identification and quantification of these species were suspect. These data were rejected from further analysis. Data for two of the five nitriles (acetonitrile and propanenitrile) were deemed useable.
Butanenitrile	109-74-0		
Pentanenitrile	110-59-8	Issue identified with butanenitrile indicated potential concern with the nitrile analysis	
Hexanenitrile	628-73-9		
Nitrosodimethylamine	62-75-9	Data had multiple flags, including “B,” “L,” “a,” and “c,” which indicate out of range values for concentrations in blanks and low level standards, out of range spike recovery, and poor reproducibility	The 222-S Laboratory analytical management reviewed the analysis reports and confirmed that the results were not quantitatively useable. These data were rejected from further analysis.
Nitrosomorpholine	59-89-2	Most cartridge concentration data were above the RL|DL and most headspace-A data were below RL|DL. No quality flags.	The 222-S Laboratory analytical management reviewed the analysis reports and confirmed that both sets of data were compromised, possibly by calibration and matrix issues. These data were rejected from further analysis
Acetone	67-64-1	All cartridge data and most headspace-A data had flags that included “EY,” indicating concentrations well above the upper end of the calibration range.	The 222-S Laboratory analytical management reviewed the data and found the detector in the analysis instrument was in its saturation range, making its response nonlinear and making quantification inaccurate. These data were rejected from further analysis

There were also non-COPC analytes that indicated breakthrough from Part A to Part B of the HS tubes. Three non-COPC VOCs with at least six detected values in the Series B tubes (1-propanol, acetone, and ethanol) and two additional non-COPC VOCs (allyl alcohol and methylene chloride) with one detected value in the Series B tubes. All of these analytes, except ethanol, were rejected from further analysis due to high fractions (i.e., median >40% of total mass observed on the Part B tubes). For ethanol, the mass collected on the Part A tubes ranged from 67% to 96% of the total analyte mass, with a median of 81%.

4.1.3 Non-Detections and Below Detection Limits

Many tank vapor COPCs were either not detected or detected below reporting limits in samples from HS, CT, or both, making evaluation of sampling method comparability impossible or difficult for these analytes. There were 24 out of 61 COPCs for which no data was reported. Twenty-two of these COPCs represent tentatively identified compounds (TICs)[18] that are rarely detected in tank HS samples. Sampling and analysis was conducted for these COPCs, but they were not detected. The remaining two COPCs not reported are nitrous oxide and dimethyl mercury. Nitrous oxide sampling is not compatible with the standard HS or CT sorbent tube sampling procedure. Similarly, dimethylmercury was not measured in these tests as it requires special sampling and analysis methods. Table 6 lists the 24 COPCs that were not detected or not measured. All HS and CT data for an additional 16 COPCs were either below analytical detection/reporting limits (DL/RL), which also is referred to as censored data in this analysis, or sample results were not reported,[19] making evaluation of sampling method comparability impossible.

Table 6. COPCs Not Detected or Not Measured

COPC Name	CAS No.	COPC Name	CAS No.
Nitrous Oxide[1]	10024-97-2	2-Methylene butanenitrile	1647-11-6
3-Methyl-3-butene-2-one	814-78-8	2,4-Pentadienenitrile	1615-70-9
6-Methyl-2-heptanone	928-68-7	Chlorinated Biphenyls	Varies
2-Methyl-2-butenal	1115-11-3	2-Fluoropropene	1184-60-7
2-Ethyl-hex-2-enal	645-62-5	Methyl nitrite	624-91-9
2-Ethyl-5-methylfuran	1703-52-2	Butyl nitrite	544-16-1
4-(1-Methylpropyl)-2,3-dihydrofuran	34379-54-9	Butyl nitrate	928-45-0
3-(1,1-Dimethylethyl)-2,3-dihydrofuran	34314-82-4	1,4-Butanediol, dinitrate	3457-91-8
2-Octylfuran	4179-38-8	2-Nitro-2-methylpropane	594-70-7
2-(3-Oxo-3-phenylprop-1-enyl)furan	717-21-5	1,2,3-Propanetriol, 1,3-dinitrate	623-87-0
2-(2-Methyl-6-oxoheptyl)furan	51595-87-0	Methyl Isocyanate	624-83-9
Heptanenitrile	629-08-3	Dimethyl Mercury[1]	593-74-8

[1] Not measured.

Table 7 lists the 16 COPCs that were detected below RLs (a.k.a., censored).

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[18] Tentatively Identified Compound (TIC) indicates that a mass spectrometry "peak" not associated with calibrated compounds has been tentatively assigned to a compound based on an adequate match to the analytical methods reference library. Reference standards for the compound are not available to accurately quantify, assign an analytical DL, or definitively confirm the identity of the TIC. TICs are reported when the peak area is sufficiently large, estimated as ≥5 nanograms of TIC mass, and other analytical criteria are met. TICs are measured from samples collected on the VOA/VOC sorbent tube (Carbotrap 300) and analyzed using the EPA TO-17 modified analytical laboratory method. Twenty-two COPCs are designated as TICs.

[19] Non-TIC samples that are identified as not reported indicate that the sorbent tube could not be analyzed, in most cases indicating that the tube was broken or otherwise incapable of being desorbed and analyzed.

Table 7. COPCs Detected Below Reporting Limits or Not Reported

COPC Name	CAS No.	COPC Name	CAS No.
1,3-Butadiene[1]	106-99-0	2-Pentylfuran	3777-69-3
Biphenyl	106-99-0	2-Heptylfuran	3777-71-7
1-Butanol	71-36-3	2-Propylfuran	4229-91-8
2-Propenal[2]	107-02-8	Ethylamine	75-04-7
2,3-Dihydrofuran	1191-99-7	Tributyl phosphate	126-73-8
2,5-Dihydrofuran	1708-29-8	Dibutyl butylphosphonate	78-46-6
2-Methylfuran	534-22-5	Pyridine	110-86-1
2,5-Dimethylfuran	625-86-5	2,4-Dimethylpyridine	108-47-4

[1] 11 censored, 1 not reported for both CT and HS samples

[2] 12 censored for CT, 10 censored and two not reported for HS

4.2 Comparative Analysis of COPCs

For data visualization, a box plot based on the detected observations and the unique detection limits was overlaid on a plot of the individual values in sample order (1-12). The box plot includes the 10th, 25th, 50th, 75th, and 90th percentiles of the concentration data. The center three percentiles are connected with a rectangle and the 10th and 90th percentiles are below and above the box, respectively. Individual detected values were indicated as a solid symbol (●) and censored values (those less than the detection limit) were indicated as an open symbol (∇). Single flags associated with the quality of the concentration estimate were indicated by the flag value (e.g., “E,” “a,” “L,” etc.) overlaid on the solid or open symbol. The box plot was only generated for those chemicals with at least four detected values and plots were produced if there was at least one detected value.

Statistical results are detailed in Appendix C, however, the major results for each analyte with at least six detected concentrations are summarized in a table within each section below. The tables are divided into three sections with the first section providing the analyte analytical method, OEL (ppm), boiling point (°F), the number of detected and censored concentrations, and a comparison of the proportion detected. The second section contains the statistical comparison of concentration medians and variance if there were at least six detected values from each sampling method. A comparison of the analytical method median sample volume and variance are also presented in the second section of the table. The percent difference between the median concentrations and sample volumes ([HS-CT]/HS %) and the ratio of the standard deviations (sCT/sHS) for the concentration and sample volume data are presented when applicable. Levene’s test was only conducted when the ratio (sCT/sHS) was greater than 1. If there were at least six detected concentrations from each sampling method, the additive and multiplicative bias were estimated and presented in the third section of the table.

4.2.1 Ammonia 7664-41-7

Ammonia was detected in the BY-110 headspace at elevated concentrations of approximately 300 ppm with both the HS and CT sampling systems. Figure 12 is a box plot depicting the 12 replicate samples from both sampling systems. All 12 samples from both sampling methods were above detection, and there were no quality flags.

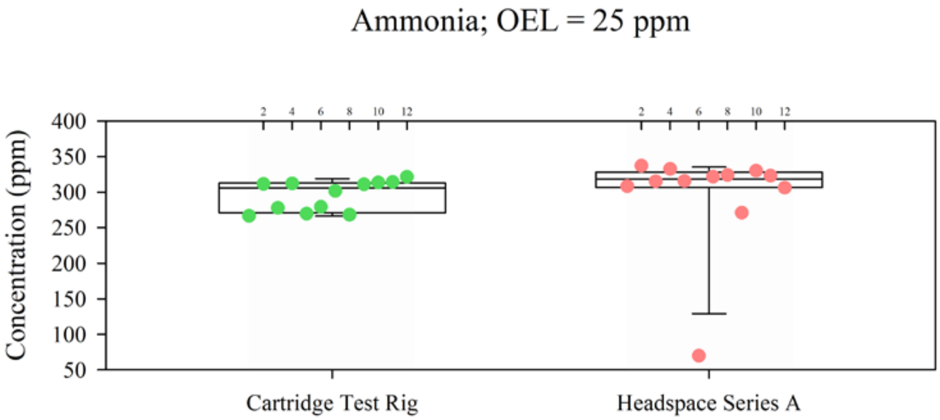

Figure 12. Box Plot of Ammonia Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

Median concentrations (Table 8), were significantly greater in HS samples compared to the CT samples based on the Mann-Whitney test (p = 0.018). However, the percent difference between medians (i.e., [HS-CT]/HS) was only 3.9%, which is relatively low compared to analytical uncertainty (±6.7%)[20] and mean precision (26.6%)[21] obtained from HS duplicate pairs analysis. The Levene's test of equal concentration variance between the two sampling methods was not conducted because the HS concentration standard deviation was more than three times greater than the CT concentration standard deviation. Thus, by the rule-of-thumb method of comparing variation,[22] the variances of the two sampling methods were not equal. The larger variance from the HS method (CV = 25%) was principally driven by the single low measurement (tube 6) which makes the CT variance so much lower (CV = 7.2%) than the HS variance. While the result from tube 6 appears like it may be an outlier (68.6 ppm versus 266-337 ppm for all others), there was no evidence of sampling or analytical errors or quality flags. Therefore, this observation was treated as a valid measurement in the statistical analysis. As a matter of exploration, however, analysis was conducted without HS tube 6, and the HS median concentration was still significantly greater (Mann-Whitney; p = 0.004) than the CT median concentration with a percent difference of 5%, but the variances were not significantly different (Levene's test; p = 0.143) with an average CV of 6.5%.

Despite a low level, but statistically observed difference in median concentrations between CT and HS samples, ammonia measured by both methods were generally equivalent, i.e., within the analytical uncertainty and sample variation. A multiplicative bias of 1.04 is derived from the HS:CT comparison assuming HS was estimated with error.

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[20] Approximate analytical uncertainty based on laboratory control standards as reported in the analytical laboratory report. For ammonia analysis, ±6.7% has a coverage factor (K)=2, representing 95% confidence (see Appendix A)

[21] Analytical precision of duplicate pairs provides a measure of analytical precision for a sampling and analysis method by calculating the absolute value of the relative difference between two identical samples. EPA has documented a precision performance criteria for analytical method TO-17 of ≤20% for duplicate pairs. Although ammonia analysis is not performed per EPA TO-17 procedure, the 12 sub-replicate samples collected in this test provide up to 66 distinct duplicate pairs that can be evaluated and compared to this well-established performance metric.

[22] The rule-of-thumb method of comparing variation uses the maximum divided by the minimum standard deviation > 1.5 as the criteria for inequality.

Table 8. Statistical Comparison of Ammonia Measurements from CT and HS Sampling

Analyte	Method	OEL (ppm)	Boiling Point (◦F)	CT Number of Observations Detected	CT Number of Observations Censored	HS Series A Number of Observations Detected	HS Series A Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Ammonia	Ammonia	25	-28	12	0	12	0	CT=HS

Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration	ppm	306	318	3.94%	Mann-Whitney	HS>CT, p = 0.018	1273%
Concentration Standard Deviation	ppm	21.3	73.6	(0.290)	Levene's Test	sCT≤sHS	
Coefficient of Variation or Relative Standard Deviation		7.2%	25%				

Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty) Additive: b+CT = HS	Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty) Multiplicative:b·CT = HS	Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty) Additive: b+CT = HS	Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty) Multiplicative:b·CT = HS
12.5 (±12.3)	1.08 (±0.05)	0.76 (±44.3)	1.04 (±0.31)

4.2.2 Benzene 7 1-43-2

Benzene was detected in all samples in the BY-110 headspace at median concentrations of approximately 2.5 ppb (0.5% of OEL) with both the HS and CT sampling systems. Figure 13 is a box plot depicting the 12 sub-replicate samples from both sampling systems. There were no quality flags.

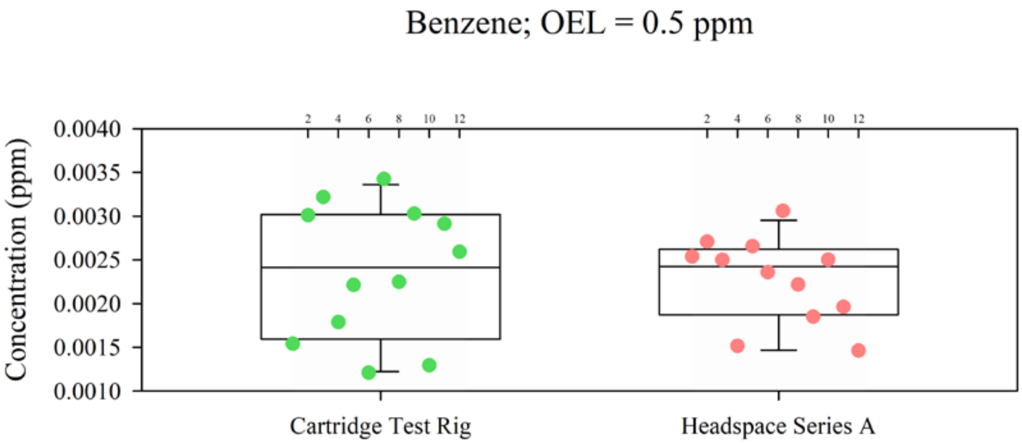

Figure 13. Box Plot of Benzene Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The median HS concentration was not significantly different from the CT concentration (Mann-Whitney test; p = 0.667) (Table 9). The percent difference between medians (i.e., [HS-CT]/HS) was 0.4%, within the analytical uncertainty for benzene analysis of approximately ±6.3%.[23] The Levene's test of equal concentration variance between the two sampling methods, however was significant (p = 0.031) with a ratio of sCT:sHS equal to 1.58 indicating that the CT concentration variance (CV = 33%) was

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[23] Approximate analytical uncertainty based on laboratory control standards (LCS) as reported in the 222-S analytical laboratory control limit report IH-LT-523-153 /L-2 dated 7/19/18. For benzene analysis, ±6.3% represents the standard deviation (1 sigma) of LCS samples (see Appendix A)

significantly greater than the HS concentration variance (CV = 22%). The mean precision obtained from HS duplicate pairs analysis was 26.4%, moderately higher than EPA TO-17 precision criteria (≤20%) for this sampling and analysis method.[24]

Benzene measured by both methods was considered equivalent, and a multiplicative bias of 0.95 can be used to estimate the HS concentration from the CT concentration.

Table 9. Statistical Comparison of Benzene Measurements from CT and HS Samples

				CT		HS Series A		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Benzene	VOC	0.5	176	12	0	12	0	CT=HS
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0024	0.0024	0.40%	Mann-Whitney	Not Significantly Different	0.5%
	Concentration Standard Deviation	ppm	0.00078	0.00049	(1.58)	Levene's Test	CT>HS, p = 0.031	
	Coefficient of Variation or Relative Standard Deviation		33%	22%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)					Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)			
Additive: b+CT = HS		Multiplicative:b·CT = HS			Additive: b+CT = HS		Multiplicative:b·CT = HS	
0.000010 (±0.00045)		1.02 (±0.20)			-0.0001 (±0.0005)		0.95 (±0.26)	

4.2.3 2-Hexanone 591-78-6

2-Hexanone was detected in the headspace of tank BY-110 at median concentrations of approximately 8 ppb (0.2% of OEL) and 4 ppb with the HS and CT sampling systems, respectively. Figure 14 is a box plot depicting the 12 replicate samples from both

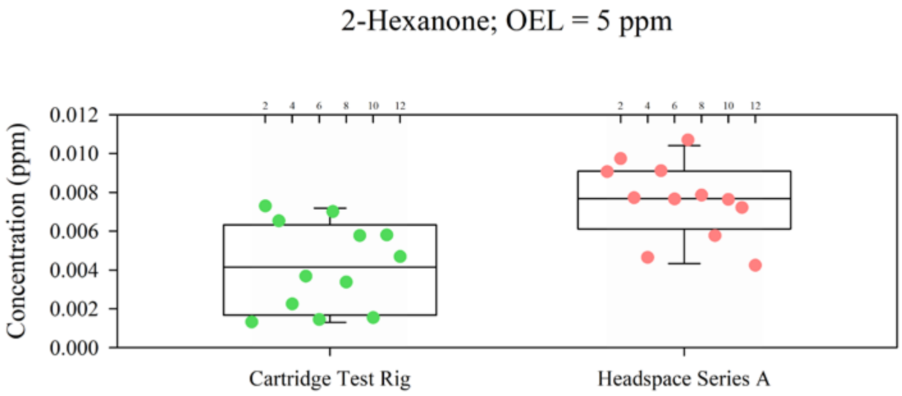

Figure 14. Box Plot of 2-Hexanone Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

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[24] Duplicate pairs analysis of the CT data had a higher mean precision of 41.2%, consistent with the higher observed concentration variance for CT versus HS sub-replicates.

Both the HS and CT sampling systems detected all 12 samples (Table 10), however, the HS median concentration was significantly greater than the CT median concentration (Mann-Whitney; p = 0.001). The percent difference between medians (i.e., [HS-CT]/HS) was 46% with the HS median concentration at 0.2% of the OEL. This difference was significantly higher than the 2-hexanone analytical uncertainty of ±7.2%.[25] The Levene's test of equal concentration variance between the two sampling methods, however, was not significant (p = 0.127). Similarly, the ratio of sCT:sHS equaled 1.15 indicating that the CT concentration variance (CV = 54%) was not different than the HS concentration variance (CV = 26%) based on the rule-of-thumb criteria. The mean precision obtained from HS duplicate pairs analysis was 31.6%, higher than EPA TO-17 precision criteria (≤20%) for this sampling and analysis method.[26]

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 1.75 can be used to estimate the HS concentration for 2-hexanone from the CT samples.

Table 10. Statistical Comparison of 2-Hexanone Measurements from CT and HS Samples

				CT		HS Series A		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
2-Hexanone	VOC	5	262	12	0	12	0	CT=HS
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	0.0041	0.0077	45.9%	Mann-Whitney	HS>CT p = 0.001	0.2%
	Concentration Standard Deviation	ppm	0.00226	0.00197	(1.15)	Levene's Test	CT>HS, p = 0.127; NS	
	Coefficient of Variation or Relative Standard Deviation		54%	26%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)					Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)			
Additive: b+CT = HS	Multiplicative:b·CT = HS				Additive: b+CT = HS		Multiplicative:b·CT = HS	
0.0035 (±0.0013)	1.83 (±0.63)				0.0034 (±0.0017)		1.75 (±1.01)	

4.2.4 Formaldehyde 50-00-0

Formaldehyde was detected in the headspace of tank BY-110 with seven out of 12 samples with both the HS and CT sampling systems. The median HS concentration was approximately 4.2 ppb (1.4% of OEL) while the median CT concentration was 1.8 ppb. Figure 15 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

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[25] Approximate analytical uncertainty based on LCS as reported in the 222-S analytical laboratory control limit report IH-LT-523-153 /L-2 dated 7/19/18. For 2-hexanone analysis, ±7.2% represents the standard deviation (1 sigma) of LCS samples (see Appendix A)

[26] Duplicate pairs analysis of the CT data had a mean precision of 68.8% significantly higher than the HS data but consistent with the higher observed concentration variance for CT versus HS sub-replicates.

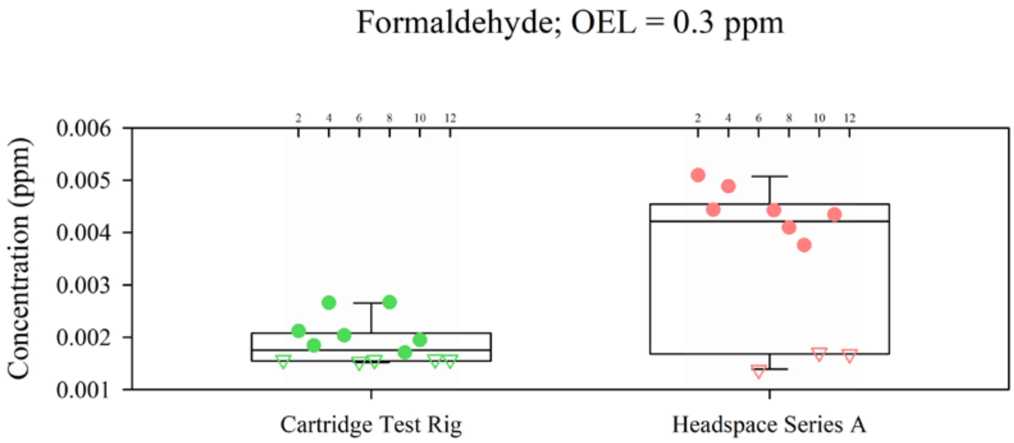

Figure 15. Box Plot of Formaldehyde Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of samples detected was not significantly different (binomial test; p = 0.28) between the HS and CT sampling systems (Table 11). The HS median concentration, however, was significantly greater than the CT median concentration (Mann-Whitney; p = 0.018). The percent difference between medians (i.e., [HS-CT]/HS) was 58% with the HS median concentration at 1.4% of the OEL. This difference in medians is significantly higher than the analytical uncertainty for formaldehyde of ±4.8%.[27] The Levene's test of equal concentration variance between the two sampling methods was not conducted because sCT was less than sHS with a ratio of 0.29. However, the ratio of sHS:sCT equaled 3.48 indicating that the HS concentration variance (CV = 40%) was greater than the CT concentration variance (CV = 22%) based on the rule-of-thumb criteria. The mean precision obtained from HS duplicate pairs analysis was 12.2%, within the EPA precision criteria (≤20%) for a similar sampling and analysis method.[28]

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 1.95 can be used to estimate the HS concentration for formaldehyde from the CT samples.

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[27] Approximate analytical uncertainty based on LCS as reported in the ALS analytical laboratory report for aldehydes analysis, ±14.5% represents the control limits (assumed 3 sigma) (see Appendix A)

[28] Formaldehyde analysis is performed to EPA-TO-11ar method procedure which does not specify a duplicate pair analysis. However, it does define a ±20% precision criteria based on collocated samples, which is similar to duplicate pairs. Duplicate pairs analysis of the CT data had a mean precision of 20.6% slightly higher than the method criteria as well as the HS data.

Table 11. Statistical Comparison of Formaldehyde Measurements from CT and HS Samples

Analyte	Method	OEL (ppm)	Boiling Point (◦F)	CT		HS Series A		Conclusion of Test of Equal Proportion Detected
				Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Formaldehyde	Aldehydes	0.3	-6	7	5	7	3	NS; p=0.28

Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
Median Concentration	ppm	0.0018	0.0042	58.3%	Mann-Whitney	HS>CT p = 0.018	1.4%
Concentration Standard Deviation	ppm	0.00041	0.00143	(0.288)	Levene's Test	sCT≤sHS	
Coefficient of Variation or Relative Standard Deviation		22%	40%				

Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)		Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)	
Additive: b+CT = HS	Multiplicative:b·CT = HS	Additive: b+CT = HS	Multiplicative:b·CT = HS
0.0025 (±0.0002)	2.24 (±0.29)	0.0017 (±0.0009)	1.95 (±0.82)

4.2.5 Acetaldehyde 75-07-0

Acetaldehyde was detected in all samples in the headspace of tank BY-110 at median concentrations of approximately 80 ppb (0.3% of OEL) and 90 ppb with both the HS and CT sampling systems, respectively. Figure 16 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

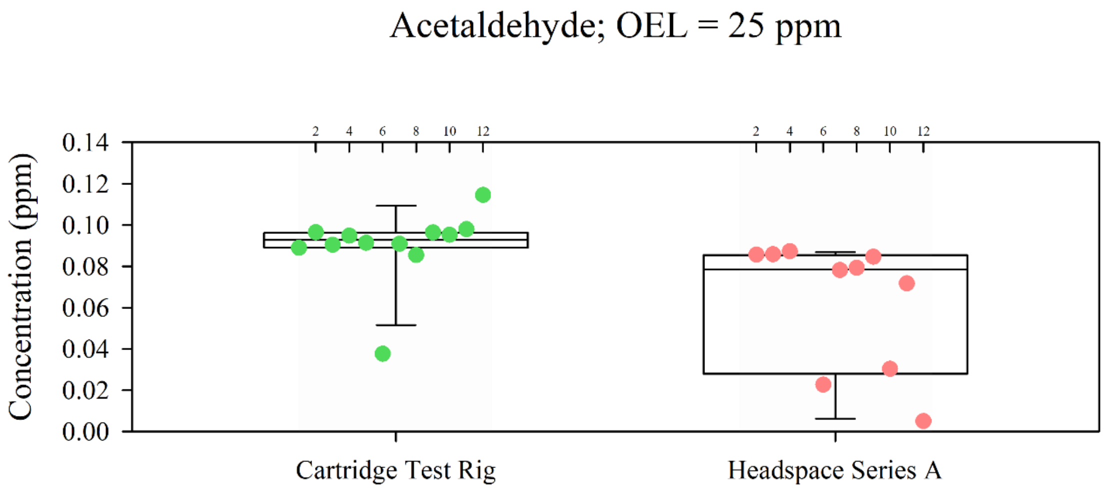

Figure 16. Box Plot of Acetaldehyde Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The CT median concentration was not significantly greater (Mann-Whitney; p = 1.00) than the HS median concentration (Table 12). The percent difference between medians (i.e., [HS-CT]/HS) was -18%. This difference in medians is significantly higher than the estimated analytical uncertainty for acetaldehyde of ±2.6%.[29] The Levene's test of equal concentration variance between the two sampling methods was not conducted because sCT was less than sHS with a ratio of 0.58. However, the ratio of

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[29] Approximate analytical uncertainty based on LCS as reported in the ALS analytical laboratory report for aldehydes analysis, ±7.9% represents the control limits (assumed 3 sigma) (see Appendix A)

sHS:sCT equaled 1.73 indicating that the HS concentration variance (CV = 50%) was greater than the CT concentration variance (CV = 20%) based on the rule-of-thumb criteria. The mean precision obtained from HS duplicate pairs analysis was 70.6%, significantly higher than the EPA precision criteria (≤20%) for a similar sampling and analysis method.[30]

The multiplicative bias of 0.85 can be used to estimate the HS concentration for acetaldehyde from the CT samples

Table 12. Statistical Comparison of Acetaldehyde Measurements from CT and HS Samples

Analyte	Method	OEL (ppm)	Boiling Point (◦F)	CT		HS Series A		Conclusion of Test of Equal Proportion Detected
				Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Acetaldehyde	Aldehydes	25	69	12	0	10	0	CT=HS

	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	0.0928	0.0784	-18.3%	Mann-Whitney	Not Significantly Different	0.3%
	Concentration Standard Deviation	ppm	0.0181	0.0312	(0.579)	Levene's Test	sCT≤sHS	
	Coefficient of Variation or Relative Standard Deviation		20%	50%				

Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)		Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)	
Additive: b+CT = HS	Multiplicative:b·CT = HS	Additive: b+CT = HS	Multiplicative:b·CT = HS
-0.014 (±0.010)	0.87 (±0.10)	-0.027 (±0.022)	0.85 (±1.89)

4.2.6 Furan 110-00-9

Furan was detected in the headspace of tank BY-110 in all but one sample with the HS sampling system and in six samples with the CT sampling system. The median HS concentrations was approximately 1.8 ppb (180% of OEL) and the median CT concentration was approximately 1.4 ppb. Figure 17 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

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[30] Acetaldehyde analysis is performed to EPA-TO-11ar method procedure which does not specify a duplicate pairs analysis. However, it does define a ±20% precision criteria based on collocated samples, which are similar to duplicate pairs. Duplicate pairs analysis of the CT data had a mean precision of 21.2% slightly higher than the method criteria and substantially lower than HS data.

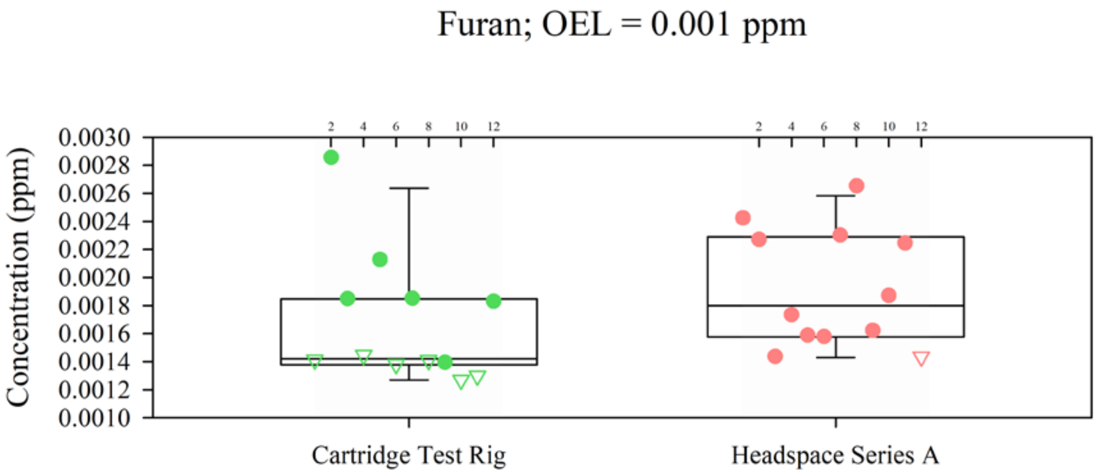

Figure 17. Box Plot of Furan Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of samples detected with the CT sampling system was significantly (binomial test; $p = 0.001$) less than the HS sampling system (Table 13). Further, the HS median concentration was significantly greater than the CT median concentration (Mann-Whitney; $p = 0.037$). The percent difference between medians (i.e., [HS-CT]/HS) was 21%. This difference in medians is moderately higher than the estimated analytical uncertainty for furan of ±11.3%.[31] The Levene's test of equal concentration variance between the two sampling methods was not significant ($p = 0.63$) with a ratio of 1.09. Likewise, the rule-of-thumb criteria (1.5) was not exceeded indicating that the HS concentration variance (CV = 22%) was similar to the CT concentration variance (CV = 28%). The mean precision obtained from HS duplicate pairs analysis was 24.7%, slightly higher than EPA TO-17 precision criteria (≤20%) for this sampling and analysis method.[32]

Table 13. Statistical Comparison of Furan Measurements from CT and HS Samples

				CT		HS Series A		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Furan	VOC	0.001	88	6	6	11	1	p < 0.001
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0014	0.0018	20.9%	Mann-Whitney	HS>CT p = 0.037	180%
	Concentration Standard Deviation	ppm	0.00046	0.00043	(1.09)	Levene's Test	CT>HS, p = 0.634; NS	
	Coefficient of Variation or Relative Standard Deviation		28%	22%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS		Multiplicative:b·CT = HS				Additive: b+CT = HS	Multiplicative:b·CT = HS	
0.00038 (±0.0003)		1.08 (±0.18)				0.00025(±0.0004)	1.15 (±0.23)	

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[31] Approximate analytical uncertainty based on LCS as reported in the 222-S analytical laboratory control limit report IH-LT-523-153 /L-2 dated 7/19/18. For furan analysis, ±11.3% represents the standard deviation (1 sigma) of LCS samples (see Appendix A)

[32] Duplicate pairs analysis of the CT data had a mean precision of 26.4% similar to that of HS data.

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 1.15 can be used to estimate the HS concentration for furan from the CT samples.

4.2.7 Acetonitrile 75-05-8

Acetonitrile was detected in all samples the headspace of tank BY-110 at median concentrations of approximately 0.9 ppm (0.5% of OEL) and 0.6 ppm with the HS and CT sampling systems, respectively. Figure 18 is a box plot depicting the 12 replicate samples from both sampling systems. Seven HS samples and four CT samples were flagged with an "E" indicating that the sorbent was near saturation. However, the analytical laboratory 222-S Laboratory considered acetonitrile, in the concentration ranges measured, to have a linear response and to be quantified without underestimation.

The HS median concentration was significantly greater (Mann-Whitney; p = 0.015) than the CT median concentration (Table 14). The percent difference between medians (i.e., [HS-CT]/HS) was 32%. This difference in medians is significantly higher than the estimated analytical uncertainty for acetonitrile of ±4.8%.[33] The Levene's test of equal concentration variance between the two sampling methods was not conducted because sCT was less than sHS with a ratio of 0.75. Likewise, the rule-of-thumb criteria (1.5) was not exceeded (ratio sCT:sHS = 1.3) indicating that the HS concentration variance (CV = 29%) was similar to the CT concentration variance (CV = 30%). The mean precision obtained from HS duplicate pairs analysis was 34.9%, higher than the EPA precision criteria (≤20%) for a similar sampling and analysis method.[34]

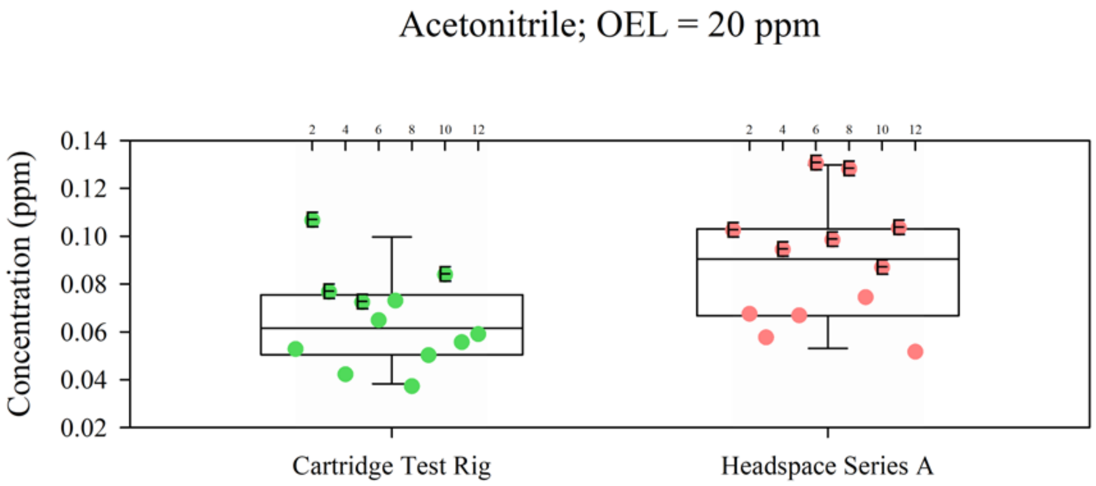

Figure 18. Box Plot of Acetonitrile Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

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[33] Approximate analytical uncertainty based on LCS as reported in the ALS analytical laboratory report for acetonitrile analysis, ±14.4% represents the control limits (assumed 3 sigma, see Appendix A). The NIOSH 1606 analytical method reports an overall method accuracy of ±16.4% (95% confidence).

[34] Although acetonitrile analysis is performed to NIOSH 1606, and does not specify a performance criterion using duplicate pairs analysis. The 12 sub-replicate samples collected in this test provide 66 distinct duplicate pairs that can be evaluated and compared to the well-established performance metric included in EPA method TO-17. Duplicate pairs analysis of the CT data had a mean precision of 34.7% similar to that of the HS data.

Table 14. Statistical Comparison of Acetonitrile Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Acetonitrile	VOC	20	179	12, 4 flagged	0	12, 7 flagged	0	CT=HS
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0616	0.0905	31.9%	Mann-Whitney	HS>CT p = 0.015	0.5%
	Concentration Standard Deviation	ppm	0.0195	0.0259	(0.752)	Levene's Test	sCT≤sHS	
	Coefficient of Variation or Relative Standard Deviation		30%	29%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS		Multiplicative:b·CT = HS				Additive: b+CT = HS	Multiplicative:b·CT = HS	
0.029 (±0.011)		1.41 (±0.25)				0.024 (±0.019)	1.38 (±0.37)	

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 1.38 can be used to estimate the HS concentration for acetonitrile from the CT concentration.

4.2.8 Propanenitrile 107-12-0

Propanenitrile was detected in the headspace of tank BY-110 in all HS samples and in 11 of 12 CT samples. The median concentration for both sampling systems was approximately 4.5 ppb (0.1% of OEL). Figure 19 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

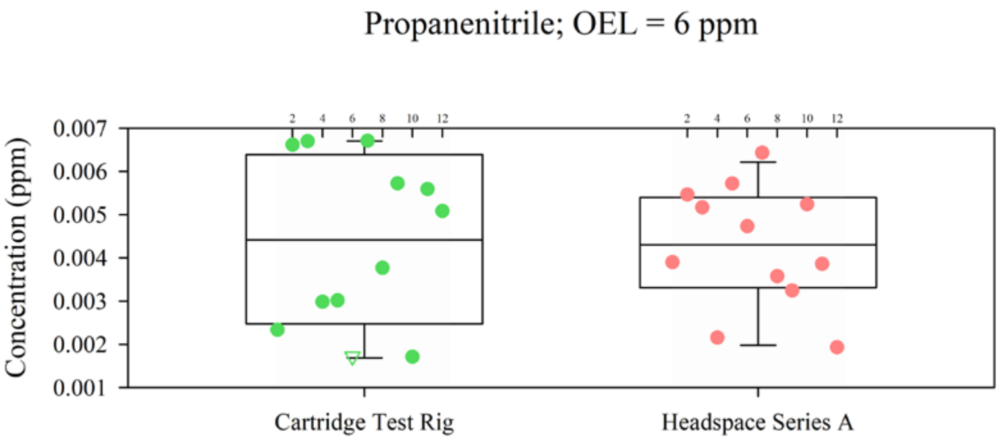

Figure 19. Box Plot of Propanenitrile Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of samples detected was not significantly different (binomial test; p = 0.11) between the HS and CT sampling systems (Table 15). Further, the HS median concentration was not significantly different than the CT median concentration (Mann-Whitney; p = 0.56). The percent difference between medians (i.e., [HS-CT]/HS) was -2.6%. This difference in medians is significantly higher than the estimated analytical uncertainty for propanenitrile of ±7.8%.[35] The CT concentration standard deviation was significantly greater (Levene's test; p = 0.032) than the HS concentration standard deviation (ratio = 1.4). However, the rule-of-thumb criteria (1.5) was not exceeded indicating that the HS concentration variance (CV = 33%) was similar to the CT concentration variance (CV = 45%). The mean precision obtained from HS duplicate pairs analysis was 41.9%, higher than the EPA precision criteria (≤20%) for a similar sampling and analysis method.[36]

The multiplicative bias of 0.98 can be used to estimate the HS concentration for propanenitrile from the CT samples.

Table 15. Statistical Comparison of Propanenitrile Measurements from CT and HS Samples

				CT		HS Series A		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Propanenitrile	VOC	6	207	11	1	12	0	NS; p=0.11
Statistical Measure		Units	CT	HS Series A	Percent Difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration		ppm	0.0044	0.0043	-2.6%	Mann-Whitney	Not Significantly Different	0.1%
Concentration Standard Deviation		ppm	0.00197	0.00142	(1.39)	Levene's Test	CT>HS, p = 0.032	
Coefficient of Variation or Relative Standard Deviation			45%	33%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS	Multiplicative:b·CT = HS					Additive: b+CT = HS	Multiplicative:b·CT = HS	
-0.000110 (±0.0011)	1.00 (±0.28)					-0.000043 (±0.0014)	0.98 (±0.46)	

4.2.9 N-Nitrosodiethylamine 55-18-5

N-Nitrosodiethylamine was detected in the headspace of tank BY-110 in all but one HS sample and in all CT samples. The median HS and CT concentrations were approximately 0.2 ppb (223% of the OEL) and 0.05 ppb with both sampling systems, respectively. Figure 20 is a box plot depicting the 12 replicate samples from both sampling systems. There were "a" quality flags on all CT samples indicating that spikes were over-recovered and that the concentrations may be over-estimated.

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[35] Approximate analytical uncertainty based on LCS as reported in the 222-S analytical laboratory control limit report IH-LT-523-153 /L-2 dated 7/19/18. For propanenitrile analysis, ±7.8% represents the standard deviation (1 sigma) of LCS samples (see Appendix A).

[36] Although propanenitrile analysis is performed to NIOSH 1606, and does not specify a performance criterion using duplicate pairs analysis. The 12 sub-replicate samples collected in this test provide up to 66 distinct duplicate pairs that can be evaluated and compared to the well-established performance metric included in EPA method TO-17. Duplicate pairs analysis of the CT data had a mean precision of 52.1%, higher than that of the HS data.

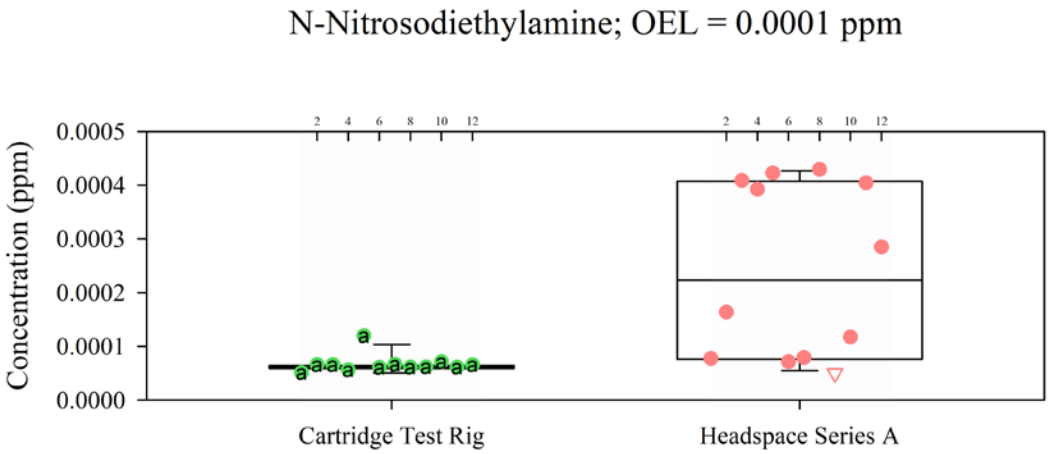

Figure 20. Box Plot of N-Nitrosodiethylamine Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The binomial test of the proportion detected was not conducted because the CT sampling system detected all 12 samples (Table 16). The HS median concentration was significantly greater (Mann-Whitney; p = 0.001) than the CT median concentration with a percent difference between medians (i.e., [HS-CT]/HS) of 72%. This difference in medians is significantly higher than the estimated analytical uncertainty for NDEA of ±7.2%.[37] The Levene's test of equal concentration variance between the two sampling methods was not conducted because sCT was less than sHS with a ratio of 0.11. However, the ratio of sHS:sCT equaled 9.3 indicating that the HS concentration variance (CV = 67%) was greater than the CT concentration variance (CV = 27%) based on the rule-of-thumb criteria. The mean precision obtained from HS duplicate pairs analysis was 76.4%, significantly higher than the EPA precision criteria (≤20%) for a similar sampling and analysis method.[38]

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 3.96 can be used to estimate the HS concentration for NDEA from the CT concentration.

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[37] Approximate analytical uncertainty based on LCS as reported in the RJ Lee Group analytical laboratory report for NDEA analysis, ±21.7% represents the control limits (assumed 3 sigma, see Appendix A). The NIOSH 2522 analytical method indicates that the method accuracy/precision has not been determined.

[38] Although NDEA analysis is performed to NIOSH 2522 method that does not specify a performance criterion using duplicate pairs analysis, the 12 sub-replicate samples collected in this test provide up to 66 distinct duplicate pairs that can be evaluated and compared to the well-established performance metric included in EPA method TO-17. Duplicate pairs analysis of the CT data had a mean precision of 19.5%, significantly lower than that of the HS data.

Table 16. Statistical Comparison of N-Nitrosodiethylamine Measurements from CT and HS Samples

Analyte	Method	OEL (ppm)	Boiling Point (◦F)	CT		HS Series A		Conclusion of Test of Equal Proportion Detected
				Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
N-Nitrosodiethylamine	Nitrosamines	0.0001	351	12, 12 flagged	0	11	1	CT≥HS

	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0001	0.0002	72.30%	Mann-Whitney	HS>CT p = 0.001	223%
	Concentration Standard Deviation	ppm	0.000017	0.00016	(0.108)	Levene's Test	sCT≤sHS	
	Coefficient of Variation or Relative Standard Deviation		27%	67%				

Additive and Multiplicative Bias (ppm) assuming HS without Error (k = 2 Uncertainty)		Additive and Multiplicative Bias (ppm) assuming HS with Error (k = 2 Uncertainty)	
Additive: b+CT = HS	Multiplicative:b·CT = HS	Additive: b+CT = HS	Multiplicative:b·CT = HS
0.00016 (±0.00001)	3.40 (±0.54)	0.00018 (±0.00009)	3.96 (±3.78)

4.2.10 N-Nitrosomethylethylamine 10595-95-6

N-Nitrosomethylethylamine was detected in the headspace of tank BY-110 in all samples of both the HS and CT sampling systems. The median HS and CT concentrations were approximately 1 ppb (357% of the OEL) and 0.1 ppb with the HS and CT sampling systems, respectively. Figure 21 is a box plot depicting the 12 replicate samples from both sampling systems. There were "a" quality flags on all CT samples indicating that spikes were over-recovered and that the concentrations may be over-estimated.

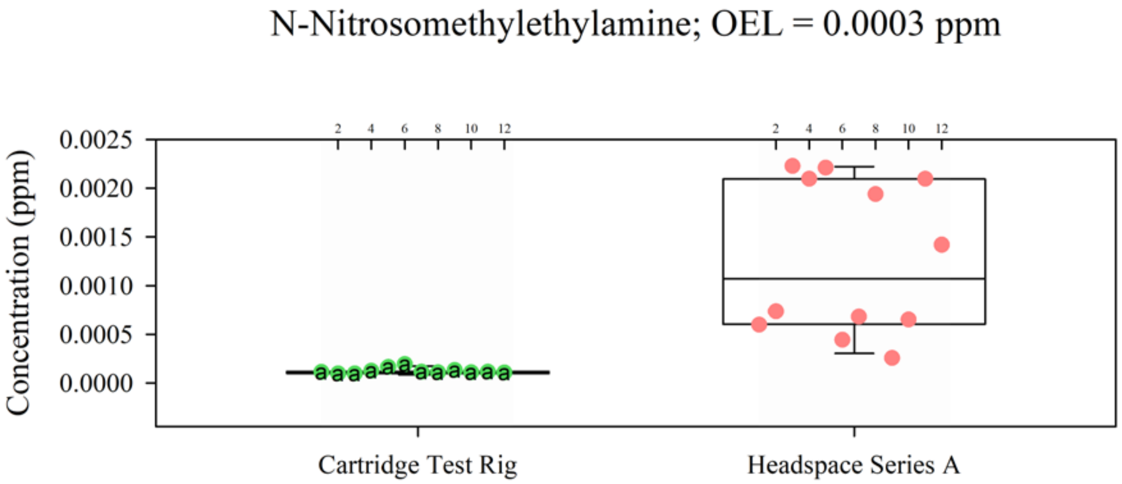

Figure 21. Box Plot of N-Nitrosomethylethylamine Concentration Measurements from Replicate Samples from the CT Rig (left) and HS (right) Systems

The HS median concentration was significantly greater (Mann-Whitney; $p < 0.001$) than the HS median concentration (Table 17). The percent difference between medians (i.e., [HS-CT]/HS) was 90%. This difference in medians is significantly higher than the estimated analytical uncertainty for NMEA of ±7.6%.[39] The Levene's test of equal concentration variance between the two sampling methods was not

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[39] Approximate analytical uncertainty based on LCS as reported in the RJ Lee Group analytical laboratory report for NMEA analysis, ±22.7% represents the control limits (assumed 3 sigma, see Appendix A). The NIOSH 2522 analytical method indicates that the method accuracy/precision has not been determined.

conducted because sCT was less than sHS with a ratio of 0.04. However, the ratio of sHS:sCT was 27, indicating that the HS concentration variance (CV = 62%) was greater than the CT concentration variance (CV = 26%) based on the rule-of-thumb criteria. The mean precision obtained from HS duplicate pairs analysis was 75.6%, significantly higher than the EPA precision criteria (≤20%) for a similar sampling and analysis method.[40]

Table 17. Statistical Comparison of N-Nitrosomethylethylamine Measurements from CT and HS Samples

				CTT)		HS Series AHS)		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
N-Nitrosomethylethylamine	Nitrosamines	0.0003	310	12, 12 flagged	0	12	0	CT=HS
Statistical Measure		Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration		ppm	0.0001	0.0011	90.4%	Mann-Whitney	HS>CT p < 0.001	357%
Concentration Standard Deviation		ppm	0.000029	0.00079	(0.037)	Levene's Test	sCT≤sHS	
Coefficient of Variation or Relative Standard Deviation			26%	62%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS	Multiplicative:b·CT = HS					Additive: b+CT = HS	Multiplicative:b·CT = HS	
0.0010 (±0.00002)	9.55 (±1.45)					0.0012 (±0.0005)	12.0 (±8.66)	

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 12 can be used to estimate the HS concentration for acetonitrile from the CT concentration.

4.3 Comparative Analysis of Non-COPC VOCs and SVOCs

In addition to COPCs, 53 non-COPC VOCs and SVOCs that are routinely sampled and evaluated using Carbotrap 150 or 300 sorbent tubes per EPA method TO-17 (modified) were considered in this study. Only 14 of the 53 non-COPCs were detected in CT or HS samples above their RLs, and subjected to quantitative or qualitative statistical analysis for this study. Table 18 provides a summary of the 14 non-COPC analytes with sufficient data available to assess and describe in this section. Ten analytes had sufficient data to conduct a statistical test of the HS and CT median concentrations. Four additional analytes had insufficient data from the CT samples to conduct full statistical analysis, but are described in this section for completeness.

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[40] Although NMEA analysis is performed to NIOSH 2522 method that does not specify a performance criterion using duplicate pairs analysis, the 12 sub-replicate samples collected in this test provide up to 66 distinct duplicate pairs that can be evaluated and compared to the well-established performance metric included in EPA method TO-17. Duplicate pairs analysis of the CT data had a mean precision of 24%, significantly lower than that of the HS data.

Table 18. Non-COPC Analytes Detected in HS and CT Samples at Sufficient Number and Data Quality to Support Quantitative or Qualitative Analysis

Non-COPC Name	**CAS No.**	**HS**			**CT**			**Statistical Test Result - Medians**	**Multiple Bias** (CT*Bias=HS)	**K = 2 Uncertainty of Bias** (±)
		# Detect.	Median Concentration (ppm)	(%OEL [a])	# Detect.	Median Concentration (ppm)	(%OEL)			
1-Propanol	71-23-8	12	0.0204	0.01%	11	0.0214	0.01%	HS=CT	1.06	1.24
2-Butanone	78-93-3	12	0.0186	0.01%	12	0.0270	0.01%	HS=CT	0.67	0.89
2-Heptanone	110-43-0	12	0.0056	0.01%	5	0.0008	0.002%	NA	NA	NA
3-Heptanone	106-35-4	12	0.0103	0.02%	7	0.0011	0.002%	HS>CT	7.15	2.87
4-Methyl-2-Pentanone	108-10-1	12	0.0037	0.01%	11	0.0027	0.01%	HS>CT	1.33	0.60
Cyclohexane	110-82-7	12	0.0076	0.01%	12	0.0071	0.01%	HS=CT	1.04	0.44
Decane	124-18-5	9	0.0012	-	0	-	-	NA	NA	NA
Dodecane	112-40-3	10	0.0009	-	1	0.0004	-	NA	NA	NA
Ethanol	64-17-5	12	0.0663	0.01%	12	0.101	0.01%	HS=CT	0.68	0.26
Hexane	110-54-3	12	0.122	0.24%	12	0.115	0.23%	HS=CT	1.09	0.41
n-Heptane	142-82-5	12	0.052	0.06%	12	0.0359	0.04%	HS>CT	1.44	0.65
Toluene	108-88-3	12	0.006	0.01%	12	0.0032	0.01%	HS>CT	1.87	0.42
Trichlorofluoromethane	75-69-4	12	0.0355	0.004%	12	0.0374	0.004%	HS=CT	0.95	0.50
Tridecane	629-50-5	8	0.0005	-	0	-	-	NA	NA	NA

[a] The threshold values used were listed as OELs in RPP-22491 Rev. 1 (Meacham et.al. 2006).
Multiplicative. bias calculated assuming mean CT and HS concentrations with error
NA – not analyzed, insufficient CT data points above detection limit.
- No data (e.g., not detected, or OEL not determined)

4.3.1 1-Propanol 71-23-8

1-Propanol was detected in the headspace of tank BY-110 in all HS samples and in all but one CT sample. Median HS and CT concentrations were approximately 0.02 ppm with both the HS and CT sampling systems. Figure 22 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

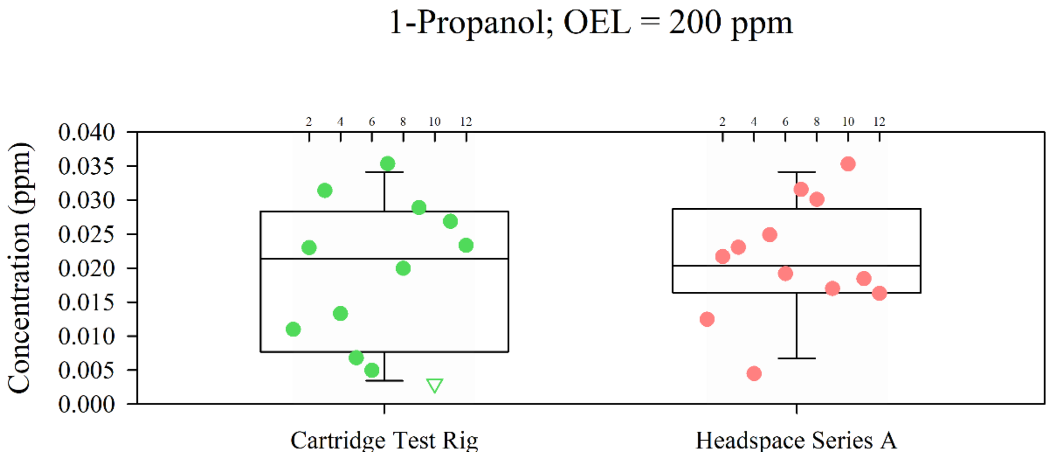

Figure 22. Box Plot of 1-Propanol Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was not significantly different (binomial test; p = 0.11) than the proportion detected with the HS sampling system (Table 19). The HS median concentration was not significantly different from the CT median concentration (Mann-Whitney; p = 0.37). The percent difference between medians (i.e., [HS-CT]/HS) was -5% with the HS median concentration less than 0.1% of the OEL. The CT concentration standard deviation was not significantly different (Levene's test; p = 0.134) than the HS concentration standard deviation (ratio = 1.27). Further, the rule-of-thumb criteria (1.5) was not exceeded indicating that the HS concentration variance (CV = 41%) was similar to the CT concentration variance (CV = 58%).

Table 19. Statistical Comparison of 1-Propanol Measurements from CT and HS Samples

Analyte	Method	OEL (ppm)	Boiling Point (◦F)	CT		HS Series A		Conclusion of Test of Equal Proportion Detected
				Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
1-Propanol	VOC	200	207	11	1	12	0	NS; p=0.11

Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration	ppm	0.0214	0.0204	-5.0%	Mann-Whitney	Not Significantly Different	0.01%
Concentration Standard Deviation	ppm	0.0110	0.0086	(1.27)	Levene's Test	CT>HS, p = 0.134; NS	
Coefficient of Variation or Relative Standard Deviation		58%	41%				

Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)		Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)	
Additive: b+CT = HS	Multiplicative:b·CT = HS	Additive: b+CT = HS	Multiplicative:b·CT = HS
-0.0010 (±0.0063)	1.08 (±0.41)	0.0022 (±0.0081)	1.06 (±1.24)

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

The multiplicative bias of 1.06 can be used to estimate the HS concentration for 1-propanol from the CT samples.

4.3.2 2-Butanone 78-93-3

2-Butanone was detected in all HS and CT samples of the headspace of tank BY-110 at median concentrations of approximately 19 ppb and 27 ppb with the HS and CT sampling systems, respectively. Figure 23 is a box plot depicting the 12 replicate samples from both sampling systems. There were four CT samples with "E" quality flags indicating that the sorbent was near saturation. These sample concentrations could be underestimated.

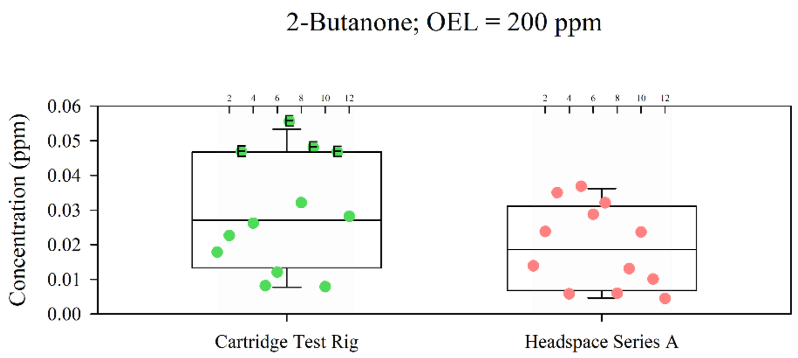

Figure 23. Box Plot of 2-Butanone Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The HS median concentration was not significantly greater (Mann-Whitney; p = 0.92) than the CT median concentration (Table 20).

Table 20. Statistical Comparison of 2-Butanone Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
2-Butanone	VOC	200	140	12, 4 flagged	0	12	0	CT=HS
Statistical Measure		Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration		ppm	0.027	0.0186	-45.2%	Mann-Whitney	Not Significantly Different	0.01%
Concentration Standard Deviation		ppm	0.0167	0.012	(1.39)	Levene's Test	CT>HS, p = 0.16; NS	
Coefficient of Variation or Relative Standard Deviation			57%	62%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)					Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)			
Additive: b+CT = HS		Multiplicative:b·CT = HS			Additive: b+CT = HS		Multiplicative:b·CT = HS	
-0.0084 (±0.010)		0.64 (±0.24)			-0.01 (±0.012)		0.67 (±0.89)	

The percent difference between medians (i.e., [HS-CT]/HS) was -45% with the HS median concentration less than 0.1% of the OEL. The CT concentration standard deviation was not significantly different (Levene's test; p = 0.16) than the HS concentration standard deviation (ratio = 1.4). Further, the rule-of-thumb criteria (1.5) was not exceeded indicating that the HS concentration variance (CV = 62%) was similar to the CT concentration variance (CV = 57%).

The analytical method for VOC sample volume and volume variance were not significantly different between the HS and CT sampling methods (p = 0.33 and 0.14, respectively). The rule-of-thumb criteria of 1.5 was exceeded (ratio = 1.7), however, suggesting that the variances in sample volume were not equal between the two sampling methods.

The multiplicative bias of 0.67 can be used to estimate the HS concentration for 2-butanone from the CT samples.

4.3.3 2-Heptanone 110-43-0

2-Heptanone was detected in all HS samples and five of 12 CT samples of the headspace of tank BY-110. The median HS and CT concentrations were approximately 5.6 ppb and 0.8 ppb with the HS and CT sampling systems, respectively. Figure 24 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

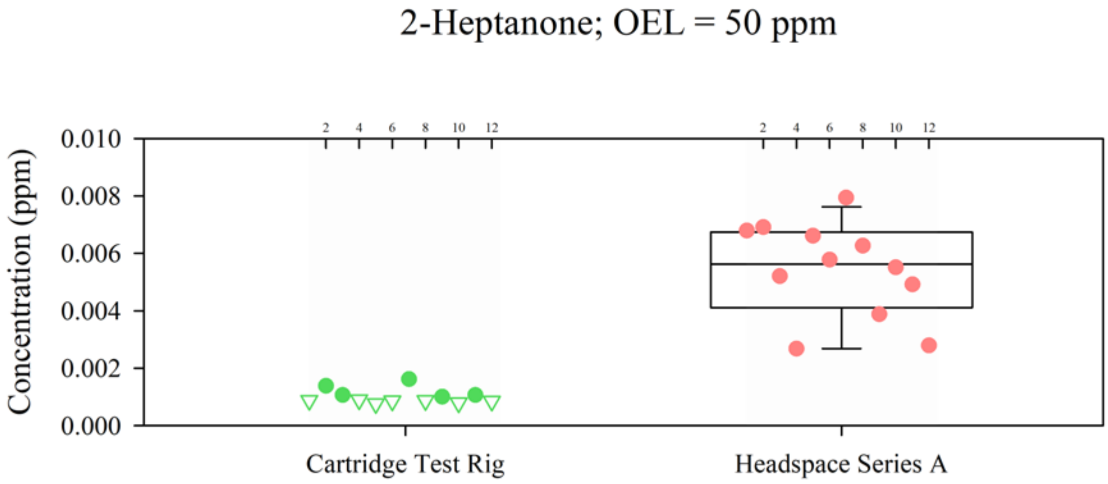

Figure 24. Box Plot of 2-Heptanone Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was significantly less (binomial test; p = 0.001) than the proportion detected with the HS sampling system (Table 21). The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with the CT sampling system.

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

Table 21. Statistical Comparison of 2-Heptanone Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
2-Heptanone	VOC	50	304	5	7	12	0	p < 0.001
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0008	0.0056	NA	Mann-Whitney	NA	0.0%
	Concentration Standard Deviation	ppm	0.0003	0.0017	NA	Levene's Test	NA	
	Coefficient of Variation or Relative Standard Deviation		27%	30%				

4.3.4 3-Heptanone 106-35-4

3-Heptanone was detected in all HS samples and seven of 12 CT samples of the headspace of tank BY-110. The median HS and CT concentrations were approximately 10 ppb and 1 ppb with the HS and CT sampling systems, respectively. Figure 25 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

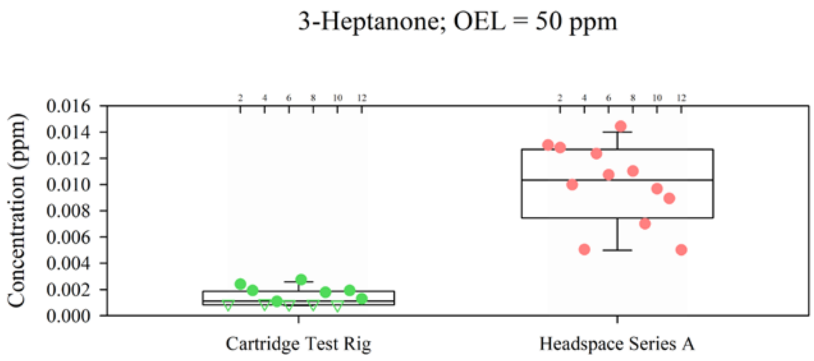

Figure 25. Box Plot of 3-Heptanone Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was significantly less (binomial test; p < 0.001) than the proportion detected with the HS sampling system (Table 22). The HS median concentration was significantly greater (Mann-Whitney; p < 0.001) than the CT median concentration with a percent difference between medians (i.e., [HS-CT]/HS) of 89%. The HS median concentration was less than 0.1% of the OEL. The Levene’s test of equal concentration variance between the two sampling methods was not conducted because sCT was less than sHS with a ratio of 0.22. However, the ratio of sHS:sCT equaled 4.6 indicating that the HS concentration variance (CV = 31%) was different than the CT concentration variance (CV = 48%) based on the rule-of-thumb criteria.

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene’s test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

The multiplicative bias of 7.15 can be used to estimate the HS concentration for 3-heptanone from the CT samples.

Table 22. Statistical Comparison of 3-Heptanone Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
3-Heptanone	VOC	50	297	7	5	12	0	$p < 0.001$
Statistical Measure		Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration		ppm	0.0011	0.0103	89.1%	Mann-Whitney	HS>CT $p < 0.001$	0.02%
Concentration Standard Deviation		ppm	0.0007	0.0031	(0.217)	Levene's Test	sCT≤sHS	
Coefficient of Variation or Relative Standard Deviation			48%	31%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS		Multiplicative:b·CT = HS				Additive: b+CT = HS		Multiplicative:b·CT = HS
0.0092 (±0.0004)		7.38 (±2.20)				0.0086 (±0.0018)		7.15 (±2.87)

4.3.5 4-Methyl-2-Pentanone 108-10-1

4-Methyl-2-pentanone was detected in all HS samples and all but one CT sample of the headspace of tank BY-110. Median HS and CT concentrations were approximately 3.7 ppb and 2.7 ppb with the HS and CT sampling systems, respectively. Figure 26 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

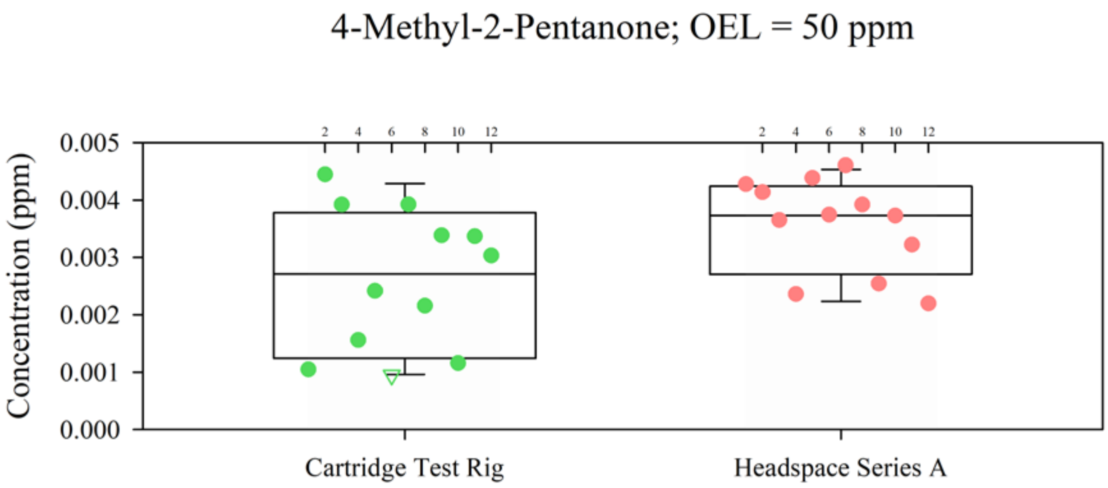

Figure 26. Box Plot of 4-Methyl-2-Pentanone Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was not significantly different (binomial test; $p = 0.11$) than the proportion detected with the HS sampling system (Table 23). The HS median concentration was significantly greater (Mann-Whitney; $p = 0.03$) than the CT median concentration with a percent difference between medians (i.e., [HS-CT]/HS) of 27%. The HS median concentration was less than 0.1% of the OEL. The Levene's test of equal concentration variance between the two sampling methods concluded that sCT was significantly greater ($p = 0.03$) than sHS with a ratio of 1.52. Further, the rule-of-thumb criteria (1.5) was exceeded indicating that the HS concentration variance (CV = 23%) was different than the CT concentration variance (CV = 48%).

Table 23. Statistical Comparison of 4-Methyl-2-Pentanone Measurements from CT and HS Samples

Analyte	Method	OEL (ppm)	Boiling Point (°F)	CT Number of Observations Detected	CT Number of Observations Censored	HS Series A Number of Observations Detected	HS Series A Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
4-Methyl-2-Pentanone	VOC	50	241	11	1	12	0	NS; p=0.11

Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration	ppm	0.0027	0.0037	27.3%	Mann-Whitney	HS>CT p = 0.03	0.01%
Concentration Standard Deviation	ppm	0.0012	0.0008	(1.52)	Levene's Test	CT>HS, p = 0.026	
Coefficient of Variation or Relative Standard Deviation		48%	23%				

Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty) Additive: b+CT = HS	Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty) Multiplicative:b·CT = HS	Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty) Additive: b+CT = HS	Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty) Multiplicative:b·CT = HS
0.00102 (±0.00072)	1.43 (±0.43)	0.00096 (±0.0009)	1.33 (±0.60)

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene’s test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

Despite a statistically observed difference in median concentrations between CT and HS samples, the mean multiplicative bias of 1.33 can be used to estimate the HS concentration for 4-methyl-2-pentanone from the CT concentration.

4.3.6 Cyclohexane 110-82-7

Cyclohexane was detected in all HS and CT samples of the headspace of tank BY-110 at a median concentration of approximately 7.5 ppb with both the HS and CT sampling systems. Figure 27 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

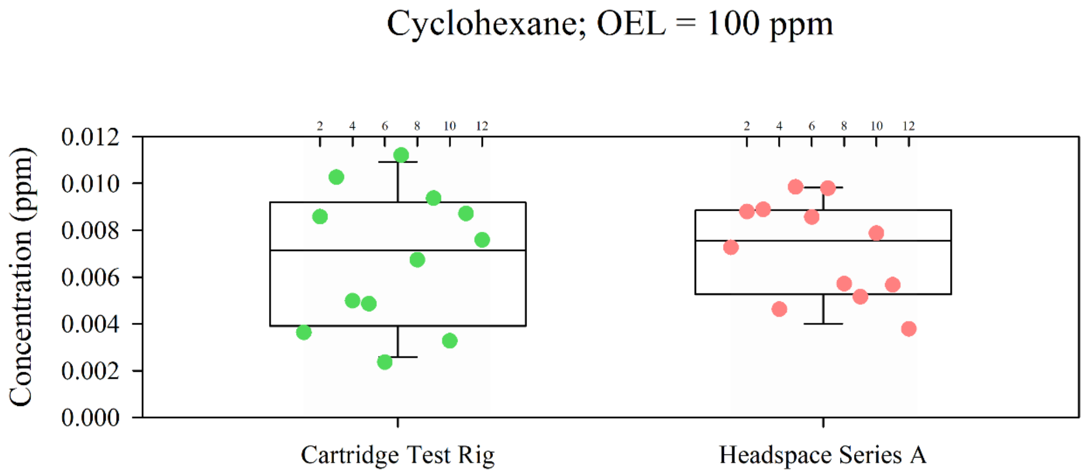

Figure 27. Box Plot of Cyclohexane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The HS median concentration was not significantly different (Mann-Whitney; p = 0.35) from the CT median concentration (Table 24). The percent difference between medians (i.e., [HS-CT]/HS) was 5.4% with the HS median concentration less than 0.1% of the OEL. The CT concentration standard deviation was not significantly greater (Levene's test; p = 0.091) than the HS concentration standard deviation (ratio = 1.4). Further, the rule-of-thumb criteria (1.5) was not exceeded indicating that the HS concentration variance (CV = 29%) was similar to the CT concentration variance (CV = 44%).

Table 24. Statistical Comparison of Cyclohexane Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Cyclohexane	VOC	100	177	12	0	12	0	CT=HS

Statistical Measure	Units	Cartridge Test Rig (CT)	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration	ppm	0.0071	0.0076	5.4%	Mann-Whitney	Not Significantly Different	0.01%
Concentration Standard Deviation	ppm	0.0029	0.0021	(1.4)	Levene's Test	CT>HS, p = 0.091; NS	
Coefficient of Variation or Relative Standard Deviation		44%	29%				

Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)		Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)	
Additive: b+CT = HS	Multiplicative:b·CT = HS	Additive: b+CT = HS	Multiplicative:b·CT = HS
0.00041 (±0.00170)	1.11 (±0.30)	0.00037 (±0.0021)	1.04 (±0.44)

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

The multiplicative bias of 1.04 can be used to estimate the HS concentration for cyclohexane from the CT samples.

4.3.7 Decane 124-18-5

Decane was detected in nine of the 12 HS samples of the headspace of tank BY-110 at a median concentration of approximately 1.2 ppb with the HS sampling system and was not detected with the CT sampling system. Figure 28 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

The proportion of detected samples with the CT sampling system was significantly less (binomial test; p < 0.001) than the proportion detected with the HS sampling system (Table 25). The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with the CT sampling system.

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

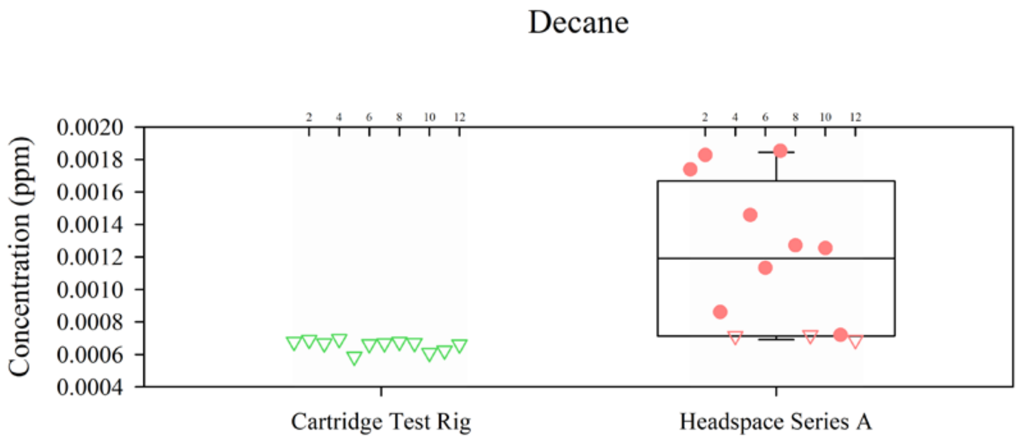

Figure 28. Box Plot of Decane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

Table 25. Statistical Comparison of Decane Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Decane	VOC			0	12	9	3	p < 0.001
	Statistical Measure	Units	CT)	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	NA	0.0012	NA	Mann-Whitney	NA	
	Concentration Standard Deviation	ppm	NA	0.0005	NA	Levene's Test	NA	
	Coefficient of Variation or Relative Standard Deviation		NA	38%				

4.3.8 Dodecane 112-40-3

Dodecane was detected in 10 of 12 HS samples and one CT sample of the headspace of tank BY-110. The median HS and CT concentrations were approximately 0.9 ppb and 0.4 ppb with the HS and CT sampling systems, respectively. Figure 29 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

The proportion of detected samples with the CT sampling system was significantly less (binomial test; p < 0.001) than the proportion detected with the HS sampling system (Table 26). The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with the CT sampling system.

The analytical method for SVOC sample volume was not significantly different between the HS and CT sampling methods (p = 0.999). The percent difference between medians volumes (i.e., [HS-CT]/HS) was -12%. The Levene’s test of equal sample volume variance between the two sampling methods was not significant (p = 0.297) even though the ratio sCT:sHS was 1.61. The rule-of-thumb criteria of 1.5 was exceeded, however, suggesting that the variances in sample volume were not equal between the two sampling methods.

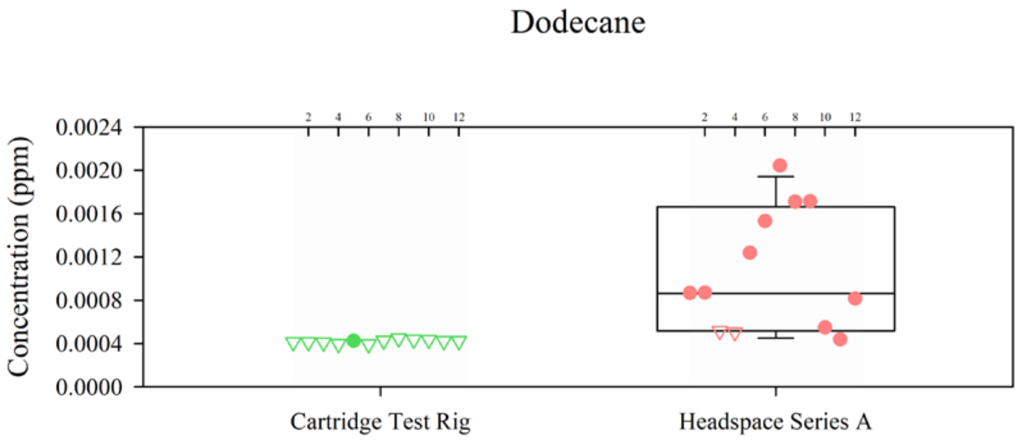

Figure 29. Box Plot of Dodecane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

Table 26. Statistical Comparison of Dodecane Measurements from the CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Dodecane	SVOC			1	11	10	2	p < 0.001
Statistical Measure		Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration		ppm	0.0004	0.0009	NA	Mann-Whitney	NA	
Concentration Standard Deviation		ppm	NA	0.0006	NA	Levene's Test	NA	
Coefficient of Variation or Relative Standard Deviation			NA	53%				

4.3.9 Ethanol 64-17-5

Ethanol was detected in all HS and CT samples of the headspace of tank BY-110. The median HS and CT concentrations were approximately 0.066 ppm and 0.10 ppm with the HS and CT sampling systems, respectively. Figure 30 is a box plot depicting the 12 replicate samples from both sampling systems. There were two CT samples with “E” flags indicating that the sorbent was near saturation and that the concentration may be underestimated.

The HS median concentration was not significantly different (Mann-Whitney; p = 0.98) from the CT median concentration (Table 27). The percent difference between medians (i.e., [HS-CT]/HS) was -53% with the HS median concentration less than 0.1% of the OEL. The CT concentration standard deviation was significantly greater (Levene’s test; p = 0.005) than the HS concentration standard deviation (ratio = 2). Further, the rule-of-thumb criteria (1.5) was exceeded indicating that the HS concentration variance (CV = 28%) was different from the CT concentration variance (CV = 40%).

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene’s test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods. The multiplicative bias of 0.68 can be used to estimate the HS concentration for ethanol from the CT samples.

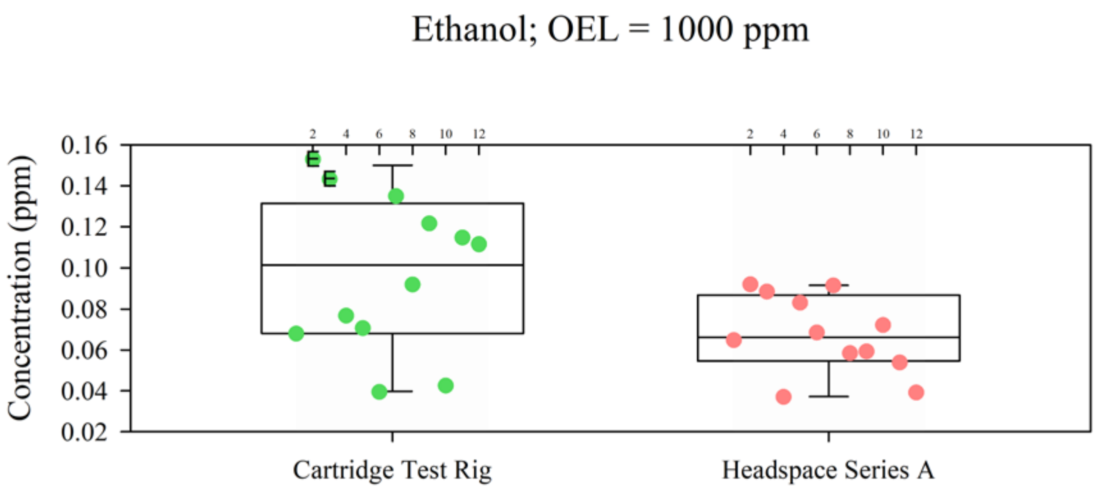

Figure 30. Box Plot of Ethanol Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

Table 27. Statistical Comparison of Ethanol Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Ethanol	VOC	1000	173	12, 2 E flagged	0	12	0	CT=HS
Statistical Measure		Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration		ppm	0.101	0.0663	-53.1%	Mann-Whitney	Not Significantly Different	0.01%
Concentration Standard Deviation		ppm	0.0384	0.019	(2.02)	Levene's Test	CT>HS, p = 0.005	
Coefficient of Variation or Relative Standard Deviation			40%	28%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty) Additive: b+CT = HS				Multiplicative:b·CT = HS			Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty) Additive: b+CT = HS Multiplicative:b·CT = HS	
-0.035 (±0.022)				0.68 (±0.16)			-0.03 (±0.025)	0.68 (±0.26)

4.3.10 Hexane 110-54-3

Hexane was detected in all HS and CT samples of the headspace of tank BY-110. The median HS and CT concentration was approximately 0.12 ppm with both the HS and CT sampling systems. Figure 31 is a box plot depicting the 12 replicate samples from both sampling systems. All HS and all but one CT sample had “E” flags indicating that the sorbent was near saturation and sample concentrations may be underestimated.

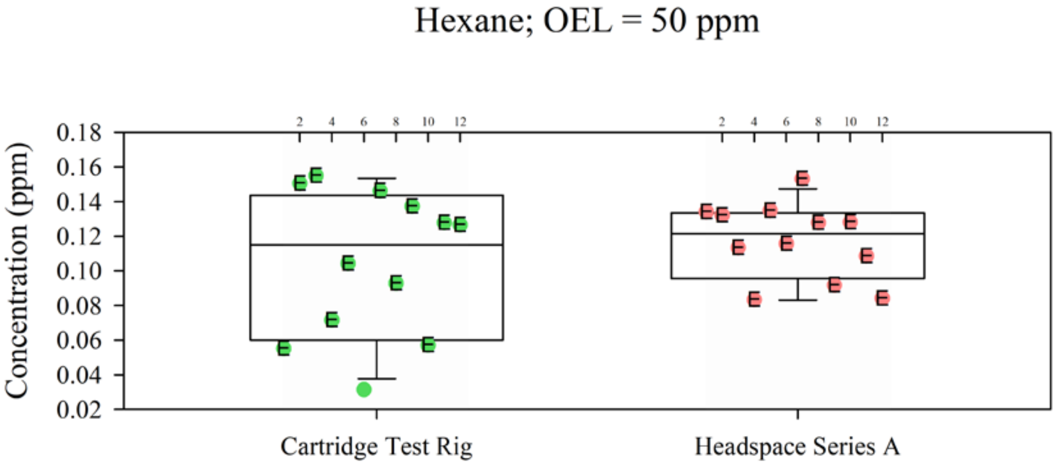

Figure 31. Box Plot of Hexane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The HS median concentration was not significantly different (Mann-Whitney; p = 0.31) from the CT median concentration (Table 28). The percent difference between medians (i.e., [HS-CT]/HS) was 5% with the HS median concentration 0.2% of the OEL. The CT concentration standard deviation was significantly greater (Levene’s test; p = 0.012) than the HS concentration standard deviation (ratio = 1.9). Further, the rule-of-thumb criteria (1.5) was exceeded indicating that the HS concentration variance (CV = 19%) was different from the CT concentration variance (CV = 41%).

The multiplicative bias of 1.09 can be used to estimate the HS concentration for hexane from the CT samples.

Table 28. Statistical Comparison of Hexane Measurements from CT and HS Samples

				CT)		HS Series A		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Hexane	VOC	50	156	12, 11 E flagged	0	12, 12 E flagged	0	CT=HS
Statistical Measure		Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
Median Concentration		ppm	0.115	0.122	5.3%	Mann-Whitney	Not Significantly Different	0.2%
Concentration Standard Deviation		ppm	0.0426	0.0221	(1.93)	Levene's Test	CT>HS, p = 0.012	
Coefficient of Variation or Relative Standard Deviation			41%	19%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
	Additive: b+CT = HS		Multiplicative:b·CT = HS				Additive: b+CT = HS	Multiplicative:b·CT = HS
	0.0065 (±0.0246)		1.17 (±0.29)				0.013 (±0.028)	1.09 (±0.41)

4.3.11 N-Heptane 142-82-5

N-Heptane was detected in all HS and CT samples of the headspace of tank BY-110. Median HS and CT concentrations were approximately 0.052 ppm and 0.036 ppm with the HS and CT sampling systems, respectively. Figure 32 is a box plot depicting the 12 replicate samples from both sampling systems. All HS samples and seven of 12 CT samples had “E” flags indicating that the sorbent was nearly saturated and the sample concentrations may be underestimated.

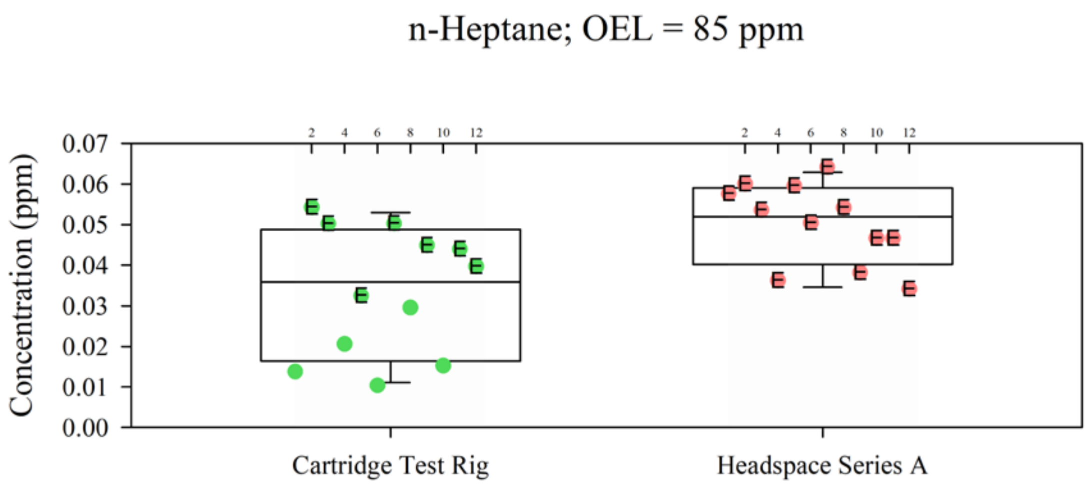

Figure 32. Box Plot of n-Heptane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The HS median concentration was significantly greater (Mann-Whitney; p = 0.005) than the CT median concentration with a percent difference between medians (i.e., [HS-CT]/HS) of 31% (Table 29). The HS median concentration was equal to 0.1% of the OEL. The Levene's test of equal concentration variance between the two sampling methods concluded that sCT was significantly greater (p = 0.03) than sHS with a ratio of 1.58. Further, the rule-of-thumb criteria (1.5) was exceeded indicating that the HS concentration variance (CV = 20%) was different than the CT concentration variance (CV = 47%).

Table 29. Statistical Comparison of n-Heptane Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
n-Heptane	VOC	85	209	12, 7 E flagged	0	12, 12 E flagged	0	CT=HS
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0359	0.052	30.9%	Mann-Whitney	HS>CT p = 0.005	0.1%
	Concentration Standard Deviation	ppm	0.0158	0.0100	(1.58)	Levene's Test	CT>HS, p = 0.029	
	Coefficient of Variation or Relative Standard Deviation		47%	20%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS			Multiplicative:b·CT = HS			Additive: b+CT = HS		Multiplicative:b·CT = HS
0.016 (±0.009)			1.55 (±0.45)			0.016 (±0.011)		1.44 (±0.65)

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 1.44 can be used to estimate the HS concentration for n-heptane from the CT concentration.

4.3.12 Toluene 108-88-3

Toluene was detected in all of the HS and CT samples of the headspace of tank BY-110. HS and CT median concentrations were approximately 6 ppb and 3 ppb with the HS and CT sampling systems, respectively. Figure 33 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

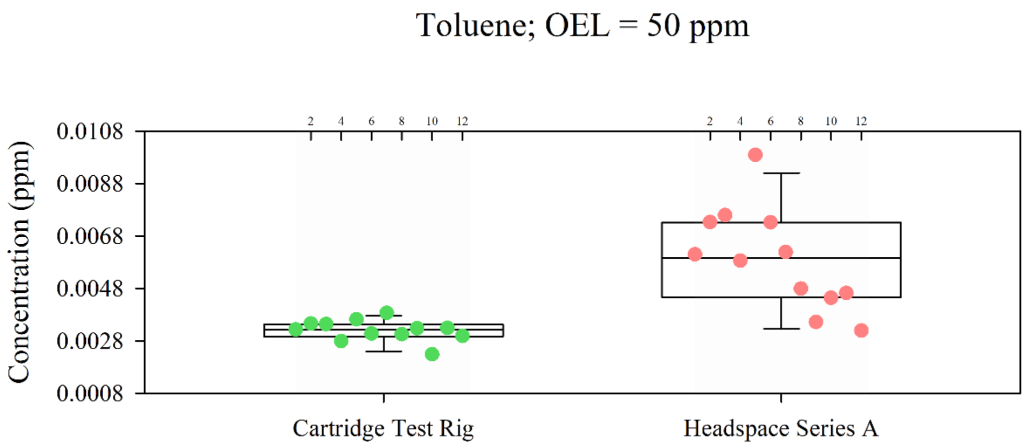

Figure 33. Box Plot of Toluene Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The HS median concentration was significantly greater (Mann-Whitney; p < 0.001) than the CT median concentration with a percent difference between medians (i.e., [HS-CT]/HS) of 46% (Table 30).

Table 30. Statistical Comparison of Toluene Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Toluene	VOC	50	231	12	0	12	0	CT=HS
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0032	0.006	45.9%	Mann-Whitney	HS>CT p < 0.001	0.01%
	Concentration Standard Deviation	ppm	0.00041	0.00194	(0.212)	Levene's Test	sCT≤sHS	
	Coefficient of Variation or Relative Standard Deviation		13%	33%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS			Multiplicative:b·CT = HS			Additive: b+CT = HS		Multiplicative:b·CT = HS
0.0027 (±0.0002)			1.88 (±0.14)			0.0027 (±0.0011)		1.87 (±0.42)

The HS median concentration was less than 0.1% of the OEL. The Levene's test of equal concentration variance between the two sampling methods was not conducted because sCT was less than sHS with a ratio of 0.212. However, the rule-of-thumb criteria (1.5) was exceeded (max s/min s = 4.7) indicating that the HS concentration variance (CV = 33%) was different than the CT concentration variance (CV = 13%).

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

Despite a statistically observed difference in median concentrations between CT and HS samples, the multiplicative bias of 1.87 can be used to estimate the HS concentration for toluene from the CT concentration.

4.3.13 Trichlorofluoromethane 75-69-4

Trichlorofluoromethane was detected in all HS and CT samples of the headspace of tank BY-110. The HS and CT median concentration was approximately 36 ppb for both sampling systems. Figure 34 is a box plot depicting the 12 replicate samples from both sampling systems. There were 10 of 12 HS samples and nine of 12 CT samples with "E" flags indicating that the sorbent was near saturation and the sample concentrations may be underestimated.

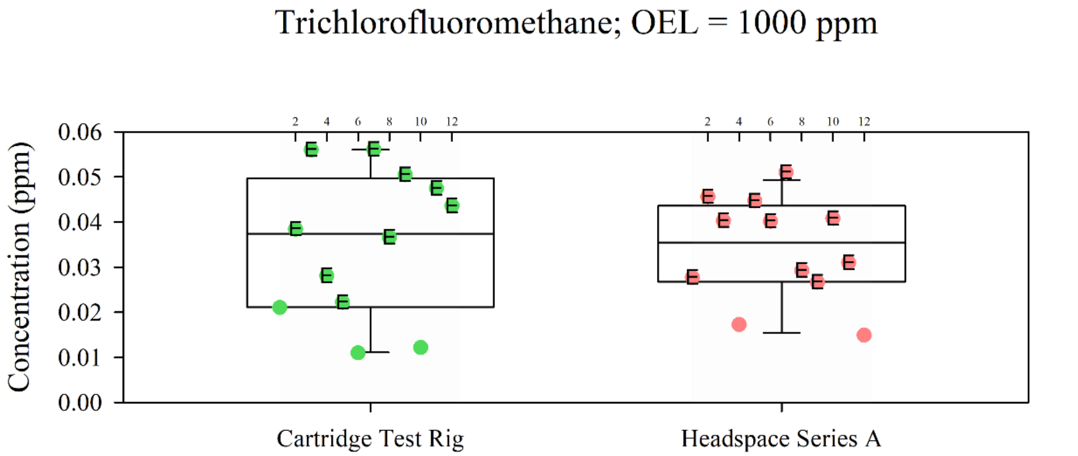

Figure 34. Box Plot of Trichlorofluoromethane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The HS median concentration was not significantly different (Mann-Whitney; p = 0.58) than the CT median concentration (Table 31). The percent difference between medians (i.e., [HS-CT]/HS) was -5.4% with the HS median concentration less than 0.1% of the OEL. The CT concentration standard deviation was not significantly different (Levene's test; p = 0.103) than the HS concentration standard deviation (ratio = 1.4). Further, the rule-of-thumb criteria (1.5) was not exceeded indicating that the HS concentration variance (CV = 34%) was similar to the CT concentration variance (CV = 46%).

Table 31. Statistical Comparison of Trichlorofluoromethane Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Trichloro-fluoromethane	VOC	1000	75	12, 10 flagged	0	12, 10 flagged	0	CT=HS
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A/OEL (%)
	Median Concentration	ppm	0.0374	0.0355	-5.40%	Mann-Whitney	Not Significantly Different	<0.1%
	Concentration Standard Deviation	ppm	0.0162	0.0114	(1.42)	Levene's Test	CT>HS, p = 0.103; NS	
	Coefficient of Variation or Relative Standard Deviation		46%	34%				
Additive and Multiplicative Bias (ppm) assuming HS without Error (k=2 Uncertainty)						Additive and Multiplicative Bias (ppm) assuming HS with Error (k=2 Uncertainty)		
Additive: b+CT = HS			Multiplicative:b·CT = HS			Additive: b+CT = HS	Multiplicative:b·CT = HS	
-0.0019 (±0.0094)			1.01 (±0.29)			-0.0011 (±0.011)	0.95 (±0.50)	

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene’s test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

The multiplicative bias of 0.95 can be used to estimate the HS concentration for trichlorofluoro-methane from the CT samples.

4.3.14 Tridecane 629-50-5

Tridecane was detected in eight of 12 HS samples and no CT samples of the headspace of tank BY-110. The median HS concentration was approximately 1 ppb with the HS sampling system. Figure 35 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

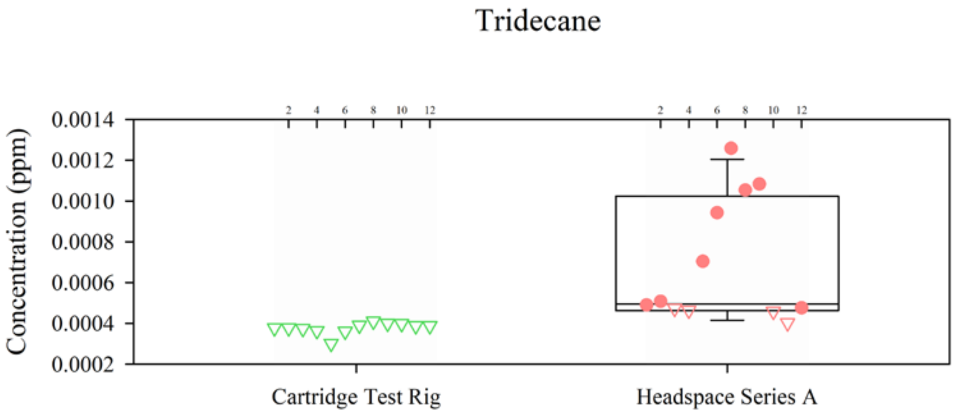

Figure 35. Box Plot of Tridecane Concentration Measurements from Replicate Samples from CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was significantly less (binomial test; $p < 0.001$) than the proportion detected with the HS sampling system (Table 32). The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with the CT sampling system.

Table 32. Statistical Comparison of Tridecane Measurements from CT and HS Samples

				CT		HS Series A		
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Tridecane	SVOC		453	0	12	8	4	p <0.001
	Statistical Measure	Units	CT	HS Series A	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	HS Series A OEL (%)
	Median Concentration	ppm	NA	0.0005	NA	Mann-Whitney	NA	
	Concentration Standard Deviation	ppm	NA	0.0003	NA	Levene's Test	NA	
	Coefficient of Variation or Relative Standard Deviation		NA	44%				

The analytical method for SVOC sample volume was not significantly different between the HS and CT sampling methods (p = 0.999). The percent difference between medians volumes (i.e., [HS-CT]/HS) was -12%. The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.297) even though the ratio sCT:sHS was 1.61. The rule-of-thumb criteria of 1.5 was exceeded, however, suggesting that the variances in sample volume were not equal between the two sampling methods.

4.4 Sample Size Analysis of Selected COPCs and Non-COPCs

The use of 12 replicates in HS and CT sampling in this test provided a unique opportunity to statistically evaluate sampling and analytical variance for analytes detected above their RLs and to estimate the number of replicates that may be valuable in future sample collection campaigns. Sample size analyses were conducted for the 10 COPCs discussed in Section 4.2 and eight selected non-COPCs from those identified in Section 4.3 with six or more samples detected above their RLs. Specifically, the information was used to predict the number of future samples that would be required to provide a mean within a given confidence interval compared to the mean using the 12-replicate set. Difference thresholds between the means were selected for illustration purposes, with 30% representing a reasonable analytical control limit and 50% representing a potential higher bound of acceptability.

The variances[41] from Section 4.2 for the 10 COPCs with at least six samples above detection are presented in Figure 36 for both HS and CT sample sets, in order of lowest to highest HS variance. The number of replicate samples needed in future testing to detect less than 30% or 50% variance from the BY-110 mean HS and CT concentrations are shown above the 30% (green) or 50% (yellow) variance lines. For example, the ammonia HS variance from BY-110 testing was 25% with a mean concentration of 296 ppm, and would require 10 replicates to be able detect a mean concentration within 30% of 296 ppm. If detection within 50% of 296 ppm were acceptable, only four replicate samples would be required. For those COPCs with significantly higher measured HS variances such as the aldehydes and nitrosamines, significantly more replicate samples would be needed to assure that a mean concentration could be detected within 30% or 50% of the previously measured mean. For these COPCs, the variance range for CT samples were greater than HS samples, despite the fact the average variance for both CT and HS samples was generally consistent.

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[41] Coefficient of variance (CV) is also known as the relative standard deviation. See Appendix C for additional descriptive statistics.

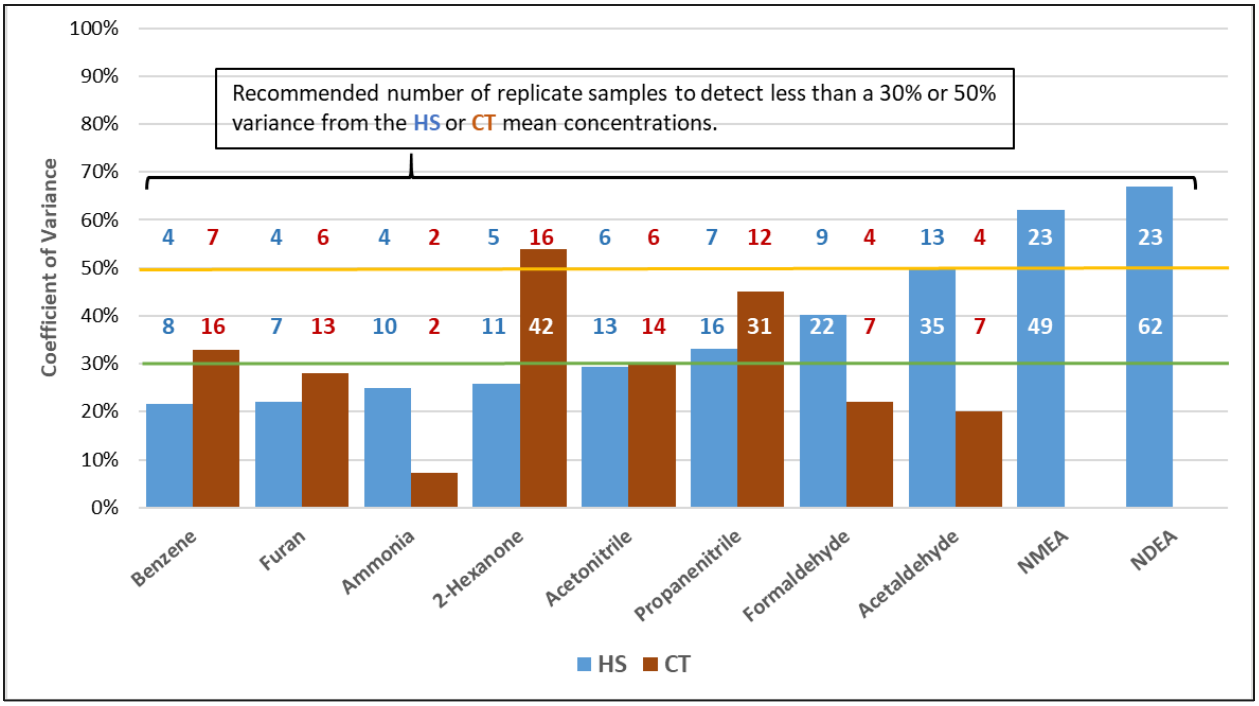

Figure 36. Plot of Measured Variances and Recommended Sample Sizes for Selected COPCs. CT nitrosamine results were suspect due to analytical quality flags and are not shown.

The variances from Section 4.3 for eight selected non-COPCs with at least six samples above detection are presented in order of lowest to highest HS variance in Figure 37 for both HS and CT sample sets. The number of replicate samples needed in future testing to detect less than 30% or 50% variance from the BY-110 mean HS and CT concentrations are shown above the 30% (green) or 50% (yellow) variance lines. For those non-COPCs with significantly higher measured HS variance, such as the aldehydes and nitrosamines, substantially more replicate samples would be needed to assure that a mean concentration within 30% or 50% of the previously measured mean could be detected. The variance of most of HS non-COPC analytes was significantly lower than CT variances for the same analytes.

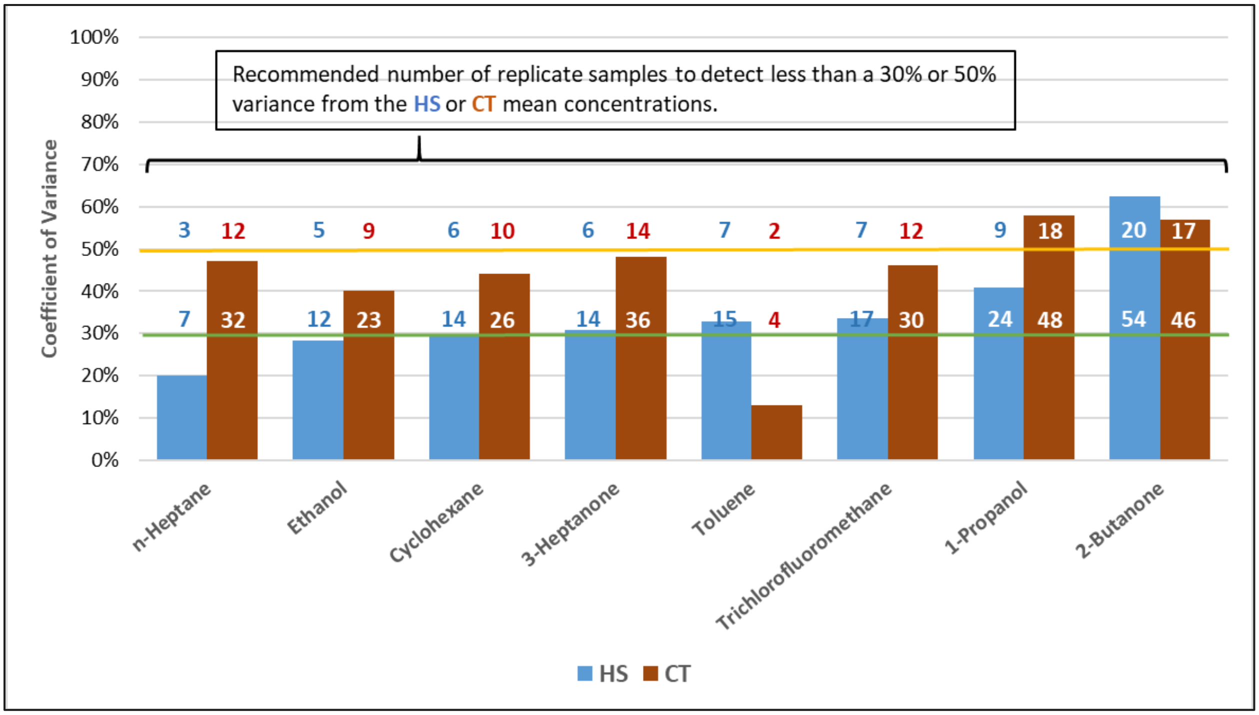

Figure 37. Plot of Measured Variances and Recommended Sample Sizes for Selected Non-COPCs

5.0 Mechanisms for Potential Bias

5.1 Compounds with Significant Bias

To determine a potential source of the bias between the CT and HS data (Table 3 and Table 18), the ratios of the mean concentrations were evaluated. Figure 38 shows the CT-HS mean ratios plotted against their corresponding boiling point values. Here, a value of 1 reflects parity between the two measurements. The error bars correspond to the standard error (k = 2 uncertainty). As seen in the plot eight analytes—five COPCs and three non-COPCs—had ratios statistically lower than parity. Six of these analytes represented higher boiling point compounds (≥209°F)—n-heptane, toluene, 2-hexanone, 3-heptanone, NEMA, and NDEA—indicating a general trend of increasing bias with higher boiling points. Formaldehyde and acetonitrile also showed statistically lower ratios but with lower boiling points (≤179°F). These results indicate that boiling point as well as other potential factors may be key contributors to the observed sampling bias. Note that the different dives (see Table 1) represented in the plot (different colored markers) did not appear to contribute bias outside of the standard deviation.

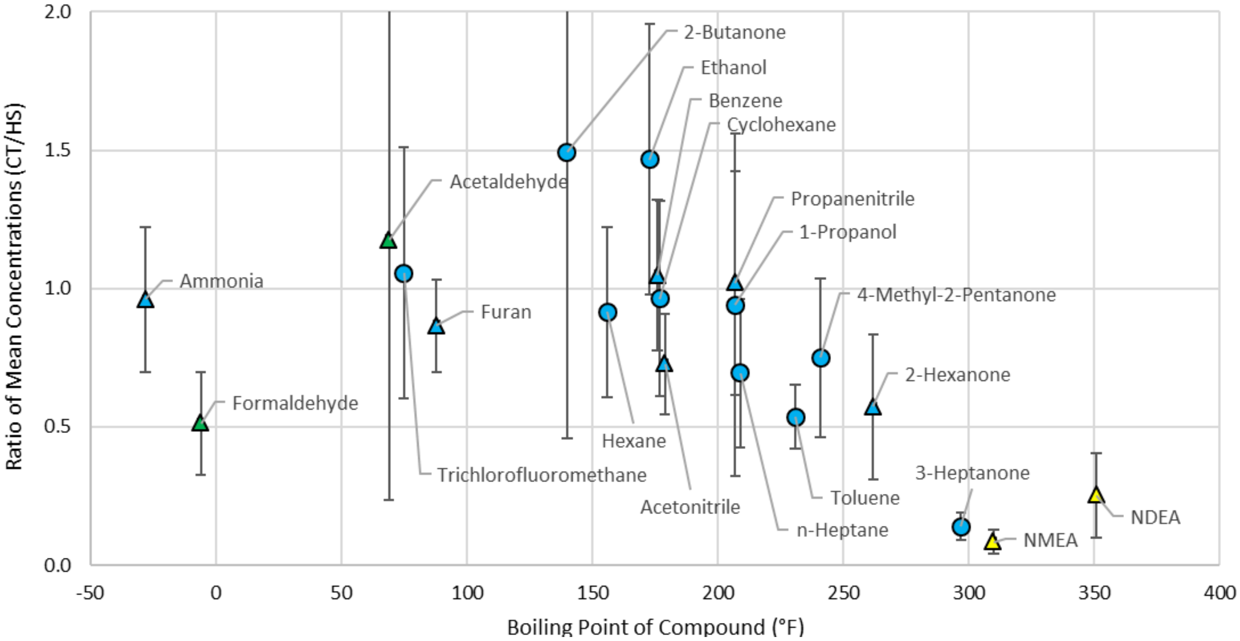

Figure 38. Plot of the Ratio of Mean Concentrations (CT/HS) versus Boiling Point. Error bars represent k=2 uncertainty. Triangular markers are COPCs and circular are non-COPCs. Colors correspond to Dives: Yellow = Dive 1, Green = Dive 3, Blue = Dive 5.

5.2 Potential Mechanisms for Observed Bias

Due to the apparent correlation of bias with boiling point, a number of mechanisms were assessed that were compatible with boiling point influences. Other mechanisms were considered as well. Table 33 summarizes five potential mechanisms, among others, that were ultimately assessed. This table references Appendix D sections with the detail around the associated analysis, along with a general summary of the assessed impact.

Table 33. Potential Causes of Observed Concentration Bias

Potential Cause of the Observed Concentration Biases	Appendix Section with the Associated Evaluation	Summary of Evaluation Conclusions
1. Sample port location/flow rate differences between rigs caused actual differences in concentrations.	D.1 Estimated impacts of sampling location differences	• The sample ports in the tank head space for each test rig were within 12 in. of one another. This difference is not expected to have a significant impact on concentration bias. • The total flow rate into the headspace rig sample port ranged from 3.6 to 12 L/min depending on the analytical tube bundles being tested. The flow into the CT rig was higher (30 to 50 L/min) because that rig is designed for respirator cartridge flow rates. These differences could have had an effect on the individual compound concentrations collected, but the magnitude of the effect could not be determined in this study.
2. The 125+ ft long extension hose required for the CT rig resulted in heat losses from the sample gas stream, thereby lowering the gas temperature, resulting in species condensation on the additional surface area.	D.2 Calculation of impacts of additional CT hose length D.3 Estimated impacts of wall adsorption/diffusion in CT hose D.4 Impacts of accumulated water	• The observed gas temperature reduction in the CT rig extension hose ranged from 6 to 22°F. Calculations and ambient temperature comparisons support this level of temperature reduction if the hose was not heated/insulated properly. There is a higher likelihood of high-boiling point compounds collecting on inner hose surfaces with this level of cooling, especially with the additional hose inner surface area. • The estimated impact of accumulated water in the system preferentially absorbing compounds was determined to be low under practical circumstances, although the degree of nitrosamine impact could not be fully assessed due to data limitations. • Diffusion of vapor species into and through the tubing was not projected to be significant – less than 3% in the most extreme circumstances.
3. The larger inline high-efficiency particulate (HEPA) filter on the CT rig allowed for condensation/ adsorption of species on the additional surface area.	D.5 Calculation of potential HEPA surface area impacts	• Sampling studies conducted during the period 1994–1996 with and without inline HEPA filters indicated the potential for statistically significant concentration differences for some analytes.

Table 33. Potential Causes of Observed Concentration Bias (continued)

Potential Cause of the Observed Concentration Biases	Appendix Section with the Associated Evaluation	Summary of Evaluation Conclusions
4. Actual sample start time differences for each rig resulted in biases due to tank headspace concentration fluctuations.	D.6 Comparison of sampling times (see also Table 1)	• There were significant sampling time differences between the two rigs for the nitrosamine/methanol dive (38 minute delay for the cartridge rig), which could have been a factor in the lower nitrosamine values. The difference in dive start times for the acetonitrile/1,3-butadiene test was also significant (26 min delay for the CT rig). All other dive start times within 11 min of one another. The impact of the time delays could not be quantified without corresponding, known, headspace concentrations.
5. Fluctuations in the flow rates to the individual analytical tubes between the two rigs resulted in the observed biases.	D.7 Comparison of analytical tube flows	• Analytical tube volume differences between the two test rigs were within 10% except for the SVOC tube (12.1% lower for the cartridge rig), the aldehyde tube (15.9% lower for the cartridge rig) and the amine tube (23% higher for the cartridge rig). These differences are not enough to explain the observed biases in COPCs and non-COPCS.
6. Differences in subsequent analytical lab steps resulted in the observed biases (e.g. analyzed on different days, used different analytical equipment and/or operators, etc.).	D.8 Estimated impacts of analytical tube location/ grouping D.9 Potential bias from laboratory analytical processes	• Possible analytical biases were identified with NDEA and NMEA, possibly linked to the associated data scatter. However, this comparison was inconclusive. • Sample grouping effects did not appear to be linked to observed biases. • The effects of sorbent tube biases were inconclusive.

Based on the evaluation of mechanisms shown in Table 33, the leading mechanism suspected of driving the observed biases in higher boiling point analytes is temperature reduction in the sample gas stream due to the 125+ ft extension hose required for the CT rig. Figure 39 shows inlet temperatures for each dive along with ambient temperature from the Hanford Meteorological station. The plot shows significant temperature losses from the CT rig extension hose, with temperatures approaching the ambient outside temperatures. Indeed, these data suggests that the hose heat tracing/insulation is not adequate for maintaining the inside gas temperatures.

Based on the other mechanisms outlined in Appendix D the ability for higher boiling point compounds to adsorb on the extension hose and other inside surfaces is possible, especially with the reduced temperatures.

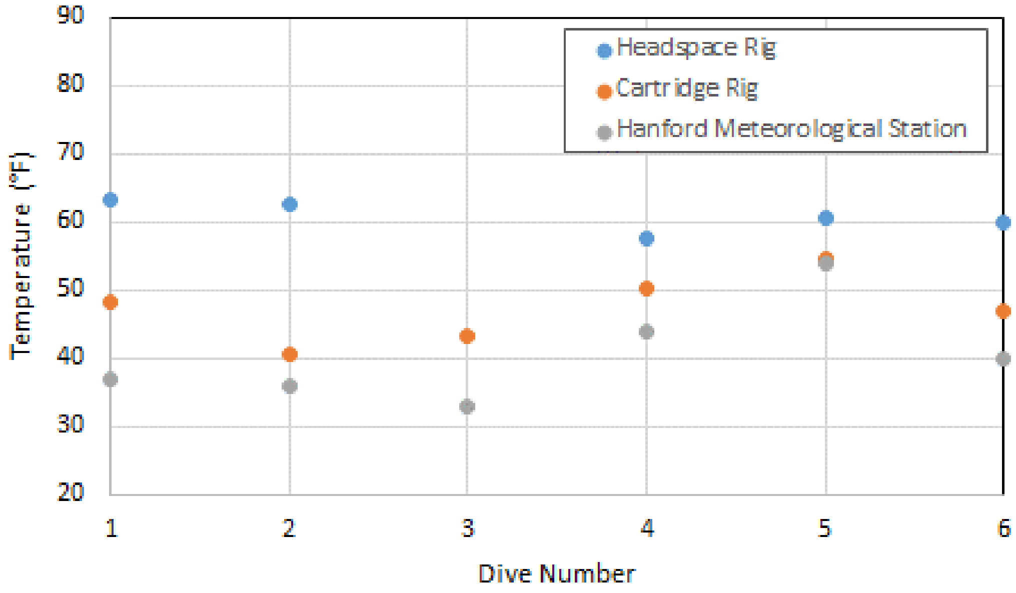

Figure 39. Plot of the Temperatures for Each Dive – HS, CT, and corresponding Hanford Meteorological Station Data. (See Figure D.2.1.)

6.0 Conclusions

Comparison testing on vapors from the BY-110 headspace consisted of simultaneous measurements using both the traditional HS method and the new CT method. Further, 12 simultaneous samples were taken for each compound (sample tube) on each test platform to quantify corresponding sampling and analytical variations. Fifty-nine of the 61 tank vapor COPCs were analyzed. Ten of the COPCs were detected at sufficient concentration in the headspace to enable comparative evaluation of the two sampling methods. Measured concentrations of these COPCs spanned a wide range, from 1 ppb to 300 ppm, and from <1% of their respective OEL to nearly 1300% of their OEL. Five of the COPCs were measured with median concentrations exceeding 10% of their OEL while the remaining five COPCs were measured with median concentrations below 2% of their OEL.

For three COPCs—benzene, acetaldehyde, and propanenitrile—the median HS and CT concentrations were found to be statistically equivalent. The median HS concentration of ammonia was statistically greater than the median CT concentration. However, the difference was within analytical uncertainty and statistical variance of the replicate samples; therefore, the two sets of concentrations were determined to be quantitatively equivalent. The HS median concentrations of the remaining six COPCs—2-hexanone, furan, formaldehyde, acetonitrile, NDEA, and NMEA—were statistically higher than their corresponding CT concentrations.

Analytical data for 53 non-COPC organic vapor analytes was also available from the comparison test sampling results. Ten analytes were detected at sufficient concentration in the headspace of BY-110 to enable quantitative comparative evaluation as a complement to the COPC analysis. These analytes were all present at concentrations below 1% of their respective OEL. Six analytes—1-propanol, 2-butanone, cyclohexane, ethanol, hexane, and trichlorofluoromethane—were found to have statistically equivalent median HS and CT concentrations. The HS median concentrations of the remaining four analytes studied—3-heptanone, 4-methyl-2-pentanone, n-heptane, and toluene—were statistically higher than their corresponding CT concentrations.

Of the 20 COPC and non-COPC analytes evaluated, half exhibited an apparent bias between the mean CT and HS measurements that warranted further analysis to understand the significance and potential mechanisms contributing to the bias. The CT/HS ratios of two analytes—furan and 4-methyl-2-pentanone—were within parity when measurement uncertainty was considered. Six of the analytes exhibiting significant bias represented higher boiling point (≥209°F) compounds indicating a general trend of increasing bias with increasing boiling points. Two COPCs—formaldehyde and acetonitrile—also showed statistically lower ratios but with lower boiling points (≤179°F). These results indicate that boiling point may be a primary contributor to the observed sampling bias, along with other factors.

Several mechanisms were evaluated as potential contributors to sampling and analytical bias. Based on this evaluation, the leading mechanism suspected of driving the observed bias in higher boiling point analytes was temperature reduction in the sample gas stream due to the 125+ ft extension hose required for the CT rig. Temperature data from the comparison test suggest that the hose heat tracing/insulation is not adequate for maintaining the inside gas temperatures, increasing the potential for higher boiling point compounds to adsorb or condense on the extension hose and other inside surfaces.

7.0 Recommendations

Based on the results of the 2018 BY-110 headspace sampling comparison test, future testing, data analysis, and implementation of HS and CT sampling, the following recommendations are offered to improve future testing:

- Based on the apparent biases identified between the CT and HS systems, it is recommended that future CT testing be performed with improved temperature conditioning on the slipstream hose between the tank riser and CT rig and its components and enclosure to maintain temperatures within one or two degrees of tank headspace temperatures. Such an improvement will likely require a combination of improved heat tracing and insulation. Once improved temperature controls are achieved on the CT system, additional CT and HS comparisons are recommended to assure that biases are minimized, especially for compounds with boiling points greater than 200°F.
- Several sampling, analysis, and data challenges impacted the ability to fully benefit from the substantial data collected during the comparison test. These challenges included large sample variances, elevated RLs, and a range of quality flags that limited the viable use of specific data. Improvements in several areas could potentially enhance the value of future headspace data collection.
- For many analytes, replicate samples produced a range of concentrations spanning well above and below analytical RLs. Additional optimization of sampling flow rates and durations is recommended to help assure quantitative results that fully support sampling objectives. For some sorbent tube methods (e.g., volatile organic analytes), consideration of multiple tubes operating with separate lower and higher collection volumes may be helpful to address situations in which one analyte was below the RL while another was well above the calibration range of the instruments.
- The sampling comparison test provided the opportunity to obtain numerous sample replicates for both the HS and CT systems. In general, for both systems, the sample variance was greater than 20% for most COPCs, and ranged up to nearly 70% in some cases. Additional efforts are recommended to understand the potential sources of these variances, especially for those analytes exhibiting variances significantly greater than their analytical uncertainty and control limits. Further, based on the data collected in this study, replicate samples are recommended going forward. For the key COPCs, four or more replicates on both sampling systems are recommended to assure that the mean concentration is within 50% of the mean of the 12-replicate mean, and eight or more to be within 30%.

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Appendix A

Raw Analytical Data

Appendix A

Raw Analytical Data

The raw analytical data is comprised of analytical laboratory reports and volume/flow files provided by WRPS that were the source of data for the calculations and statistical analysis. The analytical data represents an extensive volume of information (over 500 pages); therefore, it is provided in a separate Volume 2. Appendix A in this document (Volume 1) provides introductory information regarding the content of Volume 2, but to review the complete raw data set, readers are referred to Volume 2.

A.1 Description

This appendix includes raw data of sorbent tube sample volumes and sample analytical data for the BY-110 comparison test for both cartridge test (CT) and headspace sampling (HS) sorbent tubes. Calculations using these data are given in Appendix B.

Washington River Protection Solutions (WRPS) converted the raw sample flowrate and analytical data into Excel data spreadsheets that were transmitted to Pacific Northwest National Laboratory along with the formal analytical laboratory reports. Comments on that conversion are provided below.

The analytical measurement results were provided in both analytical report .pdf files, as well as data summary report spreadsheet .xls files in which the data were transferred from entries labeled ‘result’ in the raw analytical .pdf files to the .xls files Where a result entry was given as ‘ND’ in the .pdf, a ‘<’ symbol was used. Where a reporting limit (RL) was listed as ‘n/a,’ the result entry in the spreadsheet was set at the RL[42].

Chain-of-custody information is provided clearly in the raw analytical data .pdf files, including analyte name, sample numbers, and laboratory-assigned numbers. Chemical Abstract Service numbers were provided by the respective analytical laboratory.

The nomenclature of the sample identification (ID) was consistent for every set of chemicals, but differed between the CT and HS samples. Both CT and HS sample IDs contain a unique survey number followed by additional identifiers indicating the location or type of sample on the sampling device. Descriptions of these nomenclatures are discussed below.

For CT samples, each of the six sampling events or “dives” had a unique survey number (e.g., 18-00131), consisting of the two-digit year (18) followed by a five-digit identifier of the dive. Each dive consisted of two unique sample media that were identified as “1” or “2.” The CT sampling rig is comprised of a 12-sorbent-tube sample head on the inlet side (IN) of the cartridge housing and another 12-sorbent-tube sample head on the effluent side (EF or EFF) of the cartridge housing. Therefore, either ‘IN’ or ‘EFF’ identifiers indicated at which sample head location each tube was located. Letters A through L identified each of the sample media lines on each of the IN or EFF 12-tube sample heads.

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[42] Respirator cartridge testing results from use of the CT rig have historically used detection limit (DL) rather than reporting limit (RL) for three of the 12 analytical methods including volatile organic compound (VOC; Carbotrap 300 | EPA TO-17 Mod method), semi-volatile organic analyte (SVOA; Carbotrap 150 | EPA TO-17 Mod method), and Furans (Tenax TA | EPA TO-17 Mod method). For this comparison test, all HS and CT analytical data were reported to the RL)

'BLA'followed by a 1 or 2 indicated a blank measurement obtained for the first (1) or second (2) sample media tested for each dive. Blank indicates sorbent tubes that have not had any vapor stream passed through them. In addition, baseline 'BL' measurements were obtained for ambient air (fresh air versus tank vapor) running through the test system from the inlet (IN) or effluent (EF) locations before initiation of tank vapor testing.

The sample IDs for the CT rig embed the information given above. For example, sample ID 18-00131-1-CC-IN-A corresponds to a particular survey (18-00131) identified as the first dive with the first analyte (-1), which was methanol, on the cartridge test rig (CC), (IN) sample bundle, and the first (A) sample (1).

For HS samples, each of the 12 sorbent sampling media had a unique survey number (e.g., 18-002031), consisting of the two-digit year (18) followed by a five-digit identifier of the sample media. The HS sampling system is comprised of two-12-sorbent tube sample heads with two tubes designated A and B on each of the 12 sample lines. The 'B' tube provides a backup to the first 'A' tube to indicate potential breakthrough or overloading of the chemical on the first A tube. Numbers 001 through 012 identified each of the sample media lines on each 12-tube sample head.

'BL' indicated a blank measurement obtained for either the 'A' or 'B' tube for a specific survey. Blank indicates sorbent tubes that have not had any vapor stream passed through them.

The sample IDs for the HS sampler embed the information given above. For example, sample ID 18-00203-1-001A corresponds to a particular survey (18-00203-1) identified as the first dive with the first analyte methanol on the HS sampling system, (001) sample line, and the primary (A) sample tube. For each 001A there corresponded an 001B sample representing the backup tube.

The target slip stream flow rate from the tank riser through the CT rig was 25-30 L/min for the comparison test. The target sampling flow rates through the sorption tubes ranged between 50 and 900 mL/min for different chemicals that were being collected. WRPS provided these flow rates and conversion to total sample volumes for both the CT and HS samples in an Excel file 'Headspace Comparison Volumes.xlsx.' The volumes for each sample are documented in Section A.3.

The raw analytical data for chemicals in each analyte category are summarized in Section C.4. Some analytes are measured using more than one method (primary and secondary). A crosswalk of COPC to analyte category, media, and analytical method for both primary and secondary methods is provided in Table A.1. In general, the primary method was used for data analysis sample method comparison except in cases for which the secondary method provides improved quantitation for the specific COPC and its concentration range during a specific test.

Table A.1. Crosswalk of COPCs with Primary and Secondary Analyte Category, Media, and Analytical Method

COPC#	Analyte Name	Primary Analysis Method (Analyte Category ǀ Media ǀ Method)	Secondary Analysis Method (Analyte Category ǀ Media ǀ Method)
1	Ammonia	Ammonia ǀ Anasorb 747 ǀ OSHA-ID-188	
2	Nitrous Oxide	Not Measured	
3	Mercury	Mercury ǀ Anasorb C300 ǀ NIOSH-6009	
4	1,3-Butadiene	1,3-butadiene ǀ Charcoal ǀ NIOSH 1024	
5	Benzene	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
6	Biphenyl	SVOC ǀ Carbotrap 150 ǀ EPA TO-17 Mod	
7	1-Butanol	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
8	Methanol	Methanol ǀ Silica Gel ǀ NIOSH 2000	
9	2-Hexanone	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
10	3-Methyl-3-butene-2-one	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
11	4-Methyl-2-hexanone	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	

12	6-Methyl-2-heptanone	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
13	3-Buten-2-one	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
14	Formaldehyde	Aldehyde ǀ DNPH Treated Silica Gel ǀ EPA TO-11A	
15	Acetaldehyde	Aldehyde ǀ DNPH Treated Silica Gel ǀ EPA TO-11A	
16	Butanal/Butyraldehyde	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	Aldehyde ǀ DNPH Treated Silica Gel ǀ EPA TO-11A
17	2-Methyl-2-butenal	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
18	2-Ethyl-hex-2-enal	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
New	2-Propenal/Acrolein	Aldehyde ǀ DNPH Treated Silica Gel ǀ EPA TO-11A	
19	Furan[b]	VOC ǀ Carbotrap 300ǀ EPA TO-17 Mod	Furans ǀ Tenax TA ǀ EPA TO-17 Mod
20	2,3-Dihydrofuran	Furans ǀ Tenax TA ǀ EPA TO-17 Mod	
21	2,5-Dihydrofuran[b]	VOC ǀ Carbotrap 300ǀ EPA TO-17 Mod	Furans ǀ Tenax TA ǀ EPA TO-17 Mod
22	2-Methylfuran[b]	VOC ǀ Carbotrap 300ǀ EPA TO-17 Mod	Furans ǀ Tenax TA ǀ EPA TO-17 Mod
23	2,5-Dimethylfuran	Furans ǀ Tenax TA ǀ EPA TO-17 Mod	
24	2-Ethyl-5-methylfuran	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
25	4-(1-Methylpropyl)-2,3-dihydrofuran	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
26	3-(1,1-Dimethylethyl)-2,3-dihydrofuran	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
27	2-Pentylfuran	Furans ǀ Tenax TA ǀ EPA TO-17 Mod	
28	2-Heptylfuran	Furans ǀ Tenax TA ǀ EPA TO-17 Mod	
29	2-Propylfuran	Furans ǀ Tenax TA ǀ EPA TO-17 Mod	
30	2-Octylfuran	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
31	2-(3-Oxo-3-phenylprop-1-enyl)furan	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
32	2-(2-Methyl-6-oxoheptyl) furan	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
33	Diethylphthalate	SVOC ǀ Carbotrap 150 ǀ EPA TO-17 Mod	
34	Acetonitrile	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	Acetonitrile ǀ Charcoal ǀ NIOSH 1606
35	Propanenitrile	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
36	Butanenitrile	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
37	Pentanenitrile	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
38	Hexanenitrile	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
39	Heptanenitrile	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
40	2-Methylene butanenitrile	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
41	2,4-Pentadienenitrile	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
42	Ethylamine	Ethylamine ǀ XAD-7 ǀ OSHA-ID-34,36,40,41	
43	N-Nitrosodimethylamine	Nitrosamines ǀ Thermasorb/N ǀ NIOSH-2522 Mod	
44	N-Nitrosodiethylamine	Nitrosamines ǀ Thermasorb/N ǀ NIOSH-2522 Mod	
45	N-Nitrosomethylethylamine	Nitrosamines ǀ Thermasorb/N ǀ NIOSH-2522 Mod	
46	N-Nitrosomorpholine	Nitrosamines ǀ Thermasorb/N ǀ NIOSH-2522 Mod	
47	Tributyl phosphate	SVOC ǀ Carbotrap 150 ǀ EPA TO-17 Mod	
48	Dibutyl butylphosphonate	SVOC ǀ Carbotrap 150 ǀ EPA TO-17 Mod	
49	Chlorinated Biphenyls	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
50	2-Fluoropropene	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	

51	Pyridine	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	Pyridines ǀ Coconut Shell Charcoal ǀ NIOSH-1613
52	2,4-Dimethylpyridine	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	Pyridines ǀ Coconut Shell Charcoal ǀ NIOSH-1613
53	Methyl nitrite	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
54	Butyl nitrite	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
55	Butyl nitrate	VOC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
56	1,4-Butanediol, dinitrate	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
57	2-Nitro-2-methylpropane	VOCTIC ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
58	1,2,3-Propanetriol, 1,3-dinitrate	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
59	Methyl Isocyanate	VOCTIC[a] ǀ Carbotrap 300 ǀ EPA TO-17 Mod	
New	Dimethyl Mercury	Not Measured	

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[a] A Tentatively Identified Compound (TIC) indicates that a mass spectrometry “peak” not associated with calibrated compounds has been tentatively assigned to a compound based on an adequate match to the analytical methods reference library. Reference standards for the compound are not available to accurately quantify, assign an analytical DL, or definitively confirm the identity of the TIC. TICs are reported when the peak area is sufficiently large, estimated as ≥5 nanograms of TIC mass, and other analytical criteria are met. For the respirator cartridge testing, this mass of TIC represents an approximate concentration of <1.0 ppb, based on the average of all TICs in the COPC list. TIC compounds are measured through both the Carbotrap 300: EPA TO-17 and Carbotrap 150: EPA TO-17 modified methods. A few compounds are measured in the TIC analysis and another analytical technique. In these cases, the TIC analysis results were not retained because they are qualitative only and inferior to the other calibrated method.

[b] Furan, 2,5-dihydrofuran, and 2-methylfuran are quantified using the secondary method, as the primary method was determined to perform inadequately for these lower-boiling point furan compounds.

A.2 Miscellaneous Notes

All analytical flags assigned by each analytical laboratory are provided in Appendix B. Sample lines occasionally experienced flow control issues, and these instances are distinguished in Section A.3 of Volume 2 as yellow-highlighted cells indicating a no flow condition, and/or documented in Appendix B with a quality flag of ‘S*’ associated with the impacted data point.

A.3 Experimental Parameters – Flow Rates

See PNNL-28801, Volume 2.

A.4 Raw Data

See PNNL-28801, Volume 2.

Appendix B

Data Reduction Steps

Appendix B

Data Reduction Steps

B.1 Test Data Processing

1. Chemicals in the current Chemicals of Potential Concern (COPC) list as well as 53 non-COPC organic analytes were included in the calculated data. Nitrous oxide and dimethyl mercury were not measured in the study. Any missing COPCs were analyzed as “Tentatively Identified Compounds,” and not detected unless shown.

2. The COPCs are ordered from 1 to 61 consistent with their ranking in the Tank Operations Contractor COPC list[43], while non-COPCs were numbered from 1 to 53 alphanumerically as reported by the analytical laboratory in volatile organic analyte (VOA) and semi-volatile organic analyte analysis reports. Three separate sets of sampling tubes – Cartridge Test rig, Headspace Tube A, and Headspace Tube B, each with up to twelve replicate samples.

3. Analyte concentrations were calculated as parts per million (ppm) using their molecular weights and corresponding reported standard volume using the following equation:

   $$C = 24.14 \frac{r}{M\,V}$$

   where C is the concentration of analyte in ppmv; r is the analytical result with units of µg/sample; V is the volume of sample gas passed through the given media tube in liters; M is the species molecular weight in g/mol.

4. The reported volume measurements in Appendix A were made via DryCal devices placed downstream of each sample media tubes on each individual sampling line. This allowed for precise volume measurements through each of the tubes. The DryCal devices were set to convert the measured values to standard flow conditions. The standard flow conditions are user-defined at 70°F and 1 atm pressure.

5. The analytical detection limit (DL)—or reporting limit (RL)—for every analyte was obtained from the analytical data. Here, the maximum DL|RL is reported for each set of replicate sampling tubes, corresponding to the highest RL value of any of the twelve replicates. Because the flow rates and corresponding volumes for each sample tube vary, the calculated RL concentrations were different for each below reporting limit data point, even though some of the results are less than maximum DL|RL reported. All italicized and underlined values reported in Tables B.1 and B.2 indicate that the original readings were less than the RL.

- For ammonia and mercury, only the results obtained from the total vapors of ammonia and mercury were used.

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[43] Memorandum from K.J. Way to file, September 21, 2017. “Tank Operations Contractor – Chemicals of Potential Concern Rev. 1.” WRPS-1604188.1, Washington River Protection Solutions, Richland, Washington (unpublished).

- For furan, 2,5-dihydrofuran, and 2-methylfuran, results from the volatile organic compound (VOC) (or VOA) category were used rather than results from the furan analyte category. For acetonitrile, results from the VOC category were used. For butanal, results from the VOC category instead of the aldehydes category were used. For 2,4-dimethylpyridine and pyridine, results from the VOC category were used.

- Analytical results frequently have data qualifier flags documented for specific sample analyses. Depending on the data qualifier, specific data may be considered for deletion or removal from the analysis, or results described with appropriate clarifying language to indicate whether there are possible limitations to the data. Flags identified below were found to be associated with at least one of the COPC compounds analyzed through this effort. Here, key qualifier codes are given, along with their definitions and how they are being handled with the -testing analysis. The list does not include all flags that the analytical team may assign, but it does include the flags associated with the data set compiled within this report. In addition, specific samples were identified at the time of sampling as potentially suspect by the test operator due to potential sample volume or sample tube media issues. These samples have been flagged with a project-specific qualifier code in the data set.

Action	Flag	Flag Description
Retain (Result is treated in the analysis as a valid data point)	J	The "J" flag is applied to results that are considered estimates. Some examples of when a "J" flag are applied include (but are not limited to): • Results with concentrations greater than or equal to the method DL but less than the RL. When results are reported based on the RL, the "J" is removed from the reported data. • Unknown constituents—Tentatively Identified Compounds (TICs) or positively identified compounds.
	E	The "E" flag is applied to each analyte that exceeded the calibration range of the instrument.
	U	The "U" flag is applied to analytes that were analyzed for, but were not detected, or were detected below the method DL. If results are reported based on RL, this flag is removed from the reported data.
	N	The "N" flag is applied to compounds identified based on mass spectrometry (MS) library search. TICs (or positively identified compounds) are not target compounds, and are only an estimate and not quantitative.
	T	The "T" flag is applied to TIC compounds identified by MS library search, or identified as unknowns after an MS library search. The results are only estimates.
	H	The "H" flag is applied to all analytes in a sample where the holding time from the end of sampling to the beginning of sample analysis has been exceeded.
	D	The "D" flag is applied to all analytes in a sample that were diluted prior to analysis.
Retain/Evaluate (Result is treated in the analysis as a valid data point, but evaluated on a case-by-case basis to determine whether clarification is needed in the analysis report to document the uncertainty or potential limitations of the data)	L	The "L" flag is applied to analyte results (both detected and not detected) within a sample batch that included a low level standard with a percent recovery for that analyte that was outside the analytical method specified range.
	Y	The "Y" flag is a user-defined flag and is applied to results that require written descriptions or qualifying comments. This flag is used by the chemist, project coordinator or other technical authority to identify data that is questionable or may be inaccurate because of interferences, sampling problems, sample collection media (e.g., tubes or summa canisters) certification failures, or instrumentation limitations.

<table>
<tr><th>Action</th><th>Flag</th><th>Flag Description</th></tr>
<tr><td></td><td>S*</td><td>The “S*” flag is a project-specific user-defined flag applied to samples that were identified by the test operator as suspect due to potentially low sample volume/flow rate issues, or other sample tube media problems</td></tr>
<tr><td></td><td>a</td><td>The “a” flag is applied to all results (both detected and not detected) within a sample batch that included a laboratory control sample (LCS) with a percent recovery for that analyte that was outside the customer or analytical method specified range. The “a” flag is not applied based on laboratory control sample duplicates (LCSD) results.</td></tr>
<tr><td></td><td>B</td><td>The "B" flag is applied to each analyte in a batch where that analyte concentration is greater than or equal to the method detection limit (MDL) (or in the case of thermal desorption unit gas chromatography-MS analysis, greater than or equal to 2× the MDL or greater than or equal to the RL, whichever is less) in the preparation blank/method blank and is greater than or equal to the RL in the sample. If sample results are reported based on the MDL, then all analyte results greater than or equal to the MDL would be flagged with a “B,” provided that analyte was detected (≥MDL) in the associated blank. Samples that are “B” flagged include the blank, all field samples with the analyte present, LCS, LCSD, and low level standards.</td></tr>
<tr><td></td><td>c</td><td>The “c” flag is applied to analyte results (both detected and not detected) within a sample batch where the relative percent difference between duplicate samples (subsample aliquots carried through the sample preparation and analysis), LCSDs or matrix spike duplicates was greater than the customer or analytical method defined range. For field samples (duplicate or matrix spike duplicate) this flag is applied only to the samples that were duplicated or spiked. For LCSD relative percent difference failure, all samples within the batch are flagged.</td></tr>
<tr><td></td><td>Q</td><td>The “Q” flag is applied to results that are considered to be qualitative based on instrument and analyte specific calibration or calibration verification issues. The “Q” flag is applied to all samples contained within the analytical batch (i.e., field samples, LCS, LCSD, low-level standard, and method/preparation blank).
<table>
<tr><th></th><th><MDL</th><th>MDL≤X<RL</th><th>≥RL</th></tr>
<tr><td>% Relative standard deviation failure</td><td>Q</td><td>Q</td><td>Q</td></tr>
<tr><td>Initial calibration verification failure</td><td>Q</td><td>Q</td><td>Q</td></tr>
<tr><td>High continuing calibration verification sample/%D</td><td></td><td>Q[1]</td><td>Q</td></tr>
<tr><td>Low continuing calibration verification sample/%D</td><td>Q</td><td>Q</td><td>Q</td></tr>
<tr><td>High internal standard recovery</td><td>Q</td><td>Q</td><td>Q</td></tr>
</table></td></tr>
</table>

<table>
<tr><th>Action</th><th>Flag</th><th>Flag Description</th></tr>
<tr><td></td><td></td><td><table><tr><td>Low internal standard recovery</td><td>Q</td><td>Q</td><td>Q</td></tr></table>1. Q flag is not required when results are reported to the RL, rather than the MDL.</td></tr>
<tr><td>Delete (Result is seriously suspect and should be screened out and not reported)</td><td>N/A</td><td></td></tr>
</table>

Tables B.1 and B.2 show the calculated concentrations for each of the COPC and non-COPC measurements, respectively, conducted in this study. Italicized and underlined values reflect measurements that were below their RL. Blanks indicate that no analytical result was available (e.g., broken tube). The calculated data is organized by replicate sample sets: CT, HS Series A, and HS Series B. The maximum RL based on all replicates for a given data set is provided as DL|RL in each table. Quality flags reported in the analytical results for each replicate sample are also listed.

Table B.1. Calculated Data – COPCs

Analyte #			1	3	4	5	6	7	8	9	11	13	14	15	16	19	20
Analyte		Replicate Sample Order	Ammonia	Mercury	1,3-Butadiene	Benzene	Biphenyl	1-Butanol	Methanol	2-Hexanone	4-Methyl-2-hexanone	3-Buten-2-one	Formaldehyde	Acetaldehyde	Butanal/ Butyraldehyde	2-Propenal/Acrolein	Furan
Cartridge Test Rig	Concentration (ppm)[1]	1	2.66E+02	*4.05E-04*	*3.70E-02*	1.53E-03	*4.46E-04*	*2.58E-03*	*5.06E-01*	1.27E-03	*8.37E-04*	4.66E-03	*1.55E-03*	8.86E-02	*1.33E-03*	*8.29E-04*	*1.40E-03*
		2	3.11E+02	*4.05E-04*	*3.63E-02*	3.01E-03	*4.47E-04*	*2.62E-03*	*4.88E-01*	7.28E-03	*8.51E-04*	5.66E-03	2.10E-03	9.63E-02	*1.35E-03*	*8.40E-04*	2.86E-03
		3	2.77E+02	*3.99E-04*	*3.59E-02*	3.22E-03	*4.43E-04*	*2.54E-03*	*4.74E-01*	6.51E-03	*8.25E-04*	6.05E-03	1.83E-03	9.02E-02	*1.31E-03*	*8.43E-04*	1.85E-03
		4	3.12E+02	*4.04E-04*	*3.64E-02*	1.78E-03	*4.30E-04*	*2.65E-03*	*4.90E-01*	2.20E-03	*8.59E-04*	4.08E-03	2.65E-03	9.45E-02	*1.36E-03*	*8.44E-04*	*1.44E-03*
		5	2.69E+02	*3.89E-04*	*3.63E-02*	2.20E-03	*3.55E-04*	*2.23E-03*	*4.16E-01*	3.64E-03	*7.24E-04*	2.16E-03	2.02E-03	9.11E-02	*1.15E-03*	*8.33E-04*	2.12E-03
		6	2.79E+02	*4.05E-04*		1.20E-03	*4.26E-04*	*2.52E-03*	*5.13E-01*	1.40E-03	*8.19E-04*	3.89E-03	*1.51E-03*	3.72E-02	*1.30E-03*	*8.11E-04*	*1.37E-03*
		7	3.01E+02	*4.01E-04*	*3.63E-02*	3.42E-03	*4.62E-04*	*2.55E-03*	5.02E-01	6.99E-03	*8.26E-04*	7.18E-03	*1.55E-03*	9.06E-02	*1.31E-03*	*8.28E-04*	1.85E-03
		8	2.68E+02	*4.07E-04*	*3.62E-02*	2.24E-03	*4.86E-04*	*2.58E-03*	*5.10E-01*	3.34E-03	*8.36E-04*	6.59E-03	2.66E-03	8.52E-02	*1.32E-03*	*8.37E-04*	*1.40E-03*
		9	3.11E+02	*4.01E-04*	*3.67E-02*	3.02E-03	*4.73E-04*	*2.55E-03*	*5.12E-01*	5.74E-03	*8.28E-04*	7.19E-03	1.69E-03	9.62E-02	2.95E-03	*8.40E-04*	1.39E-03
		10	3.13E+02	*4.06E-04*	*3.71E-02*	1.28E-03	*4.72E-04*	*2.32E-03*	*4.43E-01*	1.50E-03	*7.52E-04*	2.45E-03	1.93E-03	9.50E-02	*1.19E-03*	*8.48E-04*	*1.26E-03*
		11	3.14E+02	*4.08E-04*	*3.61E-02*	2.91E-03	*4.59E-04*	*2.37E-03*	4.81E-01	5.78E-03	*7.70E-04*	6.58E-03	*1.56E-03*	9.77E-02	*1.22E-03*	*8.35E-04*	*1.29E-03*
		12	3.21E+02	*4.05E-04*	*3.66E-02*	2.59E-03	*4.58E-04*	*2.52E-03*	*4.71E-01*	4.65E-03	*8.17E-04*	7.87E-03	*1.55E-03*	1.14E-01	*1.29E-03*	*8.32E-04*	1.83E-03
	DL|RL		6.99E-01	4.08E-04	3.71E-02	1.36E-04	4.86E-04	2.65E-03	5.13E-01	8.97E-05	8.59E-04	1.75E-04	1.56E-03	1.08E-03	1.36E-03	8.48E-04	1.44E-03
	Quality Flags	1						LQYa							QY		
		2						LQYa							QY		
		3						LQYa							QY		
		4						LQYa							QY		
		5						LQYa							QY		
		6						LQYa							QY		
		7						LQYa							QY		
		8						LQYa							QY		
		9						LQYa							QY		
		10						LQYa							QY		
		11						LQYa							QY		
		12						LQYa							QY		
Headspace Series A	Concentration (ppm)[1]	1	3.08E+02	*4.03E-04*	*3.75E-02*	2.53E-03	*5.29E-04*	*2.67E-03*	5.93E-01	9.05E-03	*8.66E-04*	6.35E-03			*1.37E-03*		2.42E-03
		2	3.37E+02	*3.98E-04*	*1.88E-02*	2.70E-03	*5.03E-04*	*2.63E-03*	6.60E-01	9.73E-03	*8.54E-04*	7.30E-03	5.09E-03	8.55E-02	*1.35E-03*	*1.05E-03*	2.27E-03
		3	3.15E+02	*3.86E-04*	*3.98E-02*	2.50E-03	*5.63E-04*	*2.63E-03*	6.92E-01	7.71E-03	*8.54E-04*	6.37E-03	4.43E-03	8.56E-02	*1.35E-03*	*9.89E-04*	1.43E-03
		4	3.32E+02	5.11E-04	*1.99E-02*	1.51E-03	*5.51E-04*	*2.72E-03*	5.25E-01	4.62E-03	*8.84E-04*	5.40E-03	4.88E-03	8.70E-02	*1.40E-03*	*1.01E-03*	1.73E-03
		5	3.15E+02	*4.21E-04*	*3.99E-02*	2.65E-03	*5.24E-04*	*2.68E-03*	1.12E+00	9.10E-03	*8.71E-04*	8.04E-03			*1.38E-03*		1.58E-03
		6	6.86E+01	*3.78E-04*	*2.00E-02*	2.35E-03	*5.11E-04*	*2.48E-03*	8.70E-01	7.64E-03	*8.04E-04*	8.52E-03	*1.36E-03*	2.23E-02	*1.27E-03*	*7.29E-04*	1.57E-03
		7	3.21E+02	*3.95E-04*	*3.95E-02*	3.06E-03	*4.70E-04*	*2.67E-03*	8.24E-01	1.07E-02	9.38E-04	*1.41E-03*	4.42E-03	7.79E-02	*1.37E-03*	*9.87E-04*	2.30E-03
		8	3.24E+02	*4.01E-04*	*1.97E-02*	2.21E-03	*4.84E-04*	*2.54E-03*	5.46E-01	7.84E-03	*8.25E-04*	*1.34E-03*	4.09E-03	7.90E-02	*1.31E-03*	*9.13E-04*	2.65E-03
		9	2.71E+02	*4.23E-04*		1.84E-03	*4.98E-04*	*2.74E-03*	1.02E+00	5.75E-03	*8.90E-04*	*1.45E-03*	3.75E-03	8.44E-02	*1.41E-03*	*1.01E-03*	1.62E-03
		10	3.30E+02	*3.93E-04*		2.50E-03	*5.44E-04*	*2.75E-03*	4.84E-01	7.62E-03	*8.91E-04*	*1.45E-03*	*1.69E-03*	2.99E-02	*1.41E-03*	*9.04E-04*	1.87E-03
		11	3.23E+02	*4.22E-04*	*3.87E-02*	1.95E-03	*4.77E-04*	*2.75E-03*	6.92E-01	7.20E-03	*8.91E-04*	*1.45E-03*	4.34E-03	7.15E-02	*1.41E-03*	*9.68E-04*	2.24E-03
		12	3.06E+02	*3.79E-04*	*1.93E-02*	1.45E-03	*4.71E-04*	*2.63E-03*	*4.99E-01*	4.21E-03	*8.52E-04*	*1.39E-03*	*1.66E-03*	4.53E-03	*1.35E-03*	*8.90E-04*	*1.43E-03*
	DL|RL		7.39E-01	4.23E-04	3.99E-02	1.41E-04	5.63E-04	2.75E-03	4.99E-01	9.32E-05	8.91E-04	1.45E-03	1.69E-03	1.34E-03	1.41E-03	1.05E-03	1.43E-03
	Quality Flags	1						LQYa									
		2						LQYa							QY		
		3						LQYa							QY		
		4						LQYa							QY		
		5						LQYa							QY		
		6						LQYa							QY		
		7						L									
		8						L									
		9						L									
		10						L									
		11		a				L									
		12		a				L									
Headspace Series B	Concentration (ppm)[1]	1	*6.55E-01*	*4.03E-04*	*3.95E-02*	*1.27E-03*	*5.29E-04*	*2.67E-03*	*4.94E-01*	*9.88E-04*	*8.66E-04*	*1.41E-03*	*1.75E-03*	*1.19E-03*	*1.37E-03*	*9.37E-04*	*1.45E-03*
		2	*7.33E-01*	*3.98E-04*	*1.98E-02*	*1.25E-03*	*5.03E-04*	*2.63E-03*	*5.07E-01*	*9.73E-04*	*8.54E-04*	*1.39E-03*	*1.96E-03*	*1.34E-03*	*1.35E-03*	*1.05E-03*	*1.43E-03*
		3	*6.95E-01*	*3.86E-04*	*3.76E-02*	*1.25E-03*	*5.63E-04*	*2.63E-03*	*4.94E-01*	*9.73E-04*	*8.54E-04*	*1.39E-03*	*1.85E-03*	*1.26E-03*	*1.35E-03*	*9.89E-04*	*1.43E-03*
		4	*7.15E-01*	*4.09E-04*	*1.88E-02*	*1.29E-03*	*5.51E-04*	*2.72E-03*	*4.56E-01*	*1.01E-03*	*8.84E-04*	*1.44E-03*	*1.88E-03*	*1.28E-03*	*1.40E-03*	*1.01E-03*	*1.48E-03*
		5	*7.28E-01*	*4.21E-04*	*4.03E-02*	*1.27E-03*	*5.24E-04*	*2.68E-03*	*4.66E-01*	*9.93E-04*	*8.71E-04*	*1.42E-03*			*1.38E-03*		*1.46E-03*
		6	*6.79E-01*	*3.78E-04*	*2.02E-02*	*1.18E-03*	*5.11E-04*	*2.48E-03*	*5.12E-01*	*9.17E-04*	*8.04E-04*	*1.31E-03*	*1.36E-03*	*9.27E-04*	*1.27E-03*	*7.29E-04*	*1.35E-03*
		7	*6.48E-01*	*3.95E-04*	*2.03E-02*	*1.27E-03*	*4.70E-04*	*2.67E-03*	*4.71E-01*	*9.87E-04*	*8.66E-04*	*1.41E-03*	*1.84E-03*	*1.26E-03*	*1.37E-03*	*9.87E-04*	*1.45E-03*
		8	*7.02E-01*	*4.01E-04*	*4.06E-02*	*1.21E-03*	*4.84E-04*	*2.54E-03*	*4.55E-01*	*9.41E-04*	*8.25E-04*	*1.34E-03*	*1.70E-03*	*1.16E-03*	*1.31E-03*	*9.13E-04*	*1.38E-03*
		9	*7.24E-01*	*4.23E-04*	*3.97E-02*	*1.30E-03*	*4.98E-04*	*2.74E-03*	*4.62E-01*	*1.01E-03*	*8.90E-04*	*1.45E-03*	*1.88E-03*	*1.28E-03*	*1.41E-03*	*1.01E-03*	*1.49E-03*
		10	*7.39E-01*	*3.93E-04*	*1.99E-02*	*1.30E-03*	*5.44E-04*	*2.75E-03*	*4.61E-01*	*1.02E-03*	*8.91E-04*	*1.45E-03*	*1.69E-03*	*1.15E-03*	*1.41E-03*	*9.04E-04*	*1.49E-03*
		11	*7.16E-01*	*4.22E-04*	*3.92E-02*	*1.30E-03*	*4.77E-04*	*2.75E-03*	*4.77E-01*	*1.02E-03*	*8.91E-04*	*1.45E-03*	*1.81E-03*	*1.23E-03*	*1.41E-03*	*9.68E-04*	*1.50E-03*
		12	*7.05E-01*	*3.79E-04*	*1.96E-02*	*1.25E-03*	*4.71E-04*	*2.63E-03*	*4.99E-01*	*9.72E-04*	*8.52E-04*	*1.39E-03*	*1.66E-03*	*1.13E-03*	*1.35E-03*	*8.90E-04*	*1.43E-03*
	DL|RL		7.39E-01	4.23E-04	4.06E-02	1.30E-03	5.63E-04	2.75E-03	5.12E-01	1.02E-03	8.91E-04	1.45E-03	1.96E-03	1.34E-03	1.41E-03	1.05E-03	1.50E-03
	Quality Flags	1						LQYa							QY		
		2						LQYa							QY		
		3						LQYa							QY		
		4						LQYa							QY		
		5						LQYa							QY		
		6						L									
		7						L									
		8						L									
		9						L									
		10						L									
		11		a				L									
		12		a				L									

[1] Values italicized and underlined correspond to a value flagged as "<DL|RL".

Table B.1. Calculated Data (continued)

Analyte #			21	22	23	24	28	29	30	34	35	36	37	38	39	43
Analyte		Replicate Sample Order	2,3-Dihydrofuran	2,5-Dihydrofuran	2-Methylfuran	2,5-Dimethylfuran	2-Pentylfuran	2-Heptylfuran	2-Propylfuran	Diethylphthalate	Acetonitrile	Propanenitrile	Butanenitrile	Pentanenitrile	Hexanenitrile	Ethylamine
Cartridge Test Rig	Concentration (ppm)[1]	1	*3.35E-04*	*1.36E-03*	*1.16E-03*	*2.44E-04*	*1.70E-04*	*1.41E-04*	*2.13E-04*	*3.10E-04*	5.24E-02	2.31E-03	3.34E-03	*1.15E-03*	*9.84E-04*	*9.32E-03*
		2	*3.46E-04*	*1.39E-03*	*1.18E-03*	*2.52E-04*	*1.76E-04*	*1.46E-04*	*2.20E-04*	1.08E-03	1.07E-01	6.62E-03	1.29E-02	2.24E-03	*1.00E-03*	*9.91E-03*
		3	*3.21E-04*	*1.34E-03*	*1.15E-03*	*2.34E-04*	*1.63E-04*	*1.35E-04*	*2.04E-04*	*3.07E-04*	7.65E-02	6.70E-03	1.25E-02	1.98E-03	*9.70E-04*	*9.03E-03*
		4	*3.32E-04*	*1.40E-03*	*1.19E-03*	*2.42E-04*	*1.69E-04*	*1.40E-04*	*2.12E-04*	*2.98E-04*	4.18E-02	2.97E-03	4.73E-03	*1.18E-03*	*1.01E-03*	*4.16E-03*
		5	*3.27E-04*	*1.18E-03*	*1.01E-03*	*2.38E-04*	*1.66E-04*	*1.38E-04*	*2.08E-04*	*2.46E-04*	7.21E-02	3.00E-03	6.68E-03	1.33E-03	*8.50E-04*	*4.36E-03*
		6	*3.17E-04*	*1.33E-03*	*1.14E-03*	*2.31E-04*	*1.61E-04*	*1.33E-04*	*2.01E-04*	*2.95E-04*	6.46E-02	*1.70E-03*	2.93E-03	*1.13E-03*	*9.63E-04*	*4.36E-03*
		7	*3.38E-04*	*1.35E-03*	*1.15E-03*	*2.47E-04*	*1.71E-04*	*1.43E-04*	*2.15E-04*	*3.20E-04*	7.28E-02	6.71E-03	1.37E-02	2.17E-03	*9.71E-04*	*9.44E-03*
		8	*3.57E-04*	*1.36E-03*	*1.16E-03*	*2.60E-04*	*1.81E-04*	*1.50E-04*	*2.27E-04*	*3.37E-04*	3.68E-02	3.76E-03	*1.38E-03*	*1.15E-03*	*9.83E-04*	*9.09E-03*
		9	*3.31E-04*	*1.35E-03*	*1.15E-03*	*2.41E-04*	*1.68E-04*	*1.39E-04*	*2.10E-04*	*3.28E-04*	4.99E-02	5.72E-03	*1.37E-03*	1.89E-03	*9.73E-04*	*9.79E-03*
		10	*3.33E-04*	*1.23E-03*	*1.05E-03*	*2.43E-04*	*1.69E-04*	*1.40E-04*	*2.12E-04*	*3.27E-04*	8.37E-02	1.69E-03	*1.24E-03*	*1.03E-03*	*8.84E-04*	*4.41E-03*
		11	*3.33E-04*	*1.25E-03*	*1.07E-03*	*2.43E-04*	*1.69E-04*	*1.40E-04*	*2.12E-04*	*3.18E-04*	5.53E-02	5.59E-03	1.06E-02	1.85E-03	*9.05E-04*	*4.25E-03*
		12	*3.24E-04*	*1.33E-03*	*1.14E-03*	*2.36E-04*	*1.64E-04*	*1.37E-04*	*2.06E-04*	*3.18E-04*	5.87E-02	5.08E-03	*1.35E-03*	1.50E-03	*9.60E-04*	*4.46E-03*
	DL|RL		3.57E-04	1.40E-03	1.19E-03	2.60E-04	1.81E-04	1.50E-04	2.27E-04	3.37E-04	2.39E-03	1.70E-03	1.38E-03	1.18E-03	1.01E-03	9.91E-03
	Quality Flags	1														
		2									E					
		3									E					
		4														
		5									E					
		6														
		7														
		8														
		9														
		10									E					
		11														
		12														
Headspace Series A	Concentration (ppm)[1]	1	*3.58E-04*	*1.41E-03*	*1.20E-03*	*2.61E-04*	*1.82E-04*	*1.51E-04*	*2.28E-04*	*3.67E-04*	1.02E-01	3.89E-03	1.91E-02	2.38E-03	1.44E-03	*4.60E-03*
		2	*3.59E-04*	*1.39E-03*	*1.19E-03*	*2.62E-04*	*1.82E-04*	*1.52E-04*	*2.29E-04*	*3.49E-04*	6.73E-02	5.46E-03	1.88E-02	2.35E-03	1.25E-03	*4.53E-03*
		3	*3.56E-04*	*1.39E-03*	*1.19E-03*	*2.59E-04*	*1.80E-04*	*1.50E-04*	*2.26E-04*	*3.90E-04*	5.74E-02	5.16E-03	1.53E-02	2.05E-03	*1.00E-03*	*4.71E-03*
		4	*3.49E-04*	*1.44E-03*	*1.23E-03*	*2.54E-04*	*1.77E-04*	*1.47E-04*	*2.22E-04*	*3.82E-04*	9.43E-02	2.14E-03	8.64E-03	1.32E-03	*1.04E-03*	*4.65E-03*
		5	*3.51E-04*	*1.42E-03*	*1.21E-03*	*2.56E-04*	*1.78E-04*	*1.48E-04*	*2.24E-04*	*3.64E-04*	6.66E-02	5.72E-03	1.92E-02	2.29E-03	1.19E-03	*4.56E-03*
		6	*3.45E-04*	*1.31E-03*	*1.12E-03*	*2.52E-04*	*1.75E-04*	*1.46E-04*	*2.20E-04*	*3.55E-04*	1.31E-01	4.72E-03	1.55E-02	2.03E-03	1.10E-03	*4.65E-03*
		7	*3.49E-04*	*1.41E-03*	*1.20E-03*	*2.54E-04*	*1.77E-04*	*1.47E-04*	*2.22E-04*	*3.26E-04*	9.83E-02	6.43E-03	*1.43E-03*	2.68E-03	1.44E-03	*4.64E-03*
		8	*3.41E-04*	*1.34E-03*	*1.15E-03*	*2.49E-04*	*1.73E-04*	*1.44E-04*	*2.17E-04*	*3.36E-04*	1.28E-01	3.56E-03	*1.36E-03*	2.27E-03	1.37E-03	*4.48E-03*
		9	*3.32E-04*	*1.45E-03*	*1.24E-03*	*2.42E-04*	*1.69E-04*	*1.40E-04*	*2.12E-04*	*3.45E-04*	7.43E-02	3.23E-03	*1.47E-03*	1.53E-03	*1.05E-03*	*4.50E-03*
		10	*3.64E-04*	*1.45E-03*	*1.24E-03*	*2.65E-04*	*1.84E-04*	*1.53E-04*	*2.31E-04*	*3.78E-04*	8.68E-02	5.23E-03	*1.47E-03*	2.35E-03	1.22E-03	*4.24E-03*
		11	*3.55E-04*	*1.45E-03*	*1.24E-03*	*2.59E-04*	*1.80E-04*	*1.50E-04*	*2.26E-04*	*3.31E-04*	1.03E-01	3.85E-03	*1.47E-03*	1.84E-03	1.13E-03	*4.41E-03*
		12	*3.56E-04*	*1.39E-03*	*1.19E-03*	*2.60E-04*	*1.81E-04*	*1.50E-04*	*2.27E-04*	*3.27E-04*	5.14E-02	1.91E-03	*1.41E-03*	1.37E-03	*1.00E-03*	*4.44E-03*
	DL|RL		3.64E-04	1.45E-03	1.24E-03	2.65E-04	1.84E-04	1.53E-04	2.31E-04	3.90E-04	2.48E-03	1.85E-03	1.47E-03	1.22E-03	1.05E-03	4.71E-03
	Quality Flags	1									E					
		2														
		3														
		4									E					
		5														
		6									E					
		7									E					
		8									E					
		9														
		10									E					
		11									E					
		12														
Headspace Series B	Concentration (ppm)[1]	1	*3.58E-04*	*1.41E-03*	*1.20E-03*	*2.61E-04*	*1.82E-04*	*1.51E-04*	*2.28E-04*	*3.67E-04*	1.10E-02	*1.80E-03*	*1.43E-03*	*1.19E-03*	*1.02E-03*	*4.60E-03*
		2	*3.59E-04*	*1.39E-03*	*1.19E-03*	*2.62E-04*	*1.82E-04*	*1.52E-04*	*2.29E-04*	*3.49E-04*	1.43E-02	*1.77E-03*	*1.41E-03*	*1.17E-03*	*1.00E-03*	*4.53E-03*
		3	*3.56E-04*	*1.39E-03*	*1.19E-03*	*2.59E-04*	*1.80E-04*	*1.50E-04*	*2.26E-04*	*3.90E-04*	1.68E-02	*1.77E-03*	*1.41E-03*	*1.17E-03*	*1.00E-03*	*4.71E-03*
		4	*3.49E-04*	*1.44E-03*	*1.23E-03*	*2.54E-04*	*1.77E-04*	*1.47E-04*	*2.22E-04*	*3.82E-04*	1.89E-02	*1.83E-03*	*1.46E-03*	*1.21E-03*	*1.04E-03*	*4.65E-03*
		5	*3.51E-04*	*1.42E-03*	*1.21E-03*	*2.56E-04*	*1.78E-04*	*1.48E-04*	*2.24E-04*	*3.64E-04*	7.47E-03	*1.81E-03*	*1.44E-03*	*1.20E-03*	*1.02E-03*	*4.56E-03*
		6	*3.45E-04*	*1.31E-03*	*1.12E-03*	*2.52E-04*	*1.75E-04*	*1.46E-04*	*2.20E-04*	*3.55E-04*	1.64E-02	*1.67E-03*	*1.33E-03*	*1.10E-03*	*9.45E-04*	*4.65E-03*
		7	*3.49E-04*	*1.41E-03*	*1.20E-03*	*2.54E-04*	*1.77E-04*	*1.47E-04*	*2.22E-04*	*3.26E-04*	9.63E-03	*1.79E-03*	*1.43E-03*	*1.19E-03*	*1.02E-03*	*4.64E-03*
		8	*3.41E-04*	*1.34E-03*	*1.15E-03*	*2.49E-04*	*1.73E-04*	*1.44E-04*	*2.17E-04*	*3.36E-04*	1.82E-02	*1.71E-03*	*1.36E-03*	*1.13E-03*	*9.70E-04*	*4.48E-03*
		9	*3.32E-04*	*1.45E-03*	*1.24E-03*	*2.42E-04*	*1.69E-04*	*1.40E-04*	*2.12E-04*	*3.45E-04*	3.71E-02	*1.85E-03*	*1.47E-03*	*1.22E-03*	*1.05E-03*	*4.50E-03*
		10	*3.64E-04*	*1.45E-03*	*1.24E-03*	*2.65E-04*	*1.84E-04*	*1.53E-04*	*2.31E-04*	*3.78E-04*	1.07E-02	*1.85E-03*	*1.47E-03*	*1.22E-03*	*1.05E-03*	*4.24E-03*
		11	*3.55E-04*	*1.45E-03*	*1.24E-03*	*2.59E-04*	*1.80E-04*	*1.50E-04*	*2.26E-04*	*3.31E-04*	1.12E-02	*1.85E-03*	*1.47E-03*	*1.22E-03*	*1.05E-03*	*4.41E-03*
		12	*3.56E-04*	*1.39E-03*	*1.19E-03*	*2.60E-04*	*1.81E-04*	*1.50E-04*	*2.27E-04*	*3.27E-04*	1.90E-02	*1.77E-03*	*1.41E-03*	*1.17E-03*	*1.00E-03*	*4.44E-03*
	DL|RL		3.64E-04	1.45E-03	1.24E-03	2.65E-04	1.84E-04	1.53E-04	2.31E-04	3.90E-04	2.48E-03	1.85E-03	1.47E-03	1.22E-03	1.05E-03	4.71E-03
	Quality Flags	1														
		2														
		3														
		4														
		5														
		6														
		7														
		8														
		9														
		10														
		11														
		12														

[1] Values italicized and underline

Table B.1. Calculated Data (continued)

Analyte #			44	45	46	47	48	49	52	53
Analyte		Replicate Sample Order	N-Nitrosodimethyl-amine	N-Nitrosodiethylamine	N-Nitrosomethylethyl-amine	N-Nitrosomorpholine	Tributyl phosphate	Dibutyl butylphosphonate	Pyridine	2,4-Dimethylpyridine
Cartridge Test Rig	Concentration (ppm)[1]	1	1.39E-03	4.94E-05	1.03E-04	4.35E-05	*2.58E-04*	*2.75E-04*	*1.21E-03*	*8.92E-04*
		2	1.32E-03	6.43E-05	8.60E-05	3.91E-05	*2.59E-04*	*2.75E-04*	*1.23E-03*	*9.07E-04*
		3	1.33E-03	6.43E-05	8.59E-05	4.78E-05	*2.56E-04*	*2.73E-04*	*1.19E-03*	*8.79E-04*
		4	1.40E-03	5.46E-05	1.15E-04	4.80E-05	*2.49E-04*	*2.65E-04*	*1.24E-03*	*9.15E-04*
		5	1.46E-03	1.19E-04	1.55E-04	3.91E-05	*2.05E-04*	*2.19E-04*	*1.04E-03*	*7.71E-04*
		6	1.50E-03	5.92E-05	1.83E-04	5.20E-05	*2.46E-04*	*2.62E-04*	*1.18E-03*	*8.73E-04*
		7	1.65E-03	6.47E-05	1.04E-04	4.82E-05	*2.67E-04*	*2.85E-04*	*1.19E-03*	*8.80E-04*
		8	1.34E-03	5.94E-05	9.75E-05	4.35E-05	*2.81E-04*	*2.99E-04*	*1.21E-03*	*8.91E-04*
		9	1.62E-03	5.97E-05	1.21E-04	4.81E-05	*2.74E-04*	*2.92E-04*	*1.19E-03*	*8.82E-04*
		10	1.54E-03	6.96E-05	9.79E-05	4.81E-05	*2.73E-04*	*2.90E-04*	*1.09E-03*	*8.01E-04*
		11	1.54E-03	5.94E-05	1.03E-04	5.22E-05	*2.66E-04*	*2.82E-04*	*1.11E-03*	*8.20E-04*
		12	1.55E-03	6.40E-05	9.70E-05	4.76E-05	*2.65E-04*	*2.82E-04*	*1.18E-03*	*8.70E-04*
	DL|RL		5.49E-05	3.98E-05	4.62E-05	3.50E-05	2.81E-04	2.99E-04	1.24E-03	9.15E-04
	Quality Flags	1	BLa	a	a					
		2	BLa	a	a					
		3	BLa	a	a					
		4	BLa	a	a					
		5	BLa	a	a					
		6	BLa	a	a					
		7	BLa	a	a					
		8	BLa	a	a					
		9	BLa	a	a					
		10	BLa	a	a					
		11	BLa	a	a					
		12	BLa	a	a					
Headspace Series A	Concentration (ppm)[1]	1	2.95E-03	7.57E-05	5.92E-04	*4.16E-05*	*3.06E-04*	*3.26E-04*	*1.25E-03*	*9.23E-04*
		2	6.79E-04	1.62E-04	7.30E-04	4.33E-05	*2.91E-04*	*3.10E-04*	*1.23E-03*	*9.10E-04*
		3	1.25E-03	4.08E-04	2.23E-03	*4.08E-05*	*3.26E-04*	*3.47E-04*	*1.23E-03*	*9.10E-04*
		4	1.20E-03	3.92E-04	2.09E-03	*4.10E-05*	*3.19E-04*	*3.39E-04*	*1.28E-03*	*9.42E-04*
		5	1.37E-03	4.22E-04	2.21E-03	4.64E-05	*3.04E-04*	*3.23E-04*	*1.26E-03*	*9.28E-04*
		6	2.76E-03	6.96E-05	4.36E-04	*4.08E-05*	*2.96E-04*	*3.15E-04*	*1.16E-03*	*8.57E-04*
		7	3.18E-03	7.76E-05	6.75E-04	*4.27E-05*	*2.72E-04*	*2.90E-04*	*1.25E-03*	*9.22E-04*
		8	1.18E-03	4.29E-04	1.94E-03	*4.15E-05*	*2.80E-04*	*2.98E-04*	*1.19E-03*	*8.79E-04*
		9	1.62E-03	*4.85E-05*	2.47E-04	*4.26E-05*	*2.88E-04*	*3.07E-04*	*1.28E-03*	*9.48E-04*
		10	2.90E-03	1.16E-04	6.45E-04	*4.08E-05*	*3.15E-04*	*3.35E-04*	*1.29E-03*	*9.50E-04*
		11	1.10E-03	4.04E-04	2.09E-03	*4.18E-05*	*2.76E-04*	*2.94E-04*	*1.29E-03*	*9.50E-04*
		12	1.29E-03	2.84E-04	1.41E-03	*4.10E-05*	*2.73E-04*	*2.90E-04*	*1.23E-03*	*9.08E-04*
	DL|RL		6.11E-05	4.85E-05	5.70E-05	4.27E-05	3.26E-04	3.47E-04	1.29E-03	9.50E-04
	Quality Flags	1	BLa							
		2	BLac							
		3	BLac							
		4	BLac							
		5	BLac							
		6	BLa							
		7	BLa							
		8	BLac							
		9	BLa							
		10	BLa							
		11	BLac							
		12	BLac							
Headspace Series B	Concentration (ppm)[1]	1	*6.52E-05*	*4.73E-05*	*5.48E-05*	*4.16E-05*	*3.06E-04*	*3.26E-04*	*1.25E-03*	*9.23E-04*
		2	*6.11E-05*	*5.41E-05*	*5.70E-05*	*4.33E-05*	*2.91E-04*	*3.10E-04*	*1.23E-03*	*9.10E-04*
		3	1.30E-03	*5.10E-05*	*5.38E-05*	*4.08E-05*	*3.26E-04*	*3.47E-04*	*1.23E-03*	*9.10E-04*
		4	9.78E-04	*5.13E-05*	*5.41E-05*	*4.10E-05*	*3.19E-04*	*3.39E-04*	*1.28E-03*	*9.42E-04*
		5	1.30E-03	*5.28E-05*	*5.56E-05*	*4.22E-05*	*3.04E-04*	*3.23E-04*	*1.26E-03*	*9.28E-04*
		6	*6.40E-05*	*4.64E-05*	*5.38E-05*	*4.08E-05*	*2.96E-04*	*3.15E-04*	*1.16E-03*	*8.57E-04*
		7	*6.69E-05*	*4.85E-05*	*5.62E-05*	*4.27E-05*	*2.72E-04*	*2.90E-04*	*1.25E-03*	*9.22E-04*
		8	1.16E-03	*5.19E-05*	8.75E-05	*4.15E-05*	*2.80E-04*	*2.98E-04*	*1.19E-03*	*8.79E-04*
		9	*6.68E-05*	*4.85E-05*	*5.62E-05*	*4.26E-05*	*2.88E-04*	*3.07E-04*	*1.28E-03*	*9.48E-04*
		10	*6.39E-05*	*4.64E-05*	*5.38E-05*	*4.08E-05*	*3.15E-04*	*3.35E-04*	*1.29E-03*	*9.50E-04*
		11	1.19E-03	*5.23E-05*	*5.51E-05*	*4.18E-05*	*2.76E-04*	*2.94E-04*	*1.29E-03*	*9.50E-04*
		12	3.79E-04	*5.12E-05*	*5.40E-05*	*4.10E-05*	*2.73E-04*	*2.90E-04*	*1.23E-03*	*9.08E-04*
	DL|RL		6.69E-05	5.41E-05	5.70E-05	4.33E-05	3.26E-04	3.47E-04	1.29E-03	9.50E-04
	Quality Flags	1	BLa							
		2	Lac							
		3	BLac							
		4	BLac							
		5	BLac							
		6	BLa							
		7	BLa							
		8	BLac							
		9	BLa							
		10	BLa							
		11	BLac							
		12	BLac							

[1] Values italicized and underline

Table B.2. Calculated Data – Non-COPCs

Analyte #			1	2	3	4	5	6	7	8	9	10	11	12	13	14
Analyte		Replicate Sample Order	1,1,2,2-Tetrachloroethane	1,1,2-Trichloroethane	1,1-Dichloroethane	1,1-Dichloroethene	1,2-Dichloroethane	1,3-Dichloropropene (Total)	1,4-Dichlorobenzene	1,4-Dioxane	1-Heptanol	1-Propanol	2,6,10-Trimethyldodecane	2-Butanone	2-Heptanone	2-Methylphenol
Cartridge Test Rig	Concentration (ppm)[1]	1	*5.70E-04*	*7.17E-04*	*9.66E-04*	*9.86E-04*	*9.66E-04*	*8.62E-04*	*6.50E-04*	*1.09E-03*	*1.65E-03*	1.09E-02	*3.24E-04*	1.77E-02	8.37E-04	*6.36E-04*
		2	*5.79E-04*	*7.29E-04*	*9.82E-04*	*1.00E-03*	*9.82E-04*	*8.76E-04*	*6.61E-04*	*1.10E-03*	*1.67E-03*	2.29E-02	*3.24E-04*	2.25E-02	1.35E-03	*6.37E-04*
		3	*5.61E-04*	*7.06E-04*	*9.52E-04*	*9.72E-04*	*9.52E-04*	*8.49E-04*	*6.41E-04*	*1.07E-03*	*1.62E-03*	3.14E-02	*3.21E-04*	4.68E-02	*1.03E-03*	*6.31E-04*
		4	*5.84E-04*	*7.35E-04*	*9.91E-04*	*1.01E-03*	*9.91E-04*	*8.84E-04*	*6.67E-04*	*1.11E-03*	*1.69E-03*	1.32E-02	*3.12E-04*	2.61E-02	*8.59E-04*	*6.13E-04*
		5	*4.92E-04*	*6.19E-04*	*8.35E-04*	*8.52E-04*	*8.35E-04*	*7.45E-04*	*5.62E-04*	*9.38E-04*	*1.42E-03*	6.65E-03	*2.58E-04*	7.93E-03	*7.24E-04*	*5.06E-04*
		6	*5.57E-04*	*7.01E-04*	*9.45E-04*	*9.65E-04*	*9.45E-04*	*8.43E-04*	*6.36E-04*	*1.06E-03*	*1.61E-03*	4.80E-03	*3.09E-04*	1.19E-02	8.19E-04	*6.07E-04*
		7	*5.62E-04*	*7.07E-04*	*9.53E-04*	*9.73E-04*	*9.53E-04*	*8.50E-04*	*6.42E-04*	*1.07E-03*	*1.62E-03*	3.53E-02	*3.35E-04*	5.56E-02	*1.58E-03*	*6.59E-04*
		8	*5.69E-04*	*7.16E-04*	*9.65E-04*	*9.85E-04*	*9.65E-04*	*8.61E-04*	*6.50E-04*	*1.08E-03*	*1.64E-03*	1.99E-02	*3.53E-04*	3.20E-02	8.36E-04	*6.93E-04*
		9	*5.63E-04*	*7.08E-04*	*9.55E-04*	*9.75E-04*	*9.55E-04*	*8.52E-04*	*6.43E-04*	*1.07E-03*	*1.63E-03*	*2.88E-02*	*3.44E-04*	4.81E-02	*9.66E-04*	*6.75E-04*
		10	*5.12E-04*	*6.44E-04*	*8.68E-04*	*8.86E-04*	*8.68E-04*	*7.74E-04*	*5.84E-04*	*9.75E-04*	*1.48E-03*	2.86E-03	*3.42E-04*	7.64E-03	7.52E-04	*6.72E-04*
		11	*5.24E-04*	*6.59E-04*	*8.88E-04*	*9.07E-04*	*8.88E-04*	*7.92E-04*	*5.98E-04*	*9.98E-04*	*1.51E-03*	2.68E-02	*3.33E-04*	4.67E-02	*1.03E-03*	*6.54E-04*
		12	*5.56E-04*	*6.99E-04*	*9.42E-04*	*9.62E-04*	*9.42E-04*	*8.40E-04*	*6.34E-04*	*1.06E-03*	*1.60E-03*	2.33E-02	*3.33E-04*	2.80E-02	8.17E-04	*6.54E-04*
	DL|RL		5.84E-04	7.35E-04	9.91E-04	1.01E-03	9.91E-04	8.84E-04	6.67E-04	1.11E-03	1.69E-03	2.86E-03	3.53E-04	1.11E-02	8.59E-04	6.93E-04
	Quality Flags	1									L					
		2									L					
		3									L			E		
		4									L					
		5									L					
		6									L					
		7									L			E		
		8									L					
		9									L			E		
		10									L					
		11									L			E		
		12									L					
Headspace Series A	Concentration (ppm)[1]	1	*5.89E-04*	*7.41E-04*	*1.00E-03*	*1.02E-03*	*1.00E-03*	*8.91E-04*	*6.73E-04*	*1.12E-03*	*1.70E-03*	1.23E-02	*3.84E-04*	1.37E-02	6.79E-03	*7.55E-04*
		2	*5.81E-04*	*7.31E-04*	*9.85E-04*	*1.01E-03*	*9.85E-04*	*8.79E-04*	*6.63E-04*	*1.11E-03*	*1.68E-03*	2.16E-02	*3.65E-04*	2.37E-02	6.90E-03	*7.18E-04*
		3	*5.81E-04*	*7.31E-04*	*9.85E-04*	*1.01E-03*	*9.85E-04*	*8.78E-04*	*6.63E-04*	*1.11E-03*	*1.68E-03*	2.30E-02	*4.08E-04*	3.49E-02	5.19E-03	*8.02E-04*
		4	*6.01E-04*	*7.57E-04*	*1.02E-03*	*1.04E-03*	*1.02E-03*	*9.10E-04*	*6.87E-04*	*1.15E-03*	*1.74E-03*	4.34E-03	*4.00E-04*	5.60E-03	2.65E-03	*7.85E-04*
		5	*5.92E-04*	*7.45E-04*	*1.00E-03*	*1.03E-03*	*1.00E-03*	*8.96E-04*	*6.77E-04*	*1.13E-03*	*1.71E-03*	2.48E-02	3.81E-04	3.68E-02	6.60E-03	*7.48E-04*
		6	*5.47E-04*	*6.88E-04*	*9.28E-04*	*9.47E-04*	*9.28E-04*	*8.28E-04*	*6.25E-04*	*1.04E-03*	*1.58E-03*	1.91E-02	4.83E-04	2.87E-02	5.76E-03	*7.29E-04*
		7	*5.89E-04*	*7.41E-04*	*9.99E-04*	*1.02E-03*	*9.99E-04*	*8.91E-04*	*6.72E-04*	*1.12E-03*	*1.70E-03*	3.15E-02	6.48E-04	3.20E-02	7.94E-03	*6.70E-04*
		8	*5.61E-04*	*7.06E-04*	*9.52E-04*	*9.72E-04*	*9.52E-04*	*8.49E-04*	*6.41E-04*	*1.07E-03*	*1.62E-03*	3.01E-02	4.92E-04	5.77E-03	6.26E-03	*6.90E-04*
		9	*6.06E-04*	*7.62E-04*	*1.03E-03*	*1.05E-03*	*1.03E-03*	*9.16E-04*	*6.91E-04*	*1.15E-03*	*1.75E-03*	1.69E-02	*5.42E-04*	1.29E-02	3.86E-03	*7.10E-04*
		10	*6.06E-04*	*7.63E-04*	*1.03E-03*	*1.05E-03*	*1.03E-03*	*9.17E-04*	*6.92E-04*	*1.16E-03*	*1.75E-03*	3.53E-02	*3.95E-04*	2.35E-02	5.50E-03	*7.76E-04*
		11	*6.06E-04*	*7.63E-04*	*1.03E-03*	*1.05E-03*	*1.03E-03*	*9.17E-04*	*6.92E-04*	*1.16E-03*	*1.75E-03*	1.83E-02	*3.46E-04*	9.88E-03	4.90E-03	*6.80E-04*
		12	*5.80E-04*	*7.30E-04*	*9.83E-04*	*1.00E-03*	*9.83E-04*	*8.77E-04*	*6.62E-04*	*1.10E-03*	*1.67E-03*	*1.62E-02*	*3.42E-04*	*4.27E-03*	*2.77E-03*	*6.71E-04*
	DL|RL		6.06E-04	7.63E-04	1.03E-03	1.05E-03	1.03E-03	9.17E-04	6.92E-04	1.16E-03	1.75E-03	6.07E-04	4.08E-04	1.15E-04	8.91E-05	8.02E-04
	Quality Flags	1									L					
		2									L					
		3									L					
		4									L					
		5									L					
		6									L					
		7									L					
		8									L					
		9									L					
		10									L					
		11									L					
		12									L					
Headspace Series B	Concentration (ppm)[1]	1	*5.89E-04*	*7.41E-04*	*1.00E-03*	*1.02E-03*	*1.00E-03*	*8.91E-04*	*6.73E-04*	*1.12E-03*	*1.70E-03*	*3.29E-03*	*3.84E-04*	*1.37E-03*	*8.66E-04*	*7.55E-04*
		2	*5.81E-04*	*7.31E-04*	*9.85E-04*	*1.01E-03*	*9.85E-04*	*8.79E-04*	*6.63E-04*	*1.11E-03*	*1.68E-03*	*3.24E-03*	*3.65E-04*	*1.35E-03*	*8.54E-04*	*7.18E-04*
		3	*5.81E-04*	*7.31E-04*	*9.85E-04*	*1.01E-03*	*9.85E-04*	*8.78E-04*	*6.63E-04*	*1.11E-03*	*1.68E-03*	*3.24E-03*	*4.08E-04*	*1.35E-03*	*8.54E-04*	*8.02E-04*
		4	*6.01E-04*	*7.57E-04*	*1.02E-03*	*1.04E-03*	*1.02E-03*	*9.10E-04*	*6.87E-04*	*1.15E-03*	*1.74E-03*	*3.36E-03*	*4.00E-04*	*1.40E-03*	*8.84E-04*	*7.85E-04*
		5	*5.92E-04*	*7.45E-04*	*1.00E-03*	*1.03E-03*	*1.00E-03*	*8.96E-04*	*6.77E-04*	*1.13E-03*	*1.71E-03*	3.31E-03	*3.81E-04*	*1.38E-03*	*8.71E-04*	*7.48E-04*
		6	*5.47E-04*	*6.88E-04*	*9.28E-04*	*9.47E-04*	*9.28E-04*	*8.28E-04*	*6.25E-04*	*1.04E-03*	*1.58E-03*	1.04E-01	*3.71E-04*	*1.27E-03*	*8.04E-04*	*7.29E-04*
		7	*5.89E-04*	*7.41E-04*	*9.99E-04*	*1.02E-03*	*9.99E-04*	*8.91E-04*	*6.72E-04*	*1.12E-03*	*1.70E-03*	4.93E-02	*3.41E-04*	*1.37E-03*	*8.66E-04*	*6.70E-04*
		8	*5.61E-04*	*7.06E-04*	*9.52E-04*	*9.72E-04*	*9.52E-04*	*8.49E-04*	*6.41E-04*	*1.07E-03*	*1.62E-03*	1.31E-02	*3.51E-04*	*1.31E-03*	*8.25E-04*	*6.90E-04*
		9	*6.06E-04*	*7.62E-04*	*1.03E-03*	*1.05E-03*	*1.03E-03*	*9.16E-04*	*6.91E-04*	*1.15E-03*	*1.75E-03*	5.78E-02	*3.61E-04*	*1.41E-03*	*8.90E-04*	*7.10E-04*
		10	*6.06E-04*	*7.63E-04*	*1.03E-03*	*1.05E-03*	*1.03E-03*	*9.17E-04*	*6.92E-04*	*1.16E-03*	*1.75E-03*	4.09E-02	*3.95E-04*	*1.41E-03*	*8.91E-04*	*7.76E-04*
		11	*6.06E-04*	*7.63E-04*	*1.03E-03*	*1.05E-03*	*1.03E-03*	*9.17E-04*	*6.92E-04*	*1.16E-03*	*1.75E-03*	7.34E-02	*3.46E-04*	*1.41E-03*	*8.91E-04*	*6.80E-04*
		12	5.80E-04	7.30E-04	9.83E-04	1.00E-03	9.83E-04	8.77E-04	6.62E-04	1.10E-03	1.67E-03	1.62E-02	3.42E-04	1.35E-03	8.52E-04	6.71E-04
	DL|RL		6.06E-04	7.63E-04	1.03E-03	1.05E-03	1.03E-03	9.17E-04	6.92E-04	1.16E-03	1.75E-03	3.36E-03	4.08E-04	1.41E-03	8.91E-04	8.02E-04
	Quality Flags	1									L					
		2									L					
		3									L					
		4									L					
		5									L					
		6									L	E				
		7									L					
		8									L					
		9									L					
		10									L					
		11									L					
		12									L					

[1] Values italicized and underlined correspond to a value flagged as "<**DL**|**RL**".

Table B.2. Calculated Data – Non-COPCs (continued)

Analyte #			15	16	17	18	19	20	21	22	23	24	25	26	27	28
Analyte		Replicate Sample Order	3-Heptanone	3-Methylphenol	3-Octanone	4-Methyl-2-Pentanone	Acetone	Acetophenone	Acrylonitrile	Allyl Alcohol	Allyl Chloride	Benzonitrile	Carbon tetrachloride	Chlorobenzene	Chloroethane	Chloroform
Cartridge Test Rig	Concentration (ppm)[1]	1	8.37E-04	*6.36E-04*	*7.46E-04*	1.03E-03	3.70E-01	*7.96E-04*	*1.80E-03*	*1.65E-03*	*1.25E-03*	*9.27E-04*	*6.22E-04*	*8.50E-04*	*1.48E-03*	*8.01E-04*
		2	2.34E-03	*6.37E-04*	*7.58E-04*	4.45E-03	6.55E-01	*8.09E-04*	*1.83E-03*	*1.67E-03*	*1.27E-03*	*9.43E-04*	*6.32E-04*	*8.64E-04*	*1.51E-03*	*8.14E-04*
		3	*1.86E-03*	*6.31E-04*	*7.35E-04*	3.92E-03	8.11E-01	*7.84E-04*	*1.78E-03*	*1.62E-03*	*1.23E-03*	*9.14E-04*	*6.12E-04*	*8.37E-04*	*1.46E-03*	*7.89E-04*
		4	8.59E-04	*6.13E-04*	*7.65E-04*	1.55E-03	4.08E-01	*8.16E-04*	*1.85E-03*	*1.69E-03*	*1.28E-03*	*9.51E-04*	*6.37E-04*	*8.71E-04*	*1.52E-03*	*8.21E-04*
		5	*1.03E-03*	*5.06E-04*	*6.44E-04*	*2.41E-03*	2.49E-01	*6.88E-04*	*1.56E-03*	*1.42E-03*	*1.08E-03*	*8.01E-04*	*5.37E-04*	*7.34E-04*	*1.28E-03*	*6.92E-04*
		6	8.19E-04	*6.07E-04*	*7.29E-04*	9.34E-04	2.01E-01	*7.78E-04*	*1.76E-03*	*1.61E-03*	*1.22E-03*	*9.07E-04*	*6.08E-04*	*8.31E-04*	*1.45E-03*	*7.83E-04*
		7	*2.68E-03*	*6.59E-04*	*7.36E-04*	3.92E-03	7.31E-01	*7.85E-04*	*1.78E-03*	*1.62E-03*	*1.23E-03*	*9.15E-04*	*6.13E-04*	*8.38E-04*	*1.46E-03*	*7.90E-04*
		8	8.36E-04	*6.93E-04*	*7.45E-04*	2.15E-03	5.21E-01	*7.95E-04*	*1.80E-03*	*1.64E-03*	*1.25E-03*	*9.26E-04*	*6.21E-04*	*8.48E-04*	*1.48E-03*	*8.00E-04*
		9	*1.72E-03*	*6.75E-04*	*7.37E-04*	3.38E-03	7.19E-01	*7.87E-04*	*1.78E-03*	*1.63E-03*	*1.23E-03*	*9.16E-04*	*6.14E-04*	*8.40E-04*	*1.46E-03*	*7.92E-04*
		10	7.52E-04	*6.72E-04*	*6.70E-04*	1.14E-03	1.60E-01	*7.15E-04*	*1.62E-03*	*1.48E-03*	*1.12E-03*	*8.33E-04*	*5.58E-04*	*7.63E-04*	*1.33E-03*	*7.19E-04*
		11	1.86E-03	*6.54E-04*	*6.86E-04*	3.36E-03	6.68E-01	*7.32E-04*	*1.66E-03*	*1.51E-03*	*1.15E-03*	*8.52E-04*	*5.71E-04*	*7.81E-04*	*1.36E-03*	*7.36E-04*
		12	1.22E-03	*6.54E-04*	*7.27E-04*	3.03E-03	6.29E-01	*7.76E-04*	*1.76E-03*	*1.61E-03*	*1.22E-03*	*9.04E-04*	*6.06E-04*	*8.28E-04*	*1.45E-03*	*7.81E-04*
	DL|RL		8.59E-04	6.93E-04	7.65E-04	9.34E-04	6.75E-02	8.16E-04	1.85E-03	1.69E-03	1.28E-03	9.51E-04	6.37E-04	8.71E-04	1.52E-03	8.21E-04
	Quality Flags	1					EY			Y						
		2					EY			Y						
		3					EY			Y						
		4					EY			Y						
		5					EY			Y						
		6					EY			Y						
		7					EY			Y						
		8					EY			Y						
		9					EY			Y						
		10					EY			Y						
		11					EY			Y						
		12					EY			Y						
Headspace Series A	Concentration (ppm)[1]	1	1.30E-02	*7.55E-04*	*7.71E-04*	4.28E-03	3.26E-01	*8.23E-04*	*1.86E-03*	*1.70E-03*	*1.29E-03*	*9.59E-04*	*6.43E-04*	*8.79E-04*	*1.53E-03*	*8.29E-04*
		2	1.28E-02	*7.18E-04*	*7.60E-04*	4.14E-03	5.46E-01	*8.12E-04*	*1.84E-03*	*1.68E-03*	*1.27E-03*	*9.45E-04*	*6.34E-04*	*8.66E-04*	*1.51E-03*	*8.17E-04*
		3	9.96E-03	*8.02E-04*	*7.60E-04*	3.65E-03	5.32E-01	*8.11E-04*	*1.84E-03*	1.68E-03	*1.27E-03*	*9.45E-04*	*6.34E-04*	*8.66E-04*	*1.51E-03*	*8.17E-04*
		4	5.01E-03	*7.85E-04*	*7.87E-04*	2.35E-03	1.74E-01	*8.40E-04*	*1.90E-03*	*2.75E-03*	*1.32E-03*	*9.79E-04*	*6.56E-04*	*8.97E-04*	*1.56E-03*	*8.46E-04*
		5	1.23E-02	*7.48E-04*	*7.76E-04*	4.39E-03	5.85E-01	*8.28E-04*	*1.87E-03*	*1.71E-03*	*1.30E-03*	*9.64E-04*	*6.47E-04*	*8.84E-04*	*1.54E-03*	*8.33E-04*
		6	1.07E-02	*7.29E-04*	*7.16E-04*	3.74E-03	5.40E-01	*7.64E-04*	*1.73E-03*	*1.58E-03*	*1.20E-03*	*8.91E-04*	*5.97E-04*	*8.16E-04*	*1.42E-03*	*7.69E-04*
		7	1.44E-02	*6.70E-04*	*7.71E-04*	4.61E-03	6.24E-01	*8.23E-04*	*1.86E-03*	*1.70E-03*	*1.29E-03*	*9.59E-04*	*6.43E-04*	*8.78E-04*	*1.53E-03*	*8.28E-04*
		8	1.10E-02	*6.90E-04*	*7.35E-04*	3.92E-03	2.16E-01	*7.84E-04*	*1.78E-03*	*1.62E-03*	*1.23E-03*	*9.14E-04*	*6.13E-04*	*8.37E-04*	*1.46E-03*	*7.89E-04*
		9	6.97E-03	*7.10E-04*	*7.93E-04*	2.54E-03	2.77E-01	*8.46E-04*	*1.92E-03*	*1.75E-03*	*1.33E-03*	*9.86E-04*	*6.61E-04*	*9.03E-04*	*1.58E-03*	*8.51E-04*
		10	9.65E-03	*7.76E-04*	*7.94E-04*	3.73E-03	4.96E-01	*8.47E-04*	*1.92E-03*	*1.75E-03*	*1.33E-03*	*9.87E-04*	*6.62E-04*	*9.04E-04*	*1.58E-03*	*8.52E-04*
		11	8.91E-03	*6.80E-04*	*7.94E-04*	3.22E-03	3.07E-01	*8.47E-04*	*1.92E-03*	*1.75E-03*	*1.33E-03*	*9.87E-04*	*6.62E-04*	*9.04E-04*	*1.58E-03*	*8.53E-04*
		12	*4.97E-03*	*6.71E-04*	*7.59E-04*	*2.19E-03*	*1.20E-01*	*8.10E-04*	*1.83E-03*	*1.68E-03*	*1.27E-03*	*9.44E-04*	*6.33E-04*	*8.65E-04*	*1.51E-03*	*8.15E-04*
	DL|RL		8.91E-05	8.02E-04	7.94E-04	9.32E-05	7.01E-04	8.47E-04	1.92E-03	1.75E-03	1.33E-03	9.87E-04	6.62E-04	9.04E-04	1.58E-03	8.53E-04
	Quality Flags	1					EY			Y						
		2					EY			Y						
		3					EY			Y						
		4					EY			Y						
		5					EY			Y						
		6					EY			Y						
		7					ELY			Y						
		8					ELY			Y						
		9					ELY			Y						
		10					ELY			Y						
		11					ELY			Y						
		12					EL									
Headspace Series B	Concentration (ppm)[1]	1	*8.66E-04*	*7.55E-04*	*7.71E-04*	*9.88E-04*	*1.70E-03*	*8.23E-04*	*1.86E-03*	*1.70E-03*	*1.29E-03*	*9.59E-04*	*6.43E-04*	*8.79E-04*	*1.53E-03*	*8.29E-04*
		2	*8.54E-04*	*7.18E-04*	*7.60E-04*	*9.73E-04*	1.68E-03	*8.12E-04*	*1.84E-03*	*1.68E-03*	*1.27E-03*	*9.45E-04*	*6.34E-04*	*8.66E-04*	*1.51E-03*	*8.17E-04*
		3	*8.54E-04*	*8.02E-04*	*7.60E-04*	*9.73E-04*	*2.52E-03*	*8.11E-04*	*1.84E-03*	*1.68E-03*	*1.27E-03*	*9.45E-04*	*6.34E-04*	*8.66E-04*	*1.51E-03*	*8.17E-04*
		4	*8.84E-04*	*7.85E-04*	*7.87E-04*	*1.01E-03*	1.74E-03	*8.40E-04*	*1.90E-03*	*1.74E-03*	*1.32E-03*	*9.79E-04*	*6.56E-04*	*8.97E-04*	*1.56E-03*	*8.46E-04*
		5	*8.71E-04*	*7.48E-04*	*7.76E-04*	*9.93E-04*	2.00E-03	*8.28E-04*	*1.87E-03*	1.71E-03	*1.30E-03*	*9.64E-04*	*6.47E-04*	*8.84E-04*	*1.54E-03*	*8.33E-04*
		6	*8.04E-04*	*7.29E-04*	*7.16E-04*	*9.17E-04*	1.84E-02	*7.64E-04*	*1.73E-03*	*2.90E-03*	*1.20E-03*	*8.91E-04*	*5.97E-04*	*8.16E-04*	*1.42E-03*	*7.69E-04*
		7	*8.66E-04*	*6.70E-04*	*7.71E-04*	*9.87E-04*	1.16E-02	*8.23E-04*	*1.86E-03*	*1.70E-03*	*1.29E-03*	*9.59E-04*	*6.43E-04*	*8.78E-04*	*1.53E-03*	*8.28E-04*
		8	*8.25E-04*	*6.90E-04*	*7.35E-04*	*9.41E-04*	4.46E-03	*7.84E-04*	*1.78E-03*	*1.62E-03*	*1.23E-03*	*9.14E-04*	*6.13E-04*	*8.37E-04*	*1.46E-03*	*7.89E-04*
		9	*8.90E-04*	*7.10E-04*	*7.93E-04*	*1.01E-03*	1.41E-02	*8.46E-04*	*1.92E-03*	*1.75E-03*	*1.33E-03*	*9.86E-04*	*6.61E-04*	*9.03E-04*	*1.58E-03*	*8.51E-04*
		10	*8.91E-04*	*7.76E-04*	*7.94E-04*	*1.02E-03*	1.04E-02	*8.47E-04*	*1.92E-03*	*1.75E-03*	*1.33E-03*	*9.87E-04*	*6.62E-04*	*9.04E-04*	*1.58E-03*	*8.52E-04*
		11	*8.91E-04*	*6.80E-04*	*7.94E-04*	*1.02E-03*	1.75E-02	*8.47E-04*	*1.92E-03*	*1.75E-03*	*1.33E-03*	*9.87E-04*	*6.62E-04*	*9.04E-04*	*1.58E-03*	*8.53E-04*
		12	8.52E-04	6.71E-04	7.59E-04	9.72E-04	4.89E-03	8.10E-04	1.83E-03	1.68E-03	1.27E-03	9.44E-04	6.33E-04	8.65E-04	1.51E-03	8.15E-04
	DL|RL		8.91E-04	8.02E-04	7.94E-04	1.02E-03	1.74E-03	8.47E-04	1.92E-03	1.75E-03	1.33E-03	9.87E-04	6.62E-04	9.04E-04	1.58E-03	8.53E-04
	Quality Flags	1								Y						
		2								Y						
		3								Y						
		4								Y						
		5								Y						
		6					L			Y						
		7					L			Y						
		8					L			Y						
		9					L			Y						
		10					L			Y						
		11					L			Y						
		12					L			Y						

[1] Values italicized and underlin

Table B.2. Calculated Data – Non-COPCs (continued)

Analyte #			29	30	31	32	33	34	35	36	37	38	39	40	41	42
Analyte		Replicate Sample Order	cis-1,3-Dichloropropene	Cyclohexane	Decane	Dodecane	Ethanol	Ethyl acetate	Ethylbenzene	Hexadecane	Hexane	Methacrylonitrile	Methylene Chloride	Naphthalene	n-Butyl acetate	n-Heptadecane
Cartridge Test Rig	Concentration (ppm)[1]	1	*8.62E-04*	3.60E-03	*6.72E-04*	*4.04E-04*	6.75E-02	*1.09E-03*	*9.01E-04*	*3.04E-04*	5.46E-02	*1.43E-03*	*2.91E-03*	*7.46E-04*	*8.23E-04*	*2.86E-04*
		2	*8.76E-04*	8.57E-03	*6.83E-04*	*4.04E-04*	1.53E-01	*1.10E-03*	*9.16E-04*	*3.04E-04*	1.50E-01	*1.45E-03*	*1.14E-03*	*7.58E-04*	*8.37E-04*	*2.86E-04*
		3	*8.49E-04*	1.03E-02	*6.62E-04*	*4.01E-04*	1.43E-01	*1.07E-03*	*8.87E-04*	*3.01E-04*	1.55E-01	*1.40E-03*	*1.11E-03*	*7.35E-04*	*8.11E-04*	*2.84E-04*
		4	*8.84E-04*	4.95E-03	*6.89E-04*	3.89E-04	7.63E-02	*1.11E-03*	*9.24E-04*	*2.93E-04*	7.11E-02	*1.46E-03*	*1.15E-03*	*7.65E-04*	*8.44E-04*	*2.75E-04*
		5	*7.45E-04*	4.83E-03	*5.81E-04*	*4.18E-04*	7.02E-02	*9.38E-04*	*7.78E-04*	*2.42E-04*	1.04E-01	*1.23E-03*	*9.73E-04*	*6.45E-04*	*7.11E-04*	*2.28E-04*
		6	*8.43E-04*	2.32E-03	*6.57E-04*	*3.85E-04*	3.89E-02	*1.06E-03*	*8.81E-04*	*2.90E-04*	3.08E-02	*1.39E-03*	*1.10E-03*	*7.30E-04*	*8.05E-04*	*2.73E-04*
		7	*8.50E-04*	1.12E-02	*6.63E-04*	*4.18E-04*	1.35E-01	*1.07E-03*	*8.89E-04*	*3.15E-04*	1.46E-01	*1.41E-03*	*1.11E-03*	*7.36E-04*	*8.12E-04*	*2.96E-04*
		8	*8.61E-04*	6.71E-03	*6.71E-04*	*4.40E-04*	9.16E-02	*1.08E-03*	*9.00E-04*	*3.31E-04*	9.23E-02	*1.42E-03*	*1.12E-03*	*7.45E-04*	*8.22E-04*	*3.12E-04*
		9	*8.52E-04*	9.36E-03	*6.64E-04*	*4.28E-04*	1.21E-01	*1.07E-03*	*8.90E-04*	*3.22E-04*	1.37E-01	*1.41E-03*	*1.11E-03*	*7.37E-04*	*8.14E-04*	*3.03E-04*
		10	*7.74E-04*	3.23E-03	*6.04E-04*	*4.27E-04*	4.19E-02	*9.75E-04*	*8.09E-04*	*3.21E-04*	5.65E-02	*1.28E-03*	*1.01E-03*	*6.70E-04*	*7.39E-04*	*3.02E-04*
		11	*7.92E-04*	8.70E-03	*6.18E-04*	*4.15E-04*	1.14E-01	*9.98E-04*	*8.28E-04*	*3.12E-04*	1.27E-01	*1.31E-03*	*1.03E-03*	*6.86E-04*	*7.57E-04*	*2.94E-04*
		12	*8.40E-04*	7.57E-03	6.55E-04	4.15E-04	1.11E-01	*1.06E-03*	*8.78E-04*	*3.12E-04*	1.26E-01	*1.39E-03*	*1.10E-03*	*7.28E-04*	*8.03E-04*	*2.94E-04*
	DL | RL		8.84E-04	1.17E-02	6.89E-04	4.40E-04	1.51E-01	1.11E-03	9.24E-04	3.31E-04	1.42E-02	1.46E-03	1.15E-03	7.65E-04	8.44E-04	3.12E-04
	Quality Flags	1									E		L			
		2					E				E		L			
		3					E				E		L			
		4									E		L			
		5									E		L			
		6											L			
		7									E		L			
		8									E		L			
		9									E		L			
		10									E		L			
		11									E		L			
		12									E		L			
Headspace Series A	Concentration (ppm)[1]	1	*8.91E-04*	7.25E-03	1.74E-03	8.62E-04	6.44E-02	*1.12E-03*	*9.32E-04*	*3.60E-04*	1.34E-01	*1.47E-03*	*1.16E-03*	*7.72E-04*	*8.52E-04*	*3.39E-04*
		2	*8.79E-04*	8.79E-03	1.83E-03	*8.66E-04*	9.17E-02	*1.11E-03*	*9.18E-04*	*3.43E-04*	1.32E-01	*1.45E-03*	*1.15E-03*	*7.61E-04*	*8.39E-04*	*3.23E-04*
		3	*8.78E-04*	8.88E-03	*8.56E-04*	*5.09E-04*	8.82E-02	*1.11E-03*	*9.18E-04*	*3.83E-04*	1.13E-01	*1.45E-03*	*1.15E-03*	*7.61E-04*	*8.39E-04*	*3.61E-04*
		4	*9.10E-04*	4.60E-03	7.09E-04	4.99E-04	3.65E-02	*1.15E-03*	*9.51E-04*	*3.75E-04*	8.30E-02	*1.50E-03*	*1.19E-03*	*7.88E-04*	*8.69E-04*	*3.53E-04*
		5	*8.96E-04*	9.85E-03	1.46E-03	1.23E-03	8.27E-02	*1.13E-03*	*9.37E-04*	*3.57E-04*	1.35E-01	*1.48E-03*	*1.17E-03*	*7.76E-04*	*8.56E-04*	*3.36E-04*
		6	*8.28E-04*	8.55E-03	1.13E-03	1.53E-03	6.81E-02	*1.04E-03*	*8.65E-04*	*3.48E-04*	1.15E-01	*1.37E-03*	*1.08E-03*	*7.17E-04*	7.91E-04	*3.28E-04*
		7	*8.91E-04*	9.79E-03	1.85E-03	2.04E-03	9.12E-02	*1.12E-03*	*9.31E-04*	*3.20E-04*	1.53E-01	*1.47E-03*	*1.16E-03*	*7.71E-04*	*3.12E-03*	*3.01E-04*
		8	*8.49E-04*	5.69E-03	*1.27E-03*	1.71E-03	5.80E-02	*1.07E-03*	*8.88E-04*	*3.30E-04*	1.28E-01	*1.40E-03*	*1.11E-03*	*7.35E-04*	*8.11E-04*	*3.10E-04*
		9	*9.16E-04*	5.13E-03	7.14E-04	1.71E-03	5.88E-02	*1.15E-03*	*9.57E-04*	*3.39E-04*	9.14E-02	*1.51E-03*	*1.20E-03*	*7.93E-04*	*8.75E-04*	*3.19E-04*
		10	*9.17E-04*	7.86E-03	1.25E-03	5.42E-04	7.18E-02	*1.16E-03*	*9.59E-04*	*3.71E-04*	1.28E-01	*1.52E-03*	*1.20E-03*	*7.94E-04*	*8.76E-04*	*3.49E-04*
		11	*9.17E-04*	5.64E-03	*7.15E-04*	4.32E-04	5.34E-02	*1.16E-03*	*9.59E-04*	*3.25E-04*	1.08E-01	*1.52E-03*	*1.20E-03*	*7.94E-04*	*8.76E-04*	*3.06E-04*
		12	*8.77E-04*	*3.76E-03*	*6.84E-04*	*8.10E-04*	3.87E-02	*1.10E-03*	*9.17E-04*	*3.21E-04*	*8.38E-02*	*1.45E-03*	*1.15E-03*	*7.59E-04*	*8.38E-04*	*3.02E-04*
	DL | RL		9.17E-04	1.21E-04	7.14E-04	5.09E-04	1.57E-03	1.16E-03	9.59E-04	3.83E-04	1.48E-04	1.52E-03	1.20E-03	7.94E-04	8.76E-04	3.61E-04
	Quality Flags	1									E		L			
		2									E		L			
		3									E		L			
		4									E		L			
		5									E		L			
		6									E		L			
		7									E		L			
		8									E		L			
		9									E		L			
		10									E		L			
		11									E		L			
		12									E		L			
Headspace Series B	Concentration (ppm)[1]	1	*8.91E-04*	*1.18E-03*	*6.95E-04*	*4.79E-04*	*1.27E-02*	*1.12E-03*	*9.32E-04*	*3.60E-04*	*1.15E-03*	*1.47E-03*	*1.16E-03*	*7.72E-04*	*8.52E-04*	*3.39E-04*
		2	*8.79E-04*	*1.16E-03*	*6.85E-04*	*4.56E-04*	4.23E-03	*1.11E-03*	*9.18E-04*	*3.43E-04*	*1.13E-03*	*1.45E-03*	*1.15E-03*	*7.61E-04*	*8.39E-04*	*3.23E-04*
		3	*8.78E-04*	*1.16E-03*	*6.85E-04*	*5.09E-04*	1.02E-02	*1.11E-03*	*9.18E-04*	*3.83E-04*	*1.13E-03*	*1.45E-03*	*1.15E-03*	*7.61E-04*	*8.39E-04*	*3.61E-04*
		4	*9.10E-04*	*1.20E-03*	*7.09E-04*	*4.99E-04*	1.08E-02	*1.15E-03*	*9.51E-04*	*3.75E-04*	*1.17E-03*	*1.50E-03*	*1.19E-03*	*7.88E-04*	*8.69E-04*	*3.53E-04*
		5	*8.96E-04*	*1.18E-03*	*6.99E-04*	*4.75E-04*	1.40E-02	*1.13E-03*	*9.37E-04*	*3.57E-04*	*1.15E-03*	*1.48E-03*	1.17E-03	*7.76E-04*	*8.56E-04*	*3.36E-04*
		6	*8.28E-04*	*1.09E-03*	*6.45E-04*	*4.63E-04*	2.66E-02	*1.04E-03*	*8.65E-04*	*3.48E-04*	*1.07E-03*	*1.37E-03*	*1.89E-03*	*7.17E-04*	*7.91E-04*	*3.28E-04*
		7	*8.91E-04*	*1.17E-03*	*6.95E-04*	*4.26E-04*	2.15E-02	*1.12E-03*	*9.31E-04*	*3.20E-04*	*1.15E-03*	*1.47E-03*	*1.16E-03*	*7.71E-04*	*8.51E-04*	*3.01E-04*
		8	*8.49E-04*	*1.12E-03*	*6.62E-04*	*4.38E-04*	1.45E-02	*1.07E-03*	*8.88E-04*	*3.30E-04*	*1.09E-03*	*1.40E-03*	*1.11E-03*	*7.35E-04*	*8.11E-04*	*3.10E-04*
		9	*9.16E-04*	*1.21E-03*	*7.14E-04*	*4.51E-04*	2.94E-02	*1.15E-03*	*9.57E-04*	*3.39E-04*	*1.18E-03*	*1.51E-03*	*1.20E-03*	*7.93E-04*	*8.75E-04*	*3.19E-04*
		10	*9.17E-04*	*1.21E-03*	*7.15E-04*	*4.93E-04*	1.58E-02	*1.16E-03*	*9.59E-04*	*3.71E-04*	*1.18E-03*	*1.52E-03*	*1.20E-03*	*7.94E-04*	*8.76E-04*	*3.49E-04*
		11	*9.17E-04*	*1.21E-03*	*7.15E-04*	*4.32E-04*	2.03E-02	*1.16E-03*	*9.59E-04*	*3.25E-04*	*1.18E-03*	*1.52E-03*	*1.20E-03*	*7.94E-04*	*8.76E-04*	*3.06E-04*
		12	8.77E-04	1.16E-03	6.84E-04	4.26E-04	8.63E-03	1.10E-03	9.17E-04	3.21E-04	1.13E-03	1.45E-03	1.15E-03	7.59E-04	8.38E-04	3.02E-04
	DL | RL		9.17E-04	1.21E-03	7.15E-04	5.09E-04	4.23E-03	1.16E-03	9.59E-04	3.83E-04	1.18E-03	1.52E-03	1.20E-03	7.94E-04	8.76E-04	3.61E-04
	Quality Flags	1											L			
		2											L			
		3											L			
		4											L			
		5											L			
		6											L			
		7											L			
		8											L			
		9											L			
		10											L			
		11											L			
		12											L			

[1] Values italicized and underlin

Table B.2. Calculated Data – Non-COPCs (continued)

Analyte #			43	44	45	46	47	48	49	50	51	52	53
Analyte		Replicate Sample Order	n-Heptane	Nitrobenzene	n-Pentadecane	Styrene	Tetrachloroethene	Tetradecane	Toluene	trans-1,3-Dichloropropene	Trichloroethene	Trichlorofluoromethane	Tridecane
Cartridge Test Rig	Concentration (ppm)[1]	1	1.35E-02	*7.77E-04*	*3.24E-04*	*9.18E-04*	*5.77E-04*	*3.47E-04*	3.20E-03	*8.62E-04*	*7.28E-04*	2.09E-02	*3.73E-04*
		2	5.42E-02	*7.90E-04*	*3.24E-04*	*9.33E-04*	*5.86E-04*	*3.47E-04*	3.43E-03	*8.76E-04*	*7.40E-04*	3.83E-02	*3.73E-04*
		3	5.01E-02	*7.65E-04*	*3.21E-04*	*9.05E-04*	*5.68E-04*	*3.44E-04*	3.41E-03	*8.49E-04*	*7.17E-04*	5.60E-02	*3.70E-04*
		4	2.04E-02	*7.97E-04*	*3.12E-04*	*9.42E-04*	*5.91E-04*	*3.34E-04*	2.75E-03	*8.84E-04*	*7.46E-04*	2.80E-02	*3.59E-04*
		5	3.23E-02	*6.71E-04*	*2.58E-04*	*7.93E-04*	*4.98E-04*	*2.76E-04*	3.59E-03	*7.45E-04*	*6.29E-04*	2.21E-02	*2.97E-04*
		6	1.01E-02	*7.60E-04*	*3.09E-04*	*8.98E-04*	*5.64E-04*	*3.31E-04*	3.05E-03	*8.43E-04*	*7.12E-04*	1.08E-02	*3.56E-04*
		7	5.02E-02	*7.66E-04*	*3.35E-04*	*9.06E-04*	*5.69E-04*	*3.59E-04*	3.84E-03	*8.50E-04*	*7.18E-04*	5.61E-02	*3.86E-04*
		8	2.94E-02	*7.76E-04*	*3.53E-04*	*9.17E-04*	*5.76E-04*	*3.78E-04*	3.02E-03	*8.61E-04*	*7.27E-04*	3.65E-02	*4.06E-04*
		9	4.48E-02	*7.68E-04*	*3.44E-04*	*9.07E-04*	*5.70E-04*	*3.68E-04*	3.25E-03	*8.52E-04*	*7.19E-04*	5.04E-02	*3.96E-04*
		10	1.50E-02	*6.98E-04*	*3.42E-04*	*8.25E-04*	*5.18E-04*	*3.67E-04*	2.25E-03	*7.74E-04*	*6.54E-04*	1.20E-02	*3.94E-04*
		11	4.39E-02	*7.14E-04*	*3.33E-04*	*8.44E-04*	*5.30E-04*	*3.56E-04*	3.26E-03	*7.92E-04*	*6.69E-04*	4.75E-02	*3.84E-04*
		12	3.95E-02	*7.57E-04*	*3.33E-04*	*8.95E-04*	*5.62E-04*	*3.56E-04*	2.95E-03	*8.40E-04*	*7.10E-04*	4.36E-02	3.83E-04
	DL | RL		7.58E-03	7.97E-04	3.53E-04	9.42E-04	5.91E-04	3.78E-04	8.87E-03	8.84E-04	7.46E-04	5.53E-03	4.06E-04
	Quality Flags	1											
		2	E									E	
		3	E									E	
		4										E	
		5	E									E	
		6											
		7	E									E	
		8										E	
		9	E									E	
		10											
		11	E									E	
		12	E									E	
Headspace Series A	Concentration (ppm)[1]	1	5.76E-02	*8.03E-04*	*3.84E-04*	*9.50E-04*	*5.96E-04*	*4.11E-04*	6.08E-03	*8.91E-04*	*7.53E-04*	2.76E-02	4.87E-04
		2	6.00E-02	*7.92E-04*	*3.65E-04*	*9.36E-04*	*5.88E-04*	*3.91E-04*	7.32E-03	*8.79E-04*	*7.42E-04*	4.55E-02	*5.05E-04*
		3	5.35E-02	*7.92E-04*	*4.08E-04*	*9.36E-04*	*5.88E-04*	*4.37E-04*	7.58E-03	*8.78E-04*	*7.42E-04*	4.02E-02	*4.71E-04*
		4	3.61E-02	*8.20E-04*	*4.00E-04*	*9.69E-04*	*6.09E-04*	*4.28E-04*	5.84E-03	*9.10E-04*	*7.68E-04*	1.71E-02	4.61E-04
		5	5.95E-02	*8.08E-04*	*3.81E-04*	*9.55E-04*	*6.00E-04*	4.08E-04	9.89E-03	*8.96E-04*	*7.57E-04*	4.46E-02	7.02E-04
		6	5.04E-02	*7.46E-04*	*3.71E-04*	*8.82E-04*	*5.54E-04*	5.57E-04	7.31E-03	*8.28E-04*	*6.99E-04*	4.01E-02	9.41E-04
		7	6.41E-02	*8.03E-04*	*3.41E-04*	*9.49E-04*	*5.96E-04*	8.04E-04	6.17E-03	*8.91E-04*	*7.52E-04*	5.10E-02	1.26E-03
		8	5.41E-02	*7.65E-04*	*3.51E-04*	*9.05E-04*	*5.68E-04*	6.02E-04	4.77E-03	*8.49E-04*	*7.17E-04*	2.92E-02	1.05E-03
		9	3.80E-02	*8.26E-04*	*3.61E-04*	*9.76E-04*	*6.13E-04*	*6.96E-04*	3.49E-03	*9.16E-04*	*7.74E-04*	2.65E-02	*1.08E-03*
		10	4.65E-02	*8.27E-04*	*3.95E-04*	*9.77E-04*	*6.14E-04*	*4.23E-04*	4.42E-03	*9.17E-04*	*7.75E-04*	4.07E-02	*4.55E-04*
		11	4.66E-02	*8.27E-04*	*3.46E-04*	*9.77E-04*	*6.14E-04*	*3.71E-04*	4.60E-03	*9.17E-04*	*7.75E-04*	3.09E-02	3.99E-04
		12	*3.40E-02*	*7.90E-04*	*3.42E-04*	*9.34E-04*	*5.87E-04*	*3.66E-04*	*3.17E-03*	*8.77E-04*	*7.41E-04*	*1.48E-02*	*4.72E-04*
	DL | RL		7.87E-05	8.27E-04	4.08E-04	9.77E-04	6.14E-04	4.37E-04	9.21E-05	9.17E-04	7.75E-04	1.11E-04	9.50E-04
	Quality Flags	1	E									E	
		2	E									E	
		3	E									E	
		4	E										
		5	E									E	
		6	E									E	
		7	E									E	
		8	E									E	
		9	E									E	
		10	E									E	
		11	E									E	
		12	E										
Headspace Series B	Concentration (ppm)[1]	1	*9.87E-04*	*8.03E-04*	*3.84E-04*	*9.50E-04*	*5.96E-04*	*4.11E-04*	*1.07E-03*	*8.91E-04*	*7.53E-04*	*7.20E-04*	*4.43E-04*
		2	*9.73E-04*	*7.92E-04*	*3.65E-04*	*9.36E-04*	*5.88E-04*	*3.91E-04*	*1.06E-03*	*8.79E-04*	*7.42E-04*	*7.10E-04*	*4.21E-04*
		3	*9.73E-04*	*7.92E-04*	*4.08E-04*	*9.36E-04*	*5.88E-04*	*4.37E-04*	*1.06E-03*	*8.78E-04*	*7.42E-04*	*7.10E-04*	*4.71E-04*
		4	*1.01E-03*	*8.20E-04*	*4.00E-04*	*9.69E-04*	*6.09E-04*	*4.28E-04*	*1.10E-03*	*9.10E-04*	*7.68E-04*	*7.35E-04*	*4.61E-04*
		5	*9.92E-04*	*8.08E-04*	*3.81E-04*	*9.55E-04*	*6.00E-04*	*4.08E-04*	*1.08E-03*	*8.96E-04*	*7.57E-04*	*7.24E-04*	*4.39E-04*
		6	*9.17E-04*	*7.46E-04*	*3.71E-04*	*8.82E-04*	*5.54E-04*	*3.98E-04*	*9.97E-04*	*8.28E-04*	*6.99E-04*	*6.69E-04*	*4.28E-04*
		7	*9.86E-04*	*8.03E-04*	*3.41E-04*	*9.49E-04*	*5.96E-04*	*3.65E-04*	*1.07E-03*	*8.91E-04*	*7.52E-04*	*7.20E-04*	*3.93E-04*
		8	*9.40E-04*	*7.65E-04*	*3.51E-04*	*9.05E-04*	*5.68E-04*	*3.76E-04*	*1.02E-03*	*8.49E-04*	*7.17E-04*	*6.86E-04*	*4.05E-04*
		9	*1.01E-03*	*8.26E-04*	*3.61E-04*	*9.76E-04*	*6.13E-04*	*3.87E-04*	*1.10E-03*	*9.16E-04*	*7.74E-04*	*7.40E-04*	*4.16E-04*
		10	*1.02E-03*	*8.27E-04*	*3.95E-04*	*9.77E-04*	*6.14E-04*	*4.23E-04*	*1.10E-03*	*9.17E-04*	*7.75E-04*	*7.41E-04*	*4.55E-04*
		11	*1.02E-03*	*8.27E-04*	*3.46E-04*	*9.77E-04*	*6.14E-04*	*3.71E-04*	*1.10E-03*	*9.17E-04*	*7.75E-04*	*7.41E-04*	*3.99E-04*
		12	9.71E-04	7.90E-04	3.42E-04	9.34E-04	5.87E-04	3.66E-04	1.06E-03	8.77E-04	7.41E-04	7.08E-04	3.94E-04
	DL | RL		1.02E-03	8.27E-04	4.08E-04	9.77E-04	6.14E-04	4.37E-04	1.10E-03	9.17E-04	7.75E-04	7.41E-04	9.50E-04
	Quality Flags	1											
		2											
		3											
		4											
		5											
		6											
		7											
		8											
		9											
		10	J										
		11											
		12											

[1] Values italicized and underlin

Appendix C

Statistical Analysis

Appendix C

Statistical Analysis

C.1 Descriptive Statistics for COPCs with at Least One Detected Value

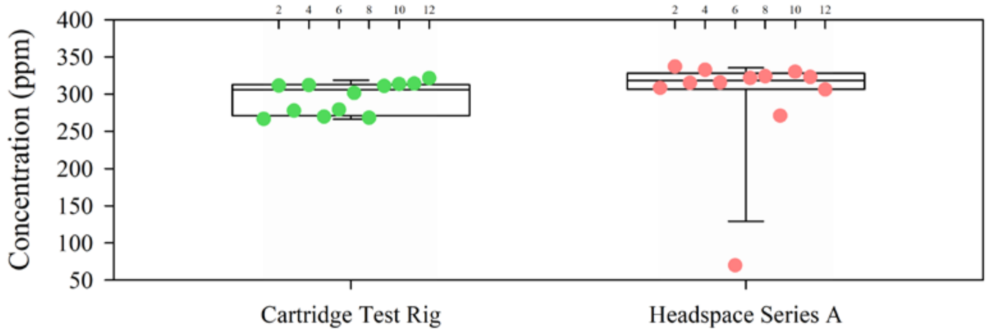
	Cartridge Test Rig									Headspace Series A								
COPCs Concentration (ppm)	Number Detected	Mean	Standard Deviation	Minimum	Q1	Median	Q3	Maximum	CV	Number Detected	Mean	Standard Deviation	Minimum	Q1	Median	Q3	Maximum	CV
Ammonia	12	295.1	21.3	266.0	271.2	305.8	312.8	321.0	7.2%	12	295.9	73.6	68.6	306.5	318.4	328.3	337.0	25%
Mercury	0	NA	NA	NA	NA	NA	NA	NA	NA	1	0.000409	NA	NA	NA	0.0004	NA	NA	NA
Benzene	12	0.0024	0.0008	0.0012	0.0016	0.0024	0.0030	0.0034	33%	12	0.0023	0.0005	0.0015	0.0019	0.0024	0.0026	0.0031	22%
Methanol	2	0.4838	NA	0.4162	NA	0.4890	NA	0.5126	NA	11	0.7100	0.2073	0.4843	0.530	0.6756	0.859	1.1183	29%
2-Hexanone	12	0.0042	0.0023	0.0013	0.0017	0.0041	0.0063	0.0073	54%	12	0.0076	0.0020	0.0042	0.0061	0.0077	0.0091	0.0107	26%
4-Methyl-2-hexanone	0	NA	NA	NA	NA	NA	NA	NA	NA	1	0.0009	NA	NA	NA	0.0009	NA	NA	NA
Formaldehyde	7	0.0019	0.0004	0.0015	0.0015	0.0018	0.0021	0.0027	22%	7	0.0036	0.0014	0.0014	0.0017	0.0042	0.0045	0.0051	40%
Acetaldehyde	12	0.0897	0.0181	0.0372	0.0890	0.0928	0.0962	0.1144	20%	10	0.0628	0.0312	0.0045	0.0280	0.0784	0.0855	0.0870	50%
Butanal/ Butyraldehyde	1	0.0014	NA	NA	NA	0.0013	NA	NA	NA	0	NA	NA	NA	NA	NA	NA	NA	NA
Furan	6	0.0017	0.0005	0.0013	0.0014	0.0014	0.0018	0.0029	28%	11	0.0019	0.0004	0.0014	0.0016	0.0018	0.0023	0.0027	22%
Diethylphthalate	1	0.0004	NA	NA	NA	0.0003	NA	NA	NA	0	NA	NA	NA	NA	NA	NA	NA	NA
Acetonitrile	12	0.0643	0.0195	0.0368	0.0505	0.0616	0.0756	0.1065	30%	12	0.0884	0.0259	0.0514	0.0668	0.0905	0.103	0.1305	29%
Propanenitrile	11	0.0043	0.0020	0.0017	0.0025	0.0044	0.0064	0.0067	45%	12	0.0043	0.0014	0.0019	0.0033	0.0043	0.0054	0.0064	33%
N-Nitrosodiethylamine	12	0.0001	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	27%	11	0.0002	0.0002	0.0000	0.0001	0.0002	0.0004	0.0004	67%
N-Nitrosomethylethylamine	12	0.0001	0.0000	0.0001	0.0001	0.0001	0.0001	0.0002	26%	12	0.0013	0.0008	0.0002	0.0006	0.0011	0.0021	0.0022	62%

C.2 Descriptive Statistics for the COPCs Sample Volume (L)

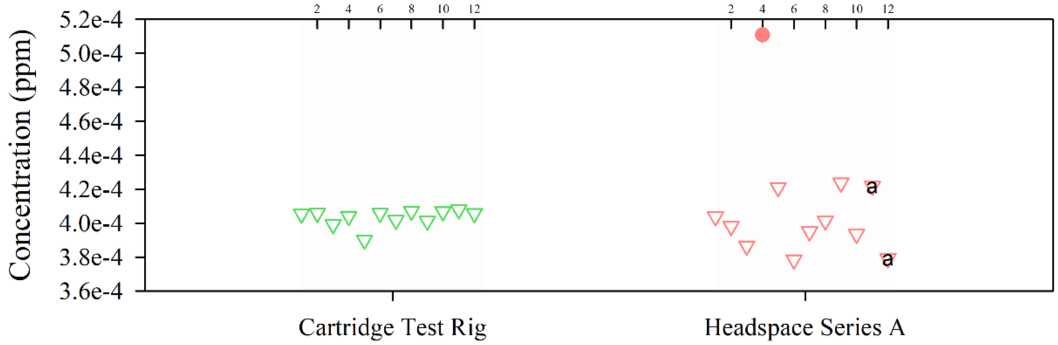
	Cartridge Test Rig									Headspace Series A								
COPCs	Number Samples	Mean	Standard Deviation	Minimum	Q1	Median	Q3	Maximum	CV	Number Samples	Mean	Standard Deviation	Minimum	Q1	Median	Q3	Maximum	CV
Ammonia	12	20.77	0.32	20.29	20.59	20.68	20.88	21.37	1.5%	12	20.19	0.87	19.17	19.50	19.97	20.76	21.87	4.3%
Mercury	12	14.94	0.19	14.77	14.82	14.85	15.01	15.45	1.3%	12	15.04	0.59	14.21	14.40	15.07	15.52	15.92	3.9%
1,3-Butadiene	11	24.49	0.24	24.05	24.32	24.58	24.64	24.84	1.0%	11	22.72	0.59	21.99	22.35	22.59	23.08	23.79	2.6%
Benzene	12	3.13	0.17	2.95	3.03	3.07	3.25	3.51	5.4%	12	2.94	0.09	2.85	2.86	2.93	2.98	3.15	3.2%
Biphenyl	12	3.53	0.31	3.22	3.34	3.46	3.62	4.41	8.8%	12	3.08	0.19	2.78	2.90	3.09	3.27	3.33	6.2%
Methanol	12	3.15	0.23	2.94	2.96	3.08	3.35	3.62	7.2%	12	3.15	0.13	2.94	3.03	3.18	3.27	3.31	4.3%
Formaldehyde	12	25.79	0.31	25.38	25.55	25.76	25.95	26.55	1.2%	11	23.03	2.45	20.52	21.42	22.23	23.82	29.55	10.6%
2,3-Dihydrofuran	12	3.21	0.10	2.99	3.17	3.21	3.29	3.37	3.2%	12	3.04	0.08	2.94	2.98	3.02	3.08	3.21	2.5%
Ethylamine	12	9.02	3.49	5.40	5.69	8.96	12.28	12.87	38.7%	12	11.82	0.35	11.36	11.53	11.78	12.02	12.64	3.0%
N-Nitrosodimethylamine	12	47.75	0.17	47.49	47.58	47.78	47.85	48.04	0.4%	12	49.90	1.01	48.02	48.87	50.04	50.87	50.96	2.0%

C.3 Data Visualization for COPCs

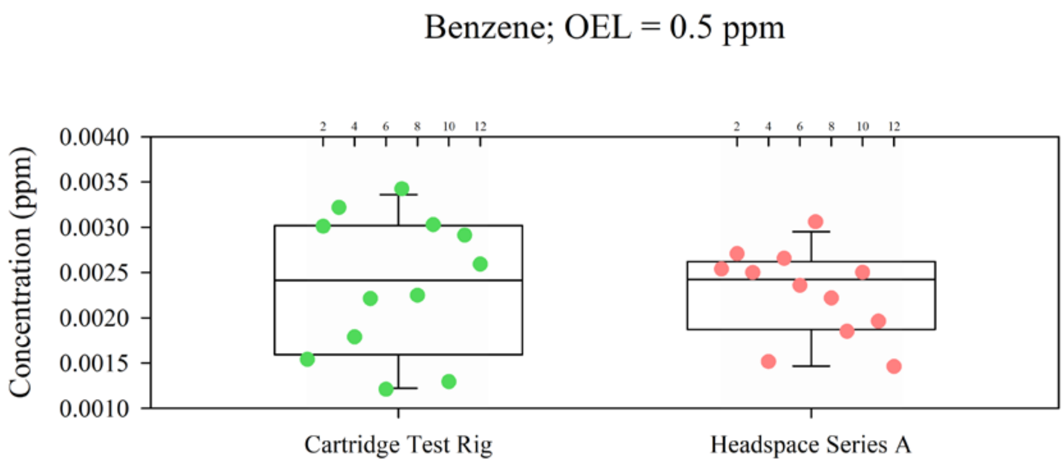
C.3.1 Ammonia


Ammonia; OEL = 25 ppm

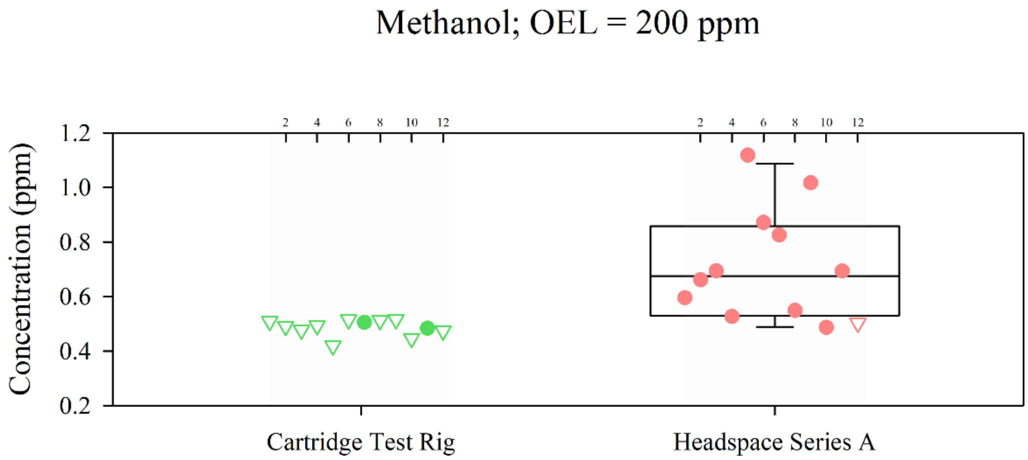
C.3.2 Mercury


Mercury; OEL = 0.003 ppm

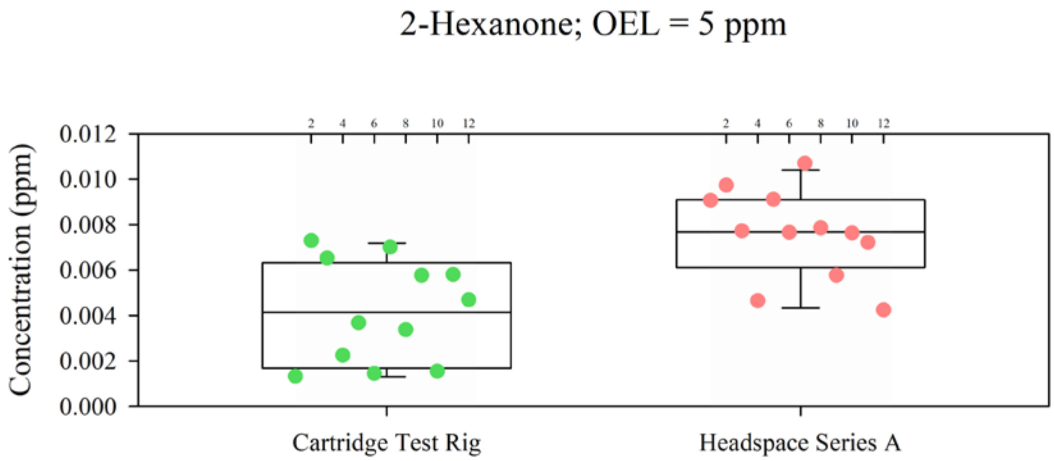
C.3.3 Benzene



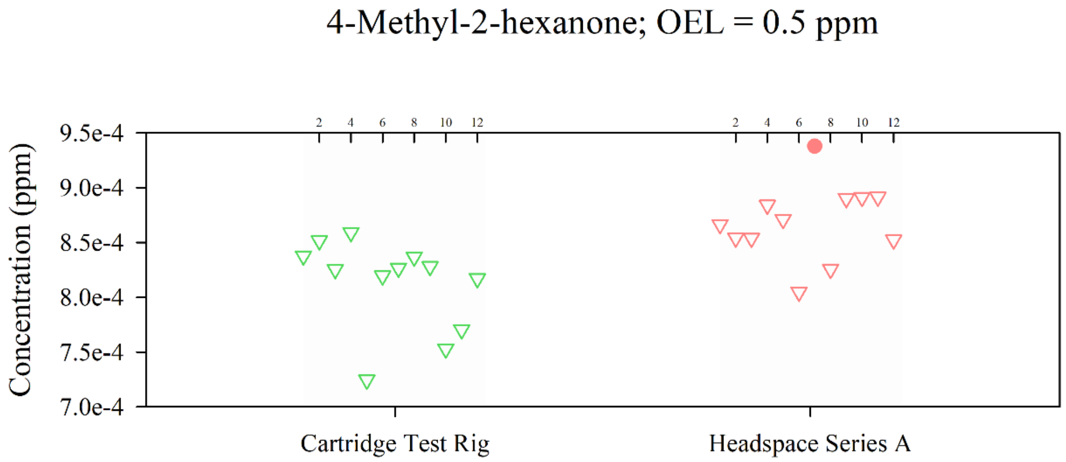
C.3.4 Methanol



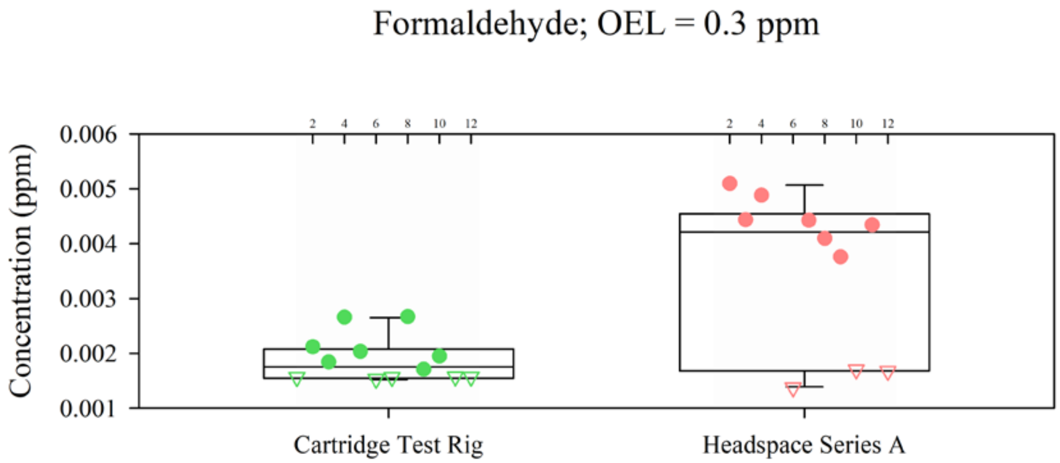
C.3.5 2-Hexanone



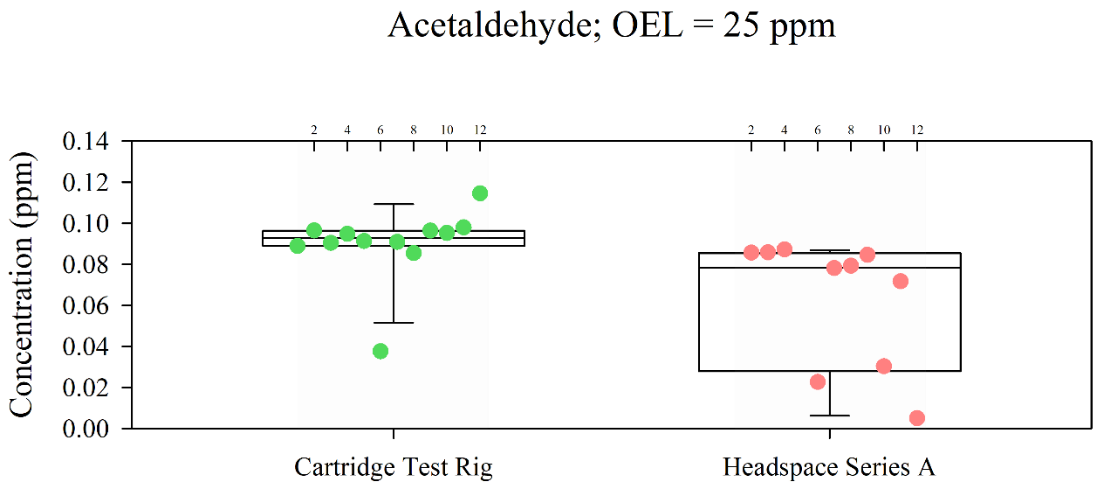
C.3.6 4-Methyl-e-hexanone



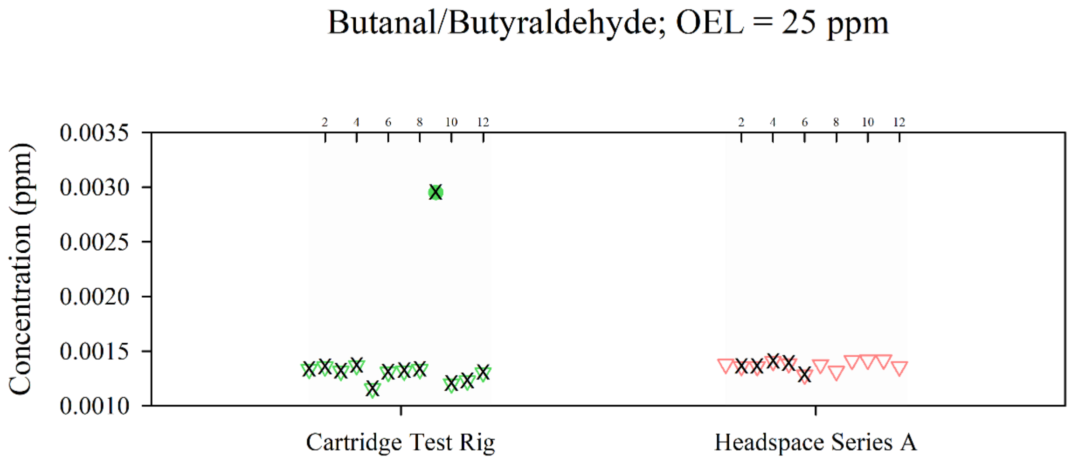
C.3.7 Formaldehyde



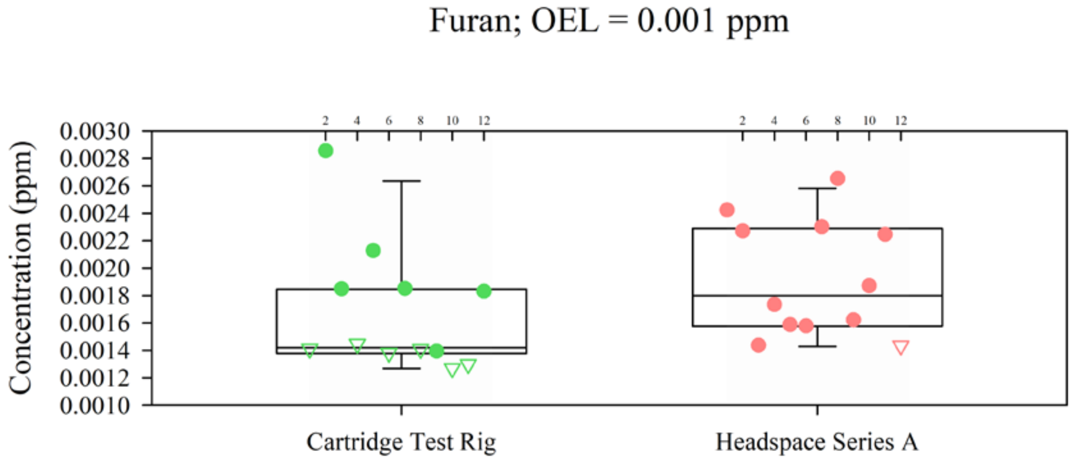
C.3.8 Acetaldehyde



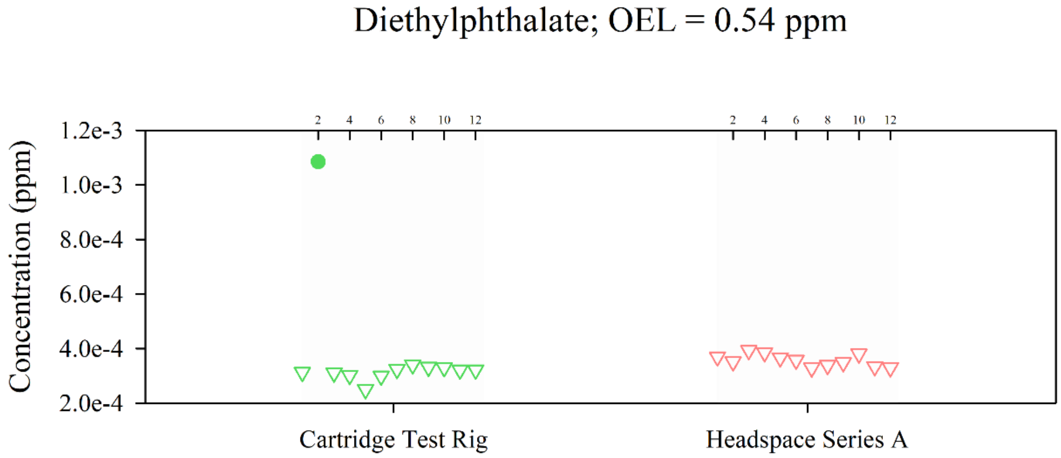
C.3.9 Butanal/Butyraldehyde



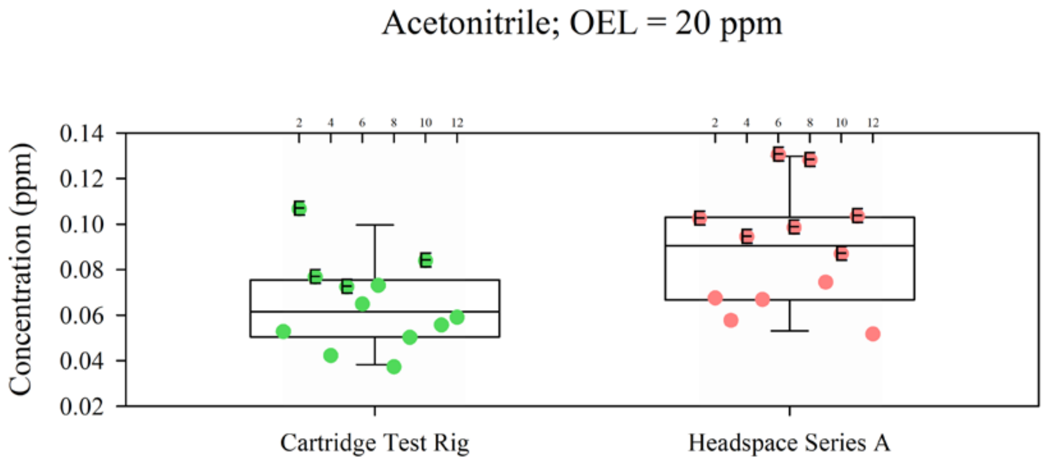
C.3.10 Furan



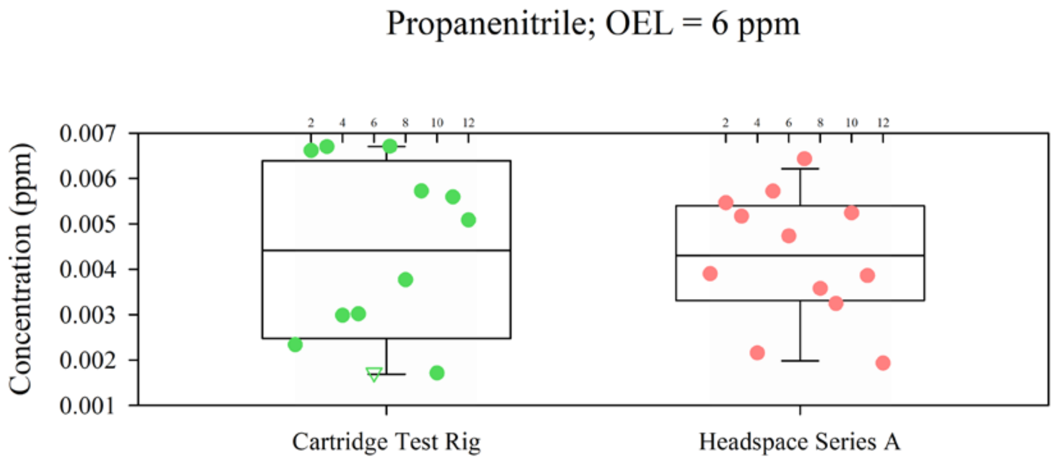
C.3.11 Diethylphthalate



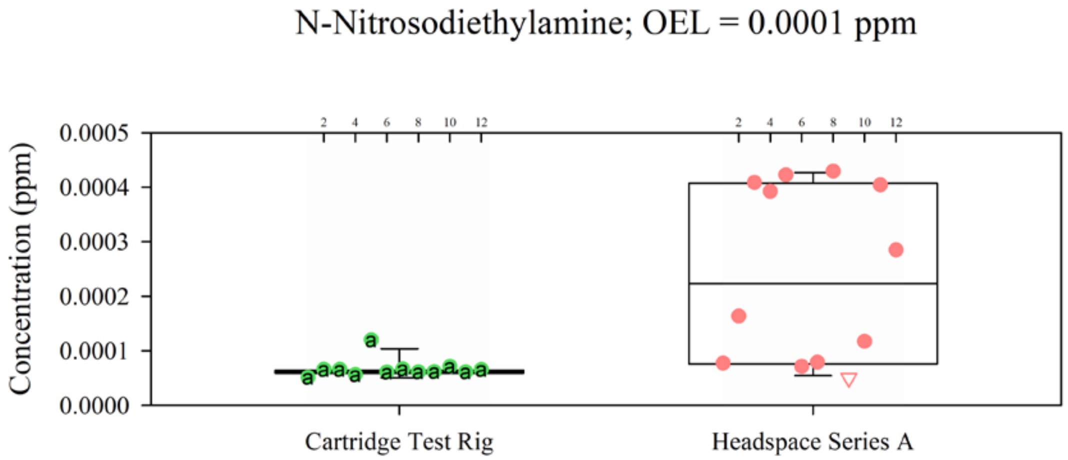
C.3.12 Acetonitrile



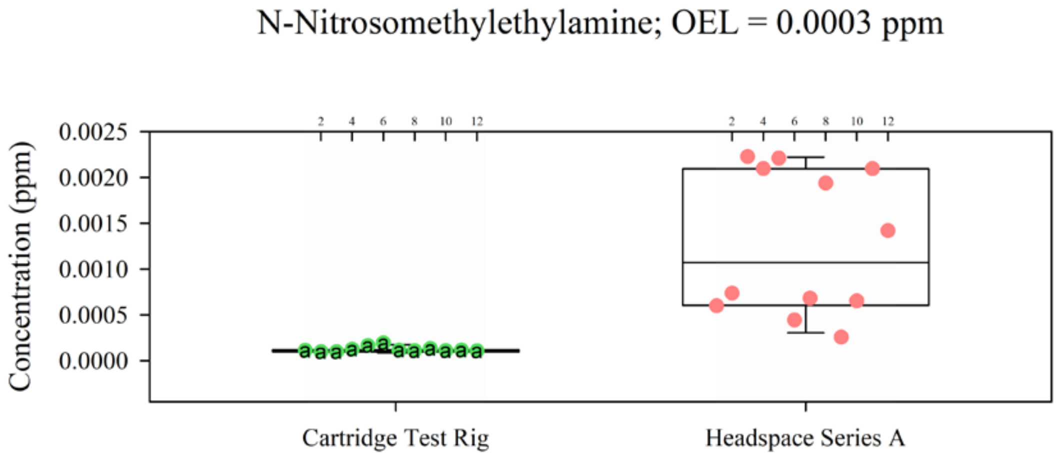
C.3.13 Propanenitrile



C.3.14 N-Nitrosodiethylamine



C.3.15 N-Nitrosomethylethylamine



C.4 Summary for COPCs with Less Than Four Detected Values for Either Sampling Method

C.4.1 Mercury 7439-97-6

Mercury was detected in only one HS sample of the headspace of tank BY-110 at a concentration of approximately 0.5 ppb with the HS sampling system and not at all with the CT sampling system**.** Figure C.1 is a box plot depicting the 12 replicate samples from both sampling systems. Two headspace censored measurements were flagged with an “a” indicating that spikes were under or over-recovered.

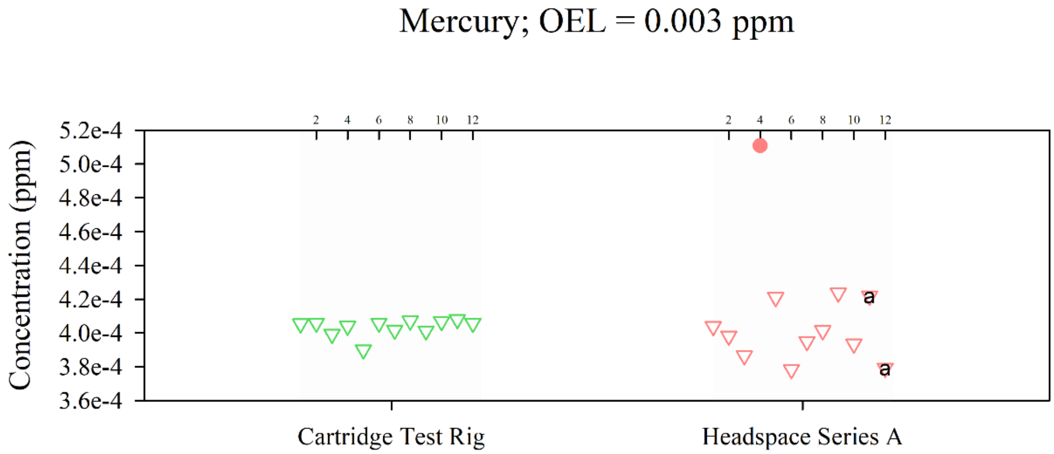


Figure C.1. Box Plot of Mercury Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT system was not significantly different (binomial test; p = 0.35) than the proportion detected with the HS system (Table C.1). The median HS concentration (including the unique detection limits in the calculation) was 13% of the OEL. However, comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with either sampling system.

The sample volume of the analytical method for mercury, however, was analyzed and the median sample volumes from both sampling methods were not statistically different (p = 0.218). The Levene's test was not conducted because the CT standard deviation was less than the HS standard deviation by approximately a third. The ratio of the maximum to the minimum standard deviation was 3.1 indicating by the rule-of-thumb criteria that the variances in sample volume were not equal between the two sampling methods (HS CV = 3.9% and CT CV = 1.3%).

Table C.1. Statistical Comparison of Mercury Measurements from CT and HS Samples

				Cartridge Test Rig (CT)		Headspace Series A (HS)		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Mercury	Mercury	0.003		0	12	1	11, 2 flagged	NS; p=0.35
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	NA	0.0004	NA	Mann-Whitney	NA	13%
	Median Sample Volume	L	14.9	15.1	1.4%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.189	0.593	(0.319)	Levene's Test	sCT≤sHS	

C.4.2 Methanol 67-56-1

Methanol was detected in the headspace of tank BY-110 in all but one sample with the HS sampling system and in only two samples with the CT sampling system. The median HS concentration was approximately 0.7 ppm. Figure C.2 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

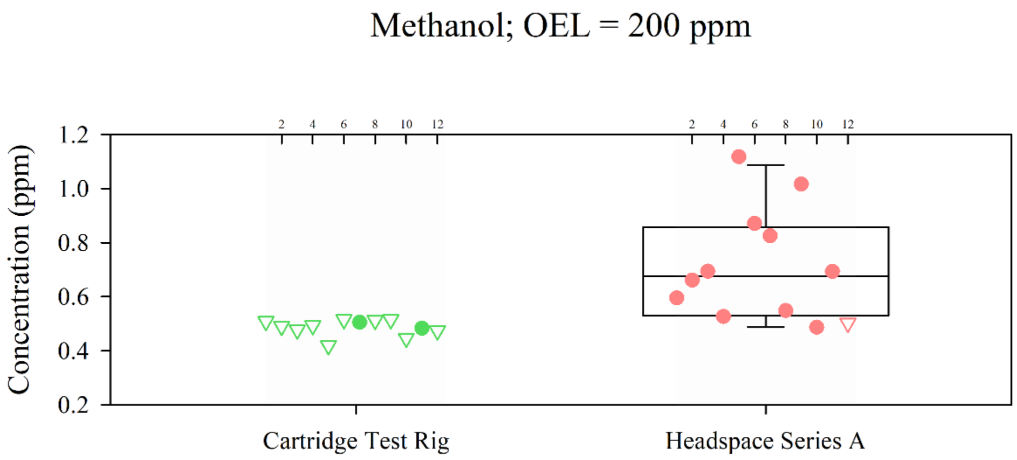


Figure C.2. Box Plot of Methanol Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems.

The proportion of CT samples above the detection limit for methanol was significantly less than the HS method ($p < 0.001$) (Table C.2). The HS median concentration was 0.3% of the OEL. Because of so few detected values in the CT samples, the Mann-Whitney test to compare median concentrations and the Levene's test to compare concentration variance between the two sampling systems was not conducted.

The analytical method for methanol sample volume and volume variance were not significantly different between the HS and CT sampling methods (p = 0.33 and 0.14, respectively). The rule-of-thumb criteria of 1.5 was exceeded (ratio = 1.7), however, suggesting that the variances in sample volume were not equal between the two sampling methods (HS CV = 4.3% and CT CV = 7.2%).

Table C.2. Statistical Comparison of Methanol Measurements from CT and HS Samples

				Cartridge Test Rig (CT)		Headspace Series A (HS)		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
Methanol	Methanol	200	148.5	2	10	11	1	p < 0.001
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	0.489	0.676	NA	Mann-Whitney	NA	0.3%
	Concentration Standard Deviation	ppm	NA	0.2073	NA	Levene's Test	NA	
	Median Sample Volume	L	3.08	3.18	3.1%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.226	0.134	(1.69)	Levene's Test	Not Significantly Different	

C.4.3 4-Methyl-2-hexanone 105-42-0

4-Methyl-2-hexanone was detected in the headspace of tank BY-110 in only one HS sample at a concentration of approximately 0.95 ppb and not at all with the CT sampling system. Figure C.3 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

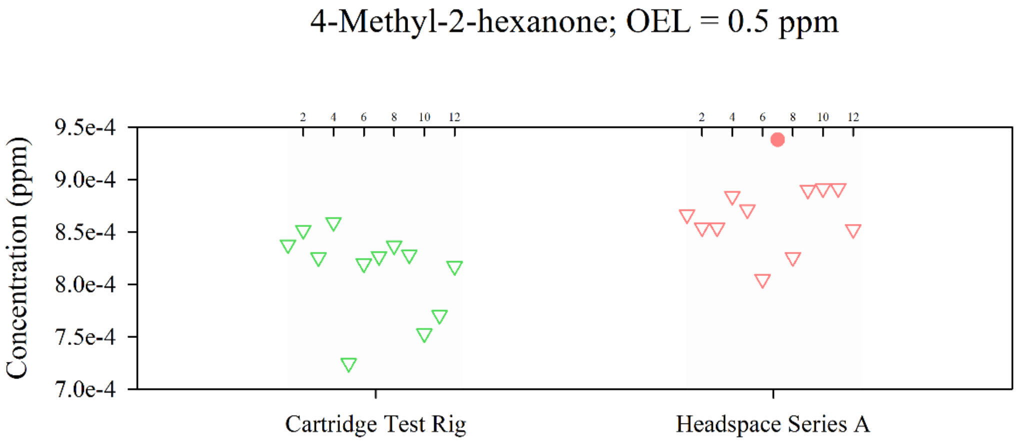


Figure C.3. Box Plot of 4-Methyl-2-hexanone Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was not significantly different (binomial test; p = 0.35) than the proportion detected with the HS sampling system (Table C.2). The median HS concentration (including the unique detection limits in the calculation) was 0.2% of the OEL. The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected observations.

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

Table C.3. Statistical Comparison of 4-Methyl-2-hexanone Measurements from CT and HS Samples

				Cartridge Test Rig (CT)		Headspace Series A (HS)		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
4-Methyl-2-hexanone	VOC	0.5		0	12	1	11	NS; p=0.35
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	NA	0.0009	NA	Mann-Whitney	NA	0.2%
	Median Sample Volume	L	3.07	2.93	-4.9%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.169	0.095	(1.78)	Levene's Test	Not Significantly Different	

C.4.4 Butanal 123-72-8

Butanal was detected in only one CT sample of the headspace of tank BY-110 at a concentration of approximately 3 ppb with the CT sampling system and not at all with the HS sampling system. Figure C.4 is a box plot depicting the 12 replicate samples from both sampling systems. All of the CT samples and five of the HS samples were marked with an "X" indicating "QY" or poor quality flags.

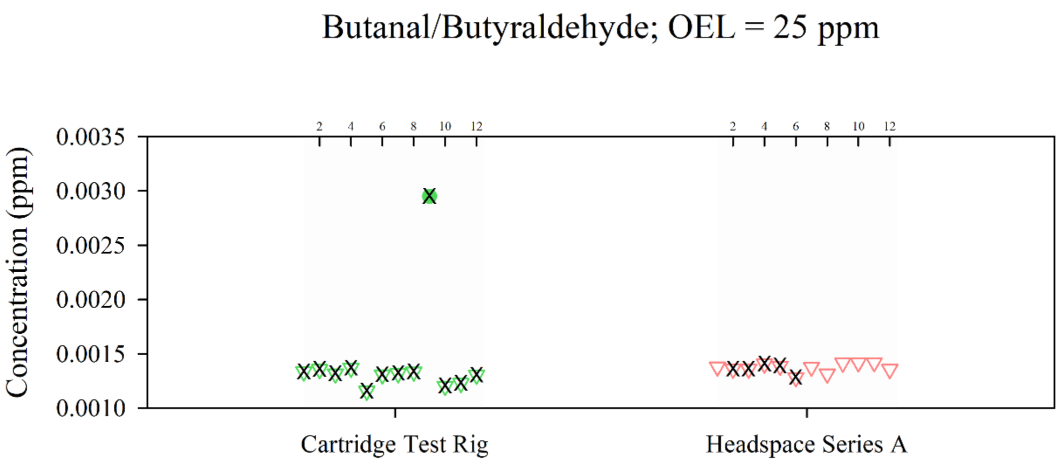


Figure C.4. Box Plot of Butanal Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

No statistical analyses were conducted on the concentration data because there were too few detected values (Table C.4).

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

Table C.4. Statistical Comparison of Butanal Measurements from CT and HS Samples

				Cartridge Test Rig (CT)		Headspace Series A (HS)		Conclusion of
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Test of Equal Proportion Detected
Butanal/Butyraldehyde	VOC	25		1, 1 flagged	11, 11 flagged	0	12, 5 flagged	CT≥HS
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	0.0013	NA	NA	Mann-Whitney	NA	NA
	Median Sample Volume	L	3.07	2.93	-4.9%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.169	0.095	(1.78)	Levene's Test	Not Significantly Different	

C.4.5 Diethylphthalate 84-66-2

Diethylphthalate was detected in the headspace of tank BY-110 in only one CT sample at a concentration of approximately 1.1 ppb and not at all with the CT sampling system. Figure C.5 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

No statistical analyses were conducted on the concentration data because there were too few detected values (Table C.5).

The analytical method for SVOC sample volume was not significantly different between the HS and CT sampling methods (p = 0.999). The percent difference between medians volumes (i.e., [HS-CT]/HS) was -12%. The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.297) even though the ratio sCT:sHS was 1.61. The rule-of-thumb criteria of 1.5 was exceeded, however, suggesting that the variances in sample volume were not equal between the two sampling methods (HS CV = 6.2% and CT CV = 8.8%).

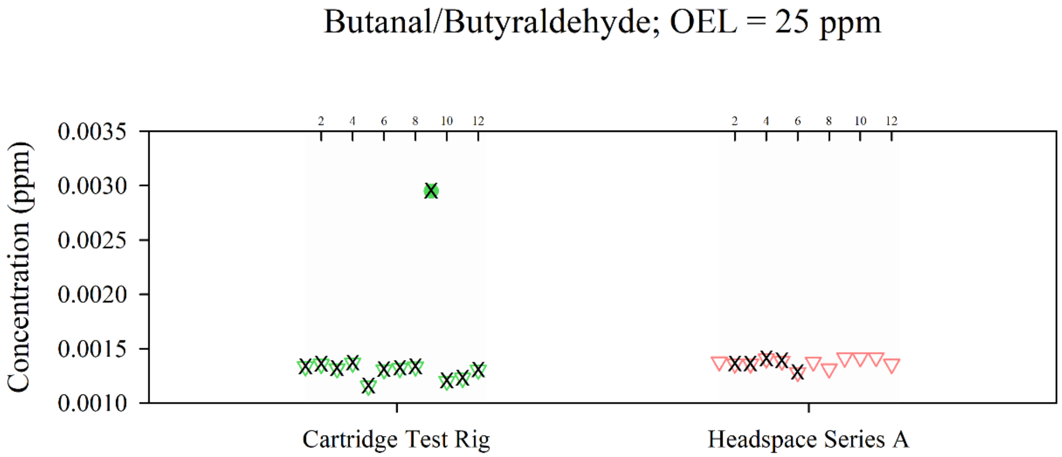


Figure C.5. Box Plot of Diethylphthalate Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

Table C.5. Statistical Comparison of Diethylphthalate Measurements from CT and HS Samples

Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Cartridge Test Rig (CT)		Headspace Series A (HS)		Conclusion of Test of Equal Proportion Detected
				Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Diethylphthalate	SVOC	0.543	563	1	11	0	12	CT≥HS

	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	0.0003	NA	NA	Mann-Whitney	NA	NA
	Median Sample Volume	L	3.46	3.09	-12.1%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.309	0.192	(1.61)	Levene's Test	Not Significantly Different	

C.5 Statistical Analysis for COPCs

C.5.1 Binomial Test

C.5.1.1 Test and CI for One Proportion for Mercury and 4-Methyl-2-hexanone

Method

p: event proportion

Exact method is used for this analysis = binomial test.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	0	0.000000	0.220922

Test

Null hypothesis H_0: p = 0.08333 = 1 detected 11 censored

Alternative hypothesis H_1: p < 0.08333

P-Value
0.352

C.5.1.2 Test and CI for One Proportion for Formaldehyde

Method

p: event proportion

Exact method is used for this analysis = binomial test.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	7	0.583333	0.818975

Test

Null hypothesis H_0: p = 0.7 = 7 detected and 3 censored

Alternative hypothesis H_1: p < 0.7

P-Value = 0.276

C.5.1.3 Test and CI for One Proportion for Propanenitrile

Method

p: event proportion

Exact method is used for this analysis = binomial test.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	11	0.916667	0.995735

Test

Null hypothesis H_0: p = 0.99 Set to 0.99 (12 detected and 0 censored)

Alternative hypothesis H_1: p < 0.99

P-Value = 0.114

C.5.1.4 Test and CI for One Proportion for Methanol

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	2	0.166667	0.438105

Test

Null hypothesis H_0: p = 0.917

Alternative hypothesis H_1: p < 0.917

P-Value = 0.000

C.5.1.5 Test and CI for One Proportion for Furan

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	6	0.500000	0.754700

Test

Null hypothesis	H_0: $p = 0.917$
Alternative hypothesis	H_1: $p < 0.917$

P-Value = 0.000

C.5.2 Mann-Whitney Test of Equal Volume Medians

C.5.2.1 Mann-Whitney: Ammonia_CT, Ammonia_HS

Method

η_1: median of Ammonia_CT

η_2: median of Ammonia_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Ammonia_CT	12	20.6812
Ammonia_HS	12	19.9650

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.7665	1.1289	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value = 188.00

P-Value = 0.987

C.5.2.2 Mann-Whitney: Mercury_CT, Mercury_HS

Method

η_1: median of Mercury_CT

η_2: median of Mercury_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Mercury_CT	12	14.8544
Mercury_HS	12	15.0670

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.147600	0.207500	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

Method	W-Value	P-Value
Not adjusted for ties	136.00	0.218
Adjusted for ties	136.00	0.218

C.5.2.3 Mann-Whitney: 1,3-Butadiene_CT, 1,3-Butadiene_HS

Method

η_1: median of 1,3-Butadiene_CT

η_2: median of 1,3-Butadiene_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
1,3-Butadiene_CT	11	24.5775
1,3-Butadiene_HS	11	22.5920

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
1.9311	2.1675	95.61%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
187.00	1.000

C.5.2.4 Mann-Whitney: Benzene_CT, Benzene_HS

Method

η_1: median of Benzene_CT

η_2: median of Benzene_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Benzene_CT	12	3.07275
Benzene_HS	12	2.92951

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.14932	0.224970	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
204.00	0.999

C.5.2.5 Mann-Whitney: Biphenyl_CT, Biphenyl_HS

Method

η_1: median of Biphenyl_CT
η_2: median of Biphenyl_HS
Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Biphenyl_CT	12	3.46016
Biphenyl_HS	12	3.08580

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.39645	0.54722	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
214.00	1.000

C.5.2.6 Mann-Whitney: Methanol_CT, Methanol_HS

Method

η_1: median of Methanol_CT

η_2: median of Methanol_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Methanol_CT	12	3.08100
Methanol_HS	12	3.17925

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0360450	0.1302	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
142.00	0.333

C.5.2.7 Mann-Whitney: Formaldehyde_CT, Formaldehyde_HS

Method

η_1: median of Formaldehyde_CT

η_2: median of Formaldehyde_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Formaldehyde_CT	12	25.7622
Formaldehyde_HS	11	22.2300

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
3.56704	4.10864	95.47%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

Method	W-Value	P-Value
Not adjusted for ties	198.00	1.000

C.5.2.8 Mann-Whitney: 2,3-Dihydrofuran_CT, 2,3-Dihydrofuran_HS

Method

η_1: median of 2,3-Dihydrofuran_CT

η_2: median of 2,3-Dihydrofuran_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
2,3-Dihydrofuran_CT	12	3.21045
2,3-Dihydrofuran_HS	12	3.02101

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.1879	0.23725	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H$_1$: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
205.00	0.999

C.5.2.9 Mann-Whitney: Ethylamine_CT, Ethylamine_HS

Method

η_1: median of Ethylamine_CT

η_2: median of Ethylamine_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Ethylamine_CT	12	8.9645
Ethylamine_HS	12	11.7795

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-3.03397	0.461845	95.01%

Test

Null hypothesis H$_0$: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H$_1$: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
142.00	0.333

C.5.2.10 Mann-Whitney: N-Nitrosodimethylamine_CT, ...osodimethylamine_HS

Method

η_1: median of N-Nitrosodimethylamine_CT

η_2: median of N-Nitrosodimethylamine_HS

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
N-Nitrosodimethylamine_CT	12	47.7794
N-Nitrosodimethylamine_HS	12	50.0430

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-2.29994	-1.4811	95.01%

Test

Null hypothesis $H_0: \eta_1 - \eta_2 = 0$

Alternative hypothesis $H_1: \eta_1 - \eta_2 < 0$

W-Value	P-Value
79.00	0.000

C.5.2.11 Power and Sample Size

2-Sample t Test
Testing mean 1 = mean 2 (versus ≠)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.6

Results

Sample Size	Power	Difference
12	0.8	0.718087

The sample size is for each group.

C.5.3 Mann-Whitney Test of Equal Concentration Medians

C.5.3.1 Mann-Whitney: Ammonia_CTR, Ammonia_HSA

Method

η_1: median of Ammonia_CTR

η_2: median of Ammonia_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Ammonia_CTR	12	305.816
Ammonia_HSA	12	318.351

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-14.9884	-2.93036	95.01%

Test

Null hypothesis $H_0: \eta_1 - \eta_2 = 0$

Alternative hypothesis $H_1: \eta_1 - \eta_2 < 0$

W-Value	P-Value
113.00	0.018

C.5.3.2 Mann-Whitney: Benzene_CTR, Benzene_HSA

Method

η_1: median of Benzene_CTR

η_2: median of Benzene_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Benzene_CTR	12	0.0024139
Benzene_HSA	12	0.0024237

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.0001803	0.0006557	95.01%

Test

Null hypothesis $H_0: \eta_1 - \eta_2 = 0$

Alternative hypothesis $H_1: \eta_1 - \eta_2 < 0$

W-Value	P-Value
157.00	0.667

C.5.3.3 Mann-Whitney: 2-Hexanone_CTR, 2-Hexanone_HSA

Method

η_1: median of 2-Hexanone_CTR

η_2: median of 2-Hexanone_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median

2-Hexanone_CTR	12	0.0041492
2-Hexanone_HSA	12	0.0076732

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0033185	-0.0018805	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
95.00	0.001

C.5.3.4 Mann-Whitney: Formaldehyde_CTR, Formaldehyde_HSA

Method

η_1: median of Formaldehyde_CTR
η_2: median of Formaldehyde_HSA
Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Formaldehyde_CTR	12	0.0017598
Formaldehyde_HSA	10	0.0042156

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0023248	0.0000000	95.37%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

Method	W-Value	P-Value
Not adjusted for ties	106.50	0.020
Adjusted for ties	106.50	0.018

C.5.3.5 Mann-Whitney: Acetaldehyde_CTR, Acetaldehyde_HSA

Method

η_1: median of Acetaldehyde_CTR

η_2: median of Acetaldehyde_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Acetaldehyde_CTR	12	0.0928221
Acetaldehyde_HSA	10	0.0784492

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.0152066	0.0364913	95.37%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
188.00	1.000

C.5.3.6 Mann-Whitney: Furan_CTR, Furan_HSA

Method

η_1: median of Furan_CTR

η_2: median of Furan_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Furan_CTR	12	0.0013249

Furan_HSA	12	0.0017993

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0003210	-0.0000000	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

Method	W-Value	P-Value
Not adjusted for ties	119.00	0.039
Adjusted for ties	119.00	0.037

C.5.3.7 Mann-Whitney: Acetonitrile_CTR, Acetonitrile_HSA

Method

η_1: median of Acetonitrile_CTR

η_2: median of Acetonitrile_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Acetonitrile_CTR	12	0.0616151
Acetonitrile_HSA	12	0.0905097

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0230831	-0.0079392	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
112.00	0.015

C.5.3.8 Mann-Whitney: Propanenitrile_CTR, Propanenitrile_HSA

Method

Note, the constant detection limit was set to 90% of the minimum detected concentration.

η_1: median of Propanenitrile_CTR

η_2: median of Propanenitrile_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Propanenitrile_CTR	12	0.0044178
Propanenitrile_HSA	12	0.0043077

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.0001520	0.0014556	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
152.00	0.557

C.5.3.9 Mann-Whitney: N-Nitrosodiethylamine_CTR, ... rosodiethylamine_HSA

Method

η_1: median of N-Nitrosodiethylamine_CTR

η_2: median of N-Nitrosodiethylamine_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
N-Nitrosodiethylamine_CTR	12	0.0000618
N-Nitrosodiethylamine_HSA	12	0.0002233

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0001393	-0.0000184	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
94.00	0.001

C.5.3.10 Mann-Whitney: N-Nitrosomethylethylamine_CTR, ... lethylamine_HSA

Method

η_1: median of N-Nitrosomethylethylamine_CTR

η_2: median of N-Nitrosomethylethylamine_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
N-Nitrosomethylethylamine_CTR	12	0.0001032
N-Nitrosomethylethylamine_HSA	12	0.0010725

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0009381	-0.0005419	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
78.00	0.000

C.5.4 Levene Test of Equal Variance for Concentrations

C.5.4.1 Test and CI for Two Variances: Benzene vs Type

Method

σ_1: standard deviation of Benzene when Type = CT

σ_2: standard deviation of Benzene when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.001	0.000	0.001
HS	12	0.000	0.000	0.000

Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.57881	1.049	1.070

Test

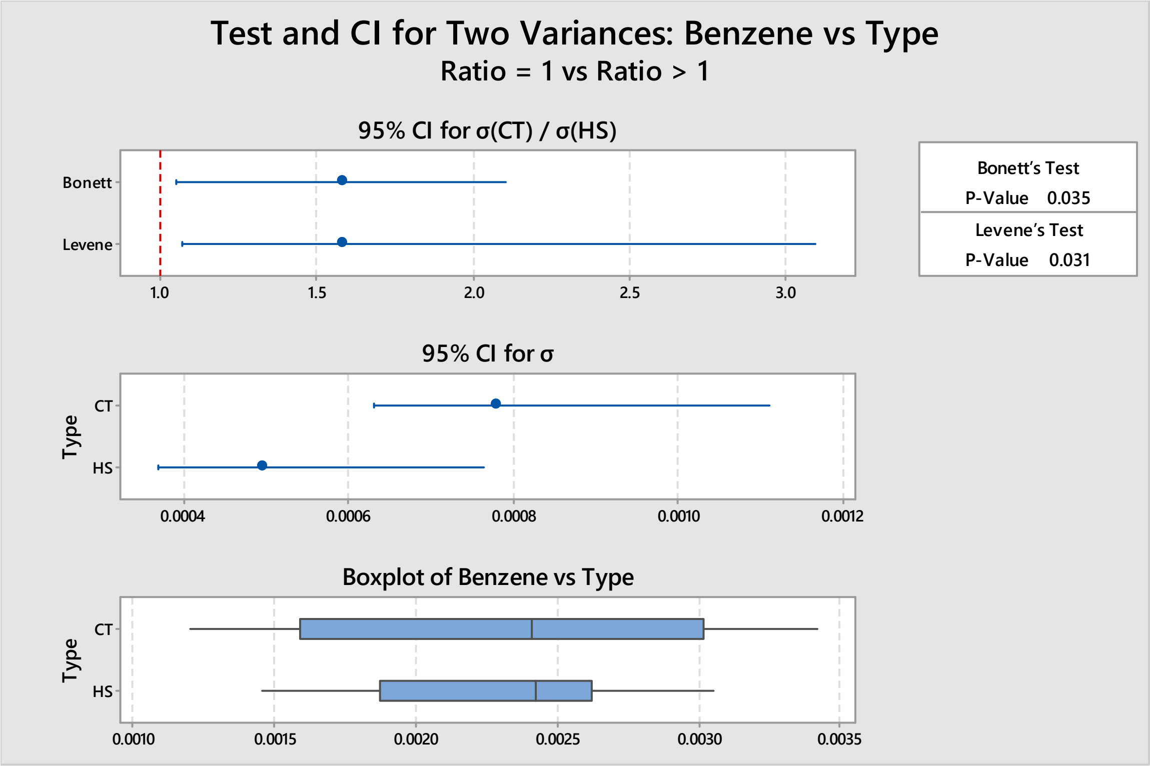
Null hypothesis H_0: $\sigma_1 / \sigma_2 = 1$

Alternative hypothesis H_1: $\sigma_1 / \sigma_2 > 1$

Significance level $\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	3.28	1		0.035

Levene	3.86	1	22	0.031



C.5.4.2 Test and CI for Two Variances: 2-Hexanone vs Type

Method

σ_1: standard deviation of 2-Hexanone when Type = CT

σ_2: standard deviation of 2-Hexanone when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.002	0.000	0.002
HS	12	0.002	0.000	0.001

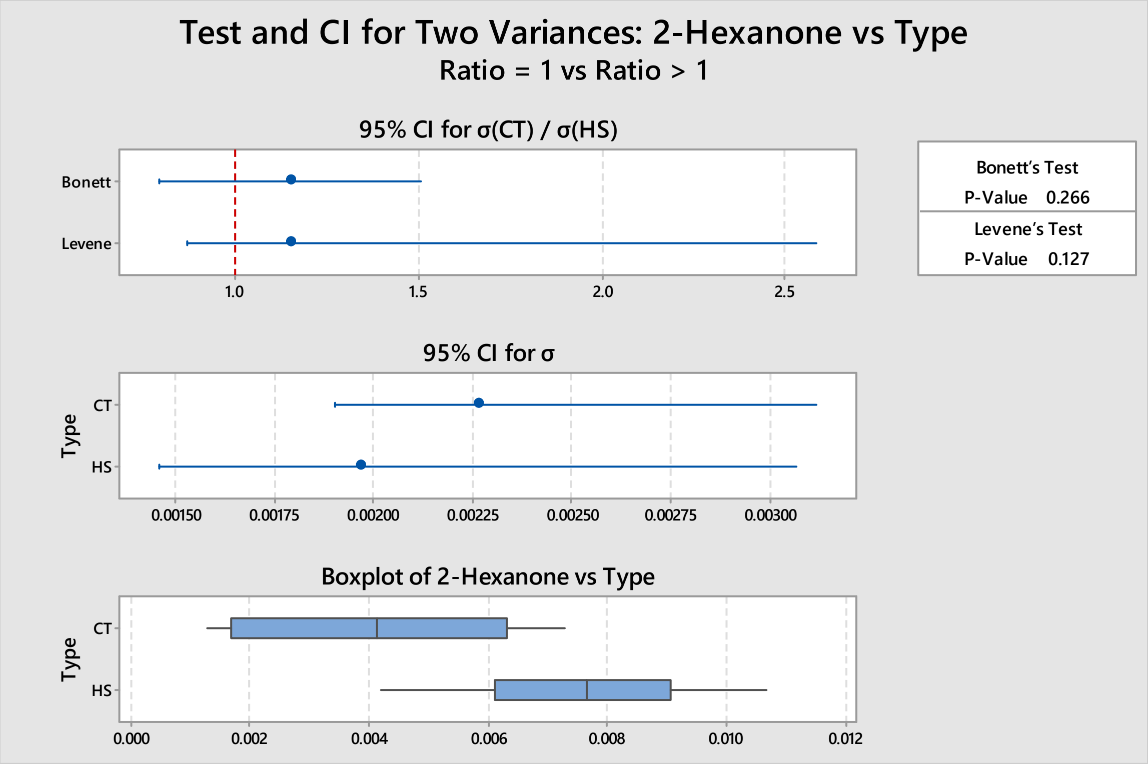
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.15136	0.794	0.868

Test

Null hypothesis	$H_0: \sigma_1 / \sigma_2 = 1$
Alternative hypothesis	$H_1: \sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	0.39	1		0.266
Levene	1.37	1	22	0.127



C.5.4.3 Test and CI for Two Variances: Furan vs Type

Method

σ_1: standard deviation of Furan when Type = CT

σ_2: standard deviation of Furan when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.000	0.000	0.000
HS	12	0.000	0.000	0.000

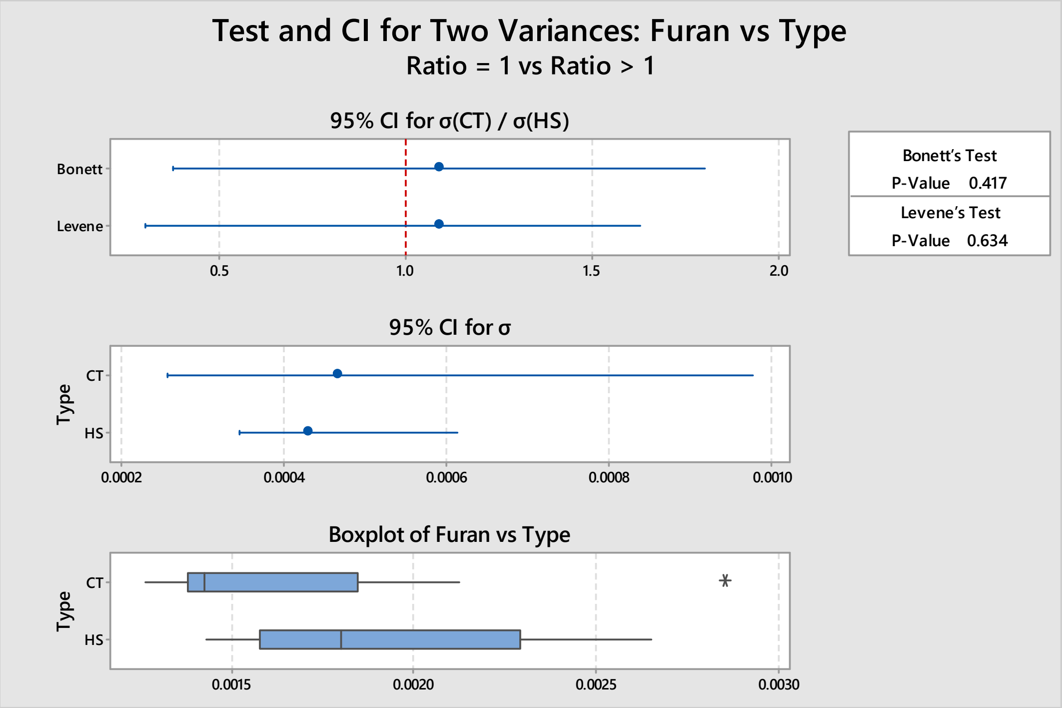
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.08870	0.375	0.298

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	0.04	1		0.417
Levene	0.12	1	22	0.634



C.5.4.4 Test and CI for Two Variances: Propanenitrile vs Type

Method

σ_1: standard deviation of Propanenitrile when Type = CT

σ_2: standard deviation of Propanenitrile when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.002	0.000	0.002
HS	12	0.001	0.000	0.001

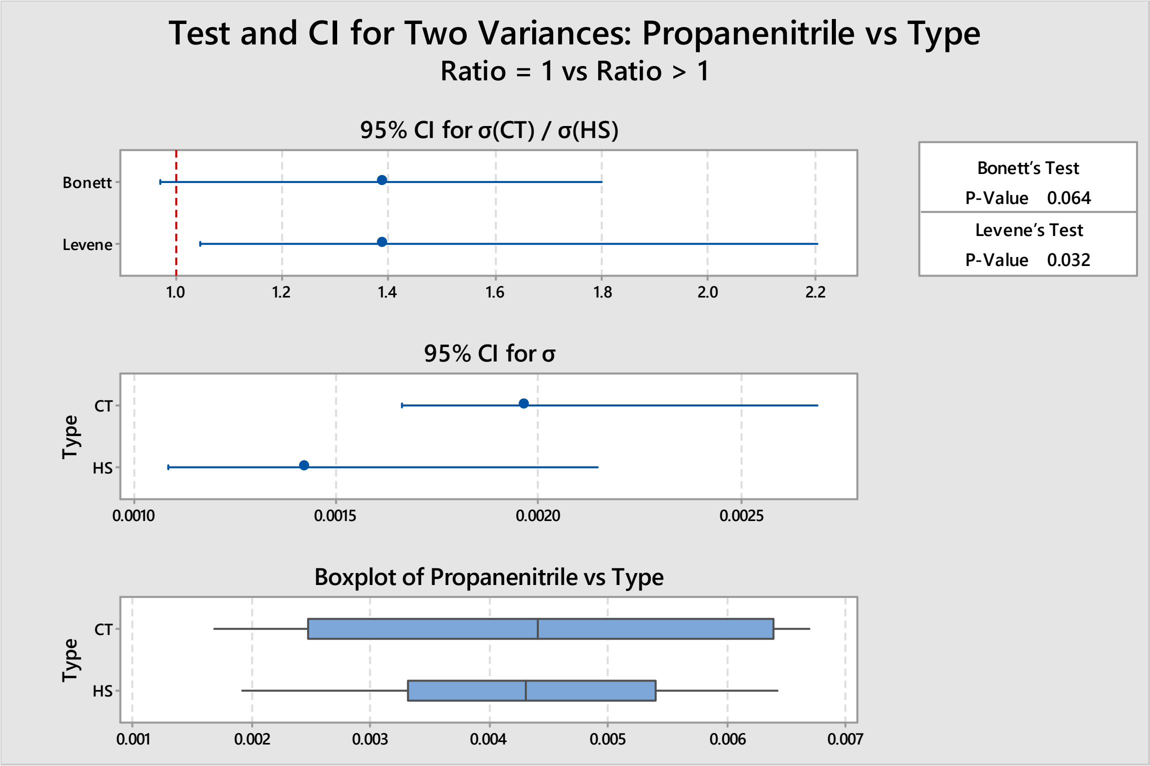
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.38630	0.971	1.047

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	2.31	1		0.064
Levene	3.78	1	22	0.032



C.5.5 Levene's Test of Equal Variance in Sample Volume

C.5.5.1 Test and CI for Two Variances: Benzene vs Type

Method

σ_1: standard deviation of Benzene when Type = CT

σ_2: standard deviation of Benzene when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.169	0.028	0.104
HS	12	0.095	0.009	0.060

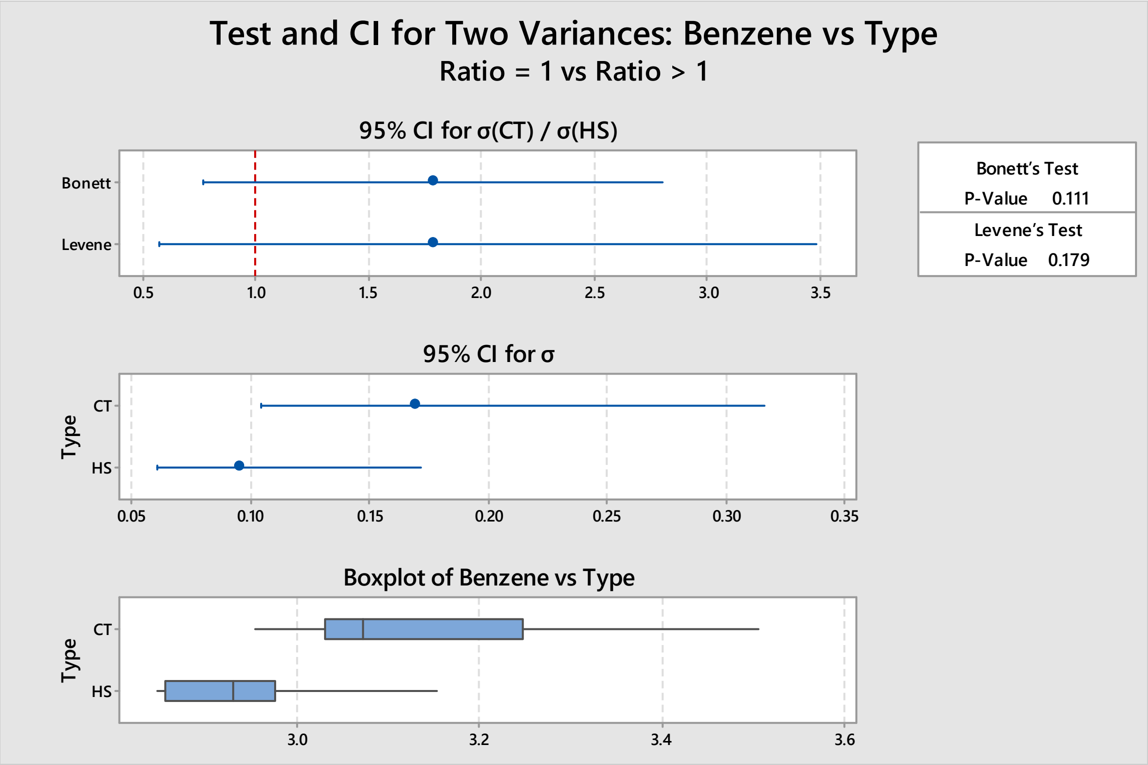
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.78221	0.760	0.570

Test

Null hypothesis	$H_0: \sigma_1 / \sigma_2 = 1$
Alternative hypothesis	$H_1: \sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	1.49	1		0.111
Levene	0.88	1	22	0.179



C.5.5.2 Test and CI for Two Variances: Biphenyl vs Type

Method

σ_1: standard deviation of Biphenyl when Type = CT

σ_2: standard deviation of Biphenyl when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.309	0.095	0.147
HS	12	0.192	0.037	0.156

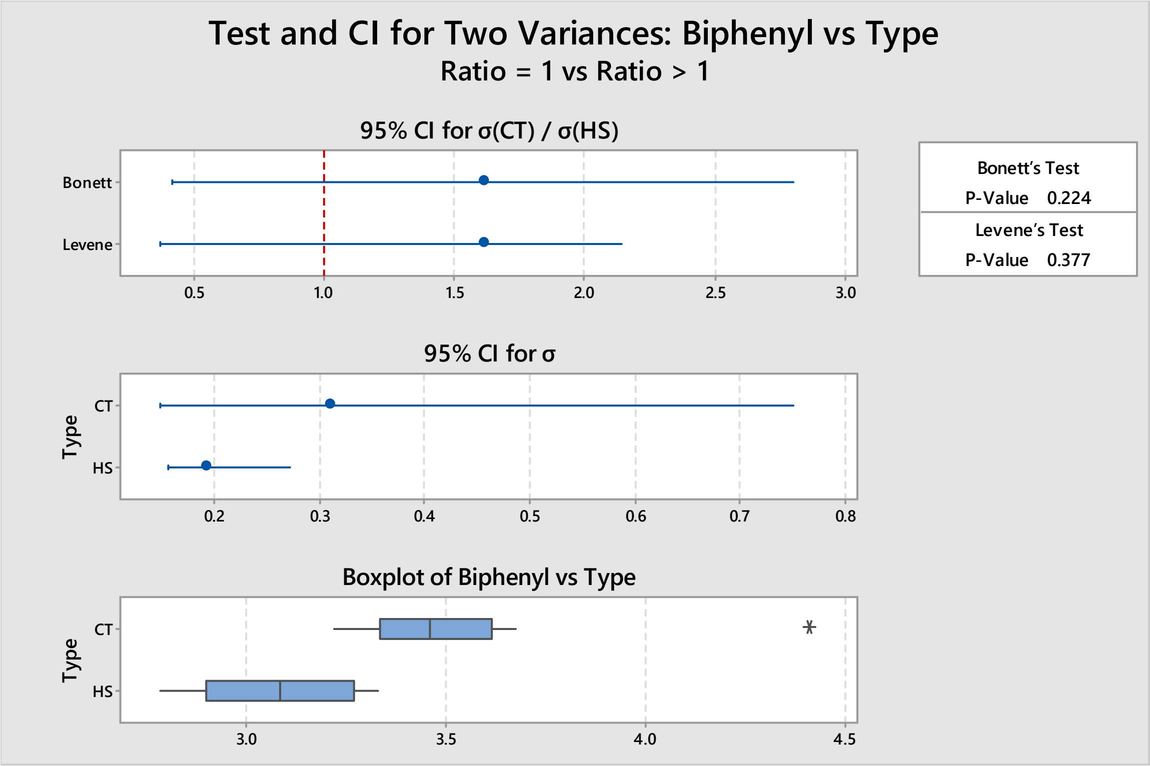
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.61302	0.420	0.367

Test

Null hypothesis	$H_0: \sigma_1 / \sigma_2 = 1$
Alternative hypothesis	$H_1: \sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	0.58	1		0.224
Levene	0.10	1	22	0.377



C.5.5.3 Test and CI for Two Variances: Methanol vs Type

Method

σ_1: standard deviation of Methanol when Type = CT

σ_2: standard deviation of Methanol when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.226	0.051	0.151
HS	12	0.134	0.018	0.111

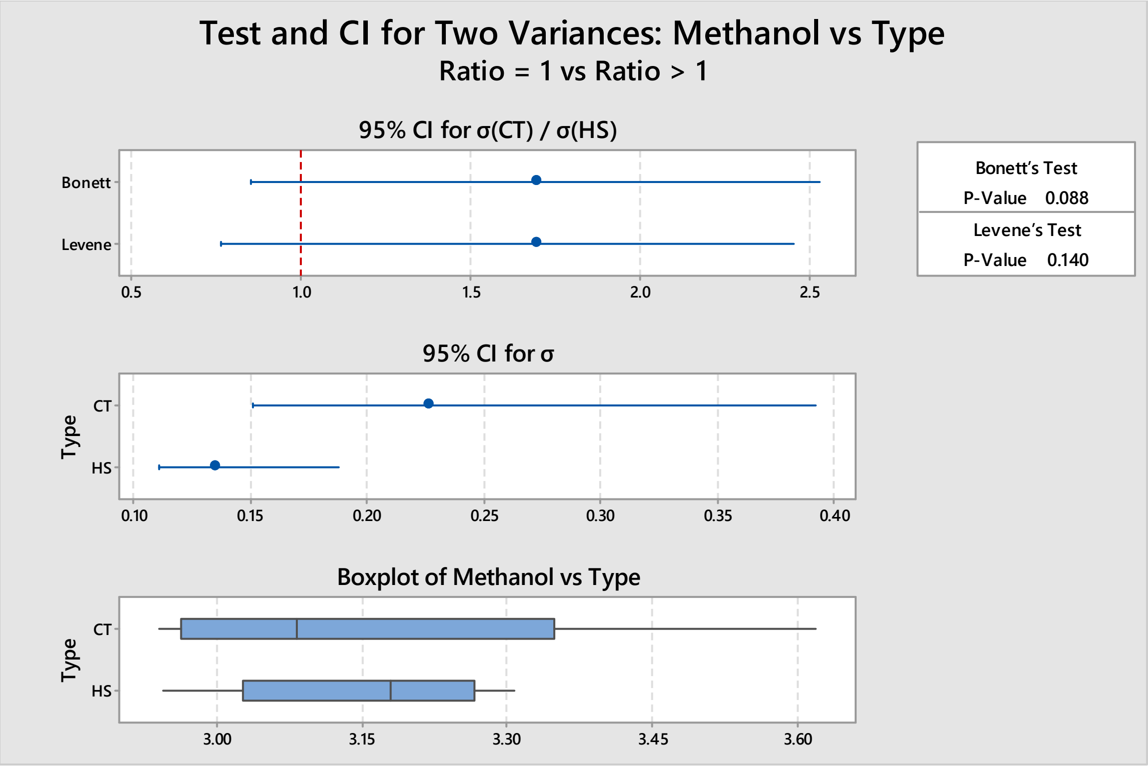
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.68918	0.848	0.763

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	1.82	1		0.088
Levene	1.23	1	22	0.140



C.5.5.4 Test and CI for Two Variances: 2,3-Dihydrofuran vs Type

Method

σ_1: standard deviation of 2,3-Dihydrofuran when Type = CT

σ_2: standard deviation of 2,3-Dihydrofuran when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.104	0.011	0.071
HS	12	0.077	0.006	0.050

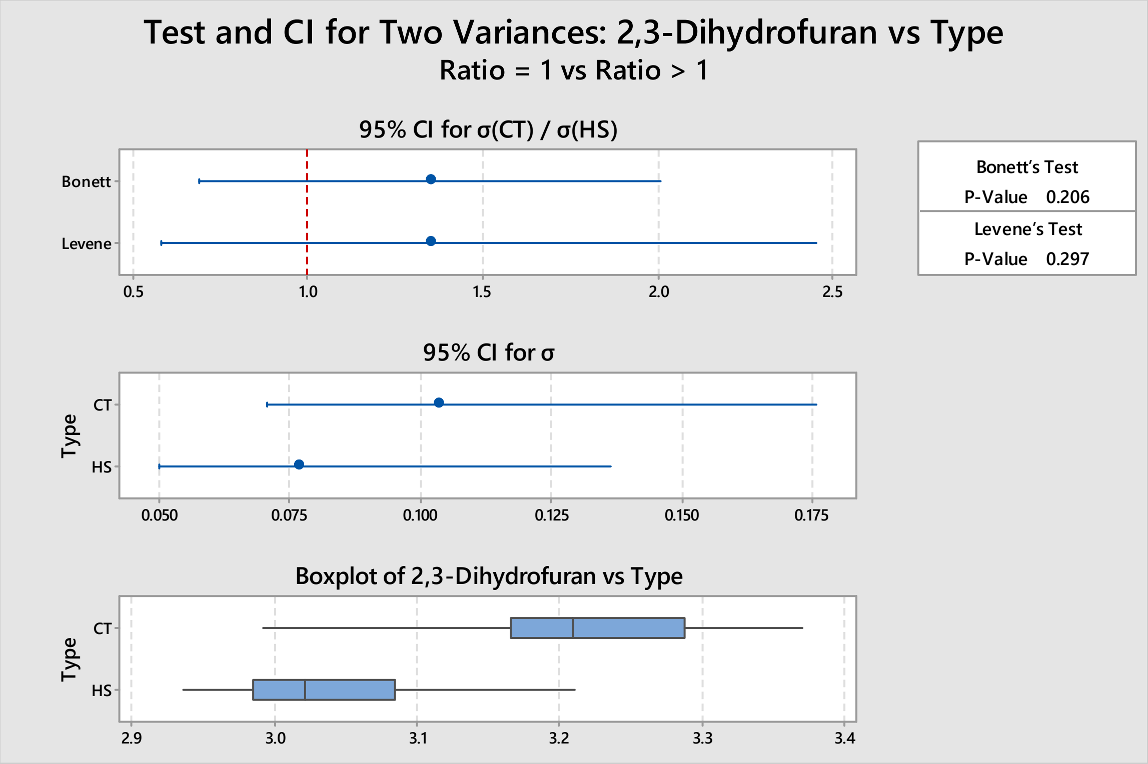
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.34916	0.687	0.579

Test

Null hypothesis	$H_0: \sigma_1 / \sigma_2 = 1$
Alternative hypothesis	$H_1: \sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	0.67	1		0.206
Levene	0.29	1	22	0.297



Test and CI for Two Variances: 2,3-Dihydrofuran vs Type

Ratio = 1 vs Ratio > 1

95% CI for σ(CT) / σ(HS)

95% CI for σ

Boxplot of 2,3-Dihydrofuran vs Type

C.5.5.5 Test and CI for Two Variances: Ethylamine vs Type

Method

σ_1: standard deviation of Ethylamine when Type = CT

σ_2: standard deviation of Ethylamine when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	3.495	12.213	3.237
HS	12	0.349	0.122	0.221

Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
10.0082	6.962	8.972

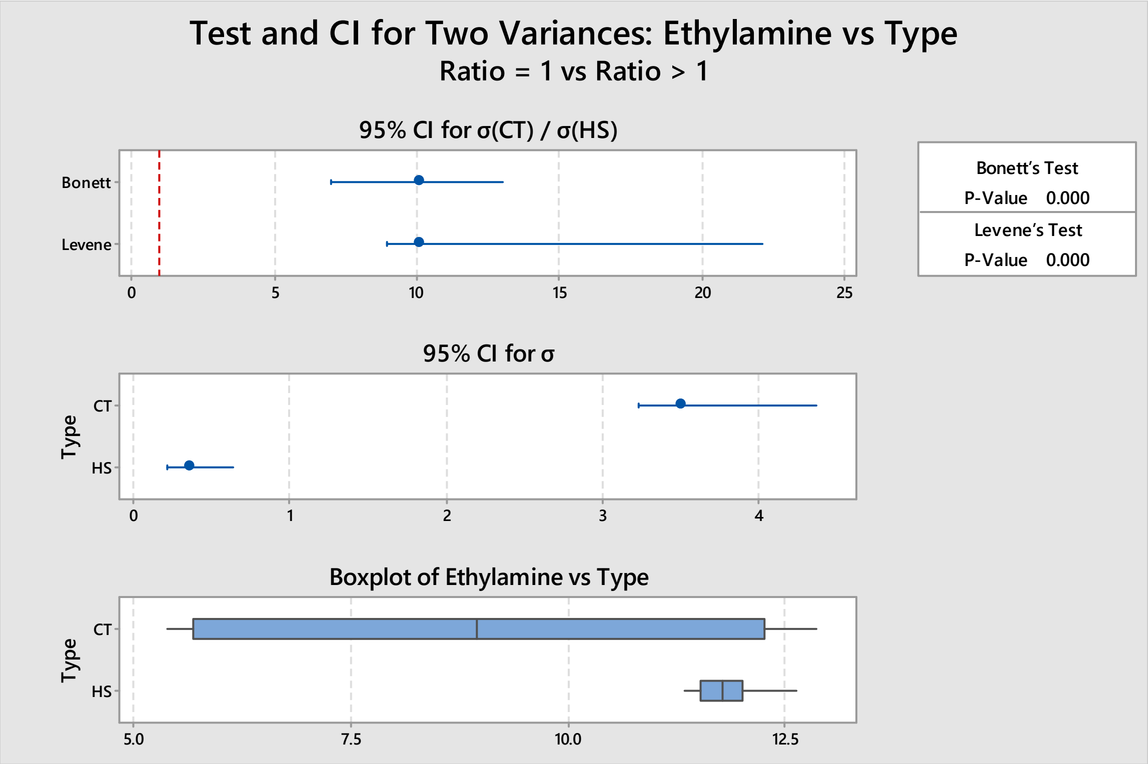
Test

Null hypothesis $H_0: \sigma_1 / \sigma_2 = 1$

Alternative hypothesis $H_1: \sigma_1 / \sigma_2 > 1$

Significance level $\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	92.74	1		0.000
Levene	932.46	1	22	0.000

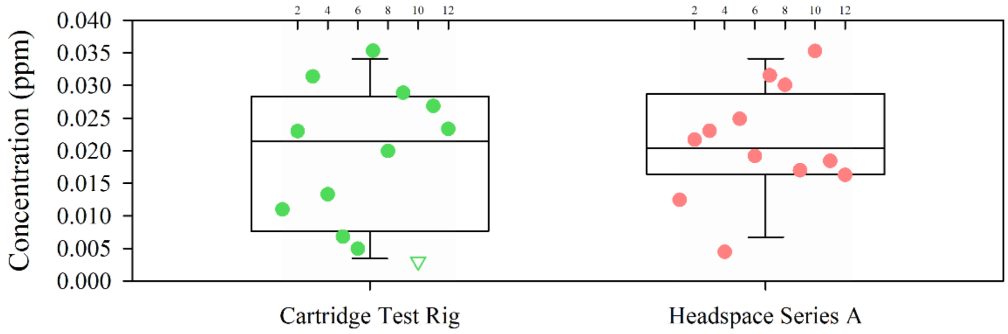


C.6 Descriptive Statistics for Non-COPCs with at Least One Detected Value

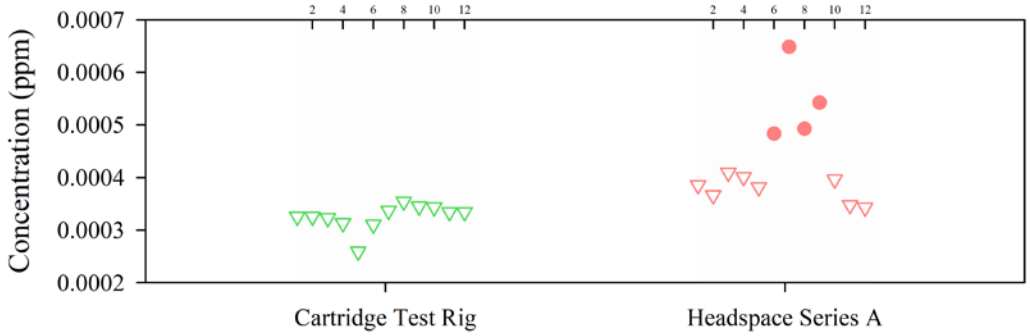
	Cartridge Test Rig									Headspace Series A								
VOCs Concentration (ppm)	Number Detected	Mean	Standard Deviation	Minimum	Q1	Median	Q3	Maximum	CV	Number Detected	Mean	Standard Deviation	Minimum	Q1	Median	Q3	Maximum	CV
1-Propanol	11	0.0189	0.0110	0.0029	0.0077	0.0214	0.0283	0.0353	58%	12	0.0211	0.0086	0.0043	0.0164	0.0204	0.0287	0.0353	41%
2,6,10-Trimethyldodecane	0	NA	NA	NA	NA	NA	NA	NA	NA	4	0.0004	0.0001	0.0003	NA	0.0004	NA	0.0006	21%
2-Butanone	12	0.0292	0.0167	0.0076	0.0133	0.0270	0.0468	0.0556	57%	12	0.0193	0.0120	0.0043	0.0068	0.0186	0.0312	0.0368	62%
2-Heptanone	5	0.0010	0.0003	0.0007	NA	0.0008	NA	0.0016	26.6%	12	0.0054	0.0017	0.0027	0.0041	0.0056	0.0067	0.0079	30.5%
3-Heptanone	7	0.0014	0.0007	0.0008	0.0008	0.0011	0.0019	0.0027	47.7%	12	0.0100	0.0031	0.0050	0.0075	0.0103	0.0127	0.0144	31%
4-Methyl-2-Pentanone	11	0.0026	0.0012	0.0009	0.0012	0.0027	0.0038	0.0044	48%	12	0.0036	0.0008	0.0022	0.0027	0.0037	0.0042	0.0046	23%
Allyl Alcohol	0	NA	NA	NA	NA	NA	NA	NA	NA	1	0.0018	NA	NA	NA	0.0017	NA	NA	NA
Cyclohexane	12	0.0068	0.0029	0.0023	0.0039	0.0071	0.0092	0.0112	44%	12	0.0071	0.0021	0.0038	0.0053	0.0076	0.0089	0.0098	29%
Decane	0	NA	NA	NA	NA	NA	NA	NA	NA	9	0.0012	0.0005	0.0007	0.0007	0.0012	0.0017	0.0019	38%
Dodecane	1	0.0004	NA	NA	NA	0.0004	NA	NA	NA	10	0.0011	0.0006	0.0004	0.0005	0.0009	0.0017	0.0020	53%
Ethanol	12	0.0970	0.0384	0.0389	0.0682	0.1014	0.1314	0.1530	40%	12	0.0670	0.0190	0.0365	0.0545	0.0663	0.0868	0.0917	28%
Hexane	12	0.1043	0.0426	0.0308	0.0601	0.1151	0.1437	0.1549	40.8%	12	0.1170	0.0221	0.0830	0.0956	0.1215	0.133	0.1529	18.9%
Methylene Chloride	1	0.0012	NA	NA	NA	0.0011	NA	NA	NA	0	NA	NA	NA	NA	NA	NA	NA	NA
n-Butyl acetate	0	NA	NA	NA	NA	NA	NA	NA	NA	1	0.0010	NA	NA	NA	0.0009	NA	NA	NA
n-Heptane	12	0.0336	0.0158	0.0101	0.0163	0.0359	0.0488	0.0542	47%	12	0.0500	0.0100	0.0340	0.0402	0.0520	0.0591	0.0641	20%
Tetradecane	0	NA	NA	NA	NA	NA	NA	NA	NA	4	0.0005	0.0001	0.0004	NA	0.0004	NA	0.0008	29%
Toluene	12	0.0032	0.0004	0.0023	0.0030	0.0032	0.0034	0.0038	13%	12	0.0059	0.0019	0.0032	0.0045	0.0060	0.0073	0.0099	33%
Trichlorofluoromethane	12	0.0352	0.0162	0.0108	0.0212	0.0374	0.0497	0.0561	46%	12	0.0340	0.0114	0.0148	0.0268	0.0355	0.0437	0.0510	34%
Tridecane	0	NA	NA	NA	NA	NA	NA	NA	NA	8	0.0007	0.0003	0.0004	0.0005	0.0005	0.0010	0.0013	44%

C.7 Data Visualization for Non-COPCs

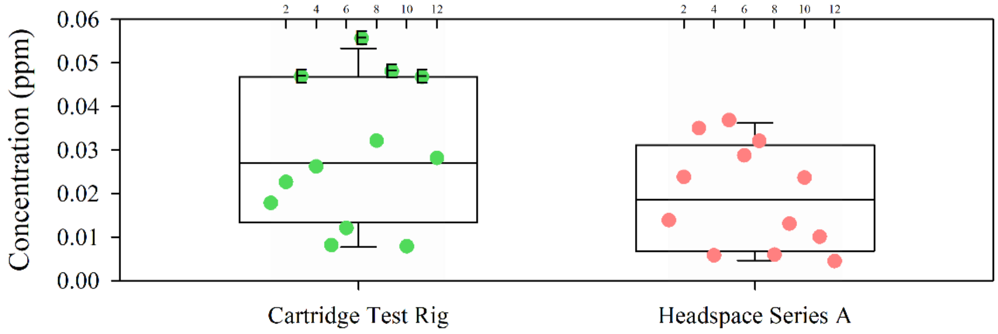
C.7.1 1-Propanol


1-Propanol; OEL = 200 ppm

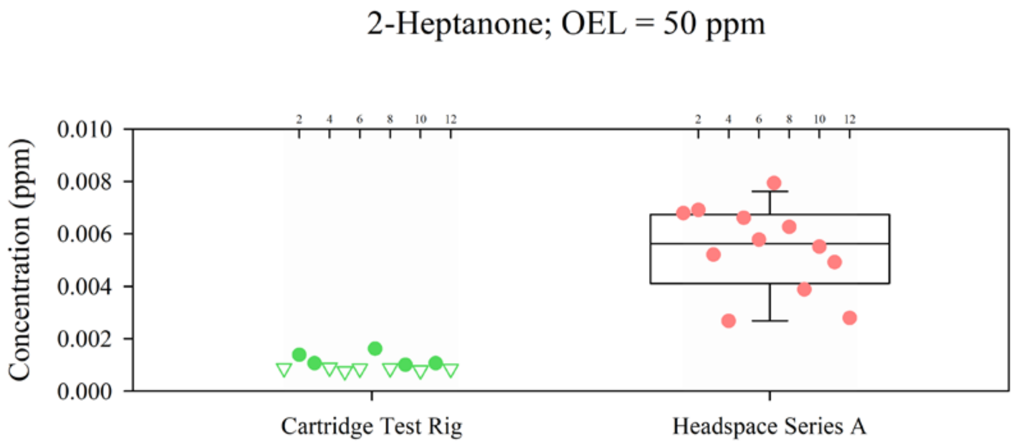
C.7.2 2,6,10-Trimethyldodecane


2,6,10-Trimethyldodecane

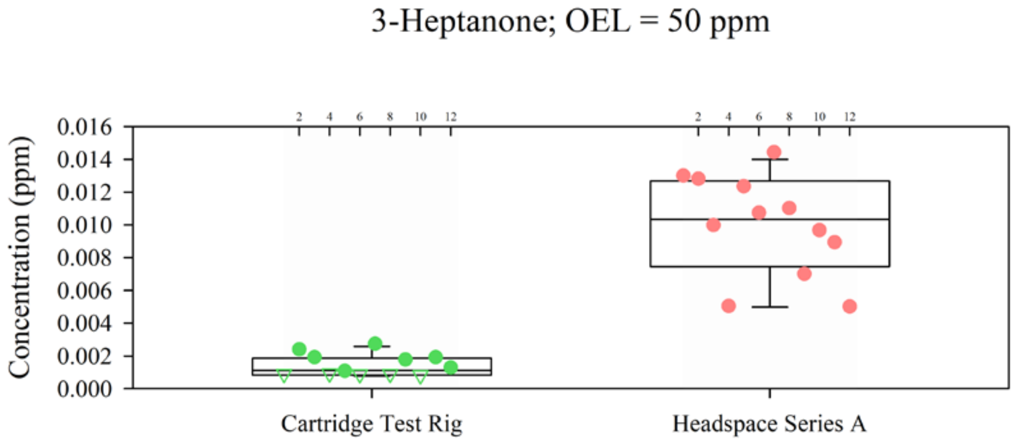
C.7.3 2-Butanone


2-Butanone; OEL = 200 ppm

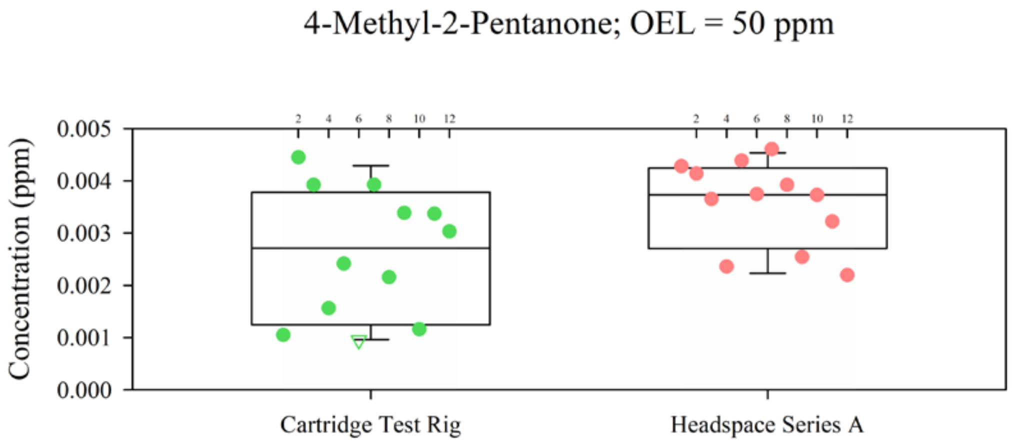
C.7.4 2-Heptanone



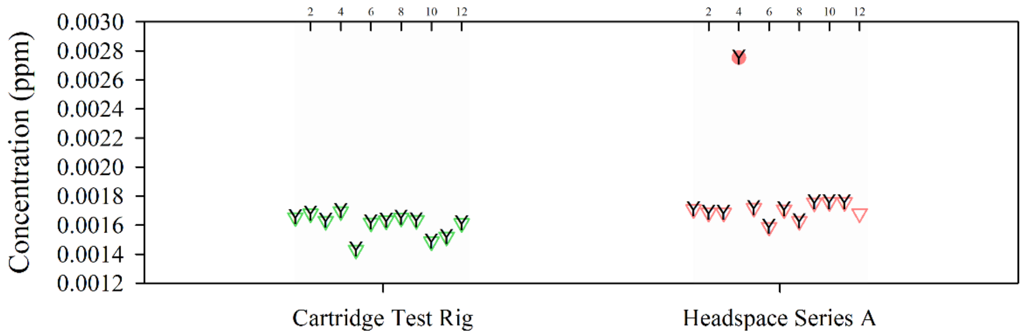
C.7.5 3-Heptanone



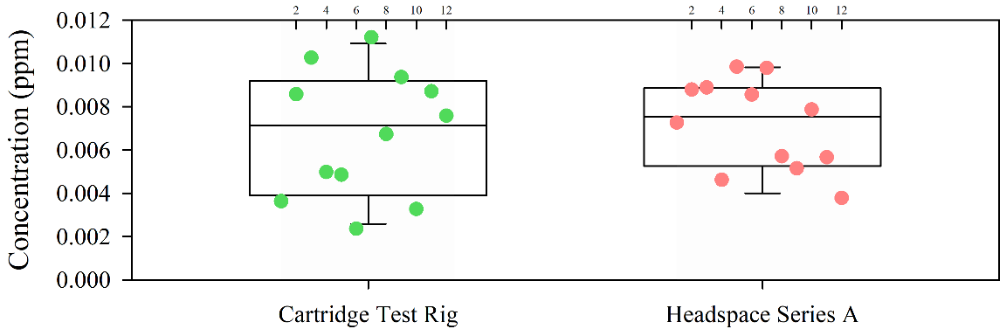
C.7.6 4-Methyl-2-Pentanone



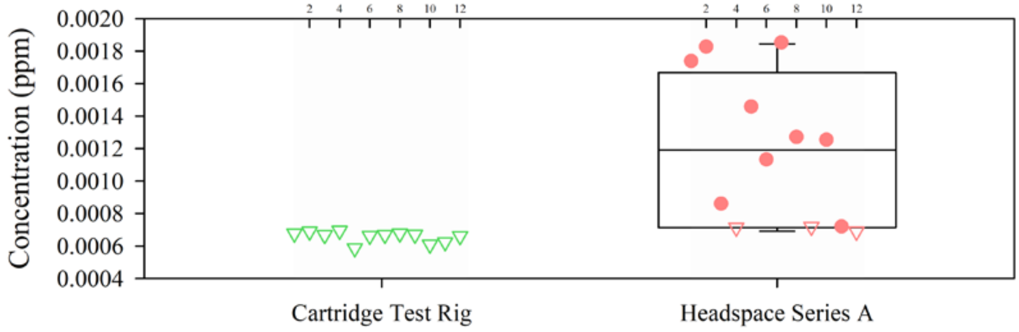
C.7.7 Ally Alcohol


Allyl Alcohol; OEL = 0.5 ppm

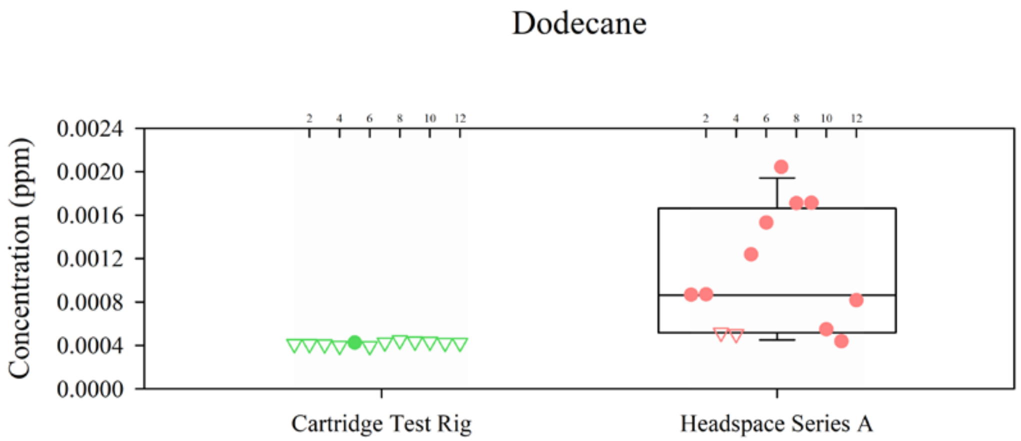
C.7.8 Cyclohexane


Cyclohexane; OEL = 100 ppm

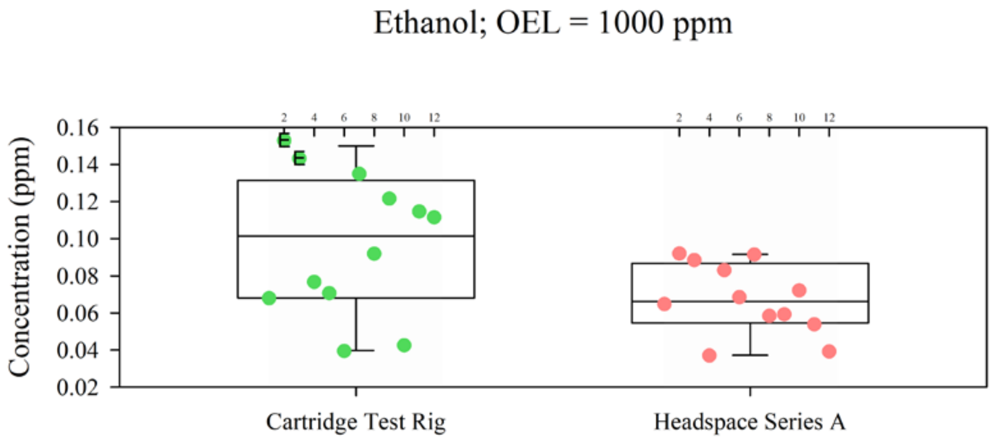
C.7.9 Decane


Decane

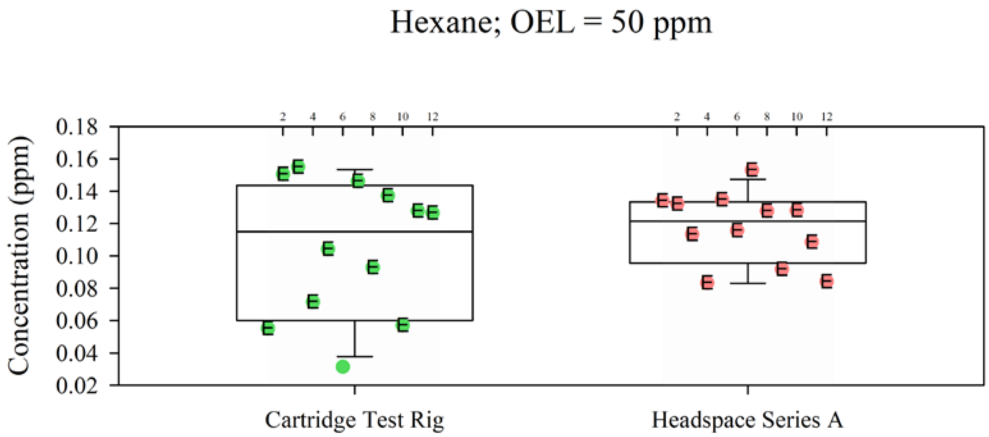
C.7.10 Dodecane



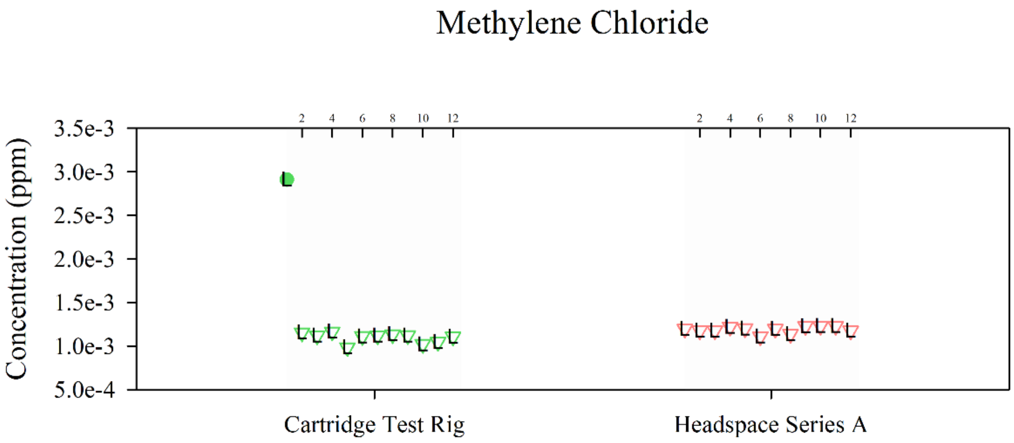
C.7.11 Ethanol



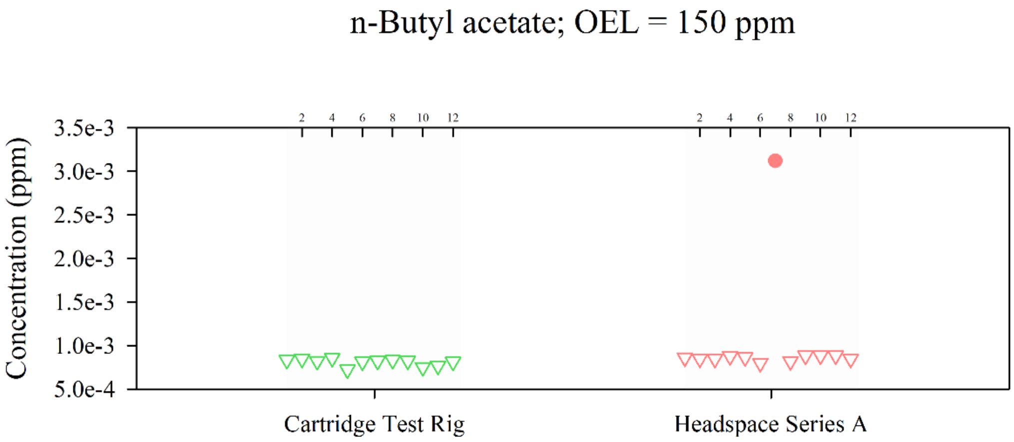
C.7.12 Hexane



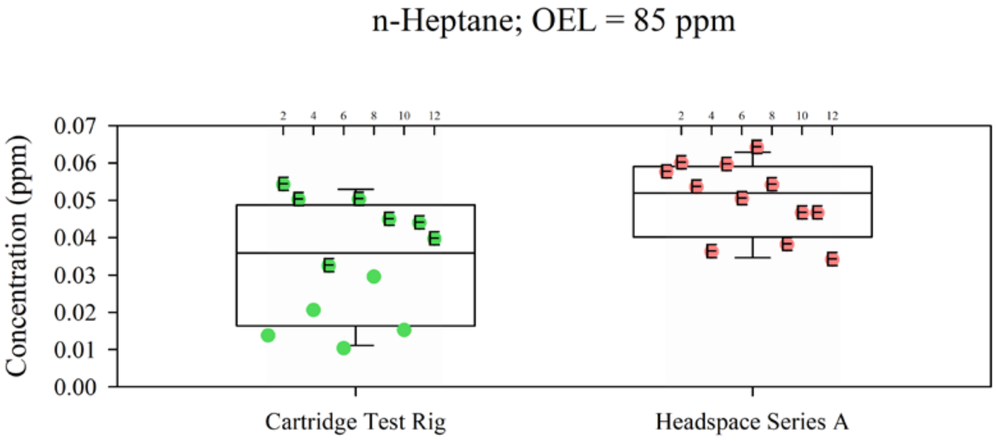
C.7.13 Methylene Chloride



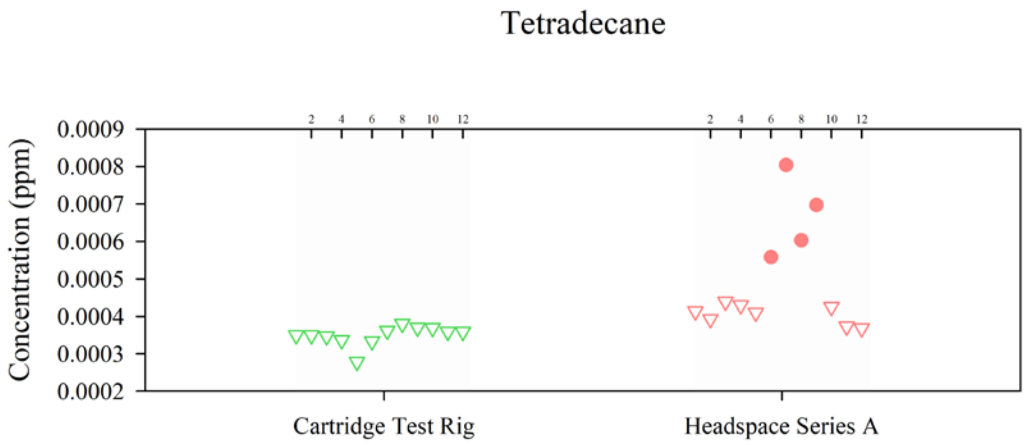
C.7.14 N-Butyl Acetate



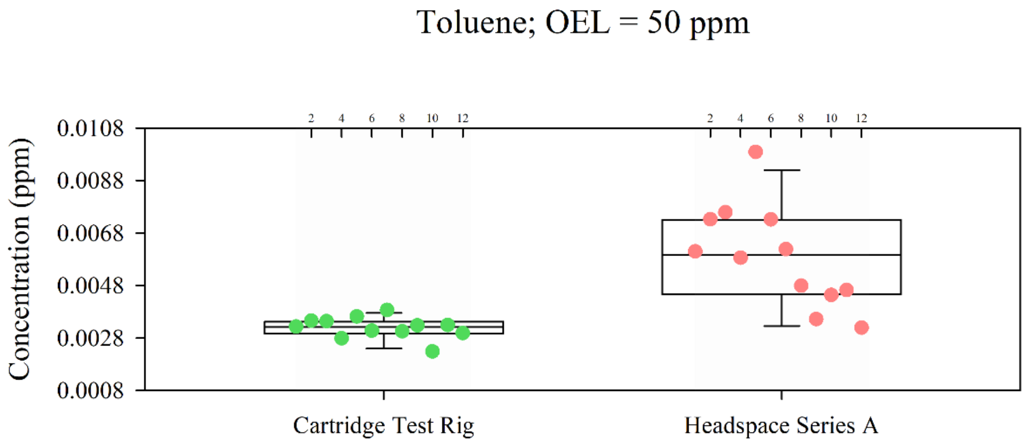
C.7.15 N-Heptane



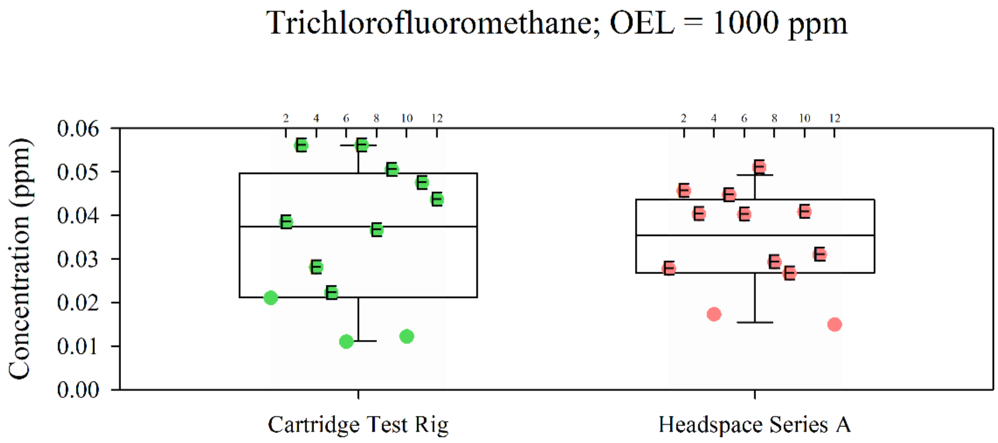
C.7.16 Tetradecane



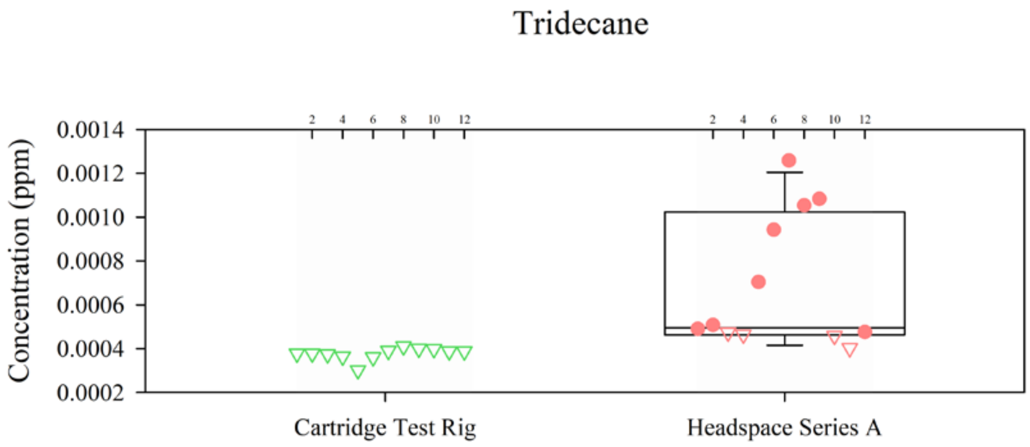
C.7.17 Toluene



C.7.18 Trichlorofluoromethane



C.7.19 Tridecane



C.8 Summary for non-COPCs with Less than Four Detected Values for Either Sampling Method

C.8.1 2,6,10-Trimethyldodecane 3891-98-3

2,6,10-Trimethyldodecane was detected in only four HS samples of the headspace of tank BY-110 at concentrations between approximately 0.5 and 0.68 ppm with the HS sampling system and not at all with the CT sampling system. Figure C.6 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

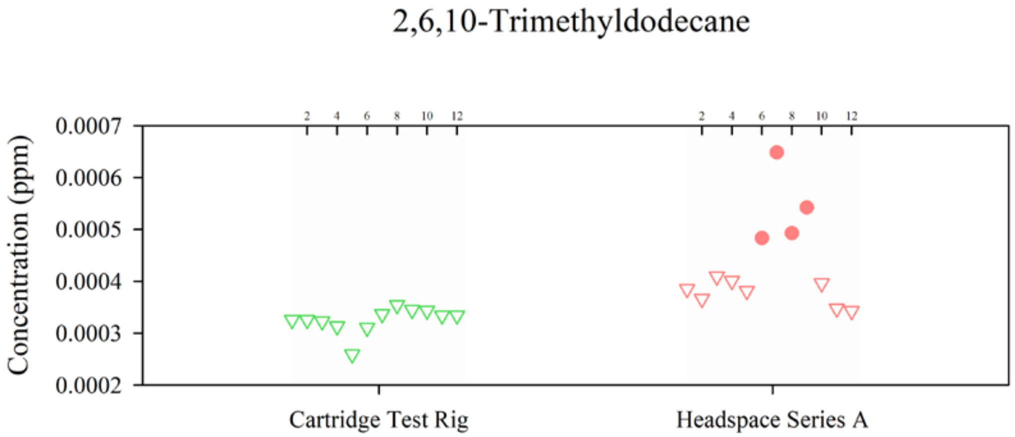


Figure C.6. Box Plot of 2,6,10-Trimethyldodecane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was significantly less (binomial test; p = 0.008) than the proportion detected with the HS sampling system (Table C.6). The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with either sampling system.

Table C.6. Statistical Comparison of 2,6,10-Trimethyldodecane Measurements from CT and HS Samples

				Cartridge Test Rig (CT)		Headspace Series A (HS)		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
2,6,10-Trimethyldodecane	SVOC			0	12	4	8	p = 0.008
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	NA	0.0004	NA	Mann-Whitney	NA	
	Median Sample Volume	L	3.46	3.09	-12.1%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.309	0.192	(1.61)	Levene's Test	Not Significantly Different	

The analytical method for SVOC sample volume was not significantly different between the HS and CT sampling methods (p = 0.999). The percent difference between medians volumes (i.e., [HS-CT]/HS) was -12%. The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.297) even though the ratio sCT:sHS was 1.61. The rule-of-thumb criteria of 1.5 was exceeded, however, suggesting that the variances in sample volume were not equal between the two sampling methods.

C.8.2 Allyl Alcohol 107-18-6

Allyl alcohol was detected in only one HS sample of the headspace of tank BY-110 at a concentration of approximately 2.8 ppb with the HS sampling system and not at all with the CT sampling method. Figure C.7 is a box plot depicting the 12 replicate samples from both sampling systems. All samples except for one HS sample had "Y" quality flags.

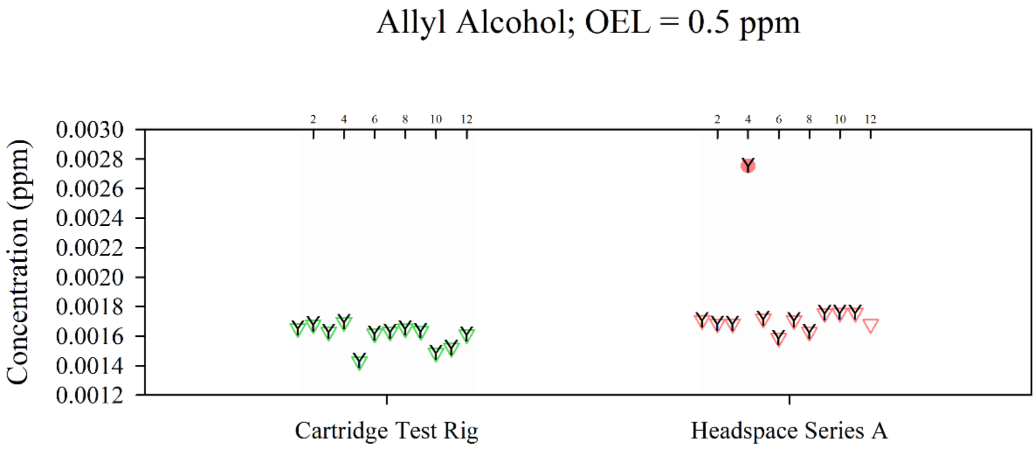


Figure C.7. Box Plot of Allyl Alcohol Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was not significantly different (binomial test; p = 0.35) than the proportion detected with the HS sampling system (Table. C.7). The median HS concentration was 0.3% of the OEL. The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with either sampling system.

Table C.7. Statistical Comparison of Allyl Alcohol Measurements from CT and HS Samples

				Cartridge Test Rig (CT)		Headspace Series A (HS)		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (°F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Allyl Alcohol	VOC	0.5		0	12, 12 flagged	1	11, 11 flagged	NS; p=0.35
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	NA	0.0017	NA	Mann-Whitney	NA	0.3%
	Median Sample Volume	L	3.07	2.93	-4.9%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.169	0.095	(1.782)	Levene's Test	Not Significantly Different	

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

C.8.3 Methylene Chloride 75-09-2

Methylene chloride was not detected in HS samples and was detected in one of 12 CT samples in the headspace of tank BY-110. The detected CT sample concentration was approximately 3 ppb with the CT sampling system. Figure C.8 is a box plot depicting the 12 replicate samples from both sampling systems. There were "L" quality flags on all HS and CT samples.

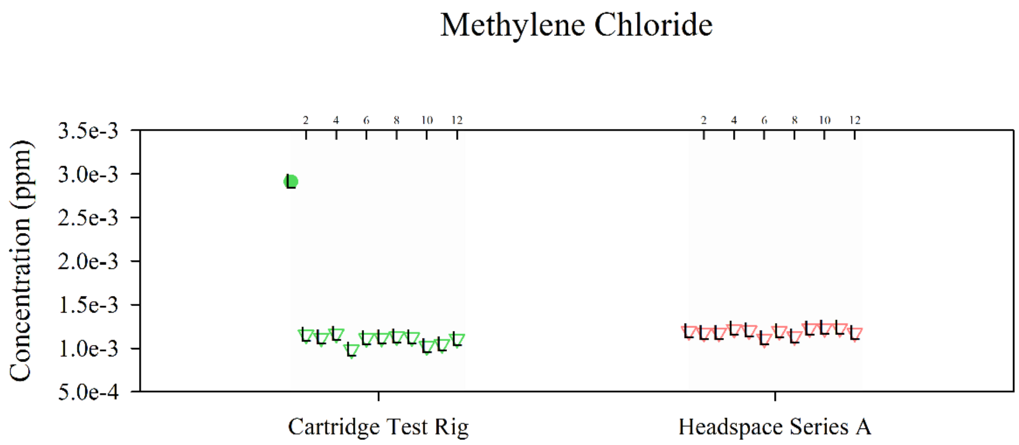


Figure C.8. Box Plot of Methylene Chloride Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

No statistical analyses were conducted on the concentration data because there were too few detected values (Table C.8).

Table C.8. Statistical Comparison of Methylene Chloride Measurements from CT and HS Samples

				Cartridge Test Rig		Headspace Series A		Conclusion of Test of Equal Proportion Detected
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Methylene Chloride	VOC			1, 1 flagged	11, 11 flagged	0	12, 12 flagged	CT≥HS
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	0.0011	NA	NA	Mann-Whitney	NA	
	Median Sample Volume	L	3.07	2.93	-4.9%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.169	0.095	(1.78)	Levene's Test	Not Significantly Different	

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene’s test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

C.8.4 n-Butyl acetate 123-86-4

n-Butyl acetate was detected in only one HS sample and no CT samples of the headspace of tank BY-110. The detected HS sample concentration was approximately 3 ppb with the HS sampling system. Figure C.9 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

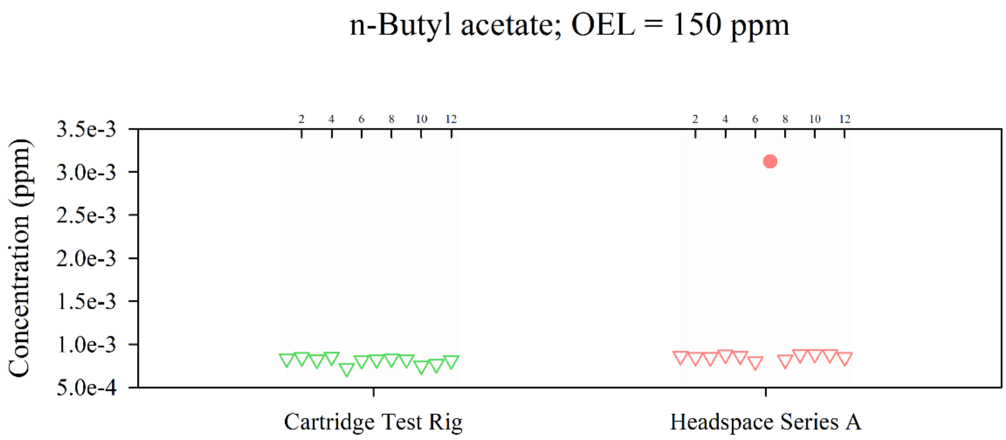


Figure C.9. Box Plot of n-Butyl acetate Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was not significantly different (binomial test; p = 0.35) than the proportion detected with the HS sampling system (Table C.9). The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with either sampling system.

Table C.9. Statistical Comparison of n-Butyl Acetate Measurements from CT and HS Samples

				Cartridge Test Rig		Headspace Series A		
Analyte	Method	OEL (ppm)	Boiling Point (◦F)	Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	Conclusion of Test of Equal Proportion Detected
n-Butyl acetate	VOC	150	259	0	12	1	11	NS; p=0.35
	Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
	Median Concentration	ppm	NA	0.0009	NA	Mann-Whitney	NA	0.0%
	Median Sample Volume	L	3.07	2.93	-4.9%	Mann-Whitney	Not Significantly Different	
	Sample Volume Standard Deviation	L	0.169	0.095	(1.782)	Levene's Test	Not Significantly Different	

The median sample volumes for the VOC analytical method were not significantly different between the two sampling methods (p = 0.999). The Levene’s test of equal sample volume variance between the two sampling methods was not significant (p = 0.179) even though the ratio sCT:sHS was 1.78. The rule-of-thumb criteria of 1.5, however, suggested that the variances in sample volume were not equal between the two sampling methods.

C.8.5 Tetradecane 629-59-4

Tetradecane was detected in four of 12 HS samples and no CT samples of the headspace of tank BY-110. Detected HS sample concentrations ranged from approximately 0.56 ppb to 0.8 ppb with the HS sampling system. Figure C.10 is a box plot depicting the 12 replicate samples from both sampling systems. There were no quality flags.

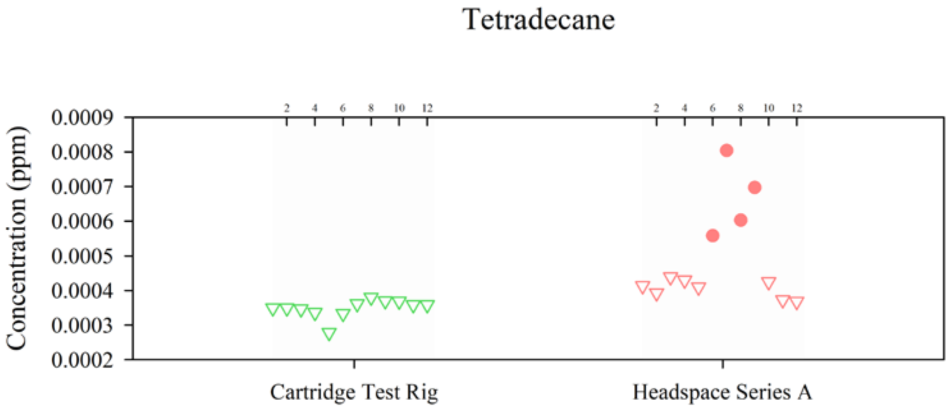


Figure C.10. Box Plot of Tetradecane Concentration Measurements from Replicate Samples from the CT (left) and HS (right) Systems

The proportion of detected samples with the CT sampling system was significantly less (binomial test; p = 0.008) than the proportion detected with the HS sampling system (Table C.10). The comparisons of the median concentrations and the concentration variance between the two sampling methods were not conducted because there were too few detected values with the CT sampling system.

Table C.10. Statistical Comparison of Tetradecane Measurements from CT and HS Samples

Analyte	Method	OEL (ppm)	Boiling Point (°F)	Cartridge Test Rig		Headspace Series A		Conclusion of Test of Equal Proportion Detected
				Number of Observations Detected	Number of Observations Censored	Number of Observations Detected	Number of Observations Censored	
Tetradecane	SVOC		488	0	12	4	8	p = 0.008

Statistical Measure	Units	Cartridge Test Rig (CT)	Headspace Series A (HS)	Percent difference (or ratio)	Statistical Test	Conclusion and Level of Significance	Headspace Series A/OEL (%)
Median Concentration	ppm	NA	0.0004	NA	Mann-Whitney	NA	
Concentration Standard Deviation	ppm	NA	0.0001	NA	Levene's Test	NA	
Median Sample Volume	L	3.46	3.09	-12.1%	Mann-Whitney	Not Significantly Different	
Sample Volume Standard Deviation	L	0.309	0.192	(1.613)	Levene's Test	Not Significantly Different	

The analytical method for SVOC sample volume was not significantly different between the HS and CT sampling methods (p = 0.999). The percent difference between medians volumes (i.e., [HS-CT]/HS) was -12%. The Levene's test of equal sample volume variance between the two sampling methods was not significant (p = 0.297) even though the ratio sCT:sHS was 1.61. The rule-of-thumb criteria of 1.5 was exceeded, however, suggesting that the variances in sample volume were not equal between the two sampling methods.

C.9 Statistical Analysis for Non-COPCs

C.9.1 Binomial Test

C.9.1.1 Test and CI for One Proportion for 1-Propanol and 4-Methyl-2-Pentanone Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	11	0.916667	0.995735

Test

Null hypothesis	H_0: p = 0.99
Alternative hypothesis	H_1: p < 0.99

P-Value = 0.114

C.9.1.2 Test and CI for One Proportion for Ally Alcohol and n-Butyl acetate

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	0	0.000000	0.220922

Test

Null hypothesis H_0: p = 0.08333

Alternative hypothesis H_1: p < 0.08333

P-Value = 0.352

C.9.1.3 Test and CI for One Proportion for 2,6,10-Trimethyldodecane and Tetradecane

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	0	0.000000	0.220922

Test

Null hypothesis H_0: p = 0.333

Alternative hypothesis H_1: p < 0.333

P-Value = 0.008

C.9.1.4 Test and CI for One Proportion for 2-Heptanone

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	5	0.416667	0.684762

Test

Null hypothesis	H_0: p = 0.99
Alternative hypothesis	H_1: p < 0.99

P-Value = 0.000

C.9.1.5 Test and CI for One Proportion for 3-Heptanone

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	7	0.583333	0.818975

Test

Null hypothesis	H_0: p = 0.99
Alternative hypothesis	H_1: p < 0.99

P-Value = 0.000

C.9.1.6 Test and CI for One Proportion for Decane

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	0	0.000000	0.220922

Test

Null hypothesis H_0: $p = 0.75$

Alternative hypothesis H_1: $p < 0.75$

P-Value = 0.000

C.9.1.7 Test and CI for One Proportion for Dodecane

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	1	0.083333	0.338681

Test

Null hypothesis H_0: $p = 0.8333$

Alternative hypothesis H_1: $p < 0.8333$

P-Value = 0.000

C.9.1.8 Test and CI for One Proportion for Tridecane

Method

p: event proportion

Exact method is used for this analysis.

Descriptive Statistics

N	Event	Sample p	95% Upper Bound for p
12	0	0.000000	0.220922

Test

Null hypothesis H_0: $p = 0.667$

Alternative hypothesis H_1: $p < 0.667$

P-Value
0.000

C.9.2 Mann-Whitney Test of Equal Concentration Medians

C.9.2.1 Mann-Whitney: 1-Propanol_CTR, 1-Propanol_HSA

Method

η_1: median of 1-Propanol_CTR

η_2: median of 1-Propanol_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
1-Propanol_CTR	12	0.0213887
1-Propanol_HSA	12	0.0203679

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0016582	0.0058492	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
144.00	0.375

C.9.2.2 Mann-Whitney: 2-Butanone_CTR, 2-Butanone_HSA

Method

η_1: median of 2-Butanone_CTR

η_2: median of 2-Butanone_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
2-Butanone_CTR	12	0.0270422
2-Butanone_HSA	12	0.0186198

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.0099959	0.0204654	95.01%

Test

Null hypothesis $H_0: \eta_1 - \eta_2 = 0$
Alternative hypothesis $H_1: \eta_1 - \eta_2 < 0$

W-Value	P-Value
174.00	0.921

C.9.3 Mann-Whitney: 3-Heptanone_CTR, 3-Heptanone_HSA

Method

η_1: median of 3-Heptanone_CTR
η_2: median of 3-Heptanone_HSA
Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
3-Heptanone_CTR	12	0.0011250
3-Heptanone_HSA	12	0.0103421

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0089188	-0.0073139	95.01%

Test

Null hypothesis $H_0: \eta_1 - \eta_2 = 0$
Alternative hypothesis $H_1: \eta_1 - \eta_2 < 0$

Method	W-Value	P-Value
Not adjusted for ties	78.00	0.000
Adjusted for ties	78.00	0.000

C.9.3.1 Mann-Whitney: 4-Methyl-2-Pentanone_CTR, ... thyl-2-Pentanone_HSA

Method

η_1: median of 4-Methyl-2-Pentanone_CTR

η_2: median of 4-Methyl-2-Pentanone_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
4-Methyl-2-Pentanone_CTR	12	0.0027159
4-Methyl-2-Pentanone_HSA	12	0.0037348

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0009069	-0.0001925	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
117.00	0.030

C.9.3.2 Mann-Whitney: Cyclohexane_CTR, Cyclohexane_HSA

Method

η_1: median of Cyclohexane_CTR

η_2: median of Cyclohexane_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Cyclohexane_CTR	12	0.0071424
Cyclohexane_HSA	12	0.0075536

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0003099	0.0014760	95.01%

Test

Null hypothesis $H_0: \eta_1 - \eta_2 = 0$

Alternative hypothesis $H_1: \eta_1 - \eta_2 < 0$

W-Value	P-Value
143.00	0.354

C.9.3.3 Mann-Whitney: Ethanol_CTR, Ethanol_HSA

Method

η_1: median of Ethanol_CTR

η_2: median of Ethanol_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Ethanol_CTR	12	0.101441
Ethanol_HSA	12	0.066264

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.0312292	0.0550364	95.01%

Test

Null hypothesis $H_0: \eta_1 - \eta_2 = 0$

Alternative hypothesis $H_1: \eta_1 - \eta_2 < 0$

W-Value	P-Value
186.00	0.982

C.9.3.4 Mann-Whitney: Hexane_CTR, Hexane_HSA

Method

η_1: median of Hexane_CTR

η_2: median of Hexane_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Hexane_CTR	12	0.115055
Hexane_HSA	12	0.121510

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0066996	0.0179660	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
141.00	0.312

C.9.3.5 Mann-Whitney: n-Heptane_CTR, n-Heptane_HSA

Method

η_1: median of n-Heptane_CTR

η_2: median of n-Heptane_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
n-Heptane_CTR	12	0.0359232
n-Heptane_HSA	12	0.0519584

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0149790	-0.0057380	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
105.00	0.005

C.9.3.6 Mann-Whitney: Toluene_CTR, Toluene_HSA

Method

η_1: median of Toluene_CTR

η_2: median of Toluene_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Toluene_CTR	12	0.0032238
Toluene_HSA	12	0.0059631

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
-0.0026649	-0.0014032	95.01%

Test

Null hypothesis H_0: $\eta_1 - \eta_2 = 0$

Alternative hypothesis H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
87.00	0.000

C.9.3.7 Mann-Whitney: Trichlorofluoromethane_CTR, ... rofluoromethane_HSA

Method

η_1: median of Trichlorofluoromethane_CTR

η_2: median of Trichlorofluoromethane_HSA

Difference: $\eta_1 - \eta_2$

Descriptive Statistics

Sample	N	Median
Trichlorofluoromethane_CTR	12	0.0374133
Trichlorofluoromethane_HSA	12	0.0354953

Estimation for Difference

Difference	Upper Bound for Difference	Achieved Confidence
0.0023632	0.0113665	95.01%

Test

Null hypothesis	H_0: $\eta_1 - \eta_2 = 0$
Alternative hypothesis	H_1: $\eta_1 - \eta_2 < 0$

W-Value	P-Value
153.00	0.580

C.9.4 Levene’s Test of Equal Variance for Concentrations

C.9.4.1 Test and CI for Two Variances: 1-Propanol vs Type

Method

σ_1: standard deviation of 1-Propanol when Type = CT

σ_2: standard deviation of 1-Propanol when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.011	0.000	0.009
HS	12	0.009	0.000	0.006

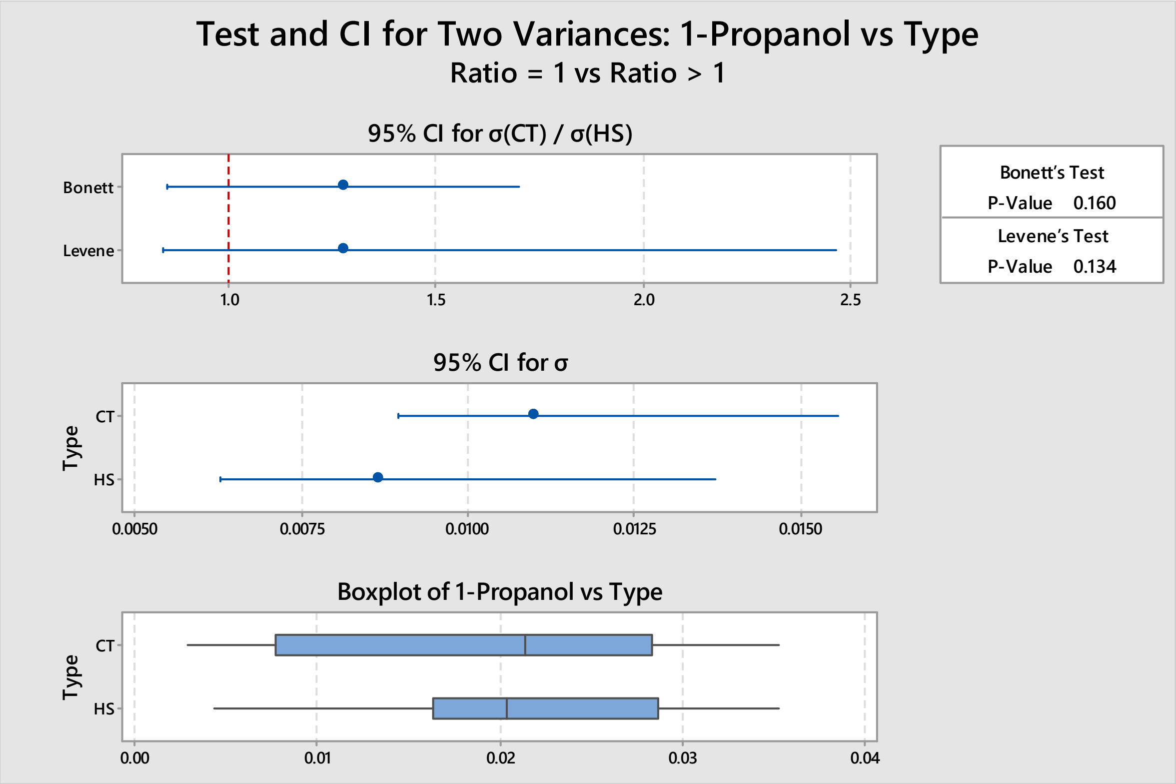
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.27271	0.846	0.839

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	0.99	1		0.160
Levene	1.29	1	22	0.134



C.9.4.2 Test and CI for Two Variances: 2-Butanone vs Type

Method

σ_1: standard deviation of 2-Butanone when Type = CT

σ_2: standard deviation of 2-Butanone when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviations	Variance	95% Lower Bound for σ
CT	12	0.017	0.000	0.014
HS	12	0.012	0.000	0.010

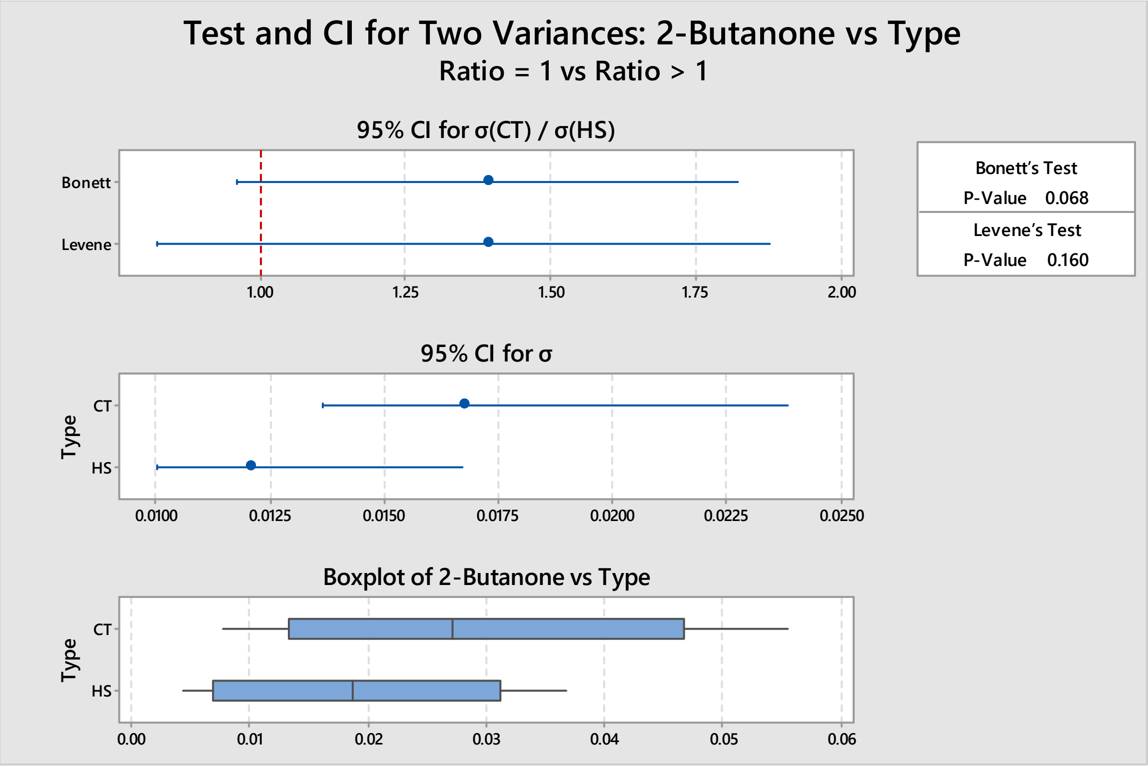
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.39183	0.959	0.822

Test

Null hypothesis	H_0: σ_1 / σ_2 = 1
Alternative hypothesis	H_1: σ_1 / σ_2 > 1
Significance level	α = 0.05

Method	Test Statistic	DF1	DF2	P-Value
Bonett	2.22	1		0.068
Levene	1.04	1	22	0.160



C.9.4.3 Test and CI for Two Variances: 4-Methyl-2-Pentanone vs Type

Method

σ_1: standard deviation of 4-Methyl-2-Pentanone when Type = CT

σ_2: standard deviation of 4-Methyl-2-Pentanone when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.001	0.000	0.001
HS	12	0.001	0.000	0.001

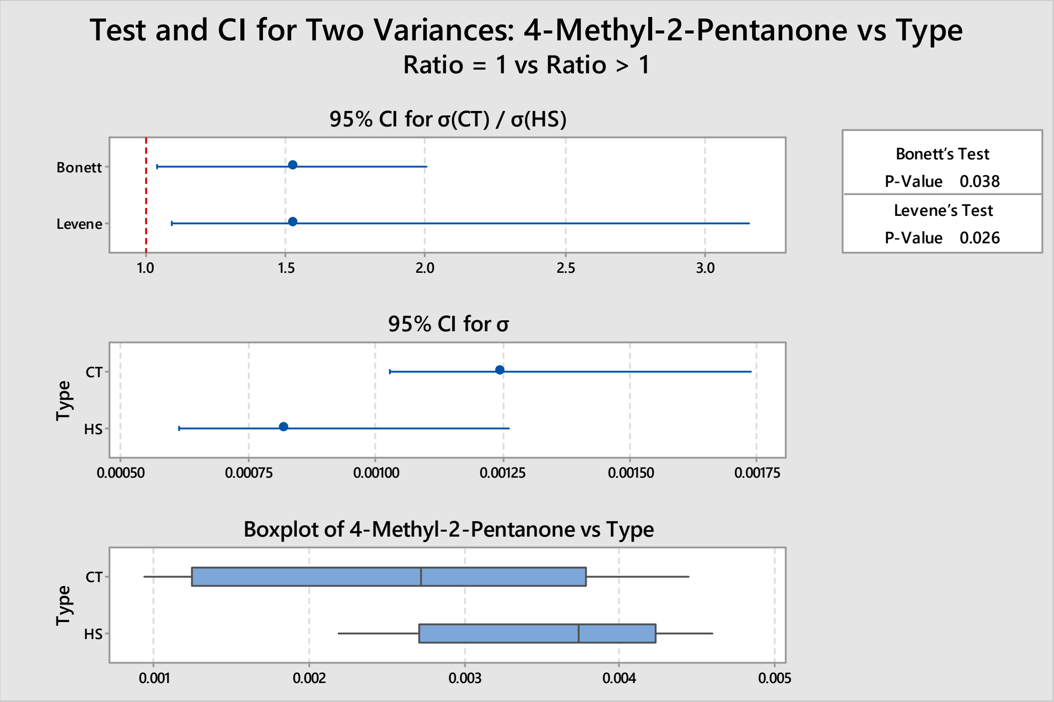
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.52142	1.036	1.091

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	3.16	1		0.038
Levene	4.19	1	22	0.026



C.9.4.4 Test and CI for Two Variances: Acetone vs Type

Method

σ_1: standard deviation of acetone when Type = CT

σ_2: standard deviation of acetone when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.225	0.051	0.181
HS	12	0.177	0.031	0.147

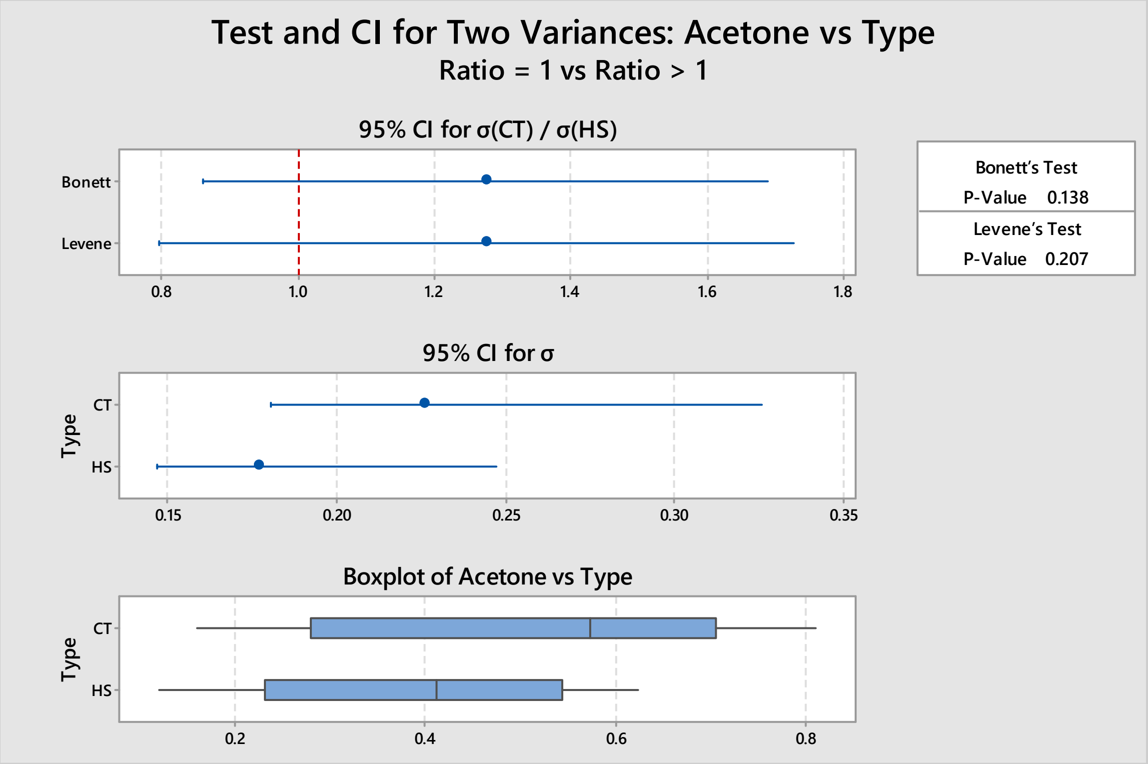
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.27468	0.859	0.794

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	1.19	1		0.138
Levene	0.69	1	22	0.207



C.9.4.5 Test and CI for Two Variances: Cyclohexane vs Type

Method

σ_1: standard deviation of Cyclohexane when Type = CT

σ_2: standard deviation of Cyclohexane when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.003	0.000	0.002
HS	12	0.002	0.000	0.002

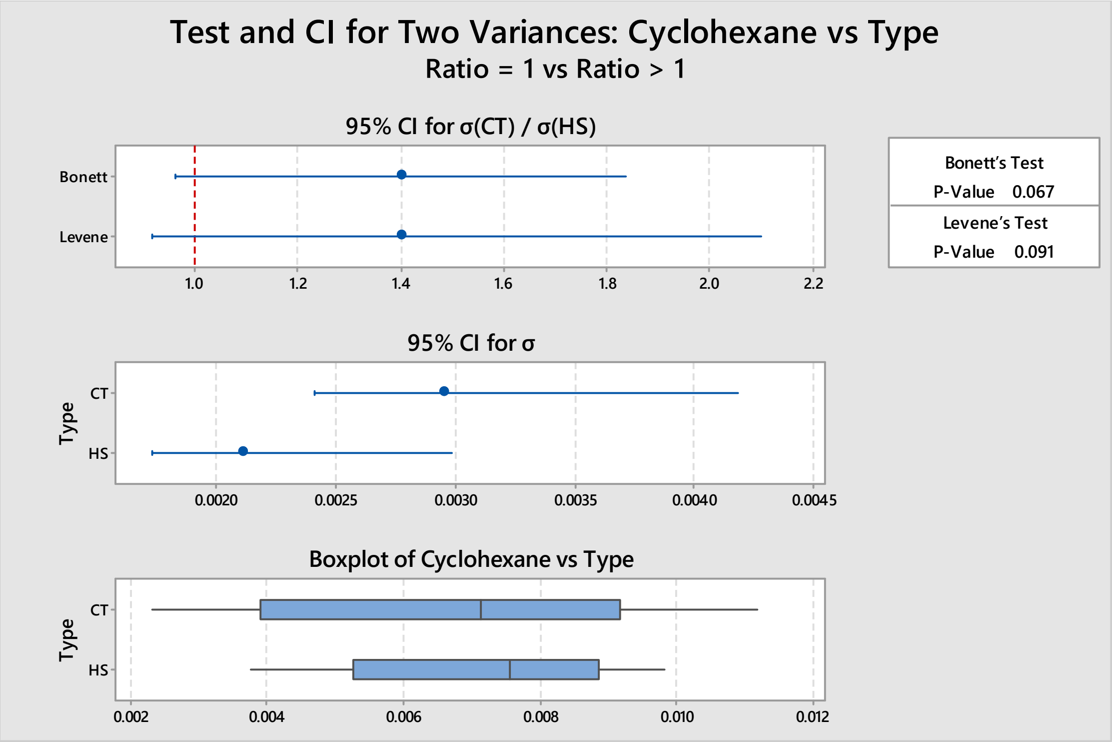
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.39963	0.961	0.918

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	2.25	1		0.067
Levene	1.90	1	22	0.091



C.9.4.6 Test and CI for Two Variances: Ethanol vs Type

Method

σ_1: standard deviation of Ethanol when Type = CT

σ_2: standard deviation of Ethanol when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.038	0.001	0.031
HS	12	0.019	0.000	0.015

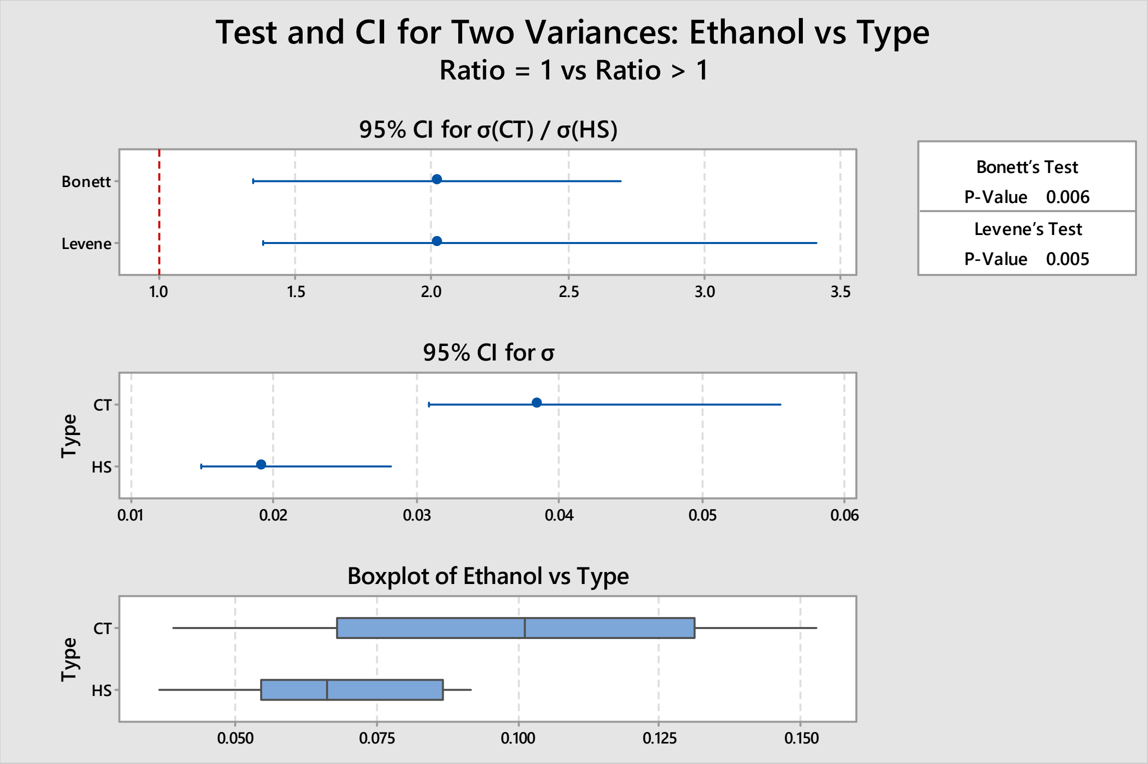
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
2.01929	1.345	1.379

Test

Null hypothesis	$H_0: \sigma_1 / \sigma_2 = 1$
Alternative hypothesis	$H_1: \sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	6.33	1		0.006
Levene	8.13	1	22	0.005



C.9.4.7 Test and CI for Two Variances: Hexane vs Type

Method

σ_1: standard deviation of Hexane when Type = CT

σ_2: standard deviation of Hexane when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.043	0.002	0.034
HS	12	0.022	0.000	0.017

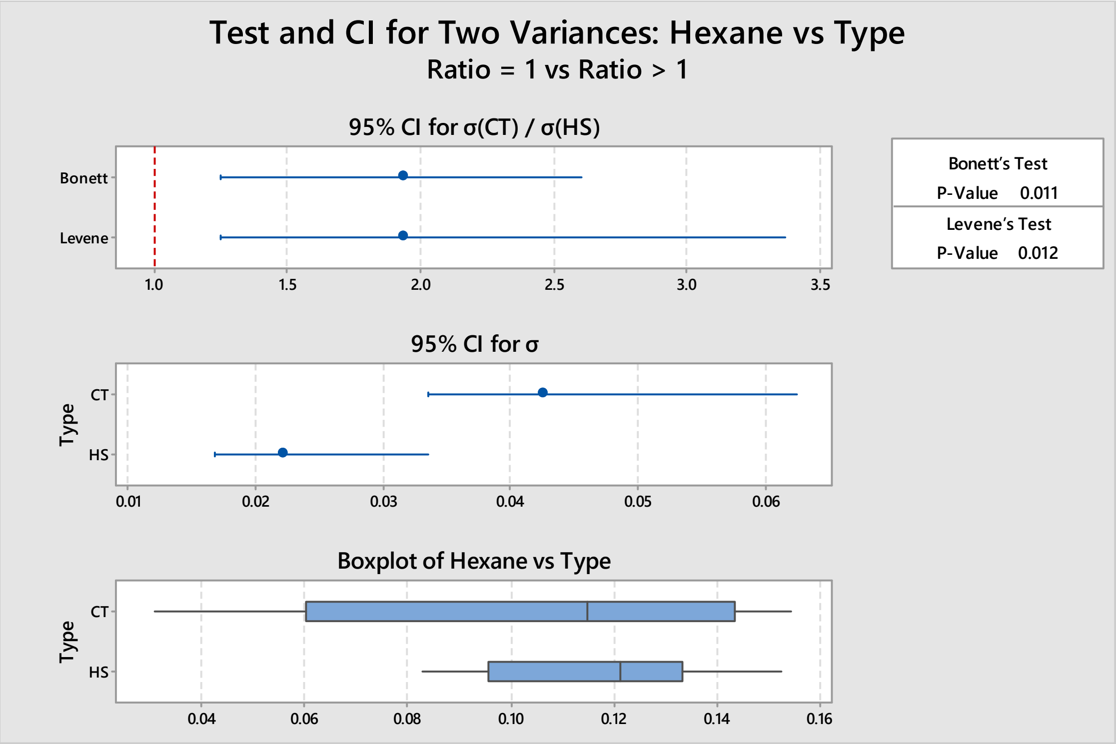
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.92868	1.249	1.250

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	5.20	1		0.011
Levene	5.86	1	22	0.012



C.9.4.8 Test and CI for Two Variances: n-Heptane vs Type

Method

σ_1: standard deviation of n-Heptane when Type = CT

σ_2: standard deviation of n-Heptane when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.016	0.000	0.013
HS	12	0.010	0.000	0.008

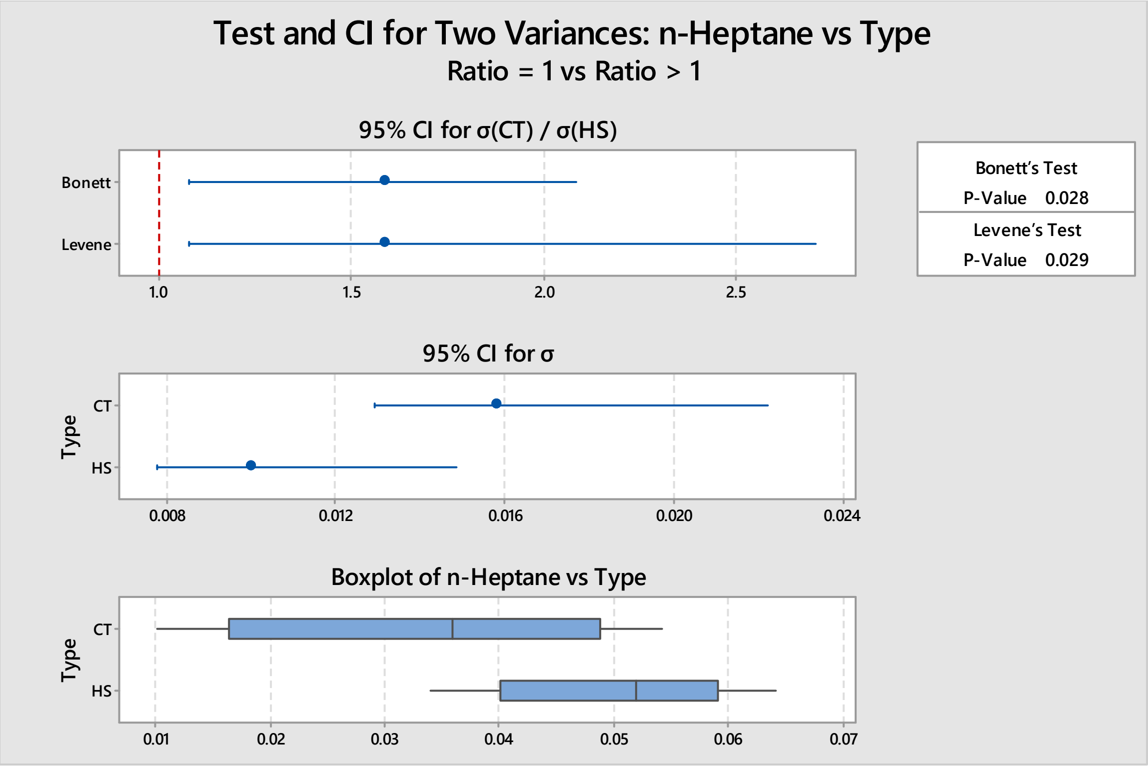
Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.58092	1.079	1.078

Test

Null hypothesis	H_0: $\sigma_1 / \sigma_2 = 1$
Alternative hypothesis	H_1: $\sigma_1 / \sigma_2 > 1$
Significance level	$\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	3.68	1		0.028
Levene	4.01	1	22	0.029



C.9.4.9 Test and CI for Two Variances: Trichlorofluoromethane versus Type

Method

σ_1: standard deviation of Trichlorofluoromethane when Type = CT

σ_2: standard deviation of Trichlorofluoromethane when Type = HS

Ratio: σ_1/σ_2

The Bonett and Levene's methods are valid for any continuous distribution.

Descriptive Statistics

Type	N	Standard Deviation	Variance	95% Lower Bound for σ
CT	12	0.016	0.000	0.013
HS	12	0.011	0.000	0.009

Ratio of Standard Deviations

Estimated Ratio	95% Lower Bound for Ratio using Bonett	95% Lower Bound for Ratio using Levene
1.41852	0.950	0.892

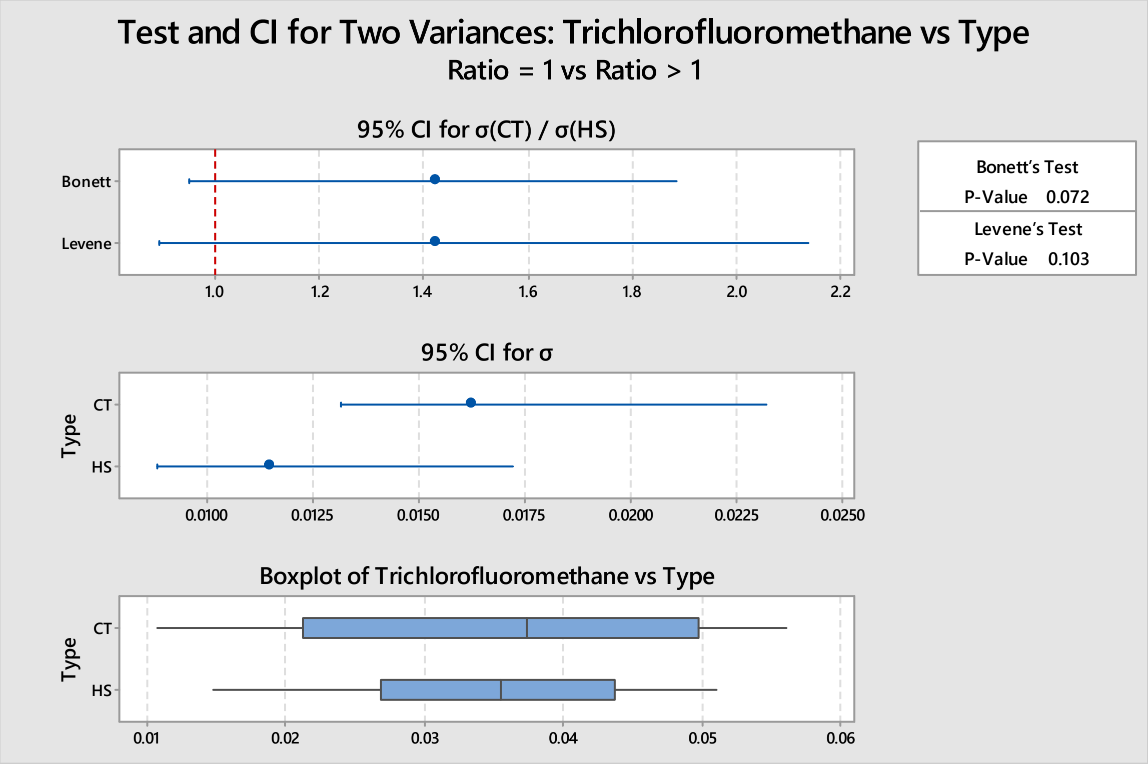
Test

Null hypothesis $H_0: \sigma_1 / \sigma_2 = 1$

Alternative hypothesis $H_1: \sigma_1 / \sigma_2 > 1$

Significance level $\alpha = 0.05$

Method	Test Statistic	DF1	DF2	P-Value
Bonett	2.13	1		0.072
Levene	1.70	1	22	0.103

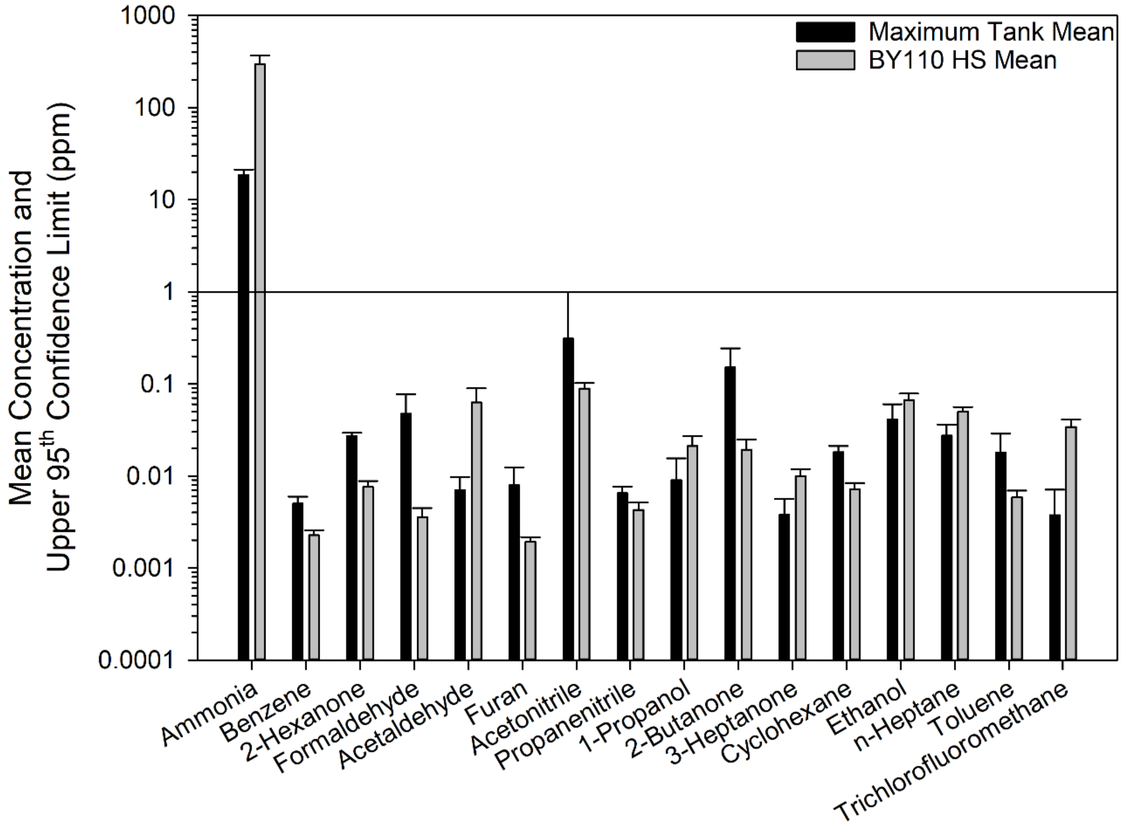


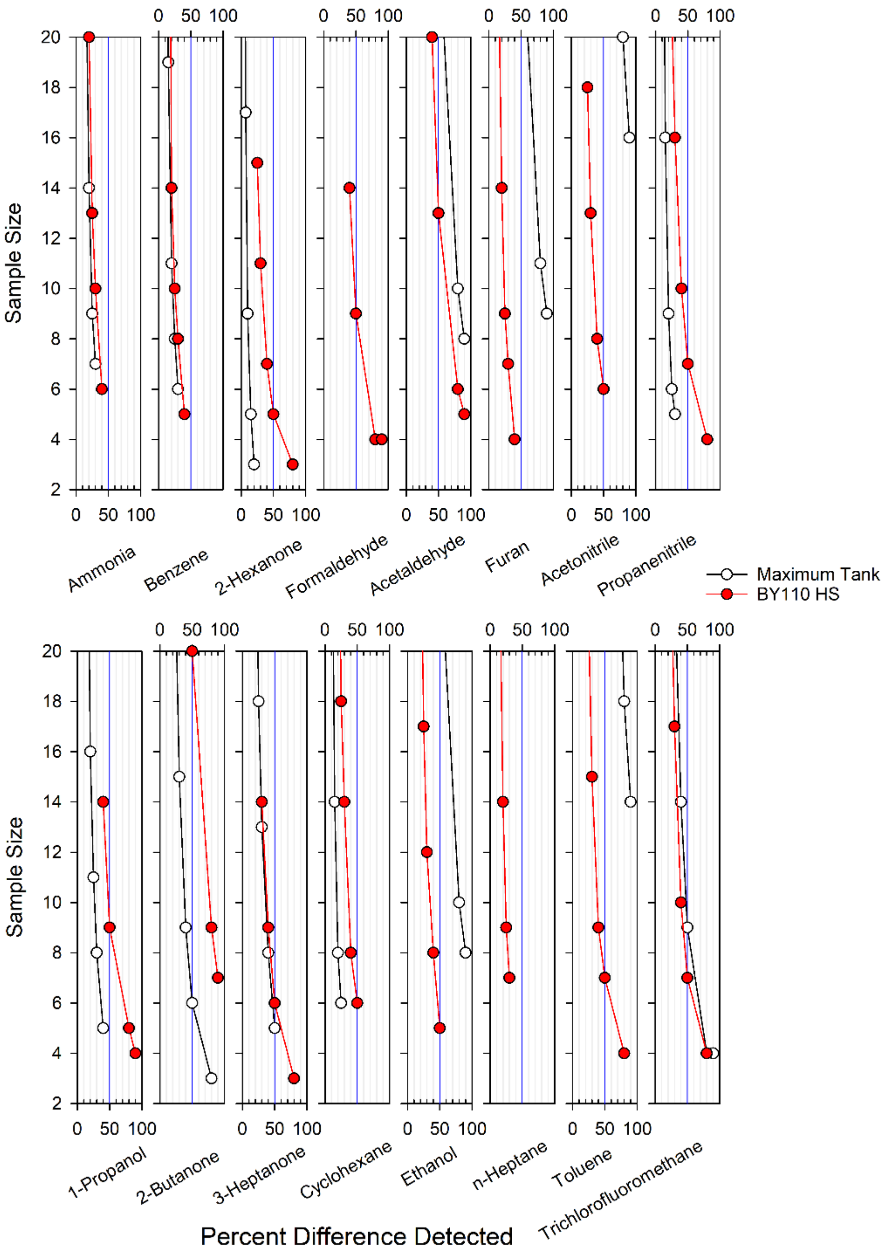
C.10 Sample Size Calculation for COPCs and Non-COPCs

For future comparison tests between the HS and CT methods, we estimated the number of samples required to detect a given percentage difference between the mean concentrations. For this purpose, SWIHDHS 050918 data were evaluated as an appropriate measure of the variance in concentration within tanks likely to be sampled with the two methods. Only SWIHDHS 050918 data greater than the detection limit, with no more than one qualifying flag, and sample volumes ≥1 L were used for analysis. Sampling dates were used as if independent and the standard deviation for a given tank (n >1) in chemical concentration was estimated for the purpose of estimating a required sample size to detect a given percentage difference between the HS and CT mean concentrations. The tank with the maximum standard deviation of the $\log_{10}$ transformed concentration (Maximum Tank) was used for the sample size calculation. Only those chemicals with greater than six detected observations in the BY110 Comparison test for both methods were used for comparison to this calculation. Sample size analysis was also conducted using the HS and CT variance for comparison.

Sample sizes were estimated from the SWIHDHS 050918 data for the tank and chemical with the maximum standard deviation of the $\log_{10}$ transformed concentration (Maximum Tank). The descriptive statistics for the Maximum Tank and the BY-110 HS needed for the sample size calculation are listed below. For visual comparative purposes, the Maximum Tank and BY110 HS mean and the upper 95% confidence limit are also presented. The confidence limits were calculated from the $\log_{10}$ transformed data and then back transformed.

Agent	Maximum Tank	Maximum Tank Stdev	Maximum Tank Mean	Maximum Tank CV	BY110 HS Stdev	BY110 HS Mean	BY110 HS CV
Ammonia	A105	3.71871	18.7	20%	73.6228	296	25%
Benzene	BY108	0.00089	0.005	18%	0.0005	0.002	22%
2-Hexanone	BY108	0.00214	0.027	8%	0.0020	0.008	26%
Formaldehyde	A102	0.05401	0.047	114%	0.0014	0.004	40%
Acetaldehyde	A104	0.0048	0.007	69%	0.0312	0.063	50%
Furan	BY108	0.00552	0.008	70%	0.0004	0.002	22%
Acetonitrile	SY102	0.30913	0.311	99%	0.0259	0.088	29%
Propanenitrile	A106	0.00105	0.007	16%	0.0014	0.004	33%
1-Propanol	A101	0.002	0.009	22%	0.0086	0.021	41%
2-Butanone	BY108	0.0509	0.163	31%	0.0120	0.019	62%
3-Heptanone	A102	0.0011	0.004	29%	0.0031	0.010	31%
Cyclohexane	BY108	0.00271	0.018	15%	0.0021	0.007	29%
Ethanol	A105	0.02772	0.041	67%	0.0190	0.067	28%
n-Heptane	A105	0.04147	0.027	151%	0.0100	0.050	20%
Toluene	A104	0.01644	0.018	92%	0.0019	0.006	33%
Trichlorofluoromethane	A104	0.0015	0.004	40%	0.0114	0.034	34%





Sample Size Required to Detect a Given Percentage Difference between the HS and CT Mean Chemical Concentrations with the Observed Variance, a 1-Sided T-Test at 80% Power, and α=0.05.

C.10.1 Maximum Tank

C.10.1.1 Power and Sample Size Ammonia Tank A105

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 3.71871

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
1.30577	7%	101	0.8	0.800101
1.86539	10%	50	0.8	0.801191
2.79808	15%	23	0.8	0.807089
3.73078	20%	14	0.8	0.826238
4.66347	25%	9	0.8	0.816027
5.59617	30%	7	0.8	0.842927

The sample size is for each group.

C.10.1.2 Power and Sample Size Benzene Tank BY108

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.000894427

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.00035	7%	82	0.8	0.802415
0.00050	10%	41	0.8	0.806400
0.00075	15%	19	0.8	0.813425
0.00100	20%	11	0.8	0.812420
0.00125	25%	8	0.8	0.844070
0.00150	30%	6	0.8	0.854384

The sample size is for each group.

C.10.1.3 Power and Sample Size 2-Hexanone Tank BY108

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.00213698

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0005433	2%	192	0.8	0.800076
0.0013583	5%	32	0.8	0.807788
0.0019017	7%	17	0.8	0.814367
0.0027167	10%	9	0.8	0.825155
0.0040750	15%	5	0.8	0.864795
0.0054333	20%	3	0.8	0.815990

The sample size is for each group.

C.10.1.4 Power and Sample Size Formaldehyde Tank A102

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0540136

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0142000	30%	180	0.8	0.800802
0.0189333	40%	102	0.8	0.802345
0.0236667	50%	66	0.8	0.804846
0.0378667	80%	26	0.8	0.801893
0.0426000	90%	21	0.8	0.807078

The sample size is for each group.

C.10.1.5 Power and Sample Size Acetaldehyde Tank A104

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.00479583

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0021	30%	66	0.8	0.804402
0.0028	40%	37	0.8	0.800282
0.0035	50%	24	0.8	0.801162
0.0056	80%	10	0.8	0.806772
0.0063	90%	8	0.8	0.802966

The sample size is for each group.

C.10.1.6 Power and Sample Size Furan Tank BY108

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.00551549

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0023738	30%	68	0.8	0.802882
0.0031650	40%	39	0.8	0.806888
0.0039562	50%	25	0.8	0.803770
0.0063300	80%	11	0.8	0.829930
0.0071213	90%	9	0.8	0.835327

The sample size is for each group.

C.10.1.7 Power and Sample Size Acetonitrile Tank SY102

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.309127

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.09342	30%	137	0.8	0.802369
0.12456	40%	77	0.8	0.800714
0.15570	50%	50	0.8	0.804023
0.24912	80%	20	0.8	0.804489
0.28026	90%	16	0.8	0.805360

The sample size is for each group.

C.10.1.8 Power and Sample Size Propanenitrile Tank A106

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.00104881

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.000455	7%	67	0.8	0.803223
0.000650	10%	33	0.8	0.801175
0.000975	15%	16	0.8	0.822383
0.001300	20%	9	0.8	0.808081
0.001625	25%	6	0.8	0.802584
0.001950	30%	5	0.8	0.849448

The sample size is for each group.

C.10.1.9 Power and Sample Size 1-Propanol Tank A101

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.002

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.00090	10%	62	0.8	0.801421
0.00135	15%	28	0.8	0.802036
0.00180	20%	16	0.8	0.800287
0.00225	25%	11	0.8	0.816632
0.00270	30%	8	0.8	0.821527
0.00360	40%	5	0.8	0.828794

The sample size is for each group.

C.10.1.10 Power and Sample Size 2-Butanone Tank BY108

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0508635

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.032500	20%	31	0.8	0.800168
0.040625	25%	21	0.8	0.815692
0.048750	30%	15	0.8	0.820085
0.065000	40%	9	0.8	0.828609
0.081250	50%	6	0.8	0.823260
0.130000	80%	3	0.8	0.819393

The sample size is for each group.

C.10.1.11 Power and Sample Size 3-Heptanone Tank A102

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.00109545

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.00057	15%	47	0.8	0.804816
0.00076	20%	27	0.8	0.808087
0.00095	25%	18	0.8	0.817133
0.00114	30%	13	0.8	0.824429
0.00152	40%	8	0.8	0.839501
0.00190	50%	5	0.8	0.803919

The sample size is for each group.

C.10.1.12 Power and Sample Size Cyclohexane Tank BY108

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.00271416

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0009083	5%	112	0.8	0.802866
0.0012717	7%	58	0.8	0.805998
0.0018167	10%	29	0.8	0.808638
0.0027250	15%	14	0.8	0.826732
0.0036333	20%	8	0.8	0.815859
0.0045417	25%	6	0.8	0.853015

The sample size is for each group.

C.10.1.13 Power and Sample Size Ethanol Tank A105

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0277167

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.012375	30%	63	0.8	0.801589
0.016500	40%	36	0.8	0.804083
0.020625	50%	24	0.8	0.814525
0.033000	80%	10	0.8	0.819986
0.037125	90%	8	0.8	0.816257

The sample size is for each group.

C.10.1.14 Power and Sample Size n-Heptane Tank A105

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0414658

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0082125	30%	316	0.8	0.800101
0.0109500	40%	178	0.8	0.800006
0.0136875	50%	115	0.8	0.802546
0.0219000	80%	46	0.8	0.807558
0.0246375	90%	36	0.8	0.802751

The sample size is for each group.

C.10.1.15 Power and Sample Size Toluene Tank A104

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0164355

Results

Difference	Percent differences	Sample Size	TargetPower	Actual Power
0.0053625	30%	117	0.8	0.800495
0.0071500	40%	67	0.8	0.805147
0.0089375	50%	43	0.8	0.804061
0.0143000	80%	18	0.8	0.819337
0.0160875	90%	14	0.8	0.809634

The sample size is for each group.

C.10.1.16 Power and Sample Size Trichlorofluoromethane Tank A104

2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0015

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0009375	25%	33	0.8	0.807007
0.0011250	30%	23	0.8	0.804856
0.0015000	40%	14	0.8	0.824086
0.0018750	50%	9	0.8	0.813834
0.0030000	80%	4	0.8	0.801534
0.0033750	90%	4	0.8	0.875645

The sample size is for each group.

C.10.2 BY110 HS Sample Size and Test of Normality

C.10.2.1 Power and Sample Size Ammonia

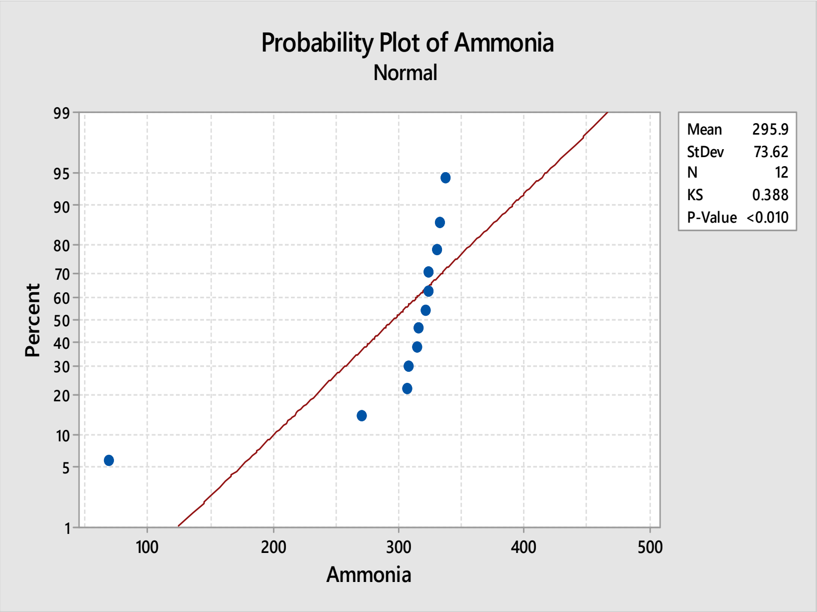
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 73.6228

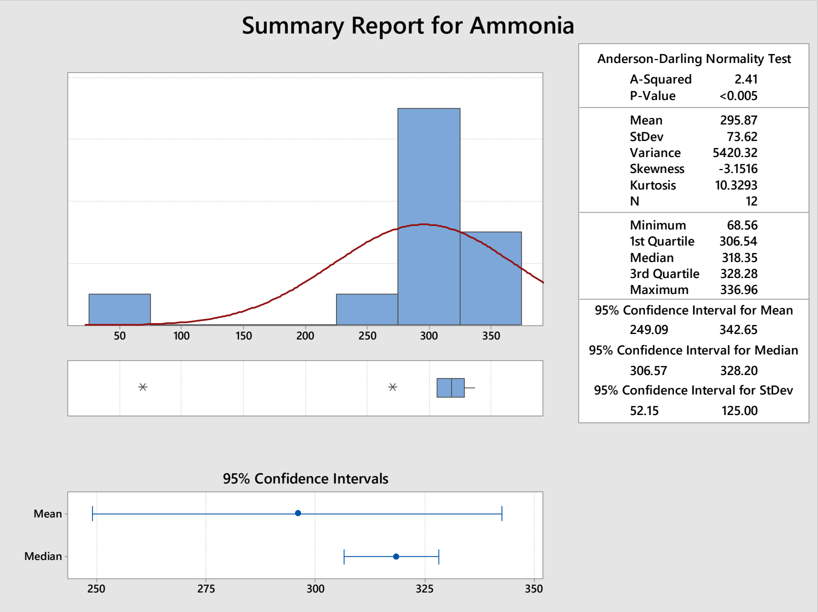
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
59.174	20%	20	0.8	0.802658
73.968	25%	13	0.8	0.800480
88.762	30%	10	0.8	0.828316
118.349	40%	6	0.8	0.827422
147.936	50%	4	0.8	0.804727

The sample size is for each group.

Ammonia significantly different from normal.





Anderson-Darling Normality Test	
A-Squared	2.41
P-Value	<0.005
Mean	295.87
StDev	73.62
Variance	5420.32
Skewness	-3.1516
Kurtosis	10.3293
N	12
Minimum	68.56
1st Quartile	306.54
Median	318.35
3rd Quartile	328.28
Maximum	336.96
95% Confidence Interval for Mean	
249.09	342.65
95% Confidence Interval for Median	
306.57	328.20
95% Confidence Interval for StDev	
52.15	125.00

C.10.2.2 Power and Sample Size Benzene

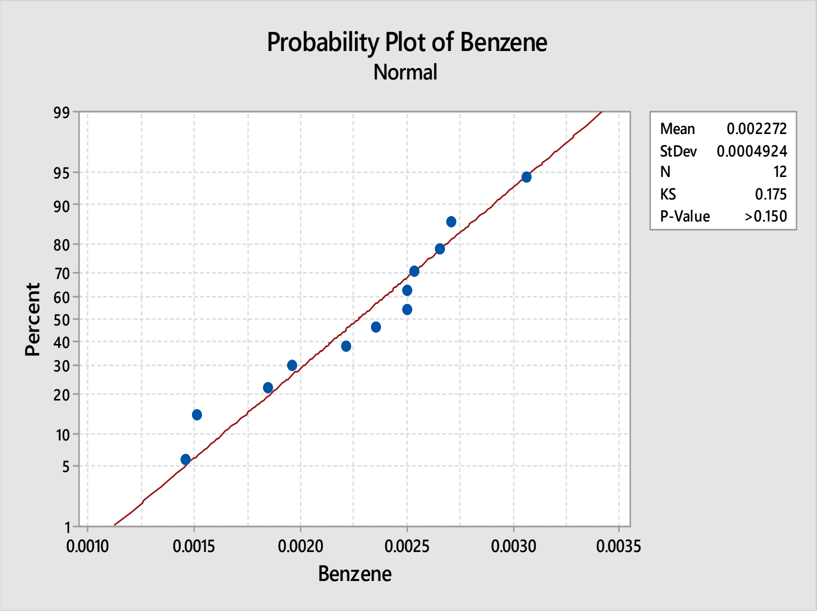
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.0005

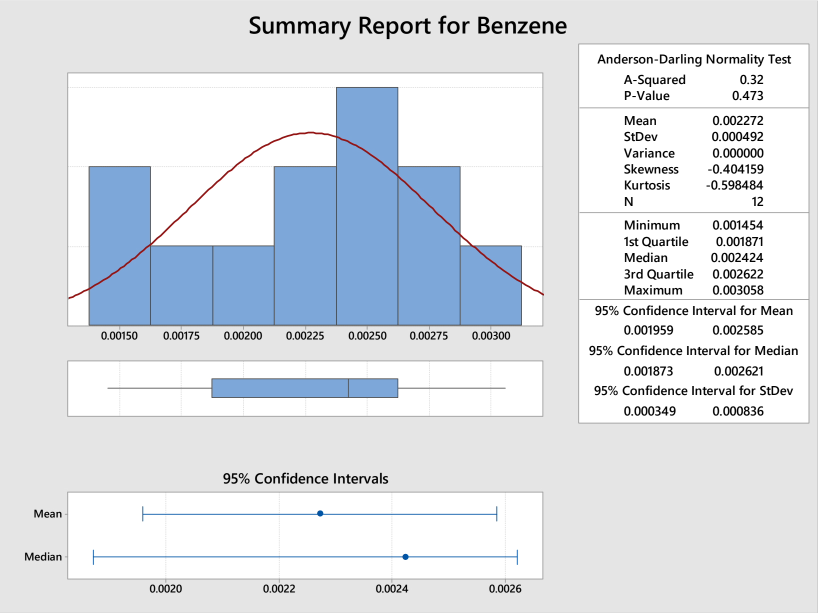
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0003	15%	36	0.8	0.809486
0.0005	20%	14	0.8	0.824086
0.0006	25%	10	0.8	0.825222
0.0007	30%	8	0.8	0.845181
0.0009	40%	5	0.8	0.828794
0.0011	50%	4	0.8	0.871558

The sample size is for each group.

Benzene no difference from Normality detected




Summary Report for Benzene

Anderson-Darling Normality Test

A-Squared	0.32
P-Value	0.473
Mean	0.002272
StDev	0.000492
Variance	0.000000
Skewness	-0.404159
Kurtosis	-0.598484
N	12
Minimum	0.001454
1st Quartile	0.001871
Median	0.002424
3rd Quartile	0.002622
Maximum	0.003058

95% Confidence Interval for Mean

0.001959 0.002585

95% Confidence Interval for Median

0.001873 0.002621

95% Confidence Interval for StDev

0.000349 0.000836

C.10.2.3 Power and Sample Size 2-Hexanone

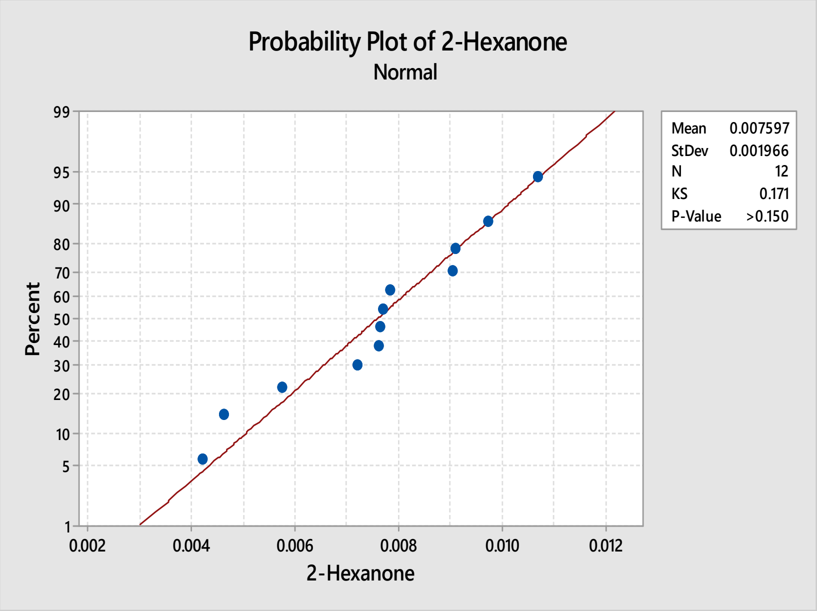
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.002

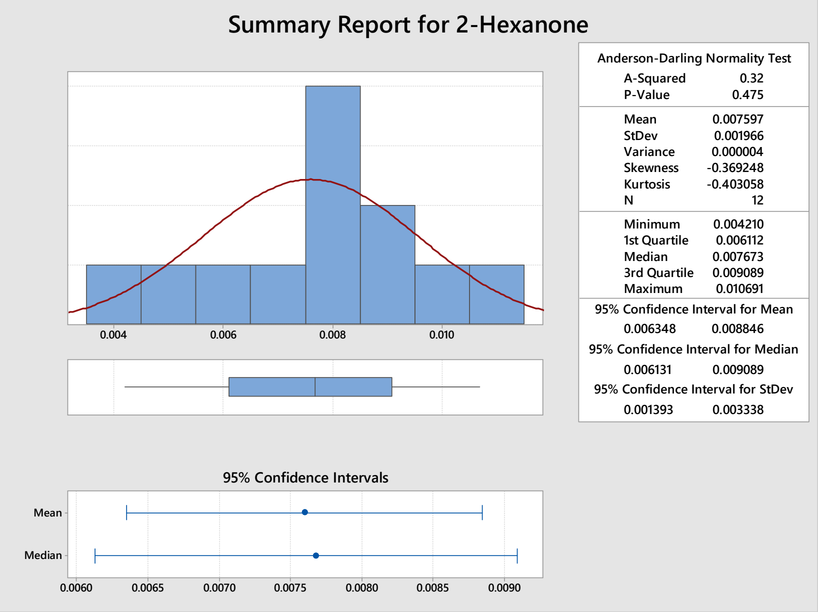
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0019	25%	15	0.8	0.814108
0.0023	30%	11	0.8	0.831257
0.0030	40%	7	0.8	0.840864
0.0038	50%	5	0.8	0.862642
0.0061	80%	3	0.8	0.917317

The sample size is for each group.

2-Hexanone no difference from Normality detected





C.10.2.4 Power and Sample Size Formaldehyde

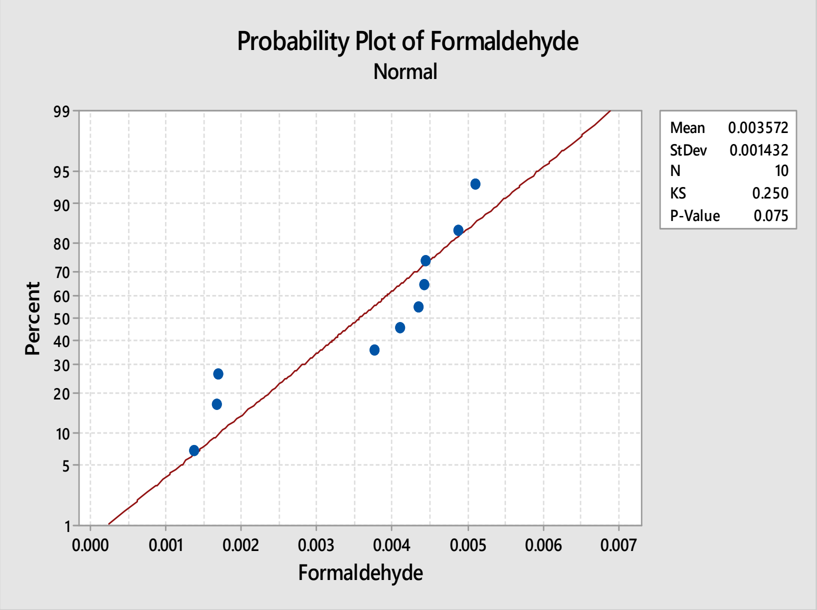
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0014

Results

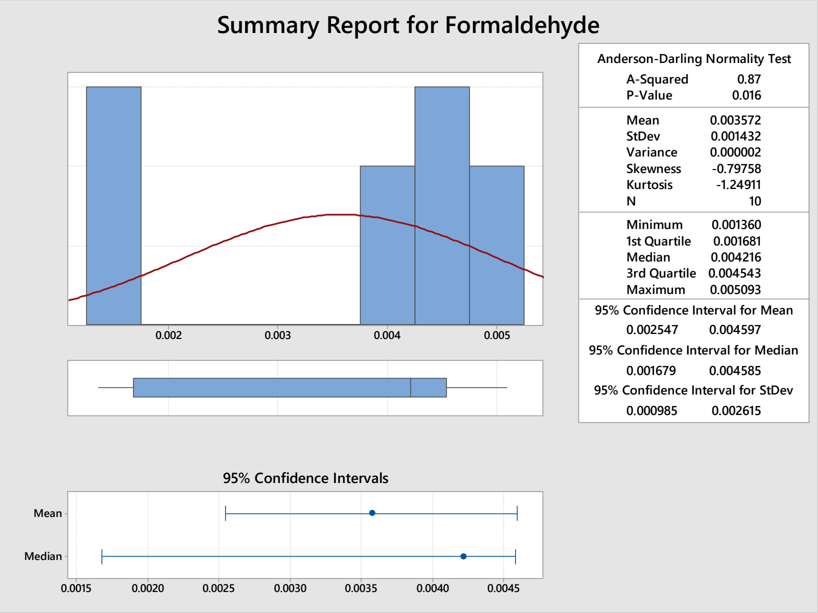
Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0011	30%	22	0.8	0.805271
0.0014	40%	14	0.8	0.824086
0.0018	50%	9	0.8	0.832590
0.0029	80%	4	0.8	0.825044
0.0032	90%	4	0.8	0.884379

The sample size is for each group.

Formaldehyde significantly different from Normal



Mean	0.003572
StDev	0.001432
N	10
KS	0.250
P-Value	0.075



Anderson-Darling Normality Test

A-Squared	0.87
P-Value	0.016
Mean	0.003572
StDev	0.001432
Variance	0.000002
Skewness	-0.79758
Kurtosis	-1.24911
N	10
Minimum	0.001360
1st Quartile	0.001681
Median	0.004216
3rd Quartile	0.004543
Maximum	0.005093

95% Confidence Interval for Mean
0.002547 0.004597
95% Confidence Interval for Median
0.001679 0.004585
95% Confidence Interval for StDev
0.000985 0.002615

C.10.2.5 Power and Sample Size Acetaldehyde

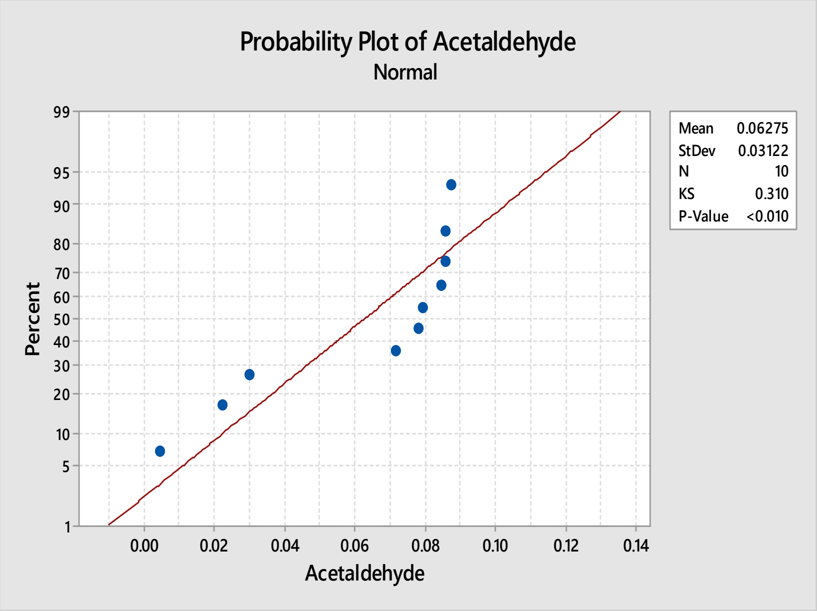
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0312

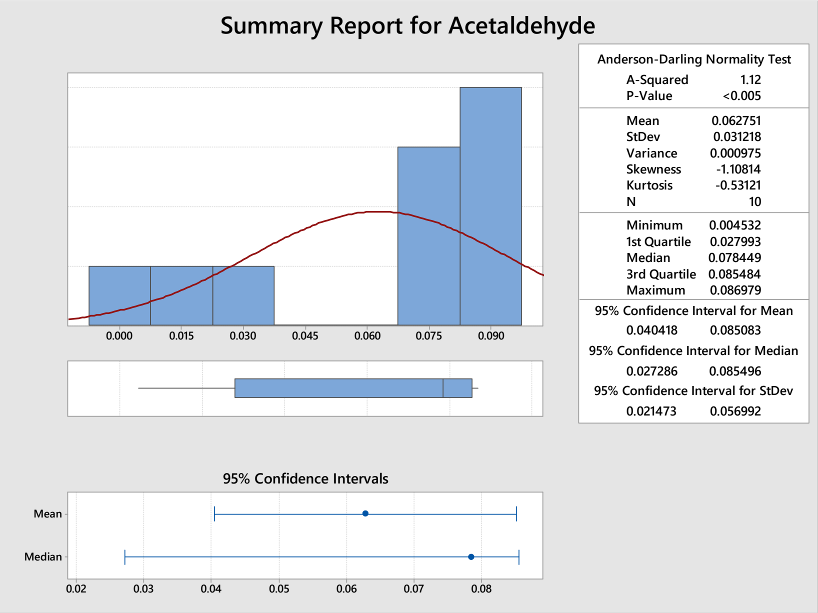
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0188	30%	35	0.8	0.802114
0.0251	40%	20	0.8	0.803292
0.0314	50%	13	0.8	0.801669
0.0502	80%	6	0.8	0.828023
0.0565	90%	5	0.8	0.832723

The sample size is for each group.

Acetaldehyde significantly different from Normal





Anderson-Darling Normality Test	
A-Squared	1.12
P-Value	<0.005
Mean	0.062751
StDev	0.031218
Variance	0.000975
Skewness	-1.10814
Kurtosis	-0.53121
N	10
Minimum	0.004532
1st Quartile	0.027993
Median	0.078449
3rd Quartile	0.085484
Maximum	0.086979
95% Confidence Interval for Mean	
0.040418	0.085083
95% Confidence Interval for Median	
0.027286	0.085496
95% Confidence Interval for StDev	
0.021473	0.056992

C.10.2.6 Power and Sample Size Furan

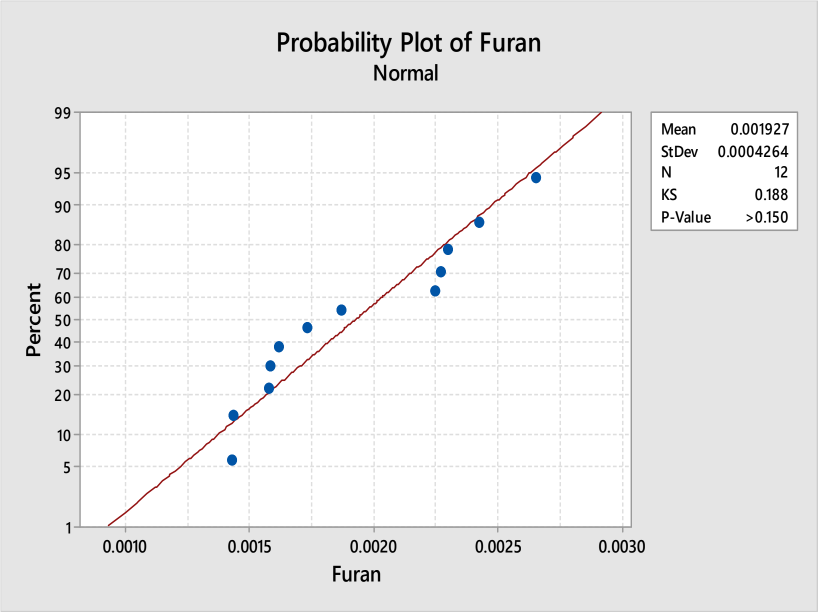
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0004

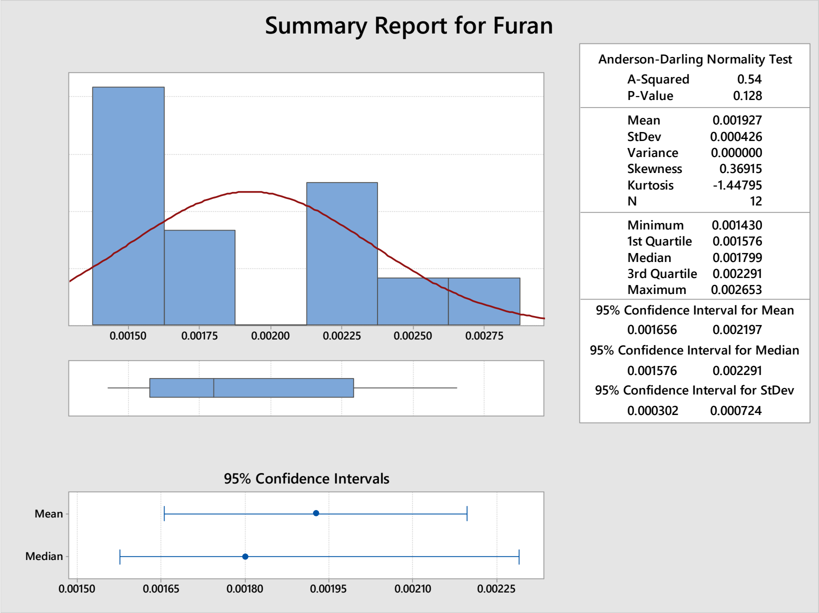
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0003	15%	23	0.8	0.804856
0.0004	20%	14	0.8	0.824086
0.0005	25%	9	0.8	0.813834
0.0006	30%	7	0.8	0.840864
0.0008	40%	4	0.8	0.801534
0.001	50%	4	0.8	0.897935

The sample size is for each group.

Furan no difference from Normality detected





```
Anderson-Darling Normality Test
   A-Squared          0.54
   P-Value           0.128

   Mean           0.001927
   StDev          0.000426
   Variance       0.000000
   Skewness        0.36915
   Kurtosis       -1.44795
   N                    12

   Minimum        0.001430
   1st Quartile   0.001576
   Median         0.001799
   3rd Quartile   0.002291
   Maximum        0.002653
95% Confidence Interval for Mean
   0.001656       0.002197
95% Confidence Interval for Median
   0.001576       0.002291
95% Confidence Interval for StDev
   0.000302       0.000724
```

C.10.2.7 Power and Sample Size Acetonitrile

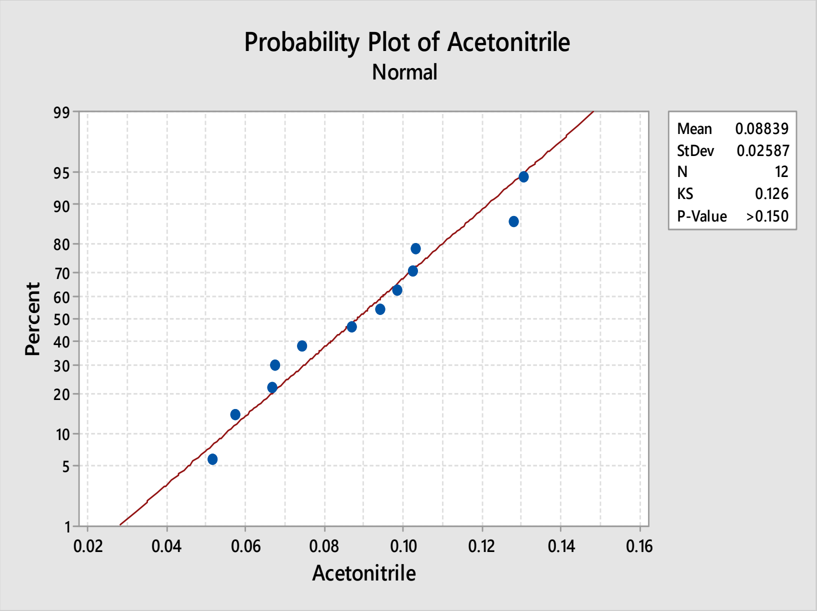
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.0259

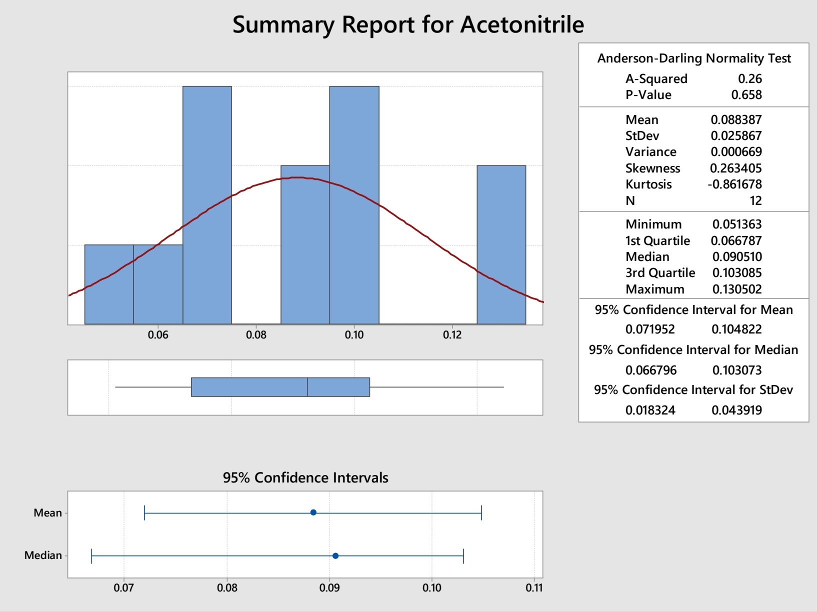
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0221	25%	18	0.8	0.806073
0.0265	30%	13	0.8	0.813014
0.0354	40%	8	0.8	0.829715
0.0442	50%	6	0.8	0.864916

The sample size is for each group.

Acetonitrile no difference from Normality detected





C.10.2.8 Power and Sample Size Propanenitrile

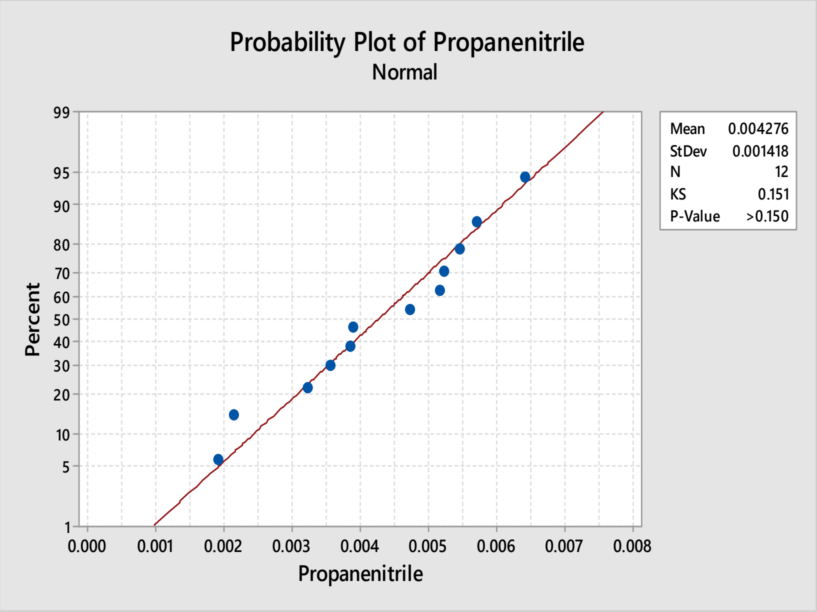
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0014

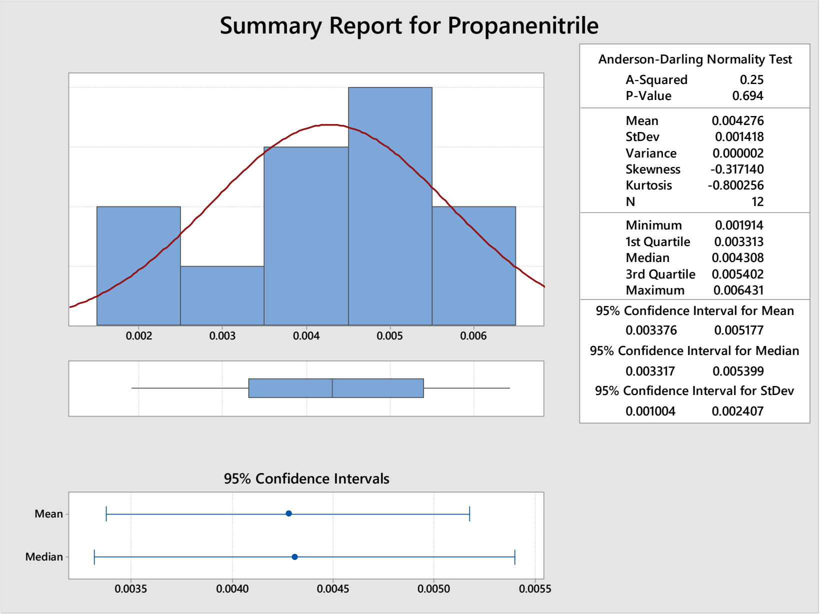
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0011	25%	21	0.8	0.804472
0.0013	30%	16	0.8	0.821624
0.0017	40%	10	0.8	0.833008
0.0021	50%	7	0.8	0.840864
0.0034	80%	4	0.8	0.914916

The sample size is for each group.

Propanenitrile no difference from Normality detected





Summary Report for Propanenitrile

Anderson-Darling Normality Test	
A-Squared	0.25
P-Value	0.694
Mean	0.004276
StDev	0.001418
Variance	0.000002
Skewness	-0.317140
Kurtosis	-0.800256
N	12
Minimum	0.001914
1st Quartile	0.003313
Median	0.004308
3rd Quartile	0.005402
Maximum	0.006431
95% Confidence Interval for Mean	
0.003376	0.005177
95% Confidence Interval for Median	
0.003317	0.005399
95% Confidence Interval for StDev	
0.001004	0.002407

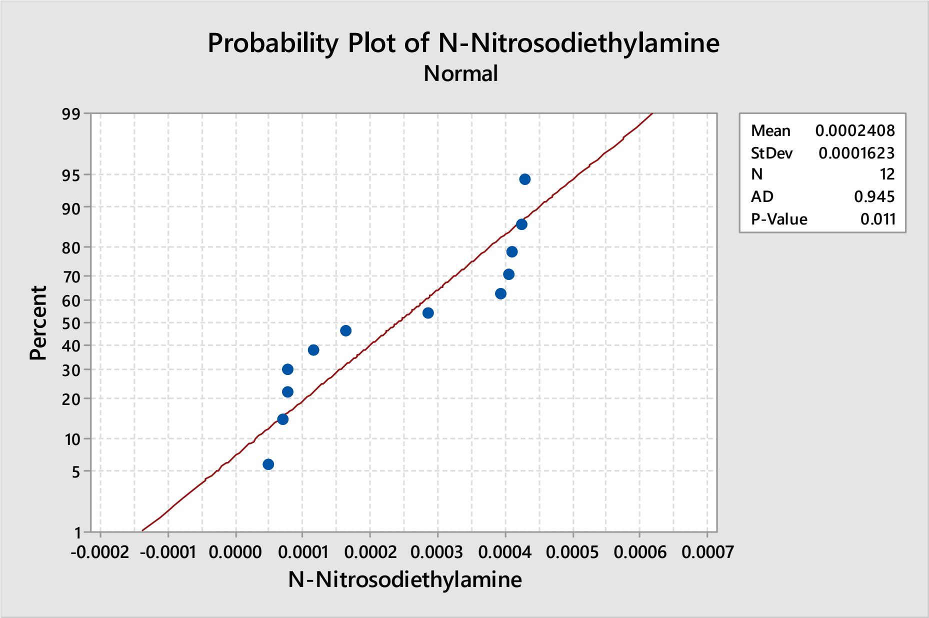
C.10.2.9 Power and Sample Size N-Nitrosodiethylamine

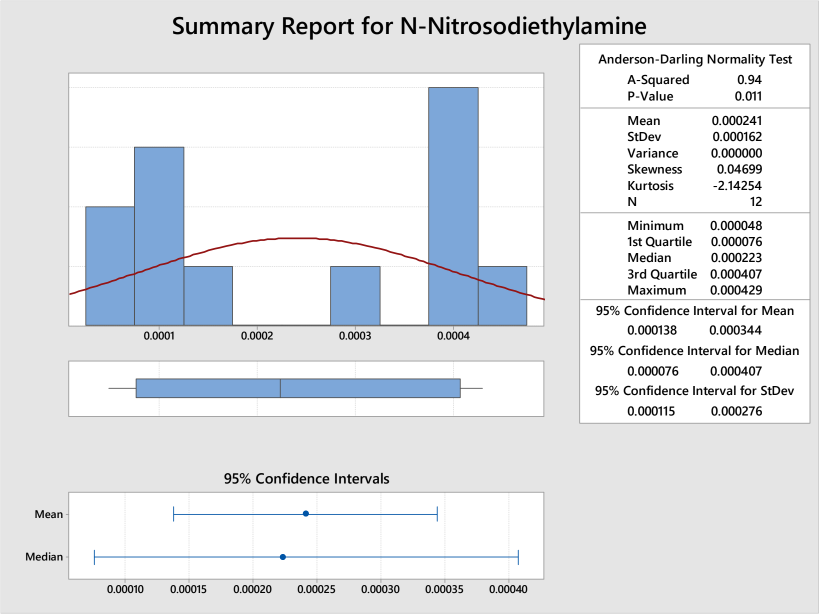
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.00016

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.000072	30%	62	0.8	0.801421
0.000092	40%	39	0.8	0.808278
0.000120	50%	23	0.8	0.804856
0.000193	80%	10	0.8	0.828657
0.000217	90%	8	0.8	0.824603

The sample size is for each group.





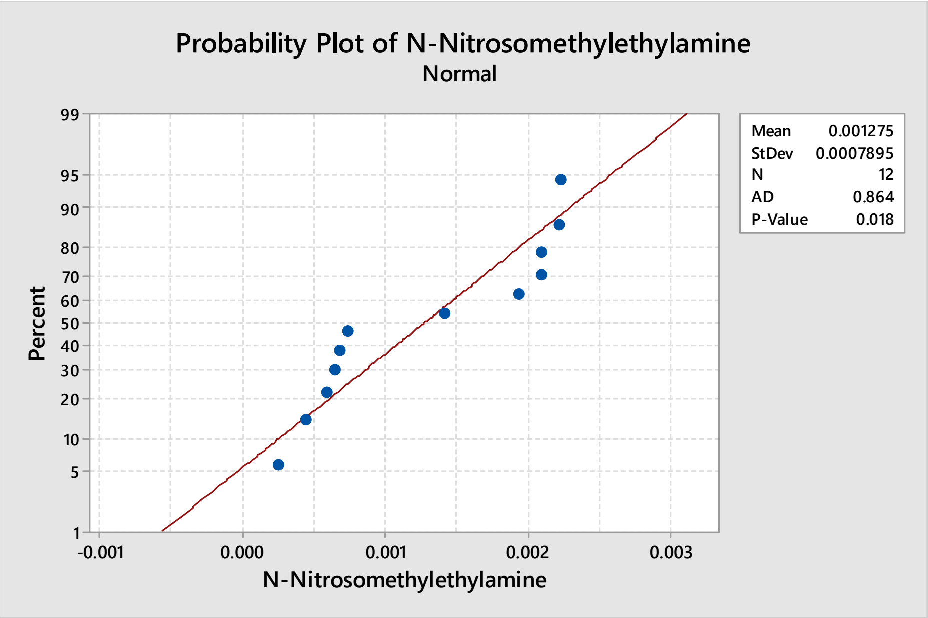
C.10.2.10 Power and Sample Size N-Nitrosomethylethylamine

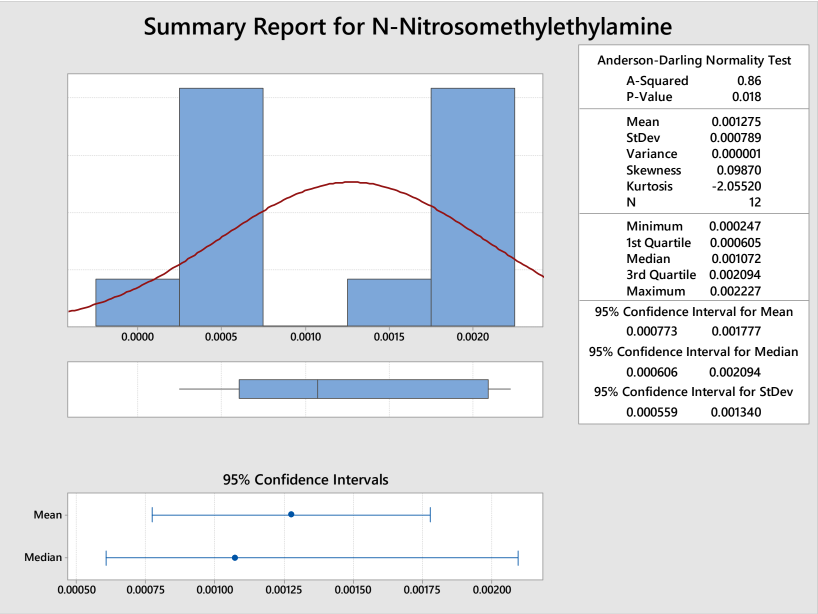
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.000789473

Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0004	30%	49	0.8	0.801024
0.0005	40%	32	0.8	0.805293
0.0006	50%	23	0.8	0.813931
0.0010	80%	9	0.8	0.822744
0.0011	90%	8	0.8	0.842154

The sample size is for each group.





Anderson-Darling Normality Test

A-Squared	0.86
P-Value	0.018
Mean	0.001275
StDev	0.000789
Variance	0.000001
Skewness	0.09870
Kurtosis	-2.05520
N	12
Minimum	0.000247
1st Quartile	0.000605
Median	0.001072
3rd Quartile	0.002094
Maximum	0.002227

95% Confidence Interval for Mean

0.000773 0.001777

95% Confidence Interval for Median

0.000606 0.002094

95% Confidence Interval for StDev

0.000559 0.001340

C.10.2.11 Power and Sample Size 1-Propanol

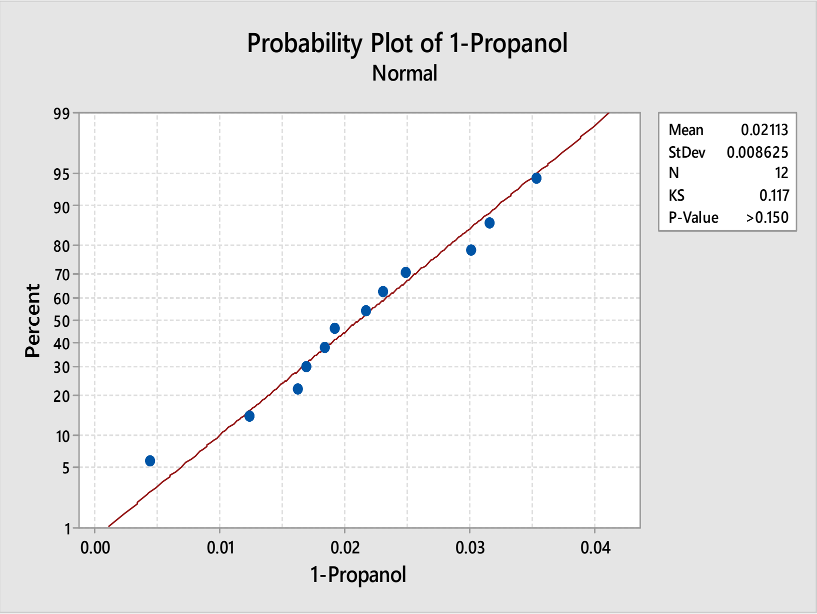
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0086

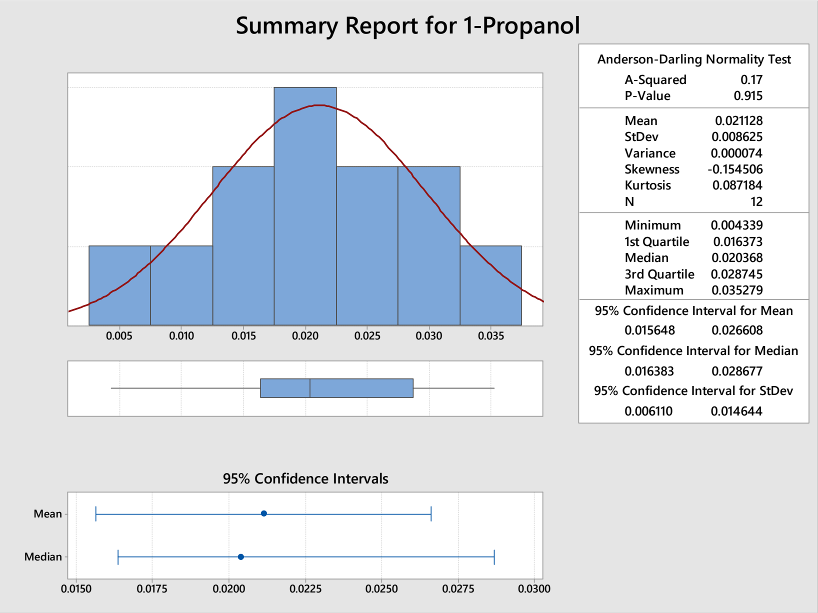
Results

Difference	Percent Differences	Sample Size	Target Power	Actual Power
0.0063	30%	24	0.8	0.801760
0.0085	40%	14	0.8	0.816237
0.0106	50%	9	0.8	0.804217
0.0169	80%	5	0.8	0.882034
0.0190	90%	4	0.8	0.865135

The sample size is for each group.

1-Propanol no difference from Normality detected





Anderson-Darling Normality Test
A-Squared 0.17
P-Value 0.915

Mean 0.021128
StDev 0.008625
Variance 0.000074
Skewness -0.154506
Kurtosis 0.087184
N 12

Minimum 0.004339
1st Quartile 0.016373
Median 0.020368
3rd Quartile 0.028745
Maximum 0.035279

95% Confidence Interval for Mean
0.015648 0.026608
95% Confidence Interval for Median
0.016383 0.028677
95% Confidence Interval for StDev
0.006110 0.014644

C.10.2.12 Power and Sample Size 2-Butanone

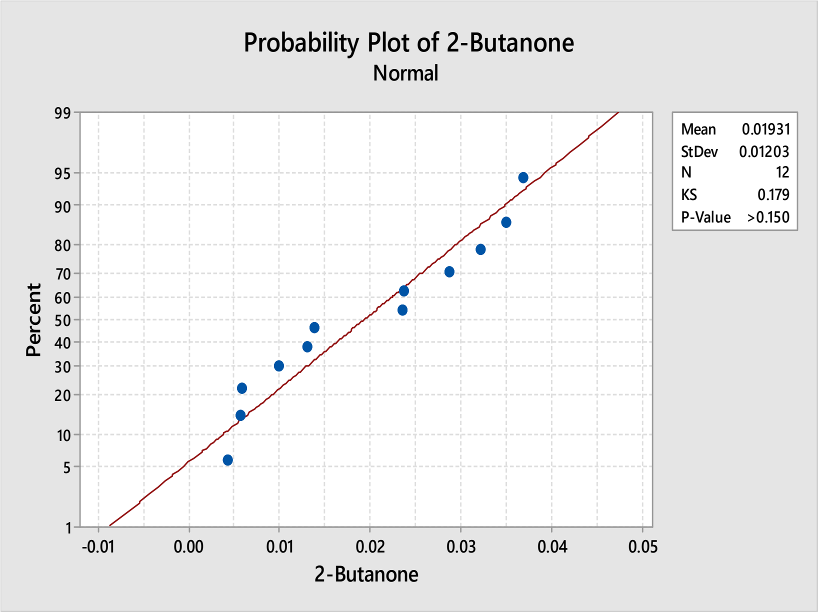
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.012

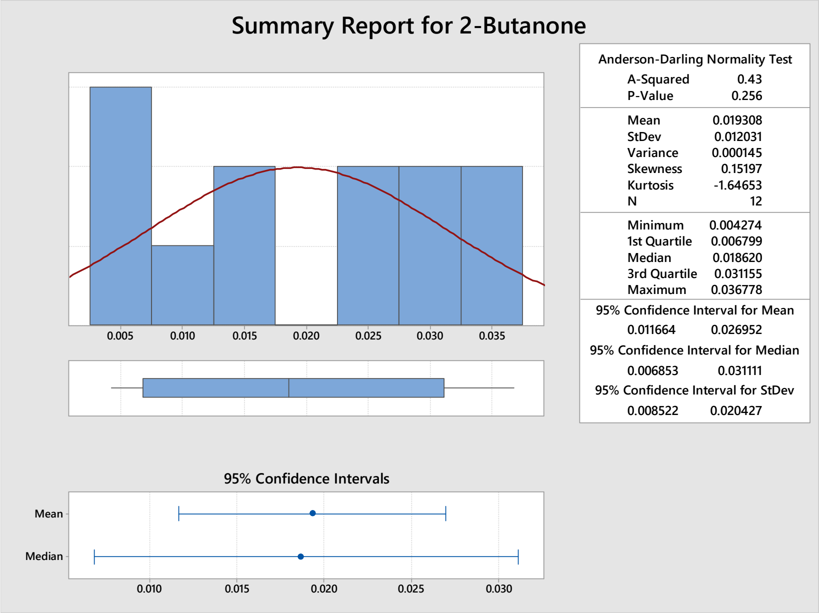
Results

Difference	Percent differences	Sample Size	Target Power	Actual Power
0.0058	30%	54	0.8	0.800717
0.0077	40%	31	0.8	0.803098
0.0097	50%	20	0.8	0.806585
0.0154	80%	9	0.8	0.831379
0.0174	90%	7	0.8	0.818650

The sample size is for each group.

2-Butanone no difference from Normality detected





C.10.2.13 Power and Sample Size 3-Heptanone

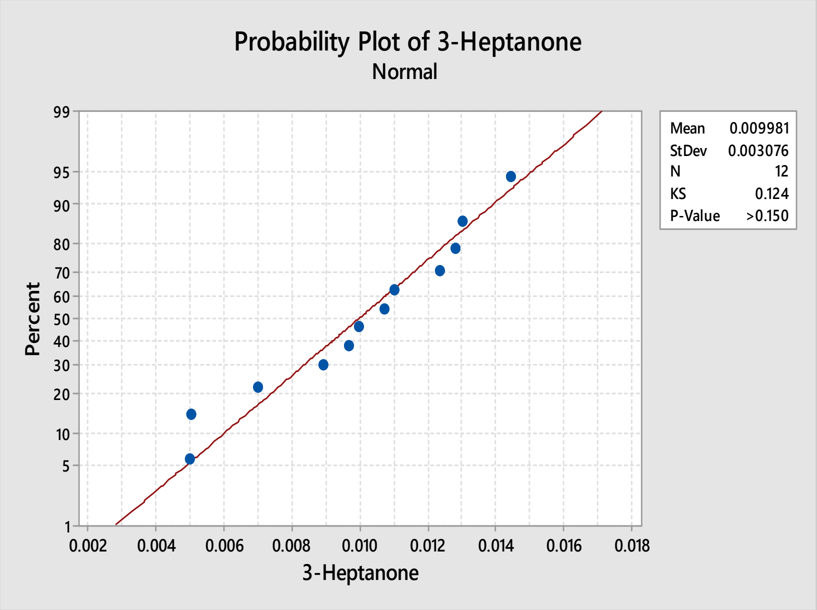
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$
Assumed standard deviation = 0.0031

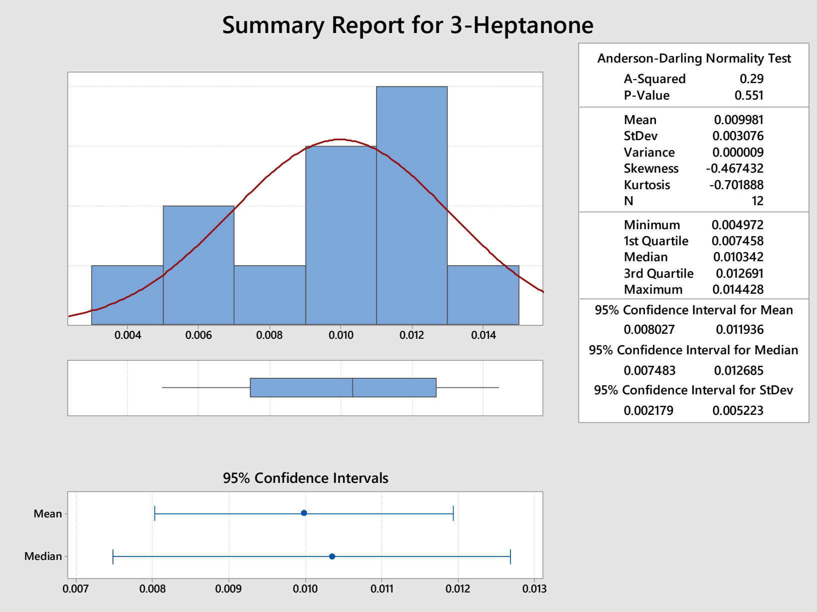
Results

Difference	Percent Differences	Sample Size	Target Power	Actual Power
0.003	30%	14	0.8	0.801785
0.004	40%	9	0.8	0.834918
0.005	50%	6	0.8	0.829623
0.008	80%	3	0.8	0.825616

The sample size is for each group.

3-Heptanone no difference from Normality detected





C.10.2.14 Power and Sample Size Cyclohexane

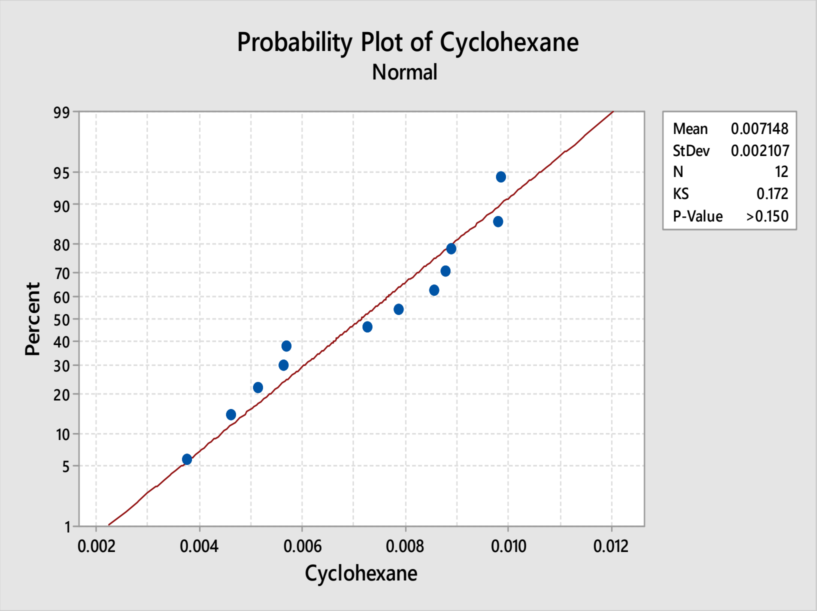
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0021

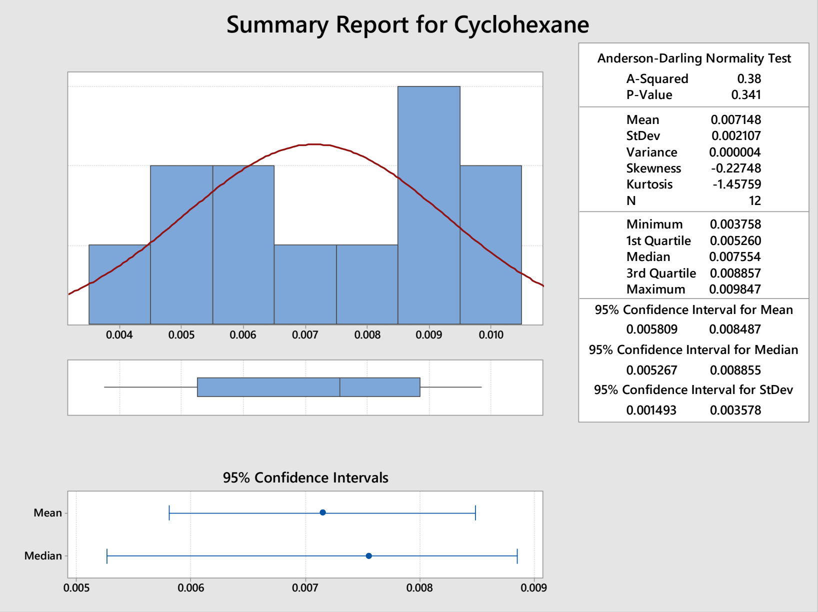
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.0014	20%	29	0.8	0.805896
0.0018	25%	18	0.8	0.809175
0.0021	30%	14	0.8	0.824086
0.0029	40%	8	0.8	0.836427
0.0036	50%	6	0.8	0.867583

The sample size is for each group.

Cyclohexane no difference from Normality detected





```
Anderson-Darling Normality Test
   A-Squared           0.38
   P-Value            0.341

   Mean            0.007148
   StDev           0.002107
   Variance        0.000004
   Skewness        -0.22748
   Kurtosis        -1.45759
   N                     12

   Minimum         0.003758
   1st Quartile    0.005260
   Median          0.007554
   3rd Quartile    0.008857
   Maximum         0.009847
95% Confidence Interval for Mean
   0.005809        0.008487
95% Confidence Interval for Median
   0.005267        0.008855
95% Confidence Interval for StDev
   0.001493        0.003578
```

C.10.2.15 Power and Sample Size Ethanol

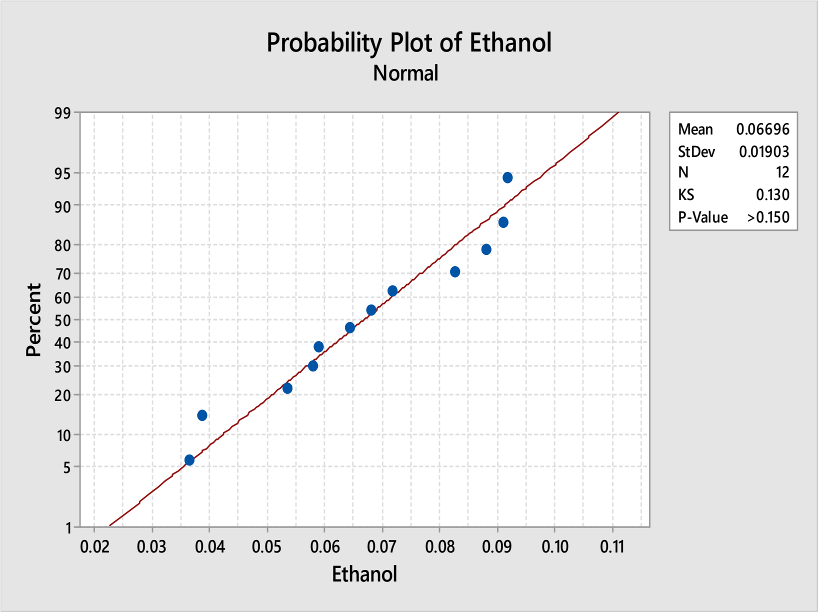
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05
Assumed standard deviation = 0.019

Results

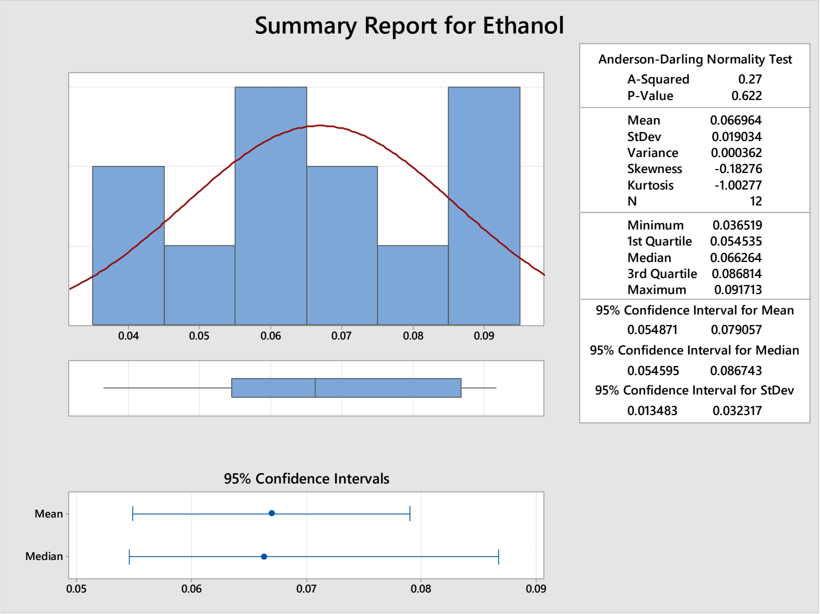
Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.0134	20%	26	0.8	0.806029
0.0167	25%	17	0.8	0.805906
0.0201	30%	12	0.8	0.806606
0.0268	40%	8	0.8	0.849884
0.0335	50%	5	0.8	0.815073

The sample size is for each group.

Ethanol no difference from Normality detected



Mean 0.06696
StDev 0.01903
N 12
KS 0.130
P-Value >0.150



Anderson-Darling Normality Test
A-Squared 0.27
P-Value 0.622

Mean 0.066964
StDev 0.019034
Variance 0.000362
Skewness -0.18276
Kurtosis -1.00277
N 12

Minimum 0.036519
1st Quartile 0.054535
Median 0.066264
3rd Quartile 0.086814
Maximum 0.091713

95% Confidence Interval for Mean
0.054871 0.079057

95% Confidence Interval for Median
0.054595 0.086743

95% Confidence Interval for StDev
0.013483 0.032317

C.10.2.16 Power and Sample Size n-Heptane

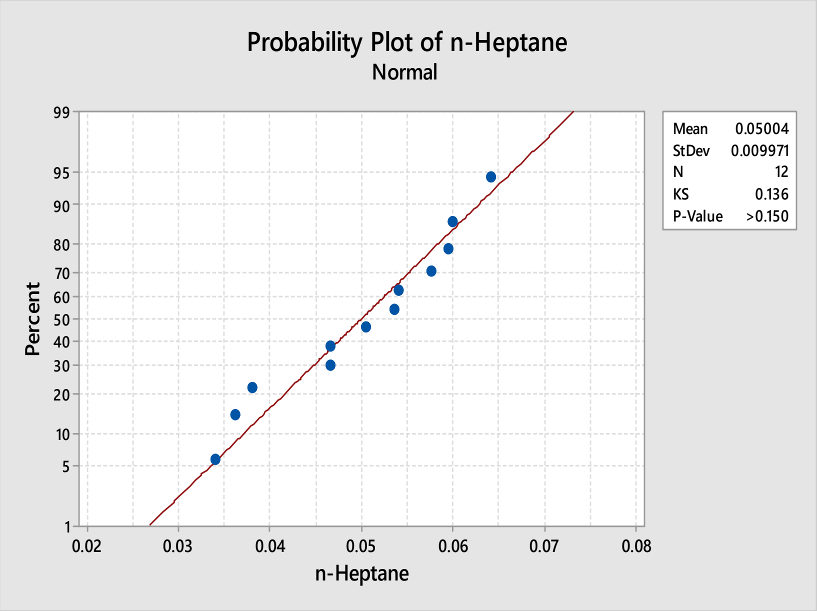
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.01

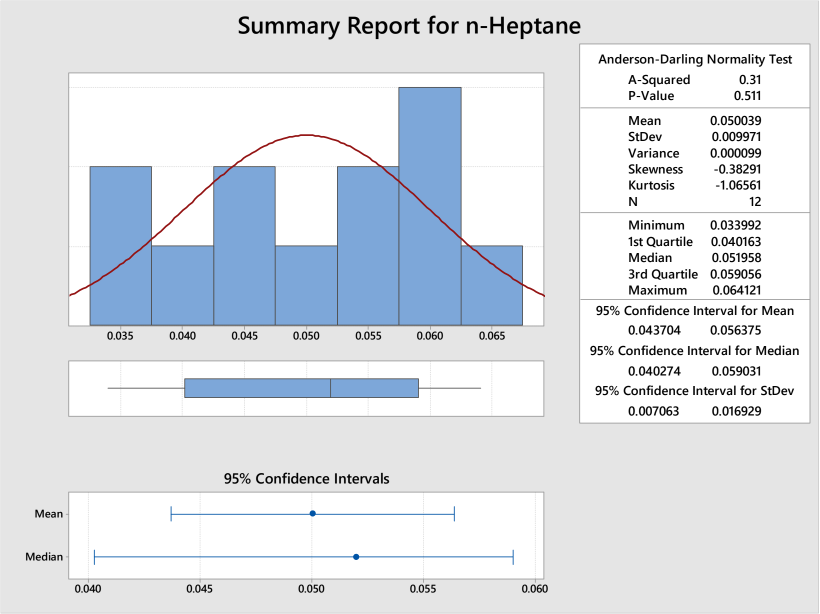
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.0050	10%	51	0.8	0.805899
0.0075	15%	23	0.8	0.804856
0.0100	20%	14	0.8	0.824086
0.0125	25%	9	0.8	0.813834
0.0150	30%	7	0.8	0.840864
0.025	50%	3	0.8	0.806789

The sample size is for each group.

n-Heptane no difference from Normality detected





Anderson-Darling Normality Test

A-Squared	0.31
P-Value	0.511
Mean	0.050039
StDev	0.009971
Variance	0.000099
Skewness	-0.38291
Kurtosis	-1.06561
N	12
Minimum	0.033992
1st Quartile	0.040163
Median	0.051958
3rd Quartile	0.059056
Maximum	0.064121

95% Confidence Interval for Mean

0.043704 0.056375

95% Confidence Interval for Median

0.040274 0.059031

95% Confidence Interval for StDev

0.007063 0.016929

C.10.2.17 Power and Sample Size Toluene

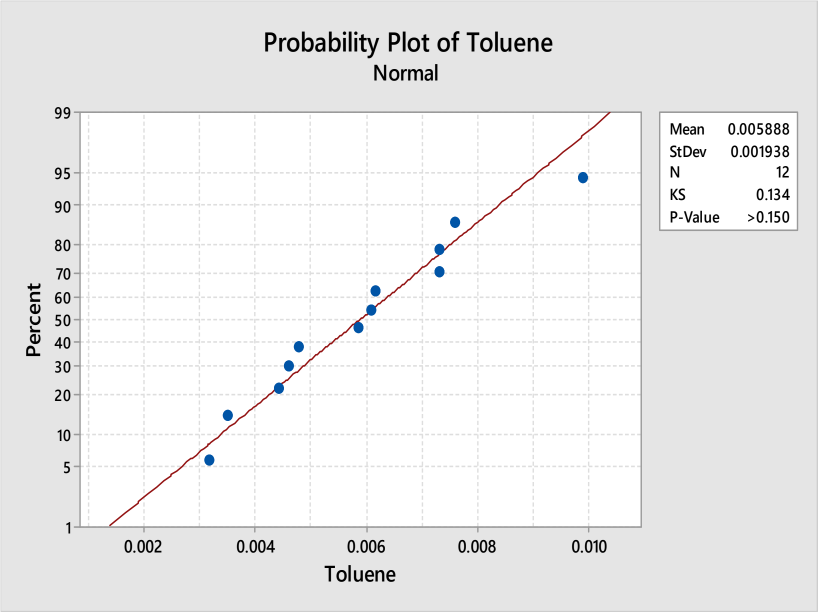
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05
Assumed standard deviation = 0.0019

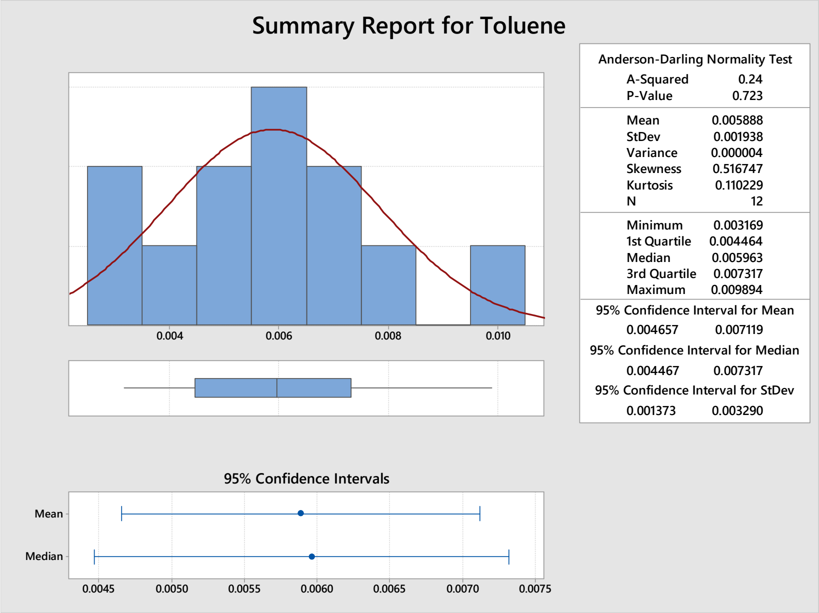
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.0015	25%	21	0.8	0.807761
0.0018	30%	15	0.8	0.812221
0.0024	40%	9	0.8	0.820891
0.0029	50%	7	0.8	0.851805
0.0047	80%	4	0.8	0.923167

The sample size is for each group.

Toluene no difference from Normality detected





C.10.2.18 Power and Sample Size Trichlorofluoromethane

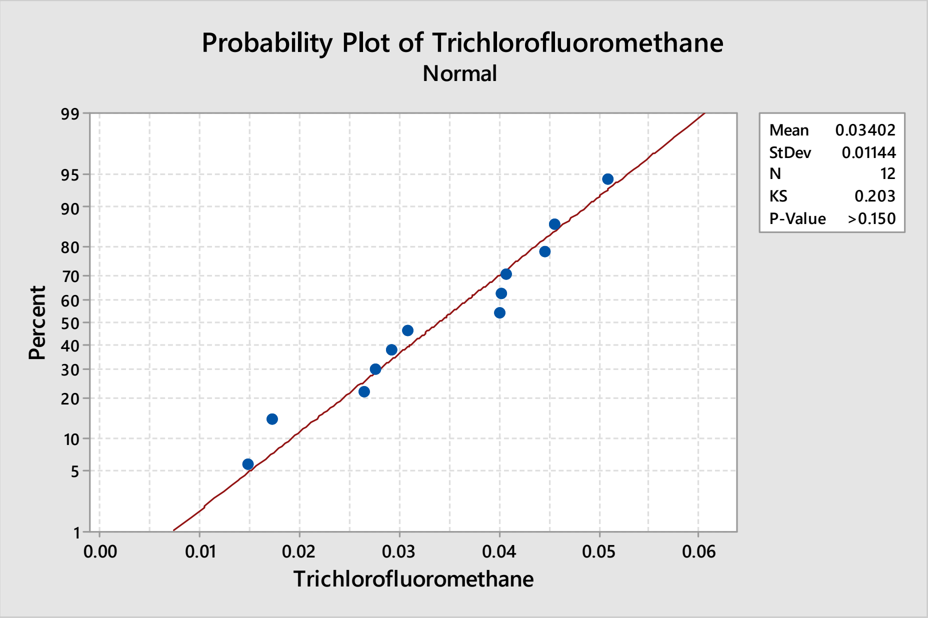
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.0114

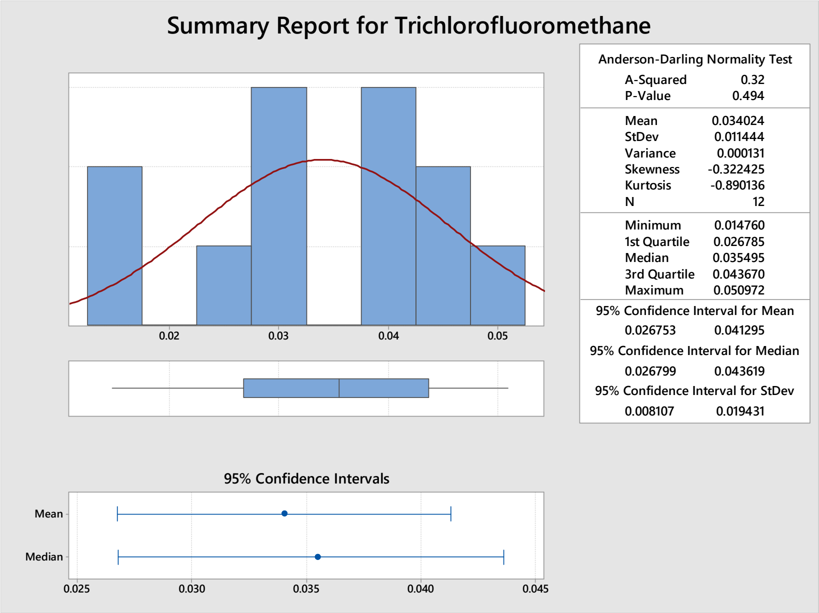
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.0085	25%	23	0.8	0.800793
0.0102	30%	17	0.8	0.818044
0.0136	40%	10	0.8	0.821315
0.0170	50%	7	0.8	0.837102
0.0272	80%	4	0.8	0.906525

The sample size is for each group.

Trichlorofluoromethane no difference from Normality detected





Summary Report for Trichlorofluoromethane

Anderson-Darling Normality Test	
A-Squared	0.32
P-Value	0.494
Mean	0.034024
StDev	0.011444
Variance	0.000131
Skewness	-0.322425
Kurtosis	-0.890136
N	12
Minimum	0.014760
1st Quartile	0.026785
Median	0.035495
3rd Quartile	0.043670
Maximum	0.050972

95% Confidence Interval for Mean

0.026753 0.041295

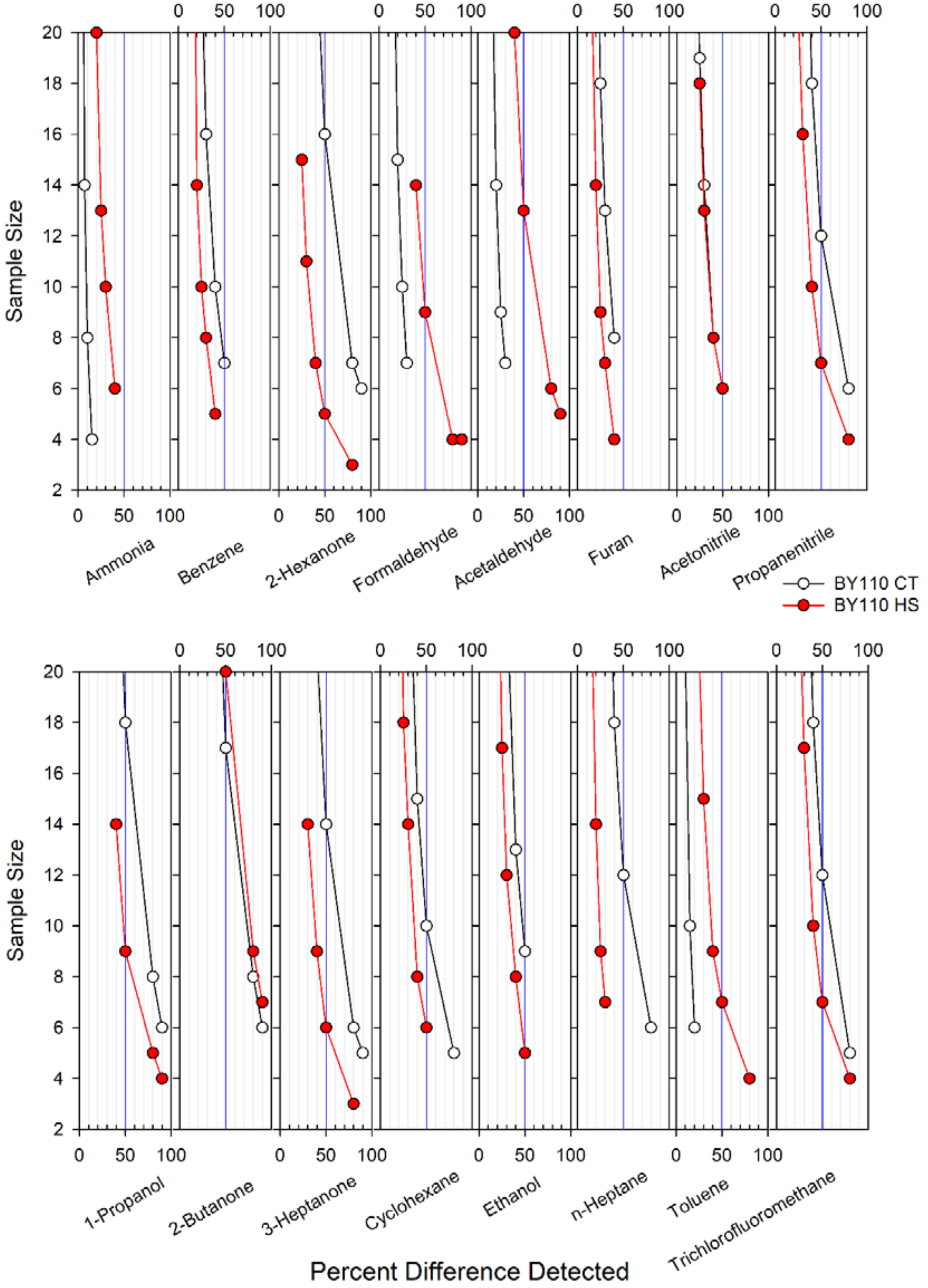
95% Confidence Interval for Median

0.026799 0.043619

95% Confidence Interval for StDev

0.008107 0.019431

C.10.3 CT Sample Size Calculation and Test of Normality



Sample Size Required to Detect a Given Percentage Difference between the HS and CT Mean Chemical Concentrations with the Observed Variance, a 1-Sided T-Test at 80% Power, and α=0.05.

C.10.3.1 Power and Sample Size Ammonia

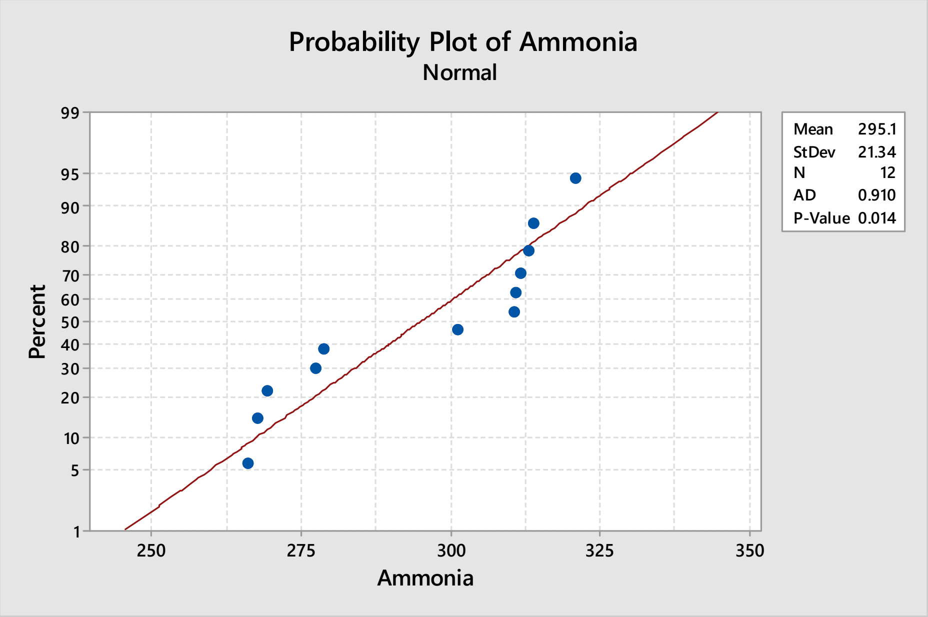
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 21.3

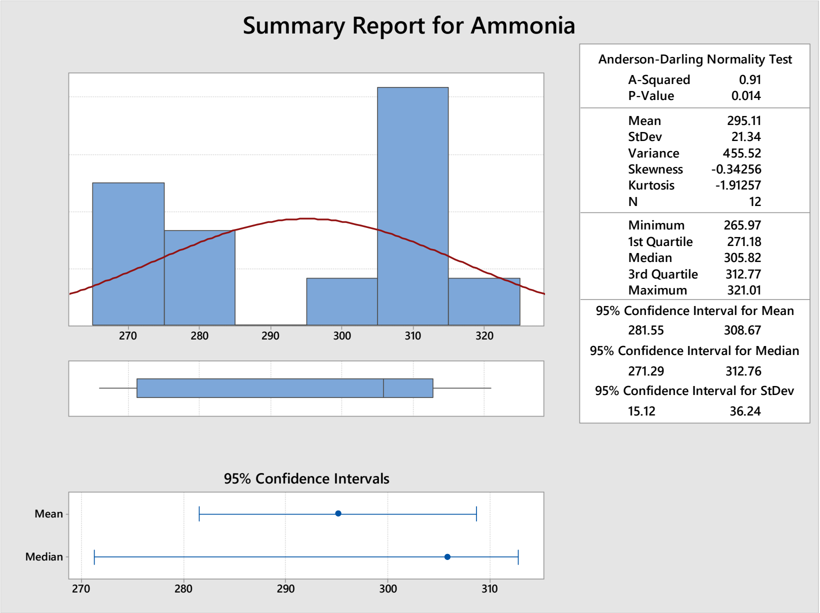
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
5.902	2%	162	0.8	0.800583
14.755	5%	27	0.8	0.807037
20.657	7%	14	0.8	0.803266
29.510	10%	8	0.8	0.838521
44.265	15%	4	0.8	0.827166
88.53	30%	2	0.8	0.825617
147.55	50%	2	0.8	0.990572

The sample size is for each group.

Ammonia significantly different from normal.





Anderson-Darling Normality Test

A-Squared	0.91
P-Value	0.014
Mean	295.11
StDev	21.34
Variance	455.52
Skewness	-0.34256
Kurtosis	-1.91257
N	12
Minimum	265.97
1st Quartile	271.18
Median	305.82
3rd Quartile	312.77
Maximum	321.01

95% Confidence Interval for Mean

281.55 308.67

95% Confidence Interval for Median

271.29 312.76

95% Confidence Interval for StDev

15.12 36.24

C.10.3.2 Power and Sample Size Benzene

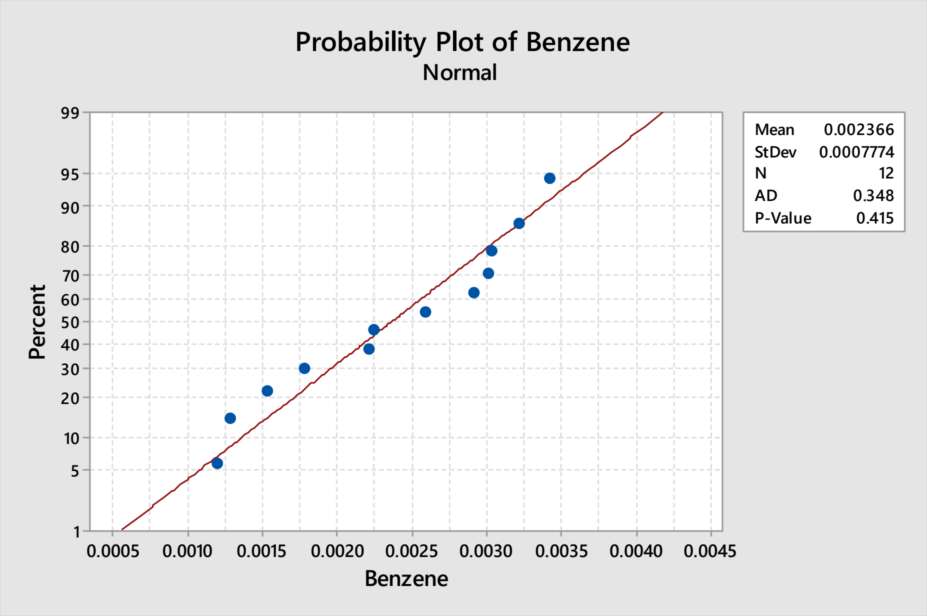
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0008

Results

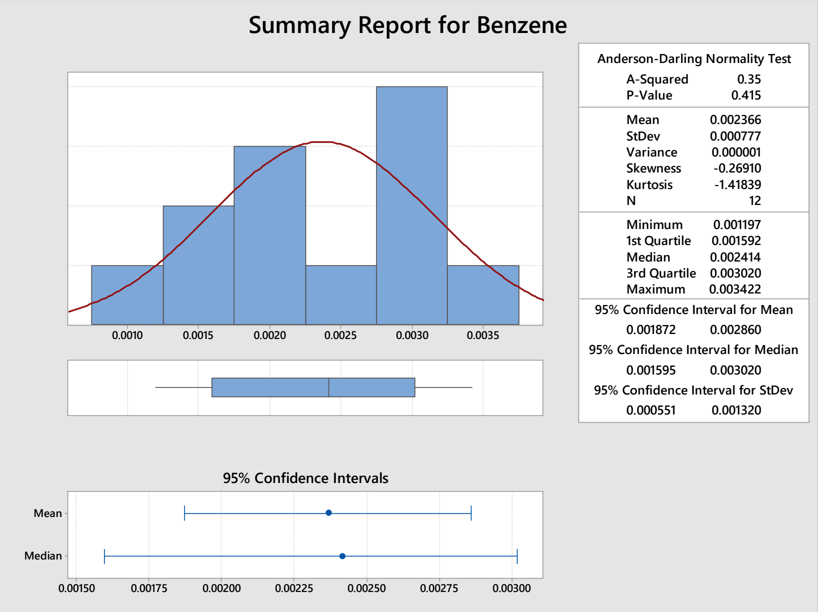
Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00048	20%	36	0.8	0.809486
0.00060	25%	23	0.8	0.804856
0.00072	30%	16	0.8	0.800287
0.00096	40%	10	0.8	0.825222
0.00120	50%	7	0.8	0.840864

The sample size is for each group.

Benzene no difference from Normality detected



Mean	0.002366
StDev	0.0007774
N	12
AD	0.348
P-Value	0.415



Anderson-Darling Normality Test

A-Squared	0.35
P-Value	0.415
Mean	0.002366
StDev	0.000777
Variance	0.000001
Skewness	-0.26910
Kurtosis	-1.41839
N	12
Minimum	0.001197
1st Quartile	0.001592
Median	0.002414
3rd Quartile	0.003020
Maximum	0.003422

95% Confidence Interval for Mean

0.001872 0.002860

95% Confidence Interval for Median

0.001595 0.003020

95% Confidence Interval for StDev

0.000551 0.001320

C.10.3.3 Power and Sample Size 2-Hexanone

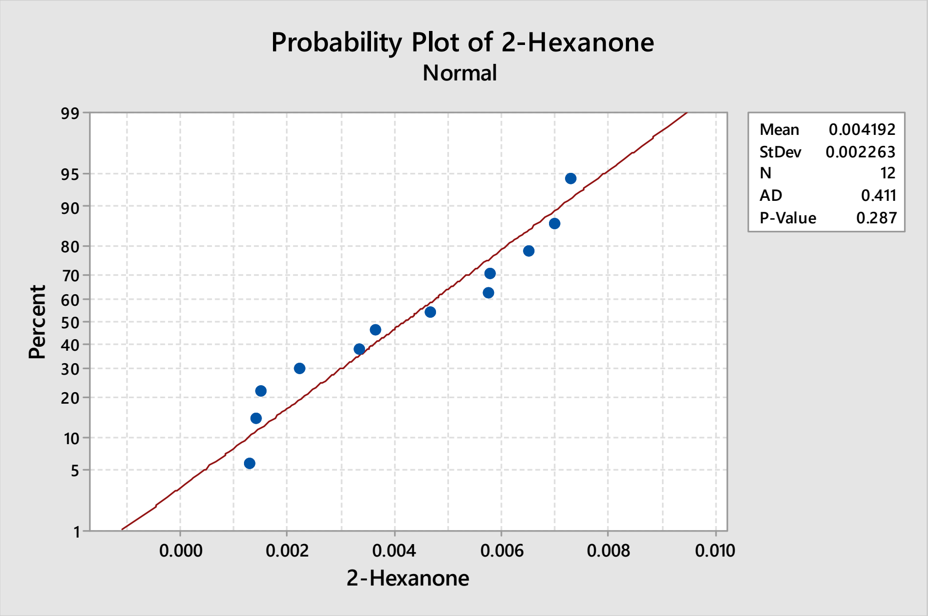
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0023

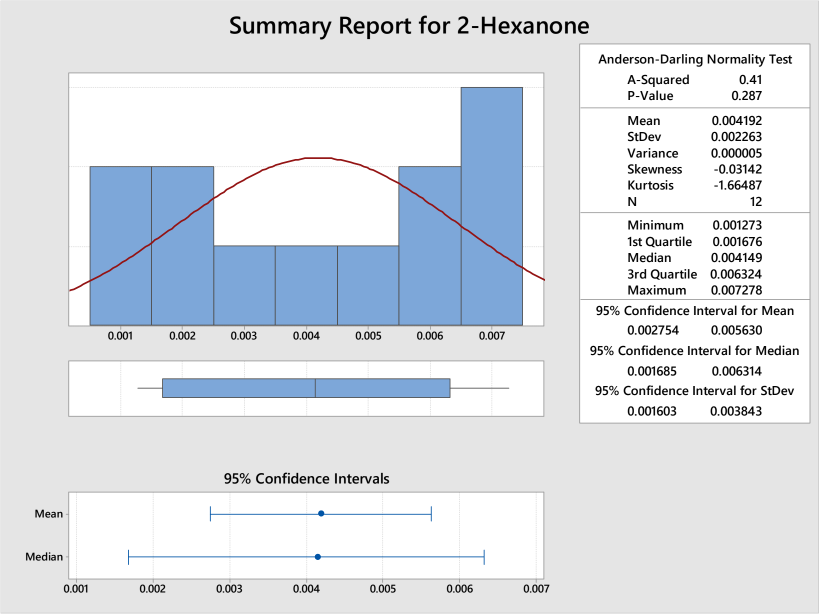
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00126	30%	42	0.8	0.800889
0.00168	40%	24	0.8	0.801766
0.00210	50%	16	0.8	0.810212
0.00336	80%	7	0.8	0.823637
0.00378	90%	6	0.8	0.841745

The sample size is for each group.

2-Hexanone no difference from Normality detected





Summary Report for 2-Hexanone

Anderson-Darling Normality Test	
A-Squared	0.41
P-Value	0.287
Mean	0.004192
StDev	0.002263
Variance	0.000005
Skewness	-0.03142
Kurtosis	-1.66487
N	12
Minimum	0.001273
1st Quartile	0.001676
Median	0.004149
3rd Quartile	0.006324
Maximum	0.007278

95% Confidence Interval for Mean
0.002754 0.005630
95% Confidence Interval for Median
0.001685 0.006314
95% Confidence Interval for StDev
0.001603 0.003843

C.10.3.4 Power and Sample Size Formaldehyde

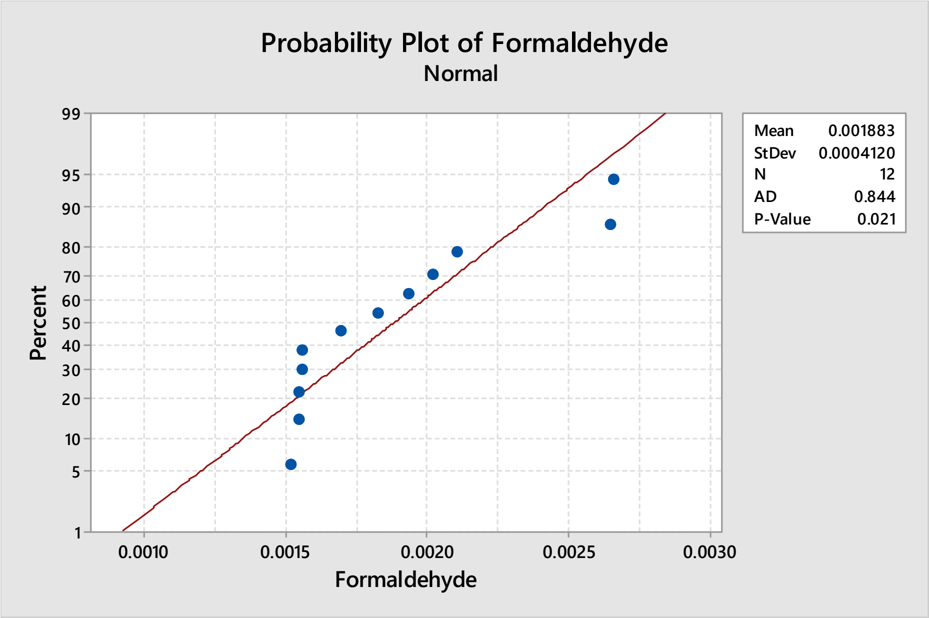
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0004

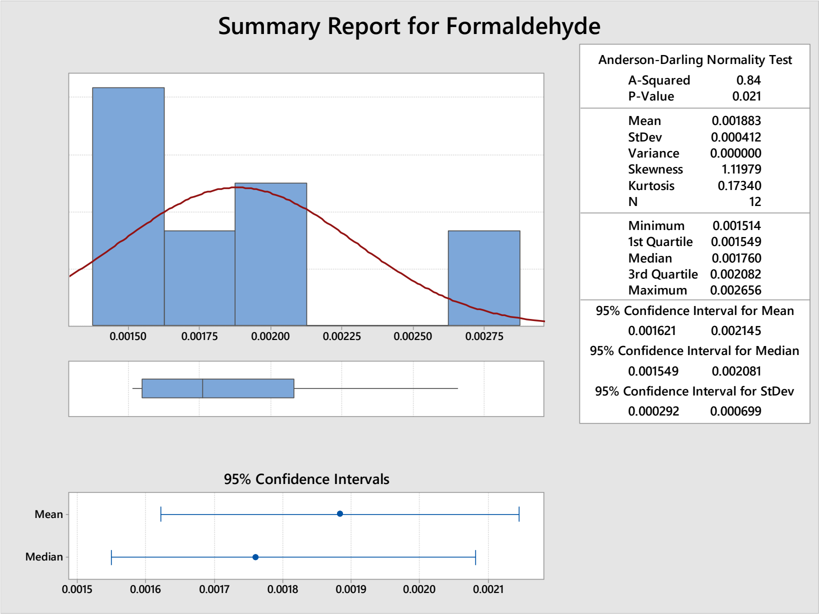
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.000190	10%	56	0.8	0.803199
0.000285	15%	26	0.8	0.813022
0.000380	20%	15	0.8	0.814108
0.000475	25%	10	0.8	0.818224
0.000570	30%	7	0.8	0.806846
0.00095	50%	4	0.8	0.904269

The sample size is for each group.

Formaldehyde significantly different from normal.





C.10.3.5 Power and Sample Size Acetaldehyde

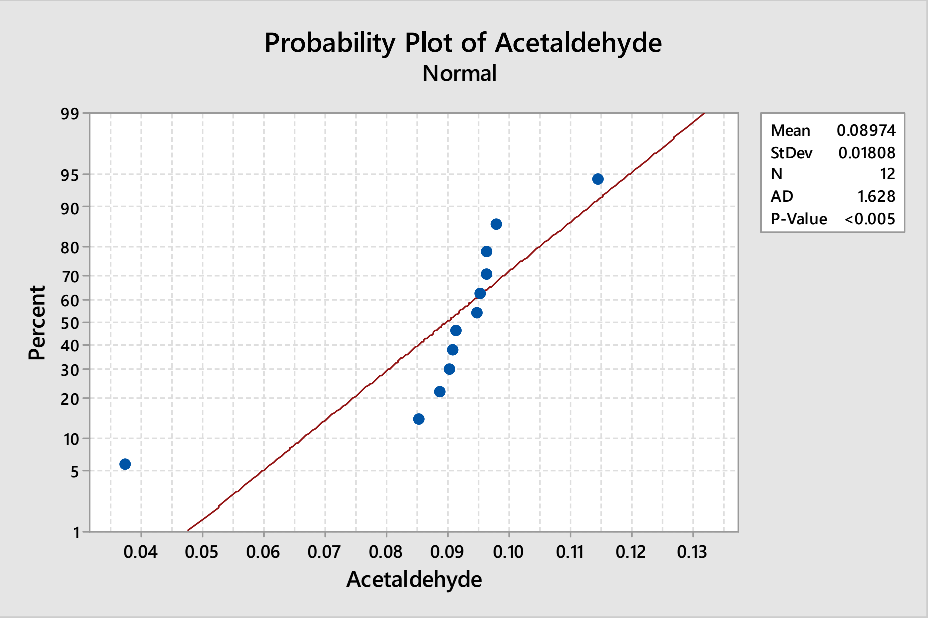
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.0181

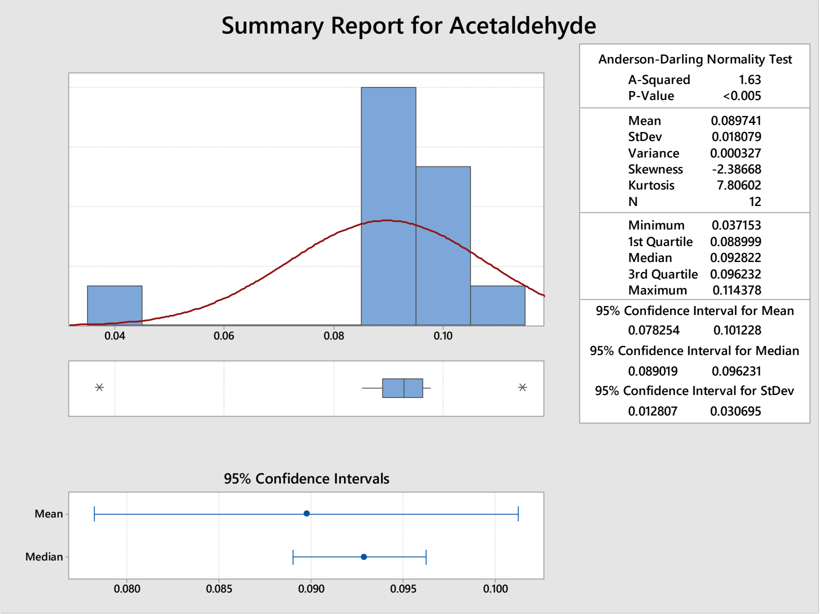
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.008970	10%	52	0.8	0.806563
0.013455	15%	24	0.8	0.813825
0.017940	20%	14	0.8	0.818139
0.022425	25%	9	0.8	0.807776
0.026910	30%	7	0.8	0.835155
0.04485	50%	4	0.8	0.923905

The sample size is for each group.

Acetaldehyde significantly different from normal.





Anderson-Darling Normality Test

A-Squared	1.63
P-Value	<0.005
Mean	0.089741
StDev	0.018079
Variance	0.000327
Skewness	-2.38668
Kurtosis	7.80602
N	12
Minimum	0.037153
1st Quartile	0.088999
Median	0.092822
3rd Quartile	0.096232
Maximum	0.114378

95% Confidence Interval for Mean

0.078254 0.101228

95% Confidence Interval for Median

0.089019 0.096231

95% Confidence Interval for StDev

0.012807 0.030695

C.10.3.6 Power and Sample Size Furan

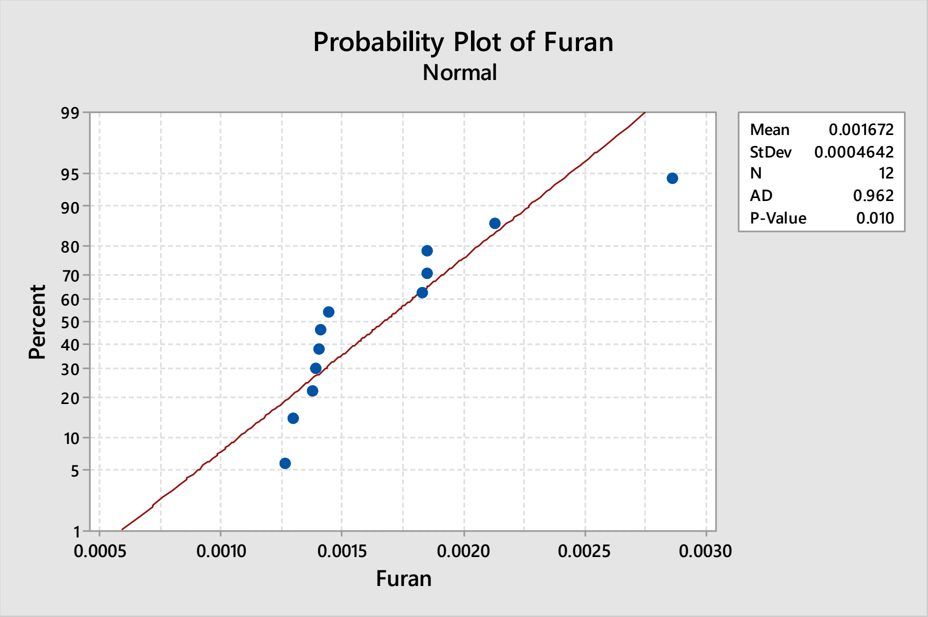
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0005

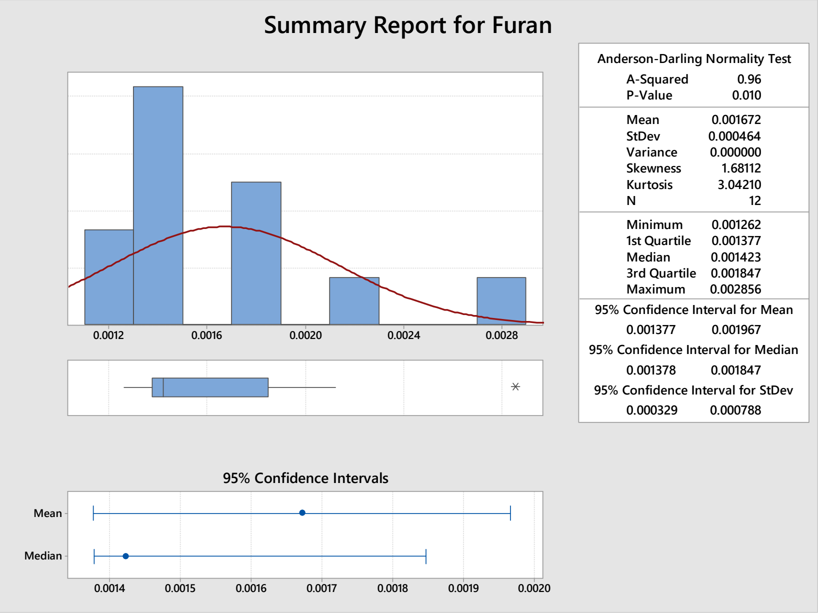
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.000255	15%	49	0.8	0.805563
0.000340	20%	28	0.8	0.807134
0.000425	25%	18	0.8	0.803412
0.000510	30%	13	0.8	0.810902
0.000680	40%	8	0.8	0.826432
0.00085	50%	6	0.8	0.862620

The sample size is for each group.

Furan significantly different from normal.





Anderson-Darling Normality Test
A-Squared 0.96
P-Value 0.010

Mean 0.001672
StDev 0.000464
Variance 0.000000
Skewness 1.68112
Kurtosis 3.04210
N 12

Minimum 0.001262
1st Quartile 0.001377
Median 0.001423
3rd Quartile 0.001847
Maximum 0.002856

95% Confidence Interval for Mean
0.001377 0.001967
95% Confidence Interval for Median
0.001378 0.001847
95% Confidence Interval for StDev
0.000329 0.000788

C.10.3.7 Power and Sample Size Acetonitrile

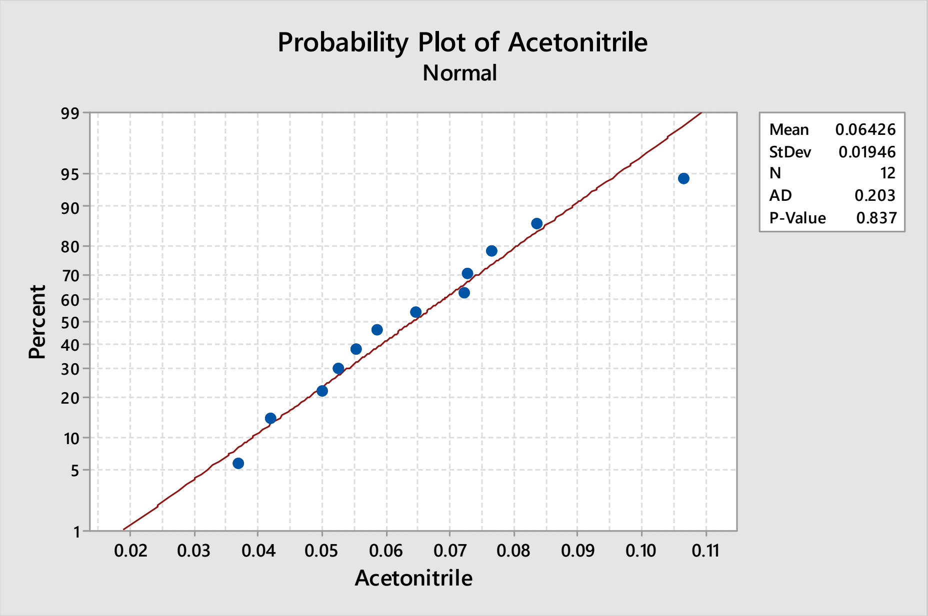
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
$\alpha = 0.05$ Assumed standard deviation = 0.0195

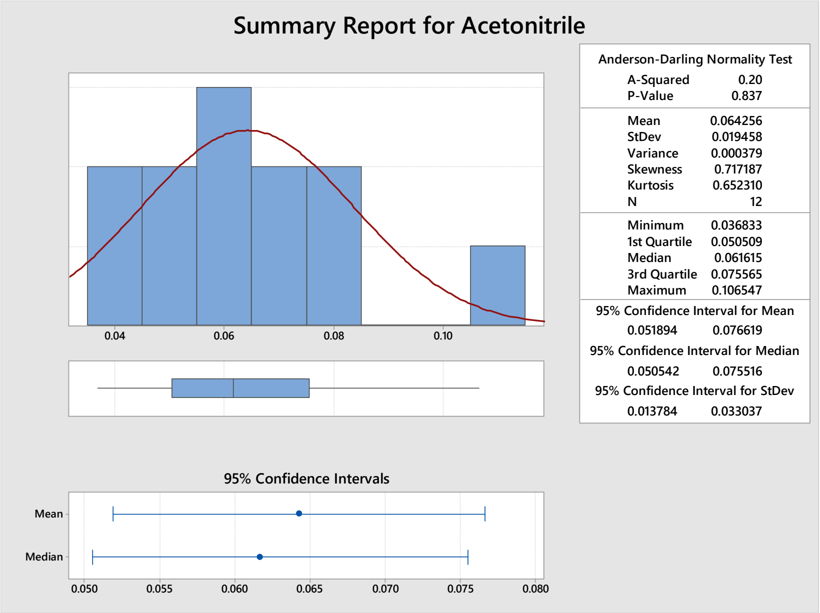
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.012860	20%	30	0.8	0.810394
0.016075	25%	19	0.8	0.801717
0.019290	30%	14	0.8	0.816824
0.025720	40%	8	0.8	0.805760
0.032150	50%	6	0.8	0.843763

The sample size is for each group.

Acetonitrile no difference from Normality detected




Summary Report for Acetonitrile

Anderson-Darling Normality Test	
A-Squared	0.20
P-Value	0.837
Mean	0.064256
StDev	0.019458
Variance	0.000379
Skewness	0.717187
Kurtosis	0.652310
N	12
Minimum	0.036833
1st Quartile	0.050509
Median	0.061615
3rd Quartile	0.075565
Maximum	0.106547
95% Confidence Interval for Mean	
0.051894	0.076619
95% Confidence Interval for Median	
0.050542	0.075516
95% Confidence Interval for StDev	
0.013784	0.033037

C.10.3.8 Power and Sample Size Propanenitrile

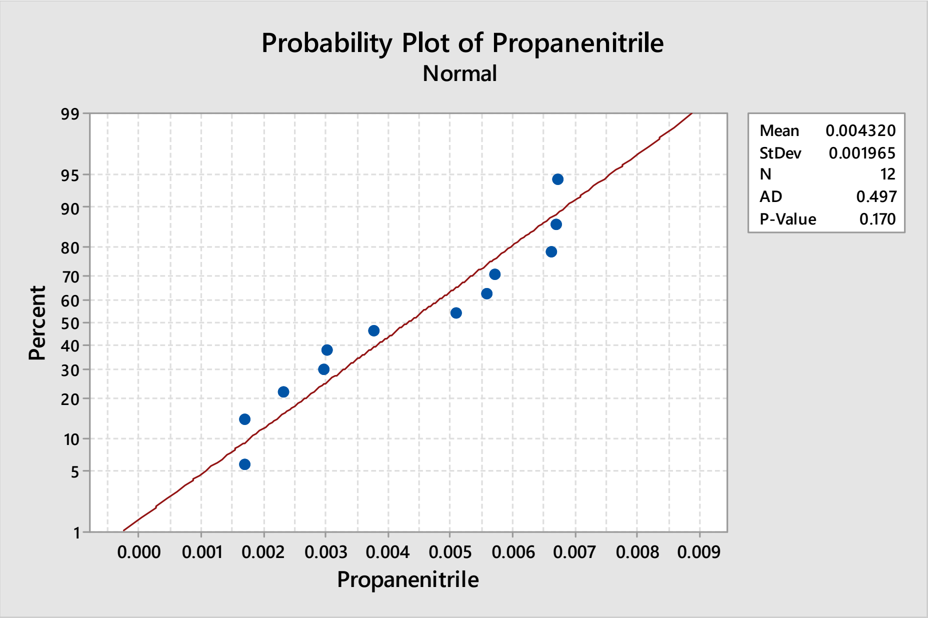
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.002

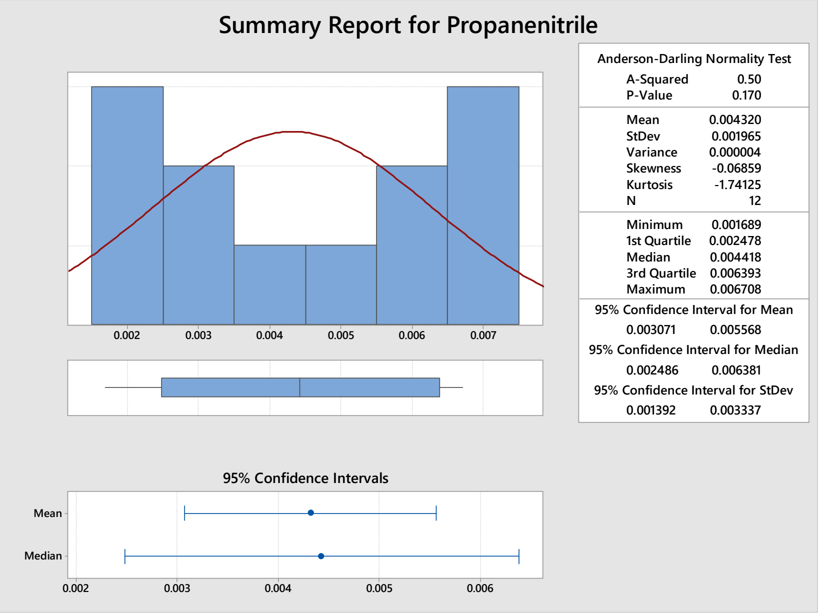
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.001075	25%	44	0.8	0.804093
0.001290	30%	31	0.8	0.806675
0.001720	40%	18	0.8	0.811451
0.002150	50%	12	0.8	0.817533
0.003440	80%	6	0.8	0.869533

The sample size is for each group.

Propanenitrile no difference from Normality detected





C.10.3.9 Power and Sample Size 1-Propanol

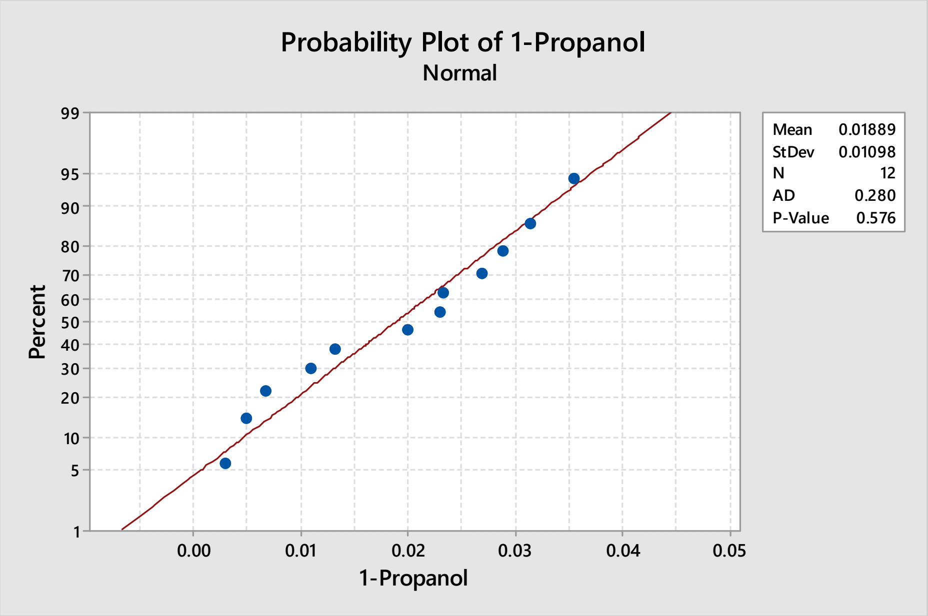
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.011

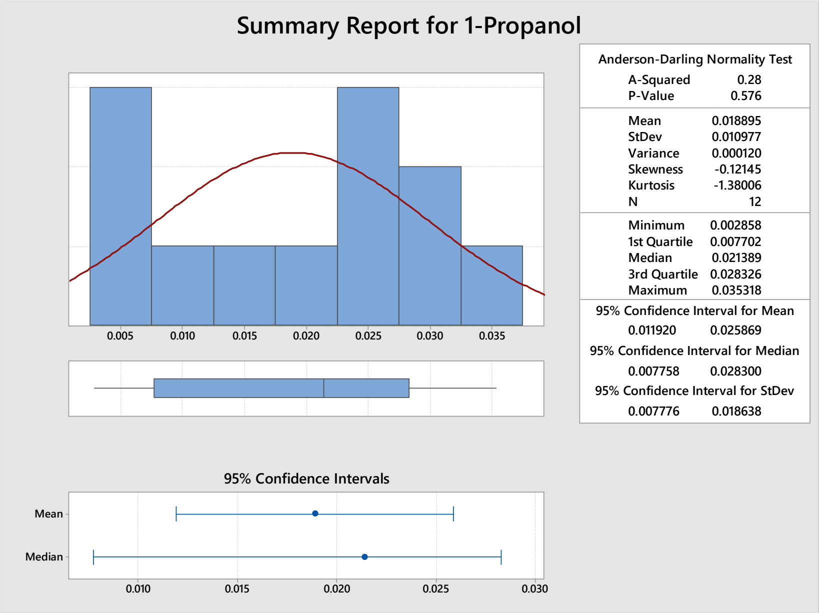
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00567	30%	48	0.8	0.805685
0.00756	40%	27	0.8	0.801578
0.00945	50%	18	0.8	0.810729
0.01512	80%	8	0.8	0.833411
0.01701	90%	6	0.8	0.801240

The sample size is for each group.

1-Propanol no difference from Normality detected





```
Anderson-Darling Normality Test
  A-Squared          0.28
  P-Value           0.576

  Mean          0.018895
  StDev         0.010977
  Variance      0.000120
  Skewness      -0.12145
  Kurtosis      -1.38006
  N                   12

  Minimum       0.002858
  1st Quartile  0.007702
  Median        0.021389
  3rd Quartile  0.028326
  Maximum       0.035318

95% Confidence Interval for Mean
  0.011920      0.025869
95% Confidence Interval for Median
  0.007758      0.028300
95% Confidence Interval for StDev
  0.007776      0.018638
```

C.10.3.10 Power and Sample Size 2-Butanone

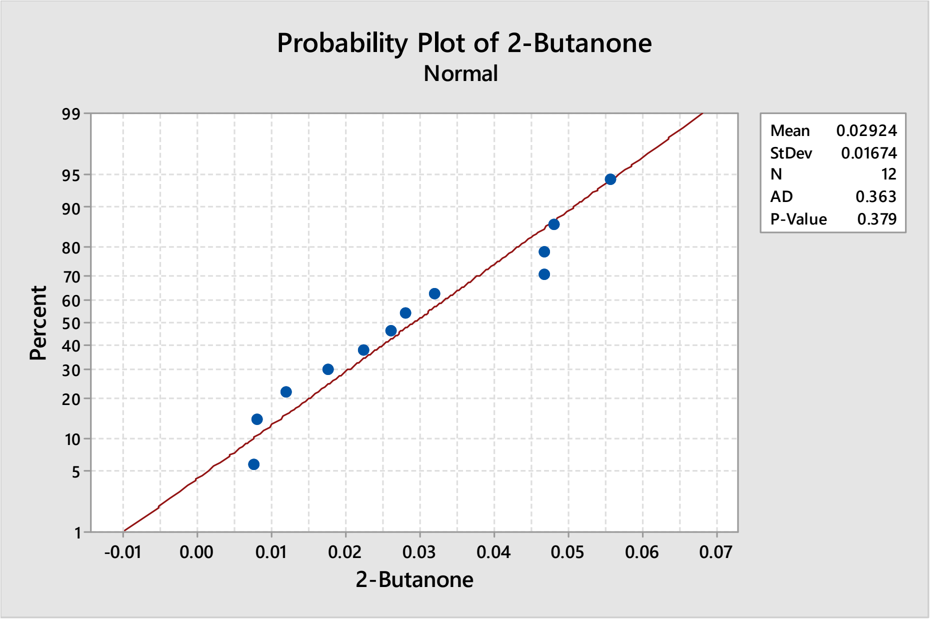
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0167

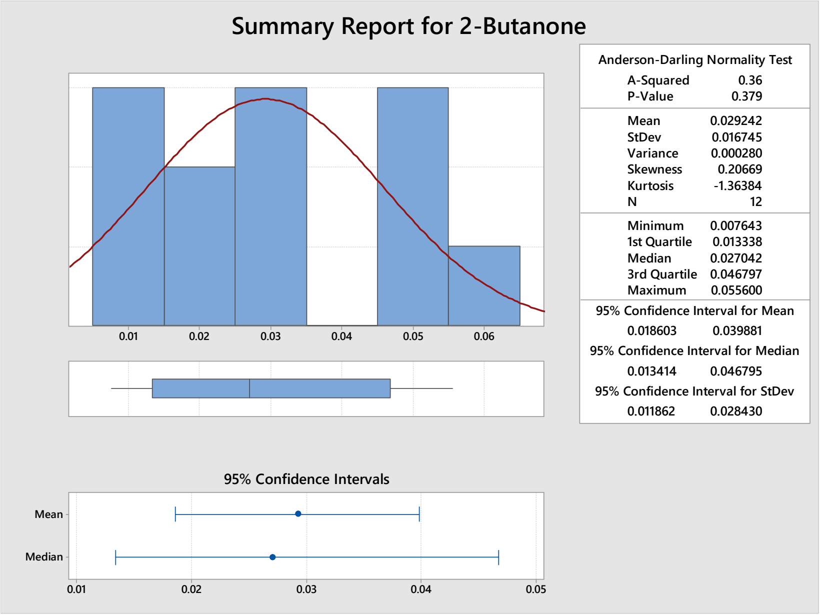
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00876	30%	46	0.8	0.802843
0.01168	40%	26	0.8	0.800249
0.01460	50%	17	0.8	0.802203
0.02336	80%	8	0.8	0.844640
0.02628	90%	6	0.8	0.813211

The sample size is for each group.

2-Butanone no difference from Normality detected





Anderson-Darling Normality Test

A-Squared	0.36
P-Value	0.379
Mean	0.029242
StDev	0.016745
Variance	0.000280
Skewness	0.20669
Kurtosis	-1.36384
N	12
Minimum	0.007643
1st Quartile	0.013338
Median	0.027042
3rd Quartile	0.046797
Maximum	0.055600

95% Confidence Interval for Mean

0.018603 0.039881

95% Confidence Interval for Median

0.013414 0.046795

95% Confidence Interval for StDev

0.011862 0.028430

C.10.3.11 Power and Sample Size 3-Heptanone

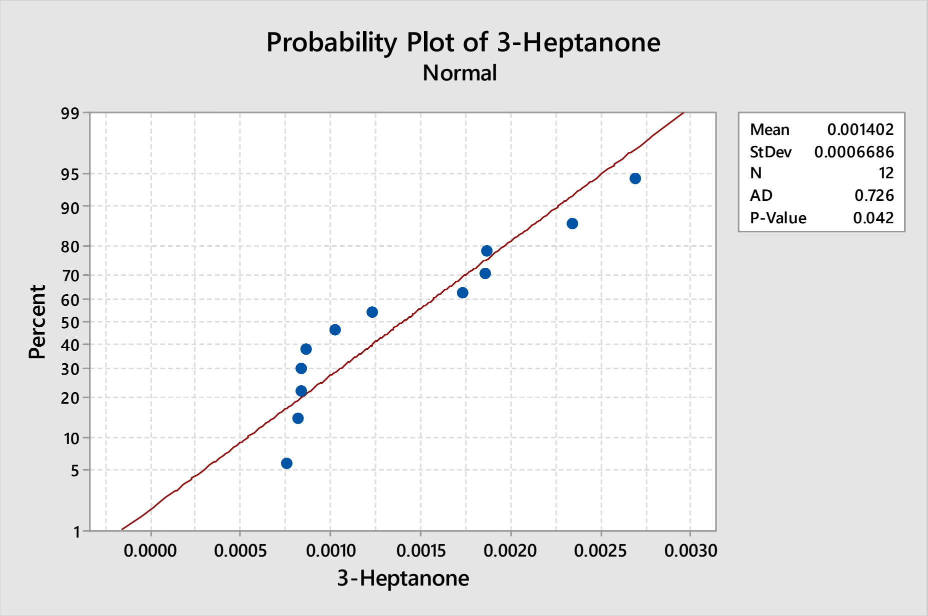
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0007

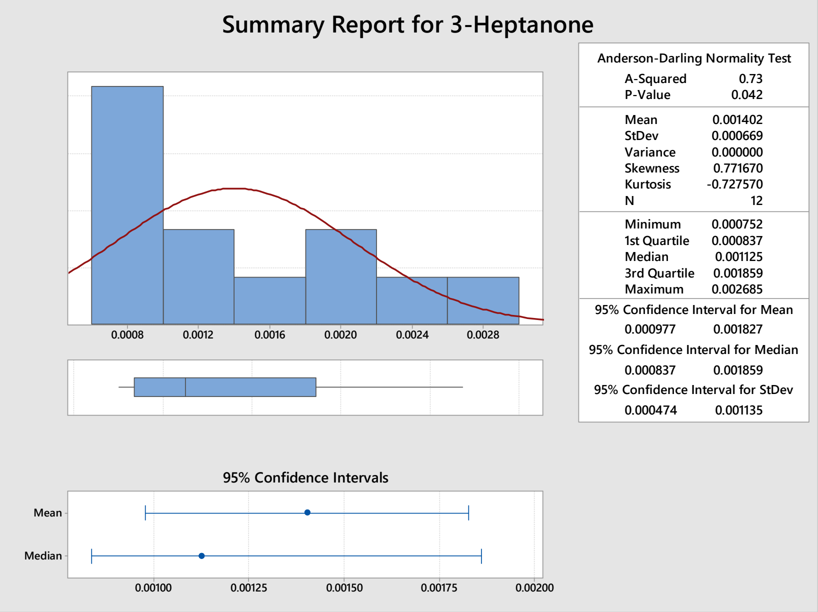
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00042	30%	36	0.8	0.809486
0.00056	40%	21	0.8	0.816788
0.00070	50%	14	0.8	0.824086
0.00112	80%	6	0.8	0.824333
0.00126	90%	5	0.8	0.828794

The sample size is for each group.

3-Heptanone significantly different from normal.





Anderson-Darling Normality Test
A-Squared 0.73
P-Value 0.042

Mean 0.001402
StDev 0.000669
Variance 0.000000
Skewness 0.771670
Kurtosis -0.727570
N 12

Minimum 0.000752
1st Quartile 0.000837
Median 0.001125
3rd Quartile 0.001859
Maximum 0.002685

95% Confidence Interval for Mean
0.000977 0.001827
95% Confidence Interval for Median
0.000837 0.001859
95% Confidence Interval for StDev
0.000474 0.001135

C.10.3.12 Power and Sample Size Cyclohexane

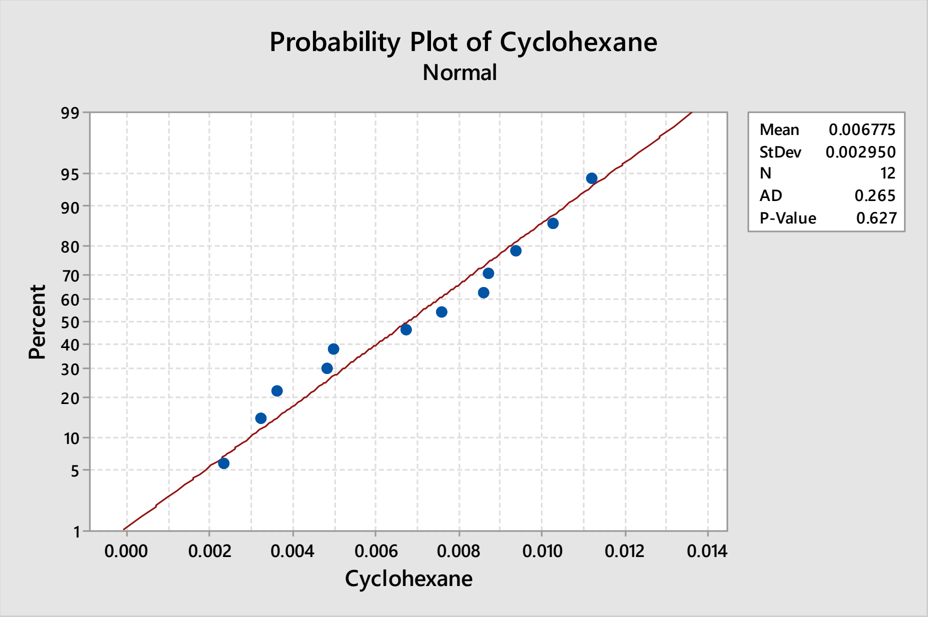
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0029

Results

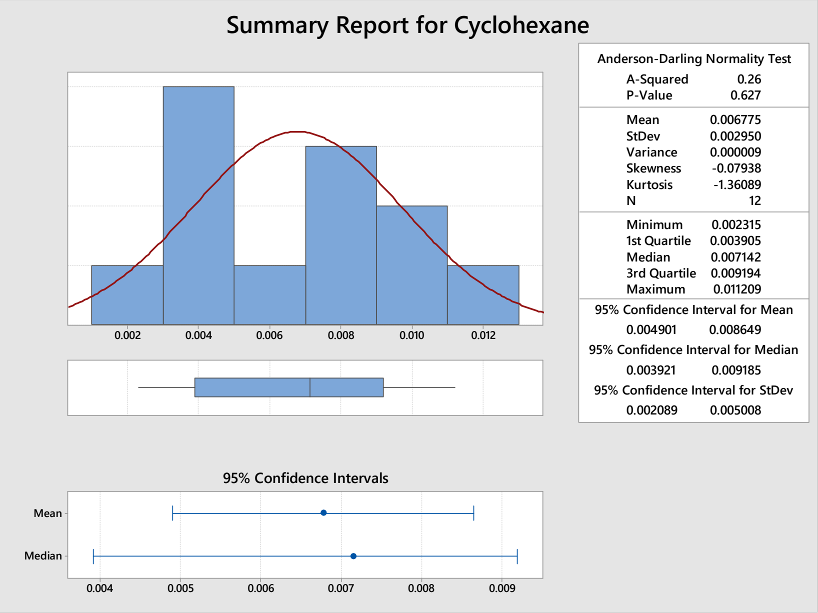
Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00170	25%	37	0.8	0.803090
0.00204	30%	26	0.8	0.804250
0.00272	40%	15	0.8	0.805358
0.00340	50%	10	0.8	0.809546
0.00544	80%	5	0.8	0.854925

The sample size is for each group.

Cyclohexane no difference from Normality detected



Mean	0.006775
StDev	0.002950
N	12
AD	0.265
P-Value	0.627



Anderson-Darling Normality Test

A-Squared	0.26
P-Value	0.627
Mean	0.006775
StDev	0.002950
Variance	0.000009
Skewness	-0.07938
Kurtosis	-1.36089
N	12
Minimum	0.002315
1st Quartile	0.003905
Median	0.007142
3rd Quartile	0.009194
Maximum	0.011209

95% Confidence Interval for Mean

0.004901 0.008649

95% Confidence Interval for Median

0.003921 0.009185

95% Confidence Interval for StDev

0.002089 0.005008

C.10.3.13 Power and Sample Size Ethanol

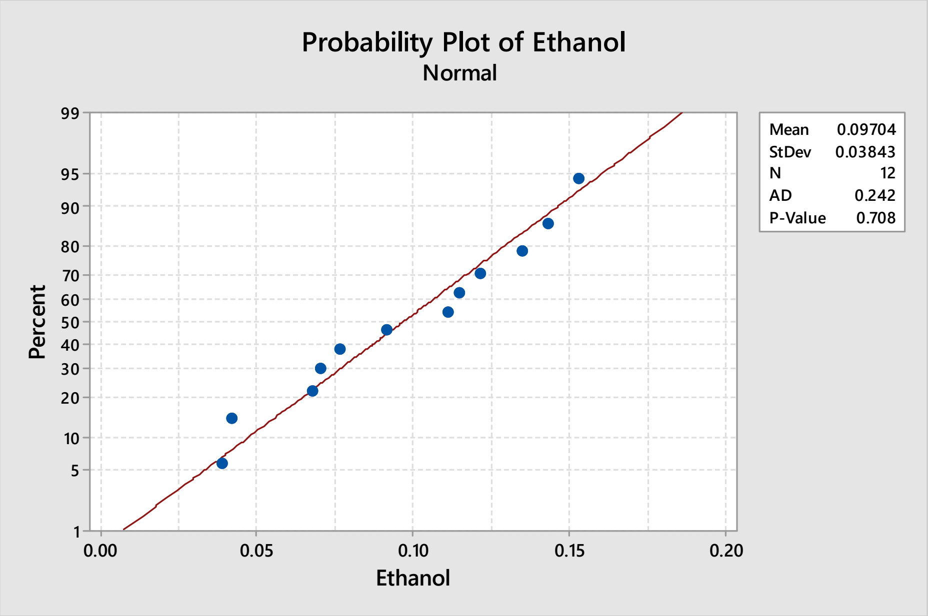
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0384

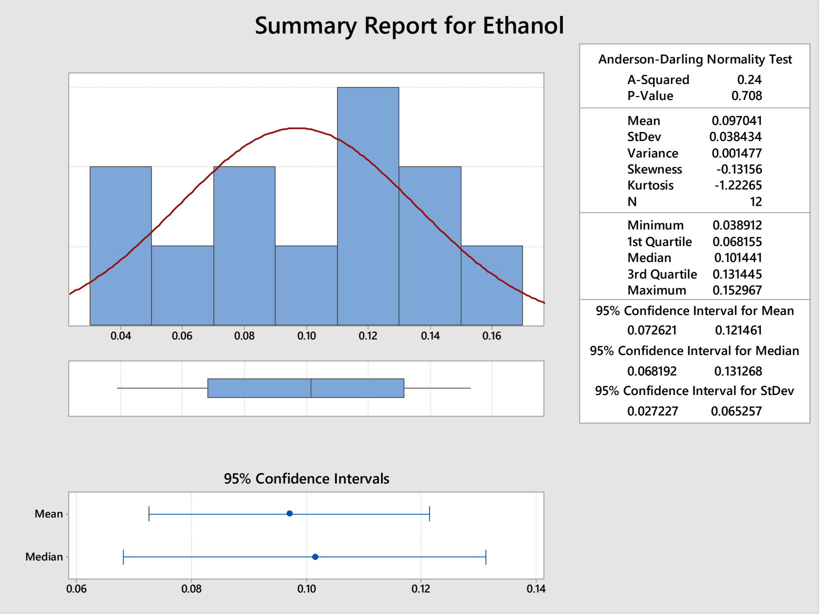
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.01940	20%	50	0.8	0.806120
0.02425	25%	32	0.8	0.803300
0.02910	30%	23	0.8	0.811968
0.03880	40%	13	0.8	0.804419
0.04850	50%	9	0.8	0.820818

The sample size is for each group.

Ethanol no difference from Normality detected





C.10.3.14 Power and Sample Size n-Heptane

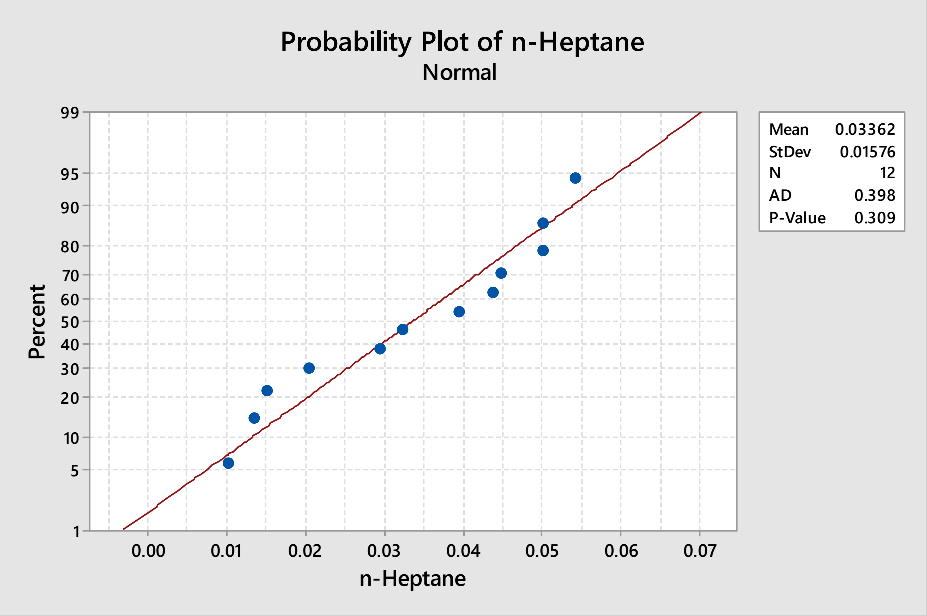
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0158

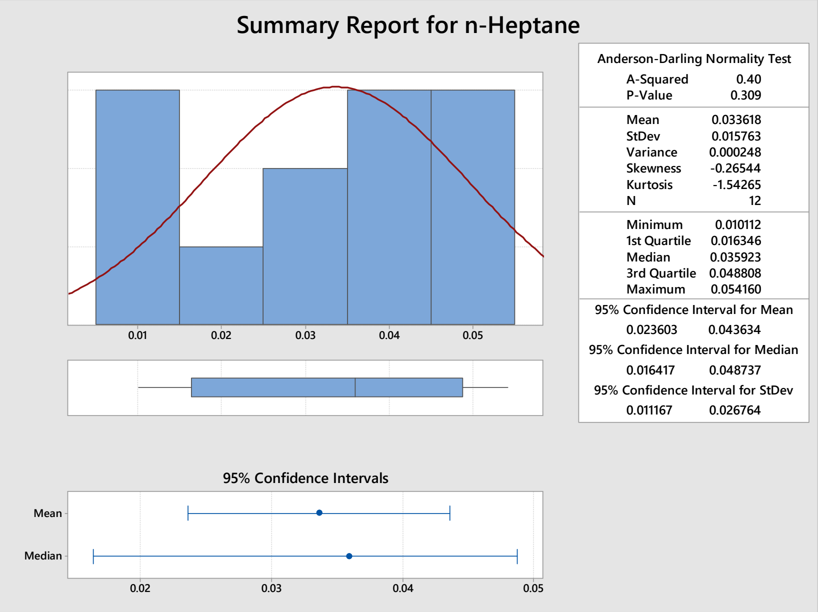
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00840	25%	45	0.8	0.804415
0.01008	30%	32	0.8	0.810309
0.01344	40%	18	0.8	0.803927
0.01680	50%	12	0.8	0.810095
0.02688	80%	6	0.8	0.863065

The sample size is for each group.

n-Heptane no difference from Normality detected





Anderson-Darling Normality Test
A-Squared 0.40
P-Value 0.309

Mean 0.033618
StDev 0.015763
Variance 0.000248
Skewness -0.26544
Kurtosis -1.54265
N 12

Minimum 0.010112
1st Quartile 0.016346
Median 0.035923
3rd Quartile 0.048808
Maximum 0.054160

95% Confidence Interval for Mean
0.023603 0.043634
95% Confidence Interval for Median
0.016417 0.048737
95% Confidence Interval for StDev
0.011167 0.026764

C.10.3.15 Power and Sample Size Toluene

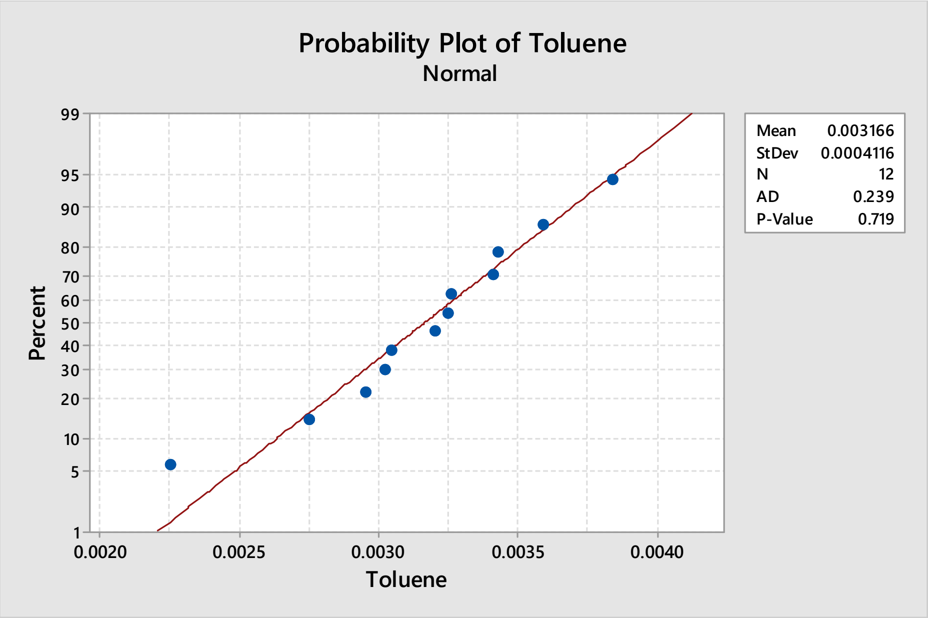
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0004

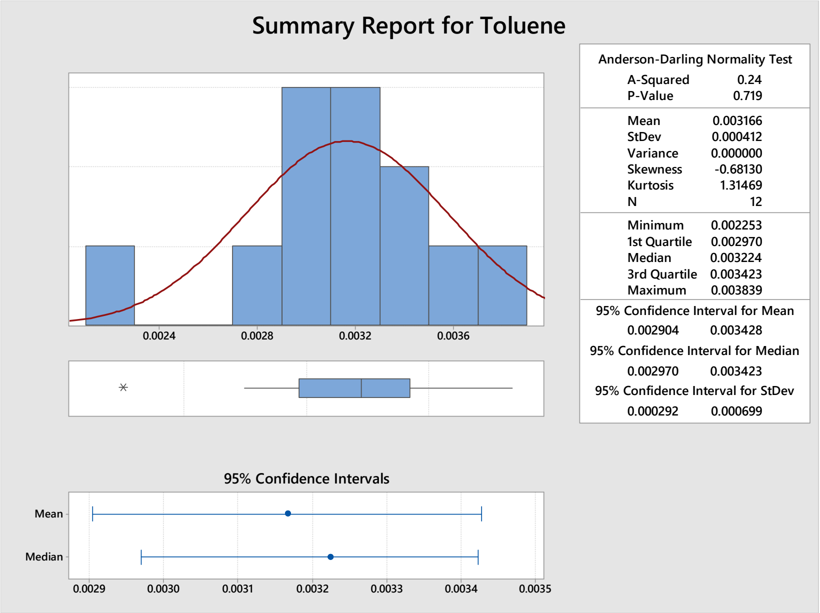
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.000160	5%	78	0.8	0.800147
0.000224	7%	41	0.8	0.807608
0.000320	10%	21	0.8	0.816788
0.000480	15%	10	0.8	0.825222
0.000640	20%	6	0.8	0.824333
0.00096	30%	4	0.8	0.909355
0.00160	50%	2	0.8	0.803159

The sample size is for each group.

Toluene no difference from Normality detected





C.10.3.16 Power and Sample Size Trichlorofluoromethane

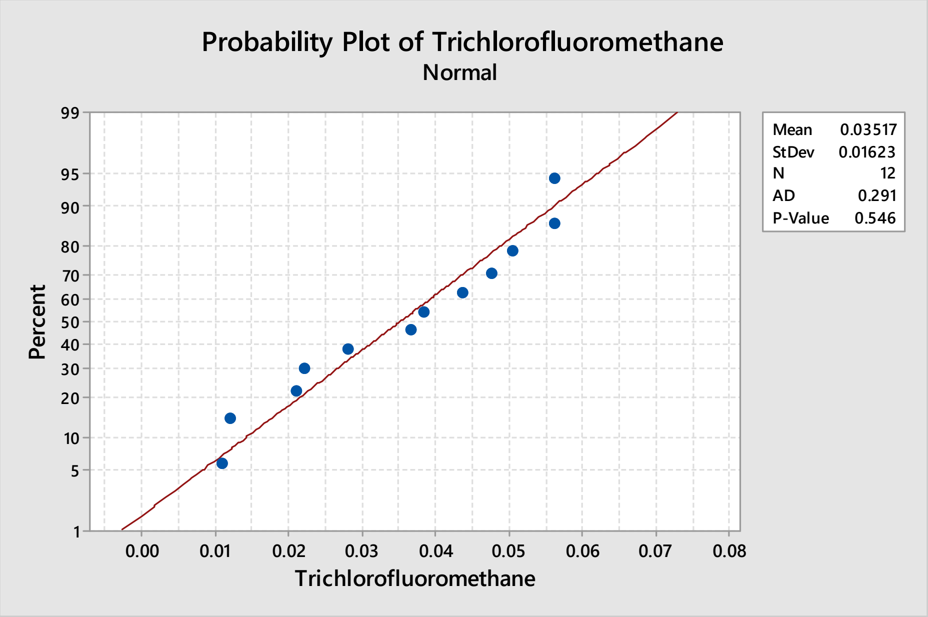
2-Sample t Test
Testing mean 1 = mean 2 (versus >)
Calculating power for mean 1 = mean 2 + difference
α = 0.05 Assumed standard deviation = 0.0162

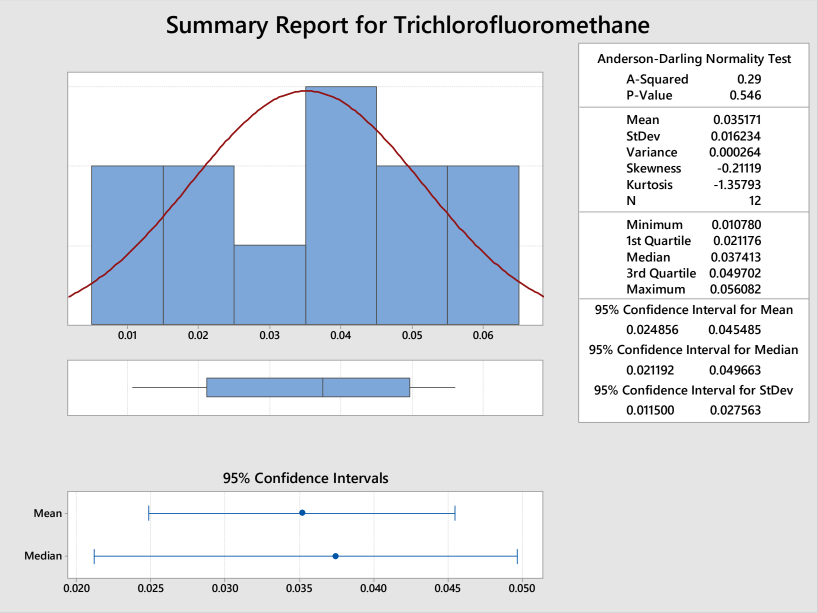
Results

Difference	Percent Difference	Sample Size	Target Power	Actual Power
0.00880	25%	43	0.8	0.803319
0.01056	30%	30	0.8	0.802374
0.01408	40%	18	0.8	0.818615
0.01760	50%	12	0.8	0.824609
0.02816	80%	5	0.8	0.805426

The sample size is for each group.

Trichlorofluoromethane no difference from Normality detected





C.11 Calculation of Bias and Uncertainty and the Sample Size for using the Bias to Estimate the HS Concentration

We used four models to estimate the bias and its associated uncertainty: additive (Model 1) and multiplicative (Model 2) bias with the median HS concentration fixed (no uncertainty) and additive (Model 3) and multiplicative (Model 4) bias with the mean HS measured with error. For the models with HS fixed, we suggest that the median (X) is the more appropriate estimate of the gas concentration in the head space. For all models, the mean or median of the CT concentrations is measured with error. Let Y be a random variable representing CT concentration values for the given analyte. We generally have 12 measured values from collected data to use for estimation purposes. The k = 2 uncertainty is defined here as 2×the estimate of the standard error of the bias estimator.

Model 1: Model with additive error structure: $y_i + \varepsilon_i = \alpha + X$ or equivalently $\alpha = y_i - X + \varepsilon_i$, where we assume $\varepsilon \sim N\left(0, \sigma_y^2\right)$. For each CT data point, we could use the model to say $a_i = y_i - X$. These a_i values represent estimates of α for each individual CT data point. Thus, $\hat{\alpha} = \bar{a} = \bar{y} - X$ and the expected value of $\hat{\alpha}$ equals $E(\hat{\alpha}) = E(\bar{y} - X) = \mu_y - X$. The variance of this estimator is $V(\hat{\alpha}) = V(\bar{y} - X) = V(\bar{y}) = \frac{\sigma_y^2}{\mathrm{n}}$ which can be estimated by $\frac{\mathrm{s}_y^2}{\mathrm{n}}$ where n is the number of CT concentration measurements. The standard error of this estimator is $SE(\hat{\alpha}) = \sqrt{\frac{\sigma_y^2}{\mathrm{n}}}$ which is estimated by $\sqrt{\frac{s_y^2}{\mathrm{n}}}$. For our purposes the $\mu_y - X$ was estimated as the median of the differences i.e., $\mathrm{Median}(y_i - X)$.

Model 2: Model with multiplicative error structure: $y_i \varepsilon_i = \alpha X$ or equivalently $= \frac{y_i \varepsilon_i}{X}$, where we assume that $\varepsilon \sim N\left(1, \sigma_y^2\right)$. For each CT data point, we could use the model to say $a_i = \frac{y_i}{X}$. These a_i values represent estimates of α for each individual CT data point. Thus, $\hat{\alpha} = \bar{a} = \frac{\bar{y}}{X}$ and the expected value of $\hat{\alpha}$ equals $E(\hat{\alpha}) = \frac{E(y)}{X} = \frac{\mu_y}{X}$, which can be estimated by $\frac{\bar{y}}{X}$. The variance of this estimator is $V(\hat{\alpha}) = \frac{V(y)}{X^2} = \frac{\sigma_y^2/\mathrm{n}}{X^2} = \frac{\sigma_y^2}{\mathrm{n}X^2}$ which can be estimated by $\frac{s_y^2}{\mathrm{n}X^2}$ where n is the number of CT concentration measurements. The standard error of this estimator is $SE(\hat{\alpha}) = \frac{\sigma_y}{X\sqrt{n}}$, which can be estimated by $\frac{s_y}{X\sqrt{n}}$.

Model 3: Model with additive error structure such that $y_i + \varepsilon_i = \beta + x_j + \delta_j$ and the unpaired data are considered independent random samples. Let *Y* be the random variable representing CT concentration values with n_1 observations and *X* be the random variable representing HS concentration values with n_2 observations for a given analyte. Let δ represent the uncertainty in *X* values (HS) and ε represent the uncertainty in the *Y* values (CT) with $\delta \sim N(0, \sigma_x^2)$ and $\varepsilon \sim N\left(0, \sigma_y^2\right)$. We use the sample means of the separate HS and CT data to estimate beta; $\hat{\beta} = \bar{y} - \bar{x}$ which has the expected value $E\left(\hat{\beta}\right) = E(\bar{y} - \bar{x}) = \mu_y - \mu_x$. The variance of this estimator is $V\left(\hat{\beta}\right) = V(\bar{y} - \bar{x}) = V(\bar{y}) + V(\bar{x}) = \frac{\sigma_y^2}{\mathrm{n}_1} + \frac{\sigma_x^2}{\mathrm{n}_2}$, which can be estimated by $\frac{s_y^2}{\mathrm{n}_1} + \frac{s_x^2}{\mathrm{n}_2}$. The standard error of this estimator is $SE\left(\hat{\beta}\right) = SE(\bar{y} - \bar{x}) = \sqrt{\frac{\sigma_y^2}{\mathrm{n}_1} + \frac{\sigma_x^2}{\mathrm{n}_2}}$, which can be estimated by $\sqrt{\frac{s_y^2}{\mathrm{n}_1} + \frac{s_x^2}{\mathrm{n}_2}}$.

Model 4: Model with multiplicative error structure $y_i \varepsilon_i = \beta x_j \delta_j$, or equivalently as $\beta = \frac{y_i \varepsilon_i}{x_j \delta_j}$, where the concentration values are lognormally distributed. A $\log_e$-transformation results in an additive model such that $\ln(\beta) = \ln(y_i) + \ln(\varepsilon_i) - \ln\left(x_j\right) - \ln(\delta_j)$ where $\delta \sim \ln N(1, \sigma_x^2)$ and $\varepsilon \sim \ln N\left(1, \sigma_y^2\right)$.

Formulas for a lognormal random variable say that for $b_i = \ln(a_i)$, $E(a_i) = \exp(\mu_b + \frac{1}{2}\sigma_b^2)$ and $V(a_i) = \exp(2\mu_b + \sigma_b^2) \cdot \left[\exp\left(\sigma_b^2\right) - 1\right]$. Let $w_i = \ln(y_i)$ and $v_i = \ln(x_i)$, thus, for $\hat{\beta} = \frac{\widehat{\mu_y}}{\widehat{\mu_x}} = \exp\left[\left(\bar{w} + \frac{1}{2}s_w^2\right) - \left(\bar{v} + \frac{1}{2}s_v^2\right)\right]$. The $V\left(\widehat{\mu_y}\right) = \exp(2\mu_w + \sigma_w^2) \cdot [\exp(\sigma_w^2) - 1]$ and the $V(\widehat{\mu_x}) = \exp(2\mu_v + \sigma_v^2) \cdot [\exp(\sigma_v^2) - 1]$. The standard error for this estimator is calculated using the expected value and variance formulas for a lognormal random variable, combined with the error propagation formula for estimating the standard error for the ratio of two random variables. Thus, the estimated standard error for this estimator is $SE\left(\hat{\beta}\right) = SE\left(\frac{\widehat{\mu_y}}{\widehat{\mu_x}}\right) = \frac{\widehat{\mu_y}}{\widehat{\mu_x}} \cdot \sqrt{\frac{V\left(\widehat{\mu_y}\right)/\mathrm{n}_1}{\left(\widehat{\mu_y}\right)^2} + \frac{V(\widehat{\mu_x})/\mathrm{n}_2}{(\widehat{\mu_x})^2}}$.

Sample Size Calculation: Calculation of the sample size required to estimate HS with a multiplicative bias developed using Model 4 was based on ensuring that the relative standard error (RSE) of the estimate $\widehat{\mathrm{HS}} = \frac{\bar{y}}{\hat{\beta}}$ was less than or equal to some designated value (say 35%). For this calculation we are assuming that the bias is known and has a known standard error and is independent of the CT samples. The standard error for this estimator was calculated by combining the error with the propagation formula for estimating the standard error for the ratio of two random variables.

Table of sample size calculations to ensure that the relative standard error (RSE) of the estimate $\widehat{\mathrm{HS}} = \frac{\bar{y}}{\boldsymbol{\beta}}$ was less than or equal to 35% where Y is a random variable representing CT concentration values with n_1 observations ($n_1 = 12$).

Analyte	Multiplicative Bias (Model 4)	CT/Bias =HS ppm	SE(Bias) from Model 4	SE(CT) = $\sqrt{\frac{s_y^2}{n_1}}$	Propagated Error	Current RSE	Sample Size
Ammonia	0.961	307.107	0.131	6.161	42.458	0.138	2
Benzene	1.048	0.002	0.135	0.0002	0.0004	0.160	3
2-Hexanone	0.573	0.007	0.131	0.001	0.002	0.277	8
Formaldehyde	0.512	0.004	0.094	0.0001	0.001	0.193	4
Acetaldehyde	1.176	0.076	0.470	0.005	0.031	0.404	17
Furan	0.866	0.002	0.083	0.0001	0.0002	0.125	2
Acetonitrile	0.726	0.088	0.091	0.006	0.014	0.153	3
Propanenitrile	1.021	0.004	0.203	0.001	0.001	0.238	6
N-Nitrosodiethylamine	0.252	0.0003	0.076	0.0001	0.0001	0.312	10
N-Nitrosomethylethylamine	0.083	0.001	0.022	0.0001	0.0004	0.272	8
1-Propanol	0.941	0.020	0.310	0.003	0.007	0.370	14
2-Butanone	1.494	0.020	0.518	0.005	0.008	0.384	15
3-Heptanone	0.140	0.010	0.025	0.0002	0.002	0.223	5
4-Methyl-2-Pentanone	0.750	0.003	0.143	0.0004	0.001	0.235	6
Cyclohexane	0.963	0.007	0.177	0.001	0.002	0.222	5
Ethanol	1.466	0.066	0.245	0.011	0.013	0.202	5
Hexane	0.915	0.114	0.154	0.012	0.023	0.205	5
n-Heptane	0.694	0.048	0.134	0.005	0.011	0.236	6
Toluene	0.535	0.006	0.058	0.0001	0.001	0.114	2
Trichlorofluoromethane	1.056	0.033	0.227	0.005	0.008	0.253	7

Table of Descriptive Statistics for the Lognormal Concentration Data (ppm) used to Calculate Bias and Uncertainty

Analyte	n1	n2	mean (a=lnCT)	mean (b=lnHS)	Var (a=lnCT)	Var (b=lnHS)	$\widehat{\mu_{CT}}$	$\widehat{\mu_{HS}}$	Var $\widehat{\mu_{CT}}$	Var $\widehat{\mu_{HS}}$
Ammonia	12	12	5.68	5.63	0.0054	0.198	295	307	469	20641
Benzene	12	12	-6.10	-6.11	0.134	0.055	0.0024	0.0023	8.21E-07	2.92E-07
2-Hexanone	12	12	-5.65	-4.92	0.434	0.082	0.0044	0.0076	1.04E-05	5.01E-06
Formaldehyde	12	10	-6.29	-5.74	0.042	0.261	0.0019	0.0037	1.51E-07	4.05E-06
Acetaldehyde	12	10	-2.44	-3.03	0.078	0.929	0.0907	0.0771	6.63E-04	9.11E-03
Furan	12	12	-6.42	-6.27	0.060	0.048	0.0017	0.0019	1.74E-07	1.84E-07
Acetonitrile	12	12	-2.79	-2.47	0.090	0.091	0.0645	0.0888	3.94E-04	7.49E-04
Propanenitrile	12	12	-5.56	-5.52	0.274	0.146	0.0044	0.0043	6.17E-06	2.96E-06
N-Nitrosodiethyl-amine	12	12	-9.66	-8.62	0.046	0.719	0.000065	0.00026	2.00E-10	7.08E-08
N-Nitrosomethyl-ethylamine	12	12	-9.12	-6.89	0.051	0.571	0.00011	0.0014	6.62E-10	1.40E-06
1-Propanol	12	12	-4.21	-3.97	0.666	0.307	0.0208	0.0221	4.08E-04	1.75E-04
2-Butanone	12	12	-3.72	-4.18	0.484	0.598	0.0307	0.0206	5.88E-04	3.47E-04
3-Heptanone	12	12	-6.67	-4.66	0.212	0.127	0.0014	0.0101	4.70E-07	1.38E-05
4-Methyl-2-Pentanone	12	12	-6.08	-5.67	0.316	0.064	0.0027	0.0036	2.67E-06	8.50E-07
Cyclohexane	12	12	-5.10	-4.99	0.258	0.103	0.0069	0.0072	1.42E-05	5.63E-06
Ethanol	12	12	-2.42	-2.74	0.210	0.096	0.0988	0.0674	0.00228	4.58E-04
Hexane	12	12	-2.36	-2.16	0.262	0.039	0.107	0.117	0.00344	5.54E-04
n-Heptane	12	12	-3.53	-3.01	0.337	0.045	0.0348	0.0502	0.00049	1.15E-04
Toluene	12	12	-5.76	-5.19	0.019	0.113	0.0032	0.0059	1.93E-07	4.20E-06
Trichlorofluoromethane	12	12	-3.48	-3.44	0.328	0.152	0.0364	0.0345	0.00052	1.95E-04

Appendix D

Assessments of Potential Bias Mechanisms

Appendix D

Assessments of Potential Bias Mechanisms

The following sections in this Appendix describe individual analyses associated with the potential causes of data bias described in Section 5. Several mechanisms may play a role in determining the magnitude of any bias. All are possible and none can be fully accepted or dismissed based on the data analyzed. However, potential contributing mechanisms may be grouped and the likelihood of the bias impact evaluated.

Note that the information provided in this appendix is "For Information Only."

D.1 Estimated Impacts of Sampling Location Differences

The configurations of both cartridge and headspace test rigs are given in Sections 2.1, 2.2, and 2.3. The locations of the inlet ports that collected headspace gases for each rig are given in Section 2.3. This description shows parallel tubes for each rig, spaced approximately 12 in. from one another, immersed 17 to 20 feet into the tank headspace. This immersion corresponds to approximately 8 ft from the top of the tank liquid level. Based on these dimensions the locations of the sampling inlets are deemed to be close enough to one another, such that biases of drawing different tank vapor concentrations due to draw location differences are unlikely.

D.2 Calculation of Impacts of Additional Cartridge Rig Hose Length

As outlined in Figure 10 of Section 2.2, the additional hose length associated with the cartridge rig was approximately 125 ft. While the hose was heat-traced to reduce heat losses, a simple lumped thermal model was created to estimate the potential gas temperature reduction if the heat tracing were completely ineffective for some reason. Table D.1 shows the assumptions and corresponding estimate of gas temperature reduction.

As shown in Table D.1 the assumed temperature of the gas entering the 125-ft long hose was 60°F. Based on the model and assumed parameters the estimated temperature of the gas exiting the hose was close to the average outside air temperature 41°F. This calculation means that if the heat trace on the hose were ineffective, the gas temperature could decrease appreciably, potentially approaching the outside air temperature.

To further assess the potential heat loss from the hose, a comparison was made between the inlet temperatures for both sample rigs, along with the ambient temperature from a local weather station. Those temperatures, for each dive, are shown in Table D.2 and plotted in Figure D.1.

Table D.1. Estimated Sample Gas Temperature Reduction from Additional Cartridge Rig Hose (assuming no line insulation or heating)

Parameter	**Value**
Inner (liner) material of the hose	Teflon
Thickness of inner liner (in.)	1/8
Outer (jacket) material of the hose	EPDM
Inner diameter of hose (in.)	0.78
Outer diameter of hose (in.)	1.30
Total length of hose (ft)	125
Inner surface area of hose (m^2)	2.8
Outer surface area of hose (m^2)	4.7
Inner volume of hose (L)	14
Sample gas flow rate through hose (L/min)	30
Average residence time of sample gas in hose (s)	28
Average outside air temperature (^{o}F)	41
Average temperature of tank headspace (^{o}F)	60
Assumed thermal conductivity of hose material (W/m·K)	0.28
Assumed natural convection heat transfer coefficient (W/m^2·K)	2.8
Overall heat transfer coefficient for pipe to air (W/m^2·K)	2.7
Assumed heat capacity of air (J/g·K)	1.0
Assumed density of air (g/L)	1.2
Estimated temperature of gas exiting hose (^{o}F)[a]	41

[a] https://physics.stackexchange.com/questions/289962/outlet-temperature-of-gas-through-a-pipe

Table D.2. Sample Gas Temperatures into Each Test Rig for Each Dive. Corresponding Atmospheric Temperatures from the Hanford Meteorological Station also are given.

			Temperatures (°F)			
Dive #	Analyte Tubes Tested	Date/ Time	Headspace Test Rig	Cartridge Test Rig	Atmospheric (Hanford Meteorological Station)	Difference: Cartridge–Headspace (°F)
1	Methanol/nitrosamines	1/16/18 ~10:00	63	48	37	-15
2	Pyridine/ethylamine	1/25/18 ~9:00	62	40	36	-22
3	Aldehyde/SVOC	2/1/18 ~9:00		43	33	
4	Acetonitrile/1,3 Butadiene	2/6/18 ~9:00	58	50	44	-7
5	VOC/ ammonia	2/8/18 ~9:00	60	54	54	-6
6	Mercury/ Furan	2/9/18 ~10:00	60	47	40	-13
					Average	-13

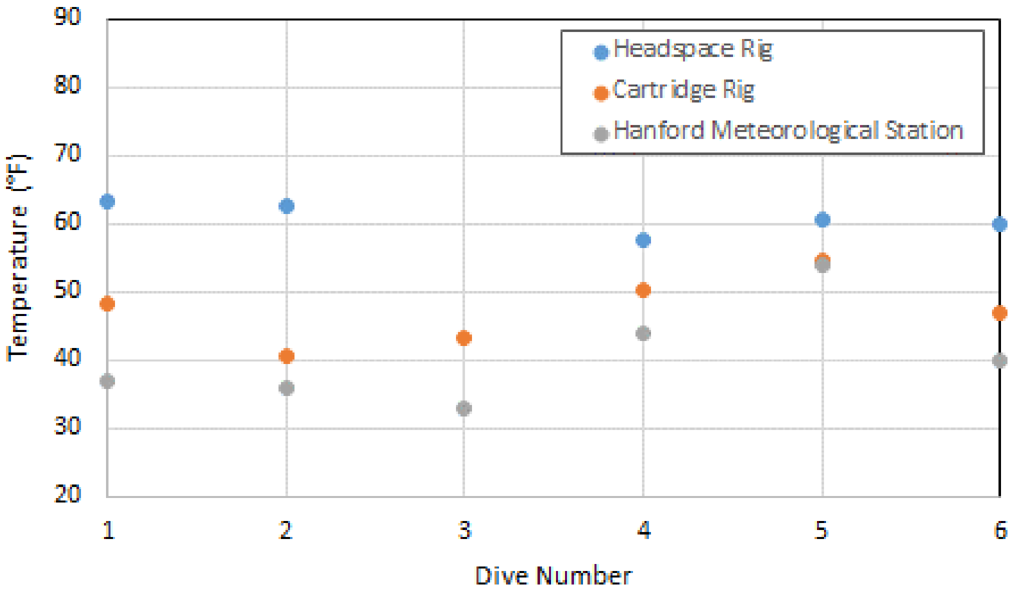


Figure D.1. Plot of Sample Gas Temperatures into Each Test Rig for Each Dive. Data from Table D.2.

As shown in Table D.2 and Figure D.1 the temperatures for the headspace rig ranged between 58 and 63°F for the six dives, compared to cartridge rig temperatures which ranged from 40 to 54°F. The wider range in temperature variability appears to be explained when the temperatures are compared to the local weather station data. Indeed, Figure D.1 shows a relatively constant set of headspace rig temperatures across dives, but a strong correlation between the cartridge rig data and the local weather station data. This comparison indicates that the heat tracing for the cartridge rig feed tube was not effective, allowing net heat losses that resulted in an average temperature reduction of 13°F. This difference is deemed to be significant toward enabling the condensation of high-boiling point volatile and semi-volatile compounds in the sample gas stream.

D.3 Estimated Impacts of Wall Adsorption/ Diffusion in Cartridge Rig Hose

As mentioned in the previous section, the hose to the cartridge rig was heat-traced to prevent or reduce condensation. The opacity of the hose and heat trace blanket did not allow for direct observation of any condensation and no condensate was observed to have drained from the hose or the lines during testing or disassembly. The inner walls of the hose and lines may have been wet—coated with condensate—or dry, or partially both. The lengths of the wet and dry segments are unknown, as are the temperatures of the walls. In the wet segment, even a thin layer of water (10 µm) may suppress, at least partially, uptake of organics by Teflon (Huang et al 2018) and enhance absorption of water soluble organics. In the dry portion, the organic’s solubility in Teflon, and diffusivity through Teflon, could be a loss mechanism.

The rest of this section discusses the relative amounts of depletion that are produced by loss mechanisms in these two (wet/dry) scenarios.

Adsorption/Absorption onto walls

As described by Guha et al. (2012), there are four stages in adsorption-desorption processes (figure not to scale) that occur at a tube wall. Given that any liquid layer present is quite thin, adsorption and absorption are interchangeable in this subsection. In stage I, the molecules of interest are adsorbing but not exiting from the transfer line to be measured by the sampling tubes. Adsorption is temporally and kinetically dynamic, but given the low surface concentrations, desorption is slower than adsorption. In stage II, molecules of interest have begun to exit the tube outlet and are measurable but adsorption is still dynamic and time dependent. The exit concentration is not at steady state. In stage III, the concentration of the molecule on the wall and the concentration emerging from the outlet are both at steady state. In stage IV, the inlet concentration is “turned off” or Figure D.2.

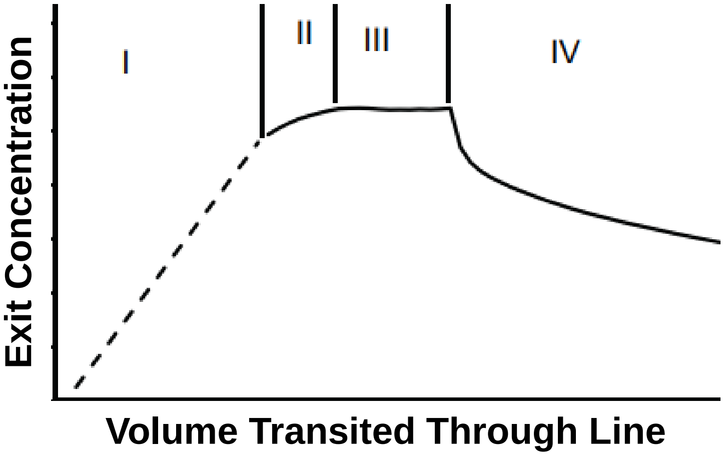


Figure D.2. Stages of Molecular Adsorption-Desorption Adapted from Guha, et al. (2012)

For all species of interest, at least some portion of the collection time must have been spent in stage I. In the absence of absorption, stage I may be very fast and have negligible effect on bias. For a flow of 30 L/min through a line that is 0.775 to 0.875 in. in diameter and ~150 ft long, flow transverses from entrance to exit in approximately 27 to 36 s, a small fraction of the approximately 3600 s during which flow is operational. This sets a minimum on the amount of time that a species spends in stage I; absorption onto or into the wall or into condensed liquid layers may increase this time for a given species. In either case, for any species measured above its detection/reporting limit, at least some portion of the collection time must have been spent outside of stage I. The analysis discussed below assumes that at the start, the tube was devoid of any of the species of interest.

For species that spend essentially all of their time in stage III (at least some time must have been spent in stages I and II), the flow of species into the tube must equal the flow of species out (because flux to the wall equals flux off the wall). In such a case, no bias would be measureable. Therefore, stage III has no bias and differentiation by chemical species cannot occur. The implication here is that for steady inlet flows that turn on at the beginning of the test in the absence of a chemical specific background, only the dynamics and timing of stage II may drive a significant bias and differentiation among species.

There is a second possibility that stages II and IV together also may be differentiating if temperature, pressure, or relative humidity swings drive both adsorption and desorption. Nominally the temperature, pressure, or relative humidity may be “constant” because the tank is large and the line heat traced, leaving this as a secondary possibility. Yet, no temperature and pressure profile in an operational environment is perfectly constant, particularly given observed variation in the flow rates and possible differences between tank temperature(s) and line temperature(s).

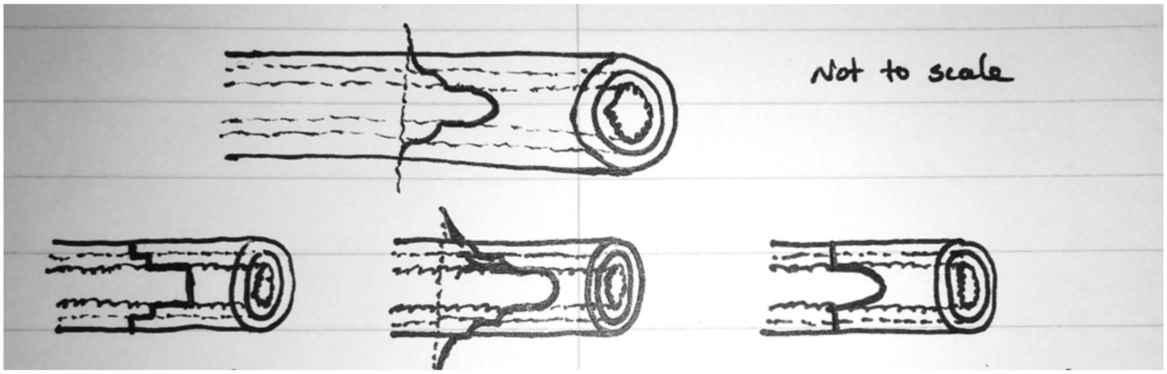
This analysis assumes that absorption/desorption does not occur prior to the start of testing. This assumption is consistent with the client indication that the pumping systems were started immediately after sampling system insertion, thus minimizing temporal offset between the start of flow and the start of collection.

Table D.3. Possible Biases from Dynamic Line Loadings

Stage	Inlet Concentration	Line Concentration	Exit Concentration	Relative Concentration
0	Same as exit	No adsorption	Same as inlet	HS=CT
I	Steady	Rising	Negligible	HS>CT, but C<DL|RL
II	Steady	Rising	Rising	HS>CT
III	Steady	Steady	Steady	HS=CT
IV	Lower	Falling	Falling	HS<CT

Observations may comprise multiple stages. HS = headspace, CT = cartridge testing rig.

To evaluate these phenomena in greater detail, we now consider three mathematical approximations to determine the governing mechanisms and provide insight into the source of biases. Concentration profiles for these three approximations are shown in Figure D.3. The first model is an equilibrium model in which mass transfer is neglected and the concentration in the wall is assumed to be completely negligible. This model is also valuable because partition coefficients are used in the remainder of the analysis. As noted above, an equilibrium model does not predict the bias because at steady state, the rate of absorption and desorption are equal and, thus, the bias must inherently be zero. When coupled with a transient time scale the equilibrium model could be used to estimate/approximate a flux and, thus, a bias. The second model is a steady flux analysis to estimate the magnitude of resistances and gain insight into the governing mass transfer mechanisms. A steady flux model may predict a bias because the composition is dynamic in contrast to the steady state of stage III, in which the concentration at the wall is constant. An estimate of time scales is also presented, which similarly gives insight into the governing mechanisms. The third and final model is a penetration analysis that treats the wall and any liquid layers as a perfect sink, so that the liquid and wall concentrations are precisely zero. This analysis provides the maximum mass transfer rates because resistances associated with the walls and liquid layers are assumed to be infinite. The second and third models, in contrast to the first model, may be used to estimate the flux to the wall, which is directly related to the bias observed.



Equilibrium **Steady Flux** **Walls as Perfect Sink**

Figure D.3. Geometry and Concentration Profiles along with Three Approximations Modeled Each Below

In the equilibrium model the interface between the gas that initially contains the species of interest and the liquid that is initially only water is evaluated. The analysis was performed in ASPEN, which permits the determination of multicomponent partition coefficients or partition coefficients for a species as influenced by all the other components in the mixture. Figure D.4 relates the geometry and concentration profiles to the ASPEN model. This model is discussed in more detail in the next section.

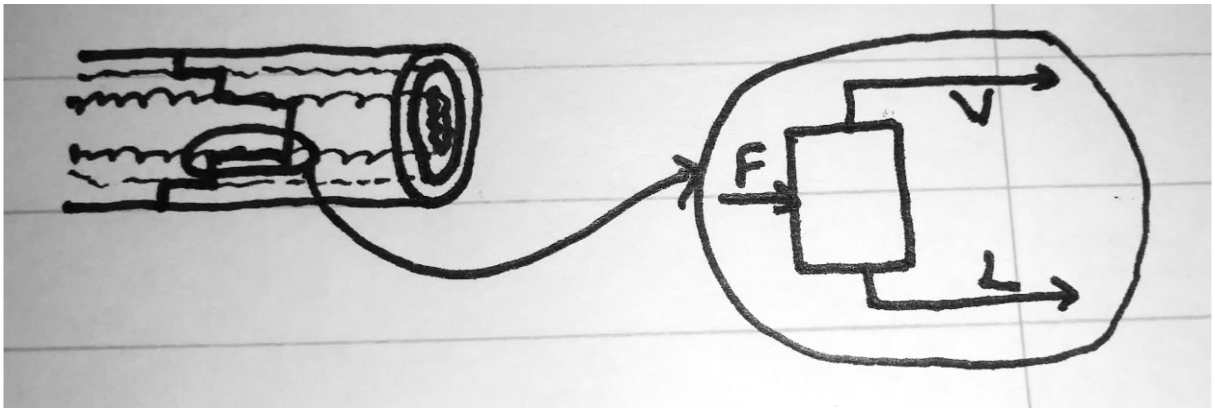


Figure D.4. Geometry and Concentration Profiles of the Equilibrium Approximation and its Representation in ASPEN as a Vapor-Liquid Equilibrium Flash Drum

The second model presented is a steady-state model to estimate the resistances of each region and predict a bias. As indicated above, a steady flux model in contrast to an equilibrium model (as part of stage III) may directly present a bias, by estimating that flux of gas phase species to the wall and any condensation layers present.

The analysis of resistances assumes radial variation to dominate over axial variation. The flow rate of a species initially in the gas phase from the center of the tube through the tube walls is given as

$$\dot{n} = \frac{c_c - \dfrac{c_\infty}{K_l K_i K_o}}{\dfrac{1}{h_i\left(2\pi r_i L\right)} + \dfrac{\ln\left(r_i/r_l\right)}{2\pi L K_l D_l} + \dfrac{\ln\left(r_o/r_i\right)}{2\pi L K_l K_i D_w} + \dfrac{1}{K_l K_i K_o h_o\left(2\pi r_o L\right)}}\ , \qquad \text{(D.1)}$$

where the concentrations along a surface or centerline are noted with c (e.g., c_c is the centerline concentration), partition coefficients as K, line radii are labeled as r, L is the pipe length, D represents diffusion constants, and h mass transfer coefficients with location and subscript defined in Figure D.5. The analysis assumes that the derivative of concentration with respect to time is negligibly small (steady state) and that Fickian expressions suffice. In this functional form, each term in the denominator is a resistance similar to the traditional and commonly known expressions for heat transfer.

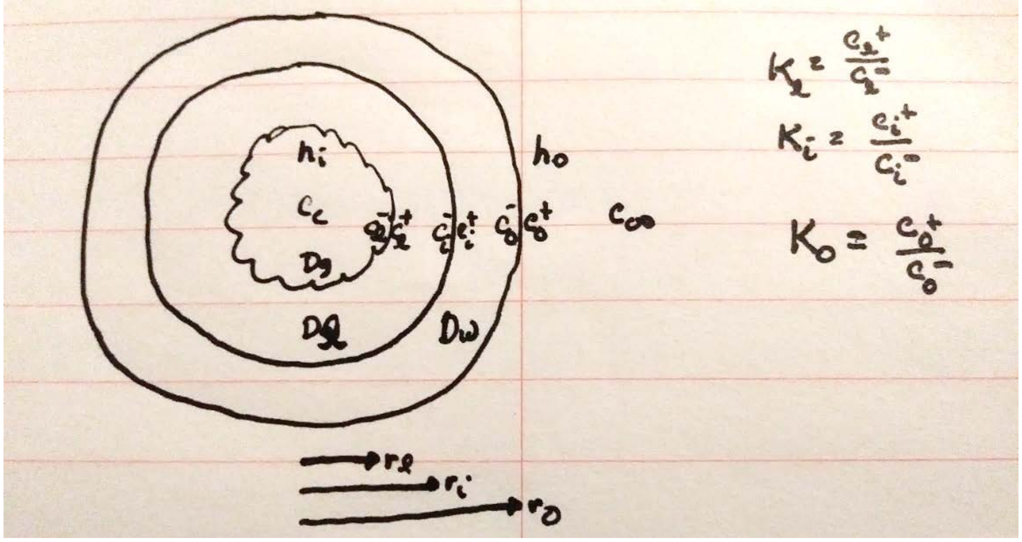


Figure D.5. Variables for the Steady-State Model

A key feature of these expressions is the inclusion of partition coefficients that play an essential role in the resistances in contrast to the resistances in heat transfer that does not have the equivalent of a partition coefficient (in the absence of interfacial resistances). Table D.4 shows that the resistances in the gas and liquid phases are much smaller than the resistances in the tube wall, raising the possibility that the penetration into the wall may be quite small, which is a conclusion that may be further appreciated from an analysis of time scales.

Table D.4. Resistances

Region	Resistance	Approximate Values (s/m^3)
Gas phase within the line	$\frac{1}{h_i\left(2\pi r_i L\right)}$	141-215
Liquid phase (if any)	$\frac{\ln\left(r_i/r_l\right)}{2\pi L K_l D_l}$	$2.0 \cdot 10^4$-$2.8 \cdot 10^9$
Tube wall	$\frac{\ln\left(r_o/r_i\right)}{2\pi L K_l K_i D_w}$	$8.2 \cdot 10^8$-$2.8 \cdot 10^{21}$
Notes: Gas phase resistance outside the line not included because likely unimportant per time scale analysis.		

Five time scales govern the losses (hence the bias) if there is no surface reaction and if species do not fully penetrate through the line. These time scales include a residence time (given above as 27-36 s), a process time scale (~ 1 h), and diffusion time scales within the gas phase within the hose, in the liquid phase, and in the hose wall. The diffusion time scales, which limit mass transfer rates, may be estimated to within an order of magnitude as:

$$t_g = \frac{r_l^2}{D_g} \text{ ,} \tag{D.2}$$

$$t_l = \frac{\left(r_i - r_l\right)^2}{D_l} \ , \tag{D.3}$$

$$t_w = \frac{\left(r_o - r_i\right)^2}{D_w} \ , \tag{D.4}$$

in the gas, liquid and wall, respectively. A formal analysis would include a factor to accommodate geometry that is typically less than a factor of three, and typically a duration equal to three to five times the longest time scale is necessary to assert steady state. The use of molecular diffusion coefficients as opposed to turbulent diffusion coefficients is justified because the Reynolds number for these flows remains less than ~1800 at 30 L/min, but turbulence is important at even marginally higher flow rates. Please note, however, that if the flow rate is only a few percent higher, turbulence may be encountered and edge/entrance instabilities may not dampen as is assumed in this analysis based on the information provided.

The diffusivity is important to this solution. The diffusivity may be estimated to first order approximation by the Stokes-Einstein equation as:

$$D = \frac{k_b T}{3\pi\mu d} \tag{D.5}$$

where k_b is the Boltzmann constant, T is absolute temperature, μ is the dynamic viscosity, and d is the molecular diameter.

The analysis shows that the time scale for mass transfer through the gas is on the same order of magnitude as the residence time of the gas within the tube. Therefore, mass transfer may not be complete and radial gradients in the concentration profile may persist. Results of the analysis in Table D.5 show that the time scale for flow within the gas phase is longer than the time scale in the liquid. This implies that the concentration in the liquid phase is no longer in flux even as the concentration gradients of the gas phase persist. This is primarily because the thickness of the liquid layer is particularly thin. Similarly, the time scale for mass transfer through the wall is much, much longer than the process time scale. This confirms that penetration through the wall (if any) is not complete. Indeed, the time scale for mass transfer through the wall may be set to the process time scale and rearranged to estimate a length scale of penetration during the process time as $l_l=(t_p D_w)^{1/2}$. For values given here, l_l=0.06-190 μm, which is much thinner than the line wall (2.6-7.7 mm).

Table D.5. Time Scales

Region	Time Scale	Approximate Values
Gas phase within the line	$t_g = \frac{r_l^2}{D_g}$	9-12 s
Liquid phase (if any)	$t_l = \frac{\left(r_i - r_l\right)^2}{D_l}$	0.013-0.045 s
Tube wall	$t_w = \frac{\left(r_o - r_i\right)^2}{D_w}$	$6.8\cdot10^{5}$-$5.9\cdot10^{13}$ s
Notes:		

The resistance analysis may be modified to estimate the corresponding flux through the wall normalized on the perimeter of inner wall diameter is given as:

$$N = \frac{\dot{n}}{2\pi r_i L} = \frac{c_c - \frac{c_\infty}{K_l K_i K_o}}{\frac{1}{h_i} + \frac{r_i \ln\left(r_i/r_l\right)}{K_l D_l} + \frac{r_i \ln\left(r_o/r_i\right)}{K_l K_i D_w} + \frac{r_i}{r_o K_l K_i K_o h_o}} . \tag{D.6}$$

The concentration lost to the wall may then be approximated as:

$$\Delta C = \frac{N A_i t_R}{V} = N \frac{2\pi r_i L}{\pi r_i^2 L} \frac{\pi r_i^2 L}{Q} , \tag{D.7}$$

where A_i is the perimeter based on the inner diameter, A_c is the cross sectional area based on the inner diameter, t_R is the residence time and Q is the volumetric flow rate through the line. This expression is simplified based on the assertion that any liquid layer is negligibly thin. This expression simplifies as:

$$\Delta C = \frac{c_c - \frac{c_\infty}{K_l K_i K_o}}{\frac{1}{h_i} + \frac{r_i \ln\left(r_i/r_l\right)}{K_l D_l} + \frac{r_i \ln\left(r_o/r_i\right)}{K_l K_i D_w} + \frac{r_i}{r_o K_l K_i K_o h_o}} \frac{2\pi r_i L}{Q} . \tag{D.8}$$

By mass balance, the concentration that exits the line is then:

$$C_{out} = C_{in} - \Delta C , \tag{D.9}$$

which supports an additive instead of a multiplicative bias. This formulation may be rearranged into a multiplicative bias as:

$$\frac{C_{out}}{C_{in}} = \frac{C_{in} - \Delta C}{C_{in}} = 1 - \frac{\Delta C}{C_{in}} . \tag{D.10}$$

Where the concentration in the wall may be neglected along with corresponding resistances and $c_c = c_{in}$, the bias becomes

$$\frac{\Delta C}{C_{in}} = \frac{1}{Q\left(\frac{1}{h_i\left(2\pi r_i L\right)} + \frac{\ln\left(r_i/r_l\right)}{2\pi L K_l D_l}\right)} . \tag{D.11}$$

Table D.6 shows that the decrements in concentration remain small, at most a few percent. Less soluble species decrement even less as may be anticipated. However, a steady flux solution may not be the best representation of the concentration profile.

The net conclusion of the analysis of resistances and time scales is that concentration gradients within the gas phase within the line and within the tube wall likely persist, even as the concentration gradients within the liquid rapidly vanish. The resistance to penetration within the wall is stiff, suggesting that perhaps mass transfer into the wall may be negligible. Therefore, an analysis that considers concentration gradients within the gas phase, but treats the liquid layer without concentration gradients, and neglects penetration into the wall may capture a majority of the mass transfer physics.

Table D.6. Biases as Estimated from Resistances

Species	$\Delta C/C_{in}$
Ammonia	$3.37 \cdot 10^{-5} – 6.61 \cdot 10^{-4}$
Benzene	$7.21 \cdot 10^{-7}$ - $1.01 \cdot 10^{-1}$
2-Hexanone	$3.28 \cdot 10^{-5} – 2.63 \cdot 10^{-3}$
Acetaldehyde	$3.55 \cdot 10^{-5} – 6.09 \cdot 10^{-3}$
Acetonitrile	$1.87 \cdot 10^{-4} – 1.65 \cdot 10^{-3}$
Propanenitrile	$8.69 \cdot 10^{-5} – 1.71 \cdot 10^{-3}$
N-Nitrosodiethylamine	$7.62 \cdot 10^{-23} – 8.61 \cdot 10^{-23}$
Notes: includes gas and liquid resistances	

Such a solution is available for laminar flow. A simple solution assuming the tube wall to be a perfect sink is recorded by Friedlander (2002). At steady state, conservation of mass within the tube is given by

$$u\frac{\partial c_i}{\partial z} = D_g\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_i}{\partial r}\right) + \frac{\partial^2 c_i}{\partial z^2}\right], \tag{D.12}$$

with boundary conditions

$$c_i = c_{io} \quad \text{at} \quad z=0, \tag{D.13a}$$

$$\frac{\partial c_i}{\partial r} = 0 \quad \text{at} \quad r=0, \tag{D.13b}$$

and

$$c_i = 0 \quad \text{at} \quad r=r_w, \tag{D.13c}$$

where c_i is the concentration of species i, c_{io} is the initial concentration, r and z are the radial and axial directions, u is the local velocity and D_g is the diffusivity. This formulation assumes that there is no bulk reaction and only the diffusivity is chemical specific. Friedlander (2002) and Hinds (1999) provide a solution that appears to depend only on the flow rate and tube length and diffusion coefficient (see Eqs. 3.74-3.75 of Friedlander or Eq. 7.29 of Hinds) assuming axial diffusion to be negligible. The penetration, here from line entrance to line exit (not radial), defined as $P=c_{out}/c_{in}$ is then

$$P = 1 - 5.50\left(\frac{D_g L}{Q}\right)^{2/3} + 3.77\left(\frac{D_g L}{Q}\right) \quad \text{for} \quad \frac{D_g L}{Q} < 0.009 \tag{D.14a}$$

and

$$P = 0.819\exp\left(-11.5\frac{D_g L}{Q}\right) + 0.0975\exp\left(-70.1\frac{D_g L}{Q}\right) \quad \text{for} \quad \frac{D_g L}{Q} \geq 0.009\,. \tag{D.14b}$$

Similarly, Cheng (1993) summarizes the work of several to find additional terms as

$$P = 1 - 2.5638\left(\pi\frac{D_g L}{Q}\right)^{2/3} + 1.2\left(\pi\frac{D_g L}{Q}\right) + 0.1767\left(\pi\frac{D_g L}{Q}\right)^{4/3} \quad \text{for} \quad \frac{\pi D_g L}{Q} < 0.02 \tag{D.15a}$$

and

$$\begin{aligned} P = {} & 0.81905\exp\left(-3.6568\pi\frac{D_g L}{Q}\right) + 0.09753\exp\left(-22.305\pi\frac{D_g L}{Q}\right) \\ & + 0.0325\exp\left(-56.961\pi\frac{D_g L}{Q}\right) + 0.01544\exp\left(-107.62\pi\frac{D_g L}{Q}\right) \end{aligned} \quad \text{for} \quad \frac{\pi DL}{Q} \geq 0.02\,. \tag{D.15b}$$

Both expressions are nearly identical.

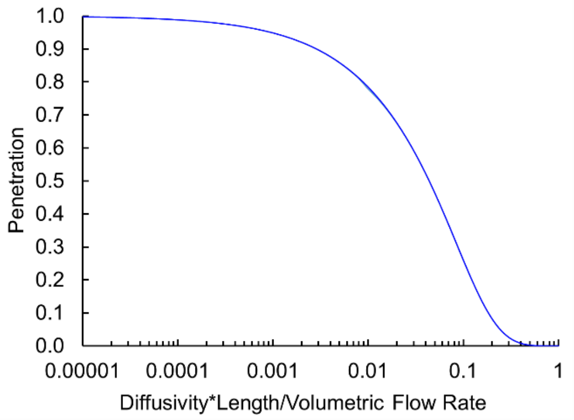


Figure D.6. Penetration, the Ratio of Outlet Concentration to Inlet Concentration versus the Dimensionless Ratio of Diffusivity, Length, and Volumetric Flow Rate

To first order approximation, c_{in} may be the concentration of the headspace and c_{out} may be the concentration of the cartridge system or both may be considered as c_{out} with a real headspace concentration unmeasured. Because diffusivities vary by species, the penetrations also vary by species. Note that this solution applies to the wall as an infinite sink that is not hindered by molecular crowding on the surface, does not depend on molecular binding, does not permit release and reentry of molecules back into the flow, and is not time dependent. It may be a reasonable approximation for relatively low surface coverages at early times.

These equations suggest that biases of species should decrease as the molecular diameter increases (less diffusion), or as flow rates increase (less residence time for diffusion losses). If either of these sorting criteria hold then we have steady state diffusion losses to an essentially infinite pipe. If we have additional chemical variation then the infinite sink with steady losses must be replaced by a more comprehensive solution.

This model as presented supports a multiplicative bias. The bias may be reformulated into an additive bias as

$$C_{bias} = C_{in}\left(1 - P\right), \tag{D.16}$$

Substitution of characteristic values (D=$1 \cdot 10^{-5}$ m^2/s, Q=$5 \cdot 10^{-4}$ m^3/s, L=45.7 m for DL/Q=0.91) finds that the penetration may be relatively small with c_{out}/c_{in}=$2.2 \cdot 10^{-5}$.

We note that each of these solutions is temperature sensitive through molecular diameters (that depend on molar volumes), diffusion coefficients, and other parameters. Therefore, the penetration is likely temperature sensitive. While the temperature may not vary dramatically within the one hour of testing, the implications for application to other conditions at different temperatures may be sensitive to the absolute temperature, diurnal variations, and seasonal changes. Therefore, the biases measured may only apply to the conditions at which they were measured.

We note that none of the mechanisms described above include surface reactions. Absorption of species onto the wall may be a significant mechanism of bias.

D.4 Impacts of Accumulated Water

Another possible mechanism that could drive concentration biases between test rigs is the effect of accumulated water in one system over the other. In order to assess the likelihood of this hypothesis a flash model was set up in Aspen Plus[44] to simulate vapor-liquid equilibrium conditions and to calculate the ratio of COPC in the vapor phase and the COPC dissolved in liquid water phase (Neroorkar and Schmidt 2011). The eight COPCs having no more than one censored concentration were selected for the study. Property analyses were performed to calculate the infinite dilute activity coefficients at 25ºC for several examples using both UNIQUAC functional-group activity coefficients (UNIFAC) and non-random two-liquid (NRTL) methods and compared with literature data to assure consistency (see Table D.7). Only pure component data exist for nitrosamines (nitrosomethylethylamine [NMEA] and nitrosodiethylamine [NDEA]) and no binary parameter with water was found with either UNIFAC or NRTL method. Therefore, NMEA and NDEA could not be accurately modeled.

Table D.7. Water Effects on the Dilution of COPCs in the Cartridge Sampling Unit

	Activity coefficient (UNIFAC)	Activity coefficient (NRTL)	*Activity coefficient (Literature)
Ammonia/Water	1.339	0.0536	0.4
2-Hexanone/Water	254.4	337.8	329.1
Acetaldehyde/Water	6.91	4.74	3.94
Acetonitrile/Water	13.08	13.43	11.1
Propanenitrile/Water	37.49	35.36	32.86^
Benzene/Water	2371	940.8	2500

*The infinite dilute activity coefficient from references Kojima et al. 1997 and Worswick et al. 1974.

^The activity coefficient was calculated using the MOSCED method in Lazzaroni et al. 2005.

The remaining COPCs were next modeled using a flash-tank model configuration in Aspen Plus, and with UNIFAC and NRTL activity coefficients for the corresponding COPCs. The feed stream contained liquid water at a range of flow rates, air (flow rates at 30 L/min) and COPCs, whose concentrations were the means obtained from the headspace test experiments. The concentrations of COPCs in the vapor outlet were used to compare with the concentrations in the feed stream (see Figure D.7).

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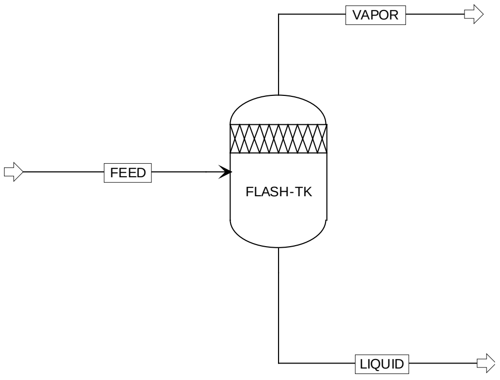
[44] Henry's law constants were from Sander 2015.



	FEED (kg/h)	FEED (ppmv)	EXPTL. (ppmv)
Ammonia	3.71E-04	2.96E+02	2.96E+02
Benzene	1.30E-08	2.27E-03	2.27E-03
2-Hexanone	5.61E-08	7.61E-03	7.60E-03
Acetaldehyde	2.04E-07	6.29E-02	6.28E-02
Acetonitrile	2.67E-07	8.83E-02	8.84E-02
Oxygen	4.83E-01	4.10E+05	*-
Nitrogen	1.57E+00	1.53E+06	*-
Water	4.40E-02	3.32E+04	*-
Propanenitrile	5.22E-08	4.29E-03	4.28E-03

*Not measured in the experiment.

Figure D.7. Aspen Plus Flash Model to Simulate Vapor-Liquid Equilibrium. The water feed flow rate shown here is 0.044 kg/h. The assumed temperature was 25 °C and pressure was 1 bar.

Multiple water flow rates (0.044 kg/h, 0.066 kg/h, 0.204 kg/h and 0.485 kg/h) were studied. The effects of water on the ratio of COPC in vapor phase versus COPC in liquid water phase, using the UNIFAC method for activity coefficient estimation, are shown in Figures D.8 and D.9. Higher ratios indicate that smaller amount of COPC dissolves in liquid water while lower ratios indicate larger amount of COPC dissolves in liquid water. In Figure D.8, the vapor ratios of nitrogen, oxygen and benzene are close to 1, which means that these chemicals stay in the vapor phase with no effect from water dissolution. Other COPCs generally show some degree of dissolution in water with increasing water flow rates. Considering the air temperature in the cartridge test is about 68°F (20°C) and the relative humidity is about 60% RH, the total amount of water into the CT rig in 1 h is about 18.6 g (30L/min, 60 min). The condensed water should be less than this values. The predicted vapor ratio from flash model, using NRTL method for activity coefficient estimation, is shown in Figure D.8. The general trend is the same for the vapor ratio as comparing with results in Figure D.9. Only some larger decrease in vapor ratio were found for chemicals such as ammonia at higher water flow rates.

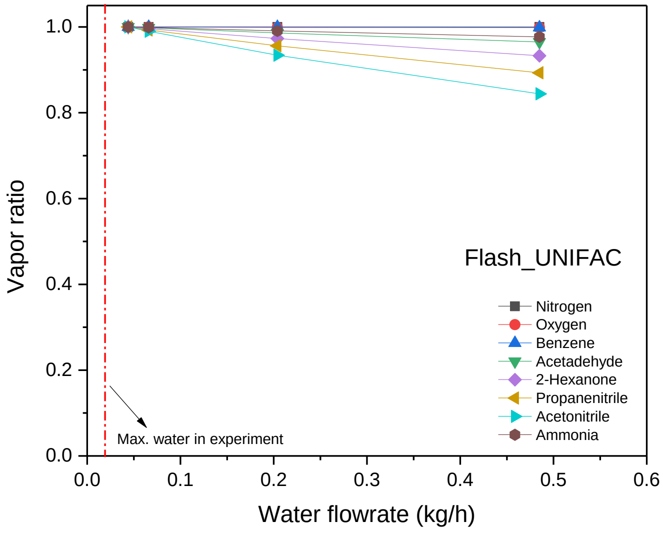


Figure D.8. Water Effects on the Dissolution of COPC in the Flash Model using UNIFAC Method

The ratios of the concentrations of the COPCs obtained from cartridge and headspace tests are calculated with uncertainties and summarized in Table D.8, along with the corresponding model predictions. As stated above, model predictions for NDEA and NMEA could not be calculated due to the lack of binary property data. The ratios of the experiment results from cartridge and headspace tests, as seen in Table D.8, are around 1, and consistent with model predictions. 2-Hexanone and NDEA had experimental ratios between the cartridge and headspace measurements that were lower than 1 with statistical significance (1σ). However, neither of these COPCs had commensurate model predictions. This may indicate that the water dissolution may not be a significant factor that will cause large difference between results obtained from CT and HS tests.

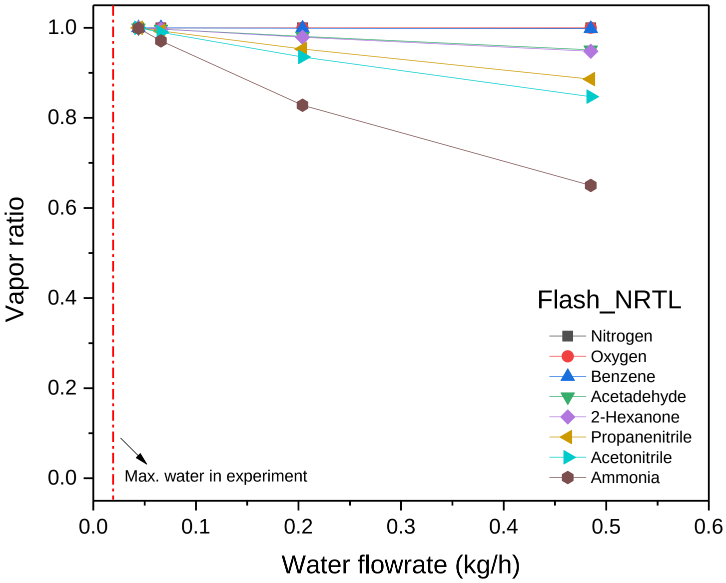


Figure D.9. Water Effects on the Dissolution of COPC in the Flash Model Using NRTL Method

Table D.8. Water Effects on the Dissolution of COPC in the CT Test

	Mass Ratio								
	Experiment	Aspen model							
	Cartridge/headspace	Vapor phase/feed							
	Mean value*	0.044 kg/h		0.066 kg/h		0.204 kg/h		0.485 kg/h	
		UNIFAC	NRTL	UNIFAC	NRTL	UNIFAC	NRTL	UNIFAC	NRTL
Ammonia	0.997± 0.258	1.000	1.000	0.999	0.971	0.991	0.828	0.977	0.649
Benzene	1.044± 0.411	1.000	1.000	1.000	1.000	1.000	0.999	0.999	0.997
2-Hexanone	0.551± 0.331	1.000	1.000	0.996	0.997	0.973	0.977	0.933	0.944
Acetaldehyde	1.430± 0.768	1.000	1.000	0.998	0.997	0.986	0.980	0.965	0.951
Acetonitrile	0.727± 0.306	1.000	1.000	0.990	0.990	0.934	0.935	0.844	0.846
Propanenitrile	1.065± 0.562	1.000	1.000	0.993	0.993	0.956	0.952	0.893	0.884
N-Nitrosodiethylamine	0.254± 0.169	N/A*	N/A	N/A	N/A	N/A	N/A	N/A	N/A
N-Nitrosomethylethylamine	0.088± 0.059	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A

*Each ratio is the arithmetic mean for cartridge data divided by that for headspace. The uncertainties were calculated using the quadratic sum rule. The nitrosamines could not be modeled due to the lack of binary interaction data with water.

D.5 Dissolution and Permeation of Chemicals in and through the Tube Walls

According to WRPS, RFRTP polytetrafluoroethylene (PTFE) Teflon-lined hose with an ethylene propylene diene monomer rubber (EPDM) cover was used in the field experiment to connect flow within the riser to the inlet of the CT rig. For a 1.30 in. (33.0 mm) outside diameter (O.D.) hose used in the field experiment, the internal diameter is 0.78 in. (19.8 mm).[45] If we assume the thickness of the PTFE layer is $^1/_8$ in. (3.2 mm), the outside polymer thickness is about 3.4 mm. Hydrocarbon and other gas molecules can dissolve in PTFE especially in amorphous fluoroplastics such as Teflon AF (Liu et al. 2017). For example, it was reported that propane can have a solubility of 7 cm^3 (STP)/(cm^3 atm) in Teflon AF 2400 and the solubility will increase for gases with higher boiling points following an exponential relationship (Freeman et al. 2006). Ammonia has a boiling point (240 K) similar to that of propane; however, ammonia is more polar than propane, making it less soluble in non-polar PTFE than propane. Using the same boiling point-solubility relationship gives 8.6 cm^3 (STP)/(cm^3 atm) as an upper bound for ammonia, the COPC that has the highest inlet concentration.

The volume of the total hose layer is 10,571 cm^3 (for the 150 ft extra length that is present for cartridge rig but not present for headspace sampling). Because the partial pressure of ammonia is about 2.96×10^{-4} atm, the equilibrium dissolved ammonia can be estimated to be about 26.9 cm^3 (STP). Because PTFE is a semi-crystalline polymer with much less free volume than the amorphous AF 2400, the dissolved gas volume can be estimated to be 1 to 10% of that of Teflon AF 2400, based on the factor of 1000 difference in CO_2 permeability[46] in the two forms of Teflon (Ono 2006). Using the upper limit of 10% for solubility, the dissolved amount of ammonia can be estimated to be about 0.012 mmol with the further assumption that the dissolved ammonia in the PTFE hose does not reach equilibrium within 1 h and is less than 10% of the equilibrium value. The total amount of ammonia entering the CT rig in 1 h is approximately 22.2 mmol. Therefore, the percentage of possible ammonia dissolved in the PTFE is less than 0.05%.

A similar analysis can be done for NDEA, whose concentrations have a statistically significant difference between the cartridge and headspace systems. The extrapolated solubility for NDEA is about 302 cm^3 (STP)/(cm^3 atm) based on its normal boiling point at 450 K. Similarly, the dissolved amount of NDEA can be estimated to be about 8.2×10^{-6} cm^3 (STP) and the percentage of possible NDEA dissolved in the PTFE is less than 1.9%. The estimated dissolved ratio of the key COPCs are shown in Figure D.10. The range of the value is from 0.05%-1.9% so the upper bound for the dissolved ratio is less than 1.9%.

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[45] Rubber Fab Technologies Group. Hose Fittings & Adapters. https://www.rubberfab.com/products/hose-fittings-adapters.

[46] Permeability is defined as the product of the solute's solubility and diffusivity.

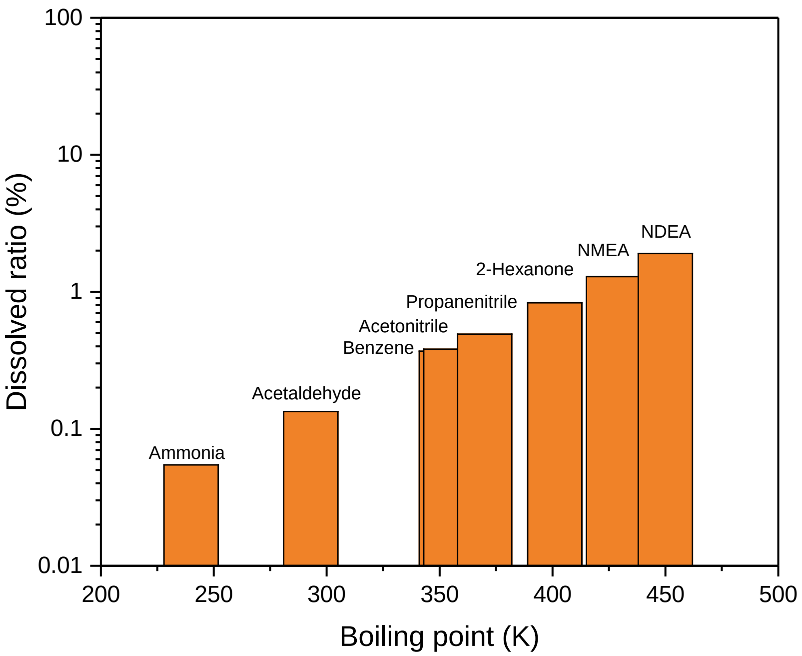

Figure D.10. Dissolved Ratio in PTFE Hose Estimated for the Key COPCs

In addition to the dissolution in the wall, permeation through the wall is another mechanism that can affect the vapor concentration. A typical water vapor transmission rate at 40 °C and 100% RH through a 1 mm semi-crystalline Teflon FEP 100 fluoropolymer resin film is about 7 g/(m^2 d), which is about 0.29 g/(m^2 h).47 The internal surface area of the hose outside of the tank headspace is 2.84 m^2. So in this case, where the water vapor pressure in the line was 55.5 mm Hg (0.0730 atm) and the air on the other side of the film was dry, the maximum water that would have permeated the FEP layer in 1 h, if the area were the same as the hose inner surface, would have been about 0.83 g. (This neglects the permeation resistance of the rubber cover.) The temperature in our case is about 20ºC and the relative humidity is about 60%, giving a water partial pressure of 10.5 mm Hg (0.0138 atm). The permeance of water is related linearly to the difference in water partial pressure, and inversely to the thickness of the Teflon layer (3.2 mm for the hose), so the amount of water that can leave the test hose in our cartridge test in 1 hr is only about 0.049 g assuming the permeation rate linearly decreased with the thickness of the Teflon layer (3.2 mm). The total amount of water flow through the CT rig in 1 h is about 18.6 g. So the percentage of permeated water is about 0.26%.

One should notice that there are several arbitrary assumptions in the above analysis and the chemicals whose transport properties are used as the basis for the analysis may not represent the exact COPCs in the field test. However, if we assume the results of ammonia and water can be applied to other chemicals as well, the analysis may indicate that the dissolution and permeation of gas into and through the extra hose surface used for the cartridge test will reduce less than 2.2% of the gas concentration assuming a simple additive effect from both hose dissolution and permeation. This difference will increase with the increase of boiling point of the gas when the partition effect is not included. However, it will not significantly affect the vapor concentration of COPCs in the cartridge test.

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[47] Teflon FEP Handbook. DuPont Company.

D.6 Calculation of Potential HEPA Surface Area Impacts

The impacts of radiation particulate filters on the headspace sampling of Hanford Waste tanks were documented in Huckaby et. al. 1996. Here, comparison tests were conducted to examine the effects of the glass fiber particulate filters[48] that have been used to remove radiological particles from the sample stream in the vapor-sampling system.[49] In laboratory testing in which sample air was passed through these filters, an important semi-volatile constituent (tributyl phosphate) was removed by the filter (Jenkins et al. 1995), and there had been concern that the filters adversely effected the measurements of other constituents. Because the filters were optional in the in situ vapor-sampling system,[50] it was possible in the study to collect sets of samples with and without the filter, allowing a direct evaluation of the effects of the filters.

The filter comparison tests were conducted on Hanford waste tanks 241-C-107 (sampled September 29, 1994), 241-BY-108 (sampled October 27, 1994), and 241-S-102 (sampled March 14, 1995). The study concluded that "… results indicated that the filters did adversely affect the collection of low volatility organic vapors… though the effect of the filters on tributyl phosphate could not be determined."

The most significant (10% or greater) impact of the filter media during the tests are summarized as follows:

- For Tank 241-C-107 – Where samples collected through the glass filter were measured at lower concentrations, the relative percent differences (RPD) were total non-methane hydrocarbons at 37%, methanol at 34%, ethanol at 20%, 1-propanol at 11%, and 2-butanone at 37%. Where samples collected by through the glass filter were measured at higher concentrations, the RPDs were acetonitrile at 21%, and propanenitrile at 12%.
- For Tank 241-BY-108 – Where samples collected by through the glass filter were measured at lower concentrations, the RPDs were acetone at 18%, tetrahydrofuran at 23%, decane at 10%, undecane at 17%, dodecane at 20%, tridecane at 23%, and tetradecane at 47%. Where samples collected by through the glass filter were measured at higher concentrations, the RPDs were 1-propanol at 22%, acetonitrile at 35%, 2-butanone at 41% and propanenitrile at 36%.
- For Tank 241-S-102 – Where the sample collected by through the glass filter were measured at lower concentrations, the RPDs were total non-methane hydrocarbons at 10%, 1-propanol at 17%, acetone at 17% to 25%, tetrahydrofuran at 14%, nonane at 11% to 19%, and 2-butanone at 18% to 21%.

Although the nature of the glass particulate filter used in the historic testing cannot be established, the historic results do indicate that particulate filters can contribute to potentially significant differences in sampling results.

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[48] The specific filter media was not identified in the report.

[49] The vapor sampling system consists of a mobile laboratory, a hot-water-jacket stainless steel probe inserted into the tank headspace, and stainless steel transfer tubing that connects the mobile laboratory with the probe. Electronically controlled heating of the tubing and manifolds at elevated temperatures prevented vapor condensation. The samples were collected into SUMMA® canisters.

[50] The in-situ vapor sampling system method was a smaller version of the current headspace sampling system. Small bundles of up to four sorbent tubes were lowered into the tank headspace with ¼-in. diameter plastic tube. The tube would be connected to a needle valve, electronic mass flow meters to monitor flow rates, and electronic totalizers. Constituents not amenable to sorbent trap sampling (e.g., gases such as hydrogen, nitrous oxide, and methane) were sampled using unheated Teflon tube that transferred the samples to SUMMA® canisters.

D.7 Comparison of Sampling Times

The timing of the cartridge and the headspace data sets were compared to evaluate the start times and the amount of overlap in the sampling windows. This information is shown in Table D.9.

Table D.9. Sampling Start Times for the Cartridge and Headspace Measurements

			Start Times				
Dive #	Analyte Tubes Tested	Date of Dive	HS Test Rig	CT Test Rig	CT–HS (min)	Overlap Time (min)	Testing Time Overlap
1	Methanol/nitrosamines	1/16/18	9:44	10:22	38	22	37%
2	Pyridine/ethylamine	1/25/18	8:57	8:58	2	59	97%
3	Aldehyde/SVOC	2/1/18	9:22	9:29	5	53	83%
4	Acetonitrile/1,3 Butadiene	2/6/18	8:40	9:06	26	34	57%
5	VOC/ammonia	2/8/18	8:55	8:48	7	54	89%
6	Mercury/Furan	2/9/18	9:47	9:36	11	49	82%

As shown in Table D.9, the methanol/nitrosamine dive had a start time difference of 38 min and a testing time overlap of only 37%. The acetonitrile/1, 3 -butadiene dive had start time difference of 26 min and a testing time overlap of 57%. The remaining dives had start times within 11 min of one another testing time overlaps that exceeded 80%.

The impact of the later start times for the CT rig cannot be fully quantified. The bias quantified for nitrosamines was significant compared to the other compounds, which could align with the start time differences, but those compounds also had high boiling points, which aligns with another potential bias mechanism. The other compound that had a statistically significant lower bias was 2-hexanone, which was measured in Dive 5 with ammonia. Because ammonia was not biased, this comparison suggests boiling point as a more likely driver than start time differences to explain the observed biases.

D.8 Comparison of Analytical Tube Flows

Table D.10 shows a comparison of the average measured flow rates through the analytical tubes for both the HS and CT sampling systems based on two methods to average the data: 1) averages provided by the client based on essentially two-point averages in (a) and 2) time-weighted averages based on the entire data set in (b). This comparison shows the largest variation (349% and 351% standard deviation for (a) and (b), respectively) in the ethylamine bundle for the CT sampling system. The flow variation for the remaining cartridge tube bundles was within a standard deviation range of 10% to 88%. The last column in Table D.10 compares the difference in average flow rates in the HS and CT sampling systems. Here, the largest difference was again with the ethylamine set, which was 23.7% and 22.4% lower for (a) and (b), respectively for the CT data compared to the HS data. SVOC and Aldehydes (the two Dive 3 tube sets) had 14.7% and 12.7% and 12.0 and 12.9% higher average tube flow for the CT system, respectively. All other average flow rates were within 8% of one another.

Table D.10. Average Flowrates for Each of the Analytical Tube Bundles Tested Based on Client-Provided and Time-Weighted Averages of the Data

(a) Client-provided Data

Tube Set	Dive #	HS			CT			(CT-HS)/HS
Methanol	1	3.1	±	13%	3.2	±	23%	0.17%
Nitrosamines	1	49.9	±	101%	47.7	±	17%	-4.3%
Ethylamine	2	11.8	±	35%	9.0	±	349%	-23.7%
SVOC	3	3.1	±	19%	3.5	±	31%	14.7%
Aldehydes	3	23.0	±	245%	25.8	±	31%	12.0%
1,3-Butadiene	4	22.7	±	59%	24.5	±	24%	7.8%
Ammonia	5	20.2	±	87%	20.8	±	32%	2.9%
VOC	5	2.9	±	9%	3.1	±	17%	6.4%
Mercury	6	15.0	±	59%	14.9	±	19%	-0.7%
Furans	6	3.0	±	8%	3.2	±	10%	5.7%

(b) Time-weighted Average Data

Tube Set	Dive #	Headspace Rig (HS)			Cartridge Rig (CT)			(CT-HS)/HS
Methanol	1	3.1	±	13%	3.1	±	23%	0.03%
Nitrosamines	1	49.5	±	146%	47.7	±	21%	-3.6%
Ethylamine	2	11.8	±	41%	9.2	±	351%	-22.4%
SVOC	3	3.1	±	20%	3.5	±	28%	12.7%
Aldehydes	3	22.7	±	174%	25.7	±	34%	12.9%
1,3-Butadiene	4	22.7	±	58%	24.6	±	16%	8.3%
Ammonia	5	20.2	±	82%	20.7	±	42%	2.5%
VOC	5	3.0	±	12%	3.1	±	15%	6.5%
Mercury	6	15.0	±	60%	14.6	±	88%	-3.2%
Furans	6	3.0	±	8%	3.2	±	16%	4.4%

Another effect related to sample tube flow rates that was evaluated was the potential for the gas volume pulled through the tubes to disproportionately impact the mass of the compounds collected. Figure D.11 shows plots of mass collected versus total gas volume for benzene. These plots show no observed trend between the sample volume and the mass of benzene collected on the tubes. This is likely due to the narrow range of volumes pulled through the tubes.

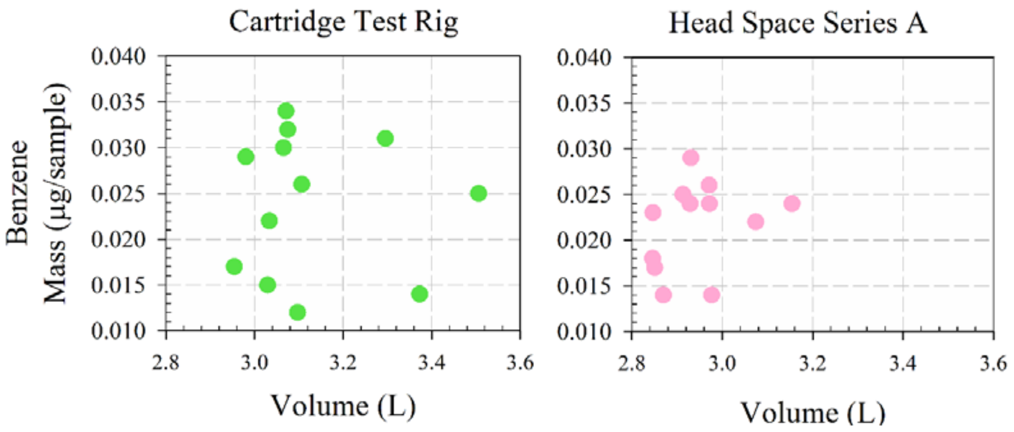

Figure D.11. Benzene Mass-to-Volume-to-Mass Comparison

Figure D.12 shows the same volume-mass plots as in Figure D.11, but for ammonia. These plots may show a slight trend between the sample volume and the mass collected. However, as with benzene, the ammonia data does not show a definitive trend that could be related to bias between the two sampling rigs.

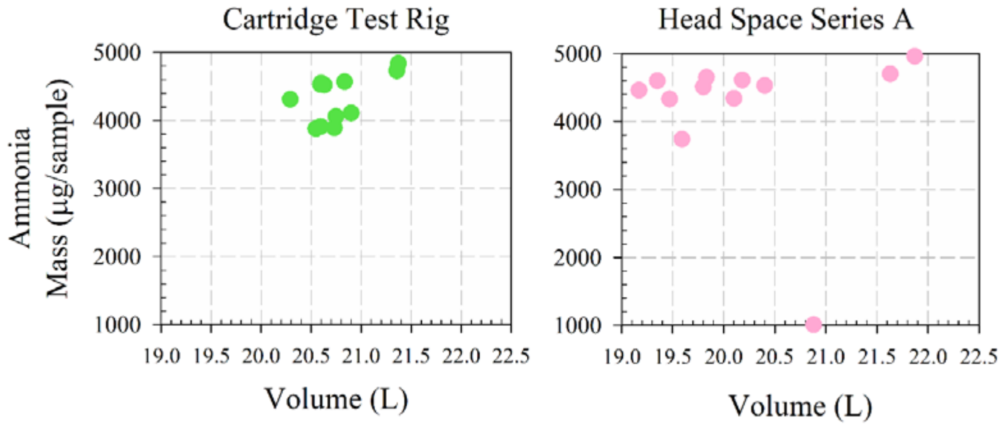

Figure D.12. Ammonia Mass-to-Sample-Volume Comparison

Estimated Impacts of Analytical Tube Location/ Grouping

The position of the analytical tubes was evaluated for the potential of causing systematic variations in the results. For the HS samples the potential that one side of the tube bundle would differentially collect tank vapors was assessed. For the CT samples the potential that the six sample tubes collected on the influent side would collect higher vapor concentration that the six tubes on the effluent side was assessed.

In the headspace bundle, the tubes were numbered 1 through 12 clockwise[51] around the circumference of the inner bundle housing. To evaluate the collection trends, the rank of several measured VOC and nitrosamine compounds[52] are shown in Table D.11. The lowest concentrations were assigned the value of 1 with the highest concentration assign a value of 12. An examination of the data did not highlight a vapor collection bias where one side (zone) of the bundle collected an observable ranking difference in vapor concentration than other zones. Table D.12 shows the corresponding data for CT sampling system locations on the influent side (before the cartridge mounting position[53]) and an additional six of the same type media tubes sampling on the effluent side (after the cartridge mounting position[2]). Here again, the data did not highlight a vapor collection bias where the tubes collected on the influent side had a significant observable difference in vapor concentration that those on the effluent side.

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[51] Sample Bundle Diagrams #1 (VOCs) and #9 (Nitrosomine) for Parent Sample number S17T006603.

[52] The VOC measurements were collected on a Carbotrap 300 TDU tube and the nitrosomines were collected on a Thermosorb/N cartridge on different dives.

[53] No cartridges were mounted in the test unit during the comparison testing.

Table D.11. Comparison of Ranked Concentrations in the Headspace for Trend Observations

Tube Position In the Bundle	Benzene	2-Hexanone	Propanenitrile	NDEA	NMEA
1	9	9	6	3	3
2	11	11	10	6	6
3	7	7	8	10	12
4	2	2	2	8	9
5	10	10	11	11	11
6	6	6	7	2	2
7	12	12	12	4	5
8	5	8	4	12	8
9	3	3	3	1	1
10	8	5	9	5	4
11	4	4	5	9	10
12	1	1	1	7	7

Table D.12. Comparison of Ranked Concentrations in the CT Rig for Trend Observation

Assigned Position	Sample Designator	Benzene	2-Hexanone	Propanenitrile
Influent Side Collected Samples				
1	IN-A	3	1	3
2	IN-B	9	12	10
3	IN-C	11	10	11
4	IN-D	4	4	4
5	IN-E	5	6	5
6	IN-F	1	2	2
Effluent Side Collected Samples				
7	EFF-A	12	11	12
8	EFF-B	6	5	6
9	EFF-C	10	8	9
10	EFF-D	2	3	1
11	EFF-E	8	9	8
12	EFF-F	7	7	7

D.9 Potential Bias from Laboratory Analytical Processes

Of the laboratory analysis mechanisms that could cause measurement bias, those considered likeliest are measurement quality problems of the types identified by data quality flags in the as-received data set; grouping of measurements into different calibration periods; and large scatter (caused by unknown mechanisms) within each data set.

D.9.1 Measurement Quality Problems

As discussed in Section 4, a number of vapor chemicals were removed from consideration in statistical analysis because of measurement quality issues that arose from the limitations of laboratory analysis methods or devices. The measurements of some other vapor chemicals also were quality-flagged, but examination showed that the data could be used. These are summarized as follows:

- NDEA and NMEA – For these chemicals, an “a” flag, indicating out of range spike recovery, appeared on all the cartridge data. A review by the 222-S Laboratory found that these data had spike recovery between 120% and 140% of the expected value, from which it can be inferred that the measured cartridge concentrations averaged about 130% of actual. Since spike recovery averaged about 100% for the HS-A concentrations, the cartridge measurements may have been even lower (compared to HS-A measurements) than was discussed in Section 4.

- Acetonitrile (by VOA method), hexane, n-heptane, and trichlorofluoromethane – Many of these measurements had “E” flags, raising the question of whether the detector was saturated for any of the measurements. The most likely effect of saturation would be a reduction in the detector response, causing the higher measurements to be underestimated. However, a review by the 222-S Laboratory found the detector response to these vapor chemicals was linear in all cases, given the range of concentrations measured and the matrix in which they were present.

Other species reviewed by the 222-S Laboratory, and found to be well identified and well quantified, were 2-hexanone, furan, propanenitrile, and toluene.(54)

D.9.2 Sample Grouping during Laboratory Analysis

Another possible cause of measurement bias comes not from limitations of the analytical method or devices, but from carrying out headspace and cartridge analyses with a recalibration in between. To check for this, the records for two types of analyses—nitrosamines and VOA—were checked by the 222-S Laboratory.

The nitrosamine HS data were all analyzed by RJ Lee in the same sequence, which ran overnight, and all had the same analyst.[55] The order in which the nitrosamine tubes were analyzed has not been checked.

The VOA analyses were performed at the 222-S Laboratory.[56] On February 26, 2018, a blank and a set of standards were run, followed by sample tubes in the following order:

- S18T004131 through 4144, in ascending order without gaps – cartridge samples:
  - 18-01142-1-CC-EFF-A and B (sample lines 7 and 8),
  - 18-01142-1-CC-EFF-BL1 (a field blank),
  - 18-01142-1-CC-EFF-C through F (sample lines 9–12),
  - 18-01142-1-CC-IN-A and B (sample lines 1 and 2),
  - 18-01142-1-CC-IN-BLA1 (a field blank),
  - 18-01142-1-CC-IN-C through F (sample lines 3–6).
- S18T004096 through 4108, in ascending order without gaps – headspace samples:
  - 18-00799-1-001A (HS-A tube 1)
  - 18-00799-1-001ABL (HS-A field blank)
  - 18-00799-1-001B (HS-B tube 1)
  - 18-00799-1-001BBL (HS-B field blank)
  - 18-00799-1-002A, 2B, 3A, 3B, 4A, 4B, 5A, 5B, 6A.

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[54] The 222-S assessments mentioned in the measurement quality section came from the following sources:
DR Hansen (222-S) to LA Mahoney, 12/26/2018, “RE: BY-110 comparison nitrosomorpholine.”
DR Hansen to LA Mahoney, 12/6/2018, “RE: 2-hexanone in BY-110 comparison study.”
DR Hansen to LA Mahoney, 11/29/2018, “RE: 3-buten-2-one in BY-110 comparison.”
DR Hansen to LA Mahoney, 11/20/2018, “RE: 3-buten-2-one in BY-110 comparison.”
DR Hansen to LA Mahoney, 10/25/2018, “RE: summary of conclusions about flagged data.”
DR Hansen, minutes from regular respirator cartridge meetings.

[55] RB Compton (of RJ Lee) to DR Hansen, 10/16/2018, “RE: Surveys with bad flags or high range of concentrations.”

[56] DR Hansen to LA Mahoney, 12/12/2018, “RE: new questions -- order of analyses.”

On February 27, 2018, a blank and a set of standards was run, followed by four "Clean Batch 180226B" samples apparently unrelated to the comparison study, followed by study-related tubes in the following order:

- S18T004109 through 4121, in ascending order without gaps – headspace samples:
  - 18-00799-1-006B, 7A, 7B, 8A, 8B, 9A, 9B, 10A, 10B, 11A, 11B, 12A, 12B.

Figure D.13 shows the concentrations of four chemicals whose concentrations were measured by VOA; the four were chosen as being COPCs that were all in about the same concentration range. All the concentrations shown are non-censored, with blanks where there were censored values. The x axis represents the sequence of analyses in the 222-S Laboratory, including standards, field blanks, and unrelated analyses (all of which are shown as blank in the figure). Lines between symbols indicate that more than one sample in a row was non-censored. Because all headspace-B samples were censored, and alternated with headspace-A samples, no lines are drawn between headspace-A samples.

Figure D.13 shows no apparent trend in the concentrations measured during the analysis sequence. The sequencing of analyses not does appear to be a cause of bias.

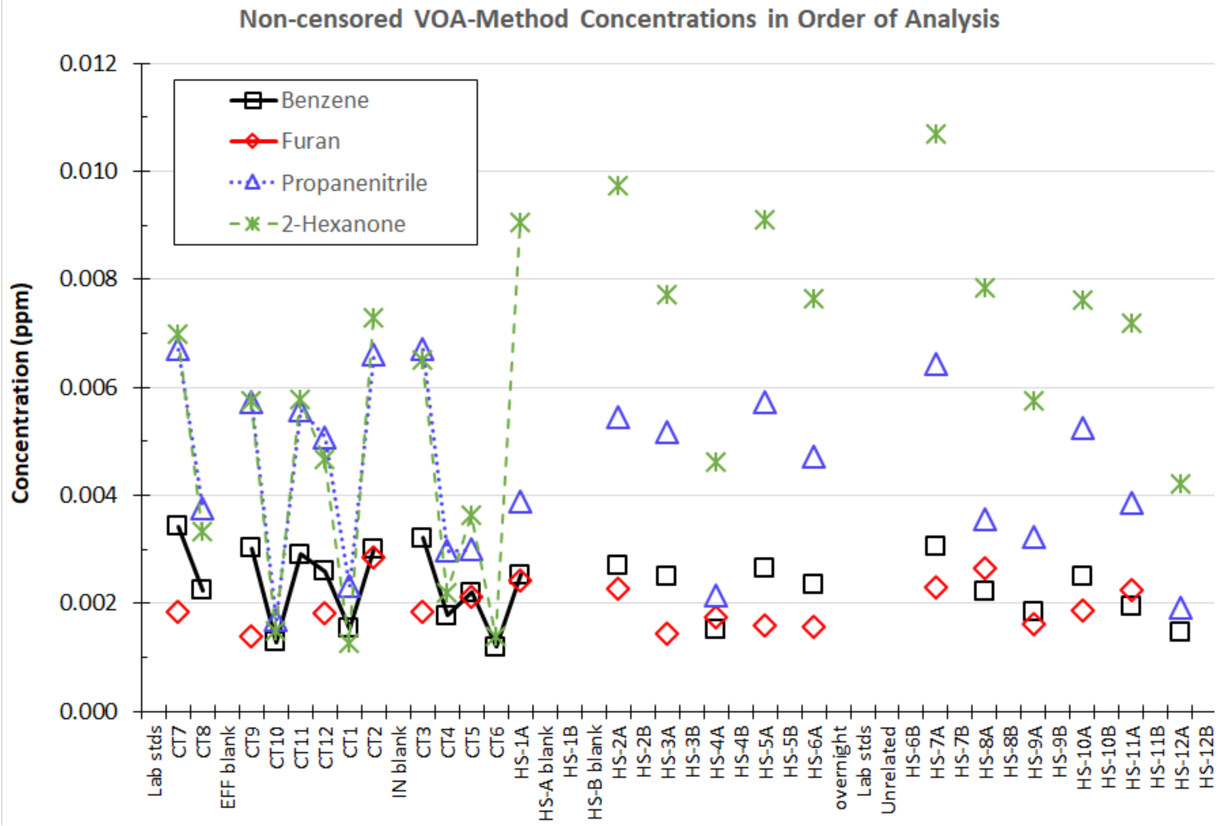
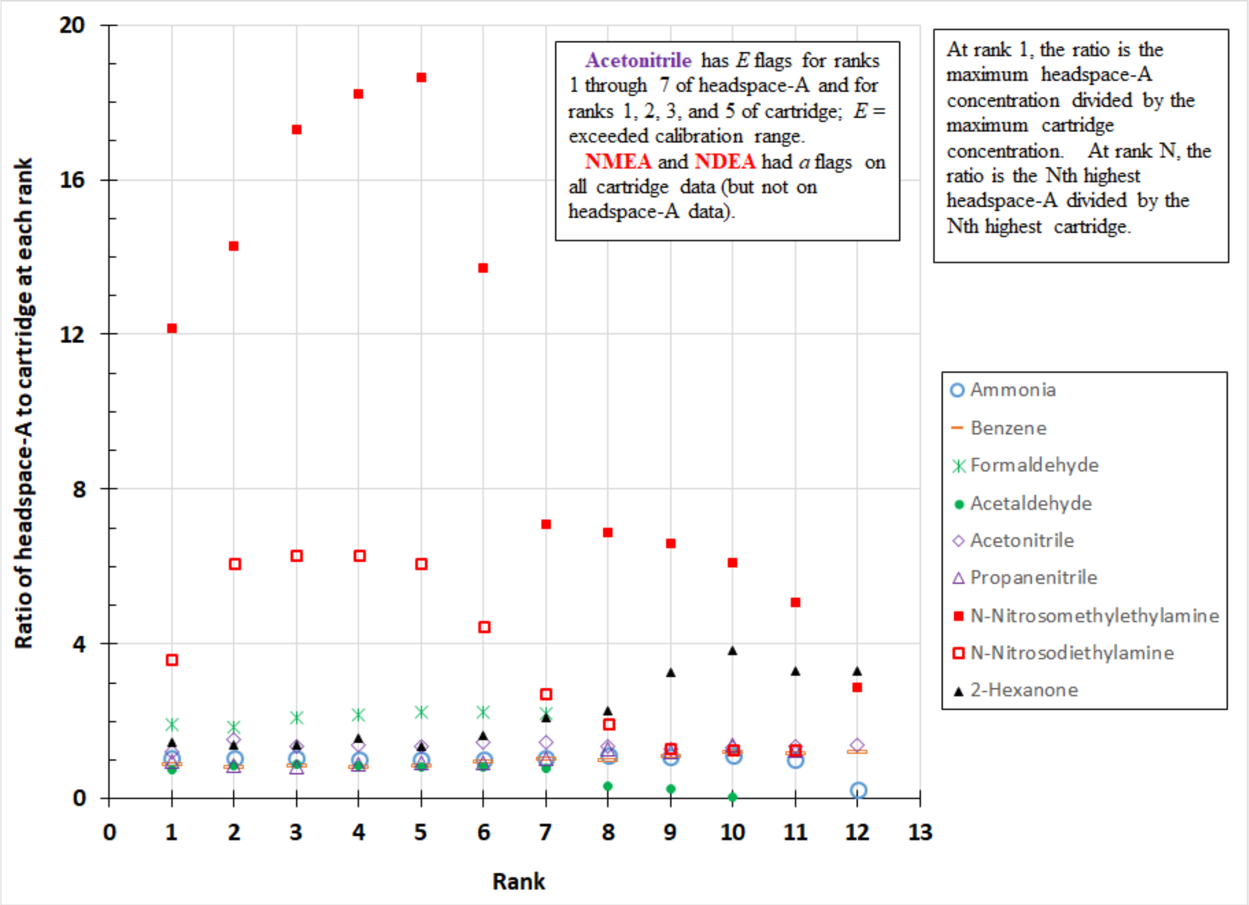


Figure D.13. Non-Censored Concentrations of Four VOA Chemicals in Sequence of Laboratory Analysis

D.9.3 Data Scatter

In many cases substantial scatter was observed within each data set—that is, within the headspace-A set or the cartridge set—in spite of the fact that the whole set was collected at the same location and over the same time period. The effect of scatter upon bias is visualized in Figure D.14 and Figure D.15.



Acetonitrile has *E* flags for ranks 1 through 7 of headspace-A and for ranks 1, 2, 3, and 5 of cartridge; *E* = exceeded calibration range.

NMEA and **NDEA** had *a* flags on all cartridge data (but not on headspace-A data).

At rank 1, the ratio is the maximum headspace-A concentration divided by the maximum cartridge concentration. At rank N, the ratio is the Nth highest headspace-A divided by the Nth highest cartridge.

Figure D.14. Ratio of Headspace-A to Cartridge Concentration at Each Rank (including only non-censored COPC concentrations)

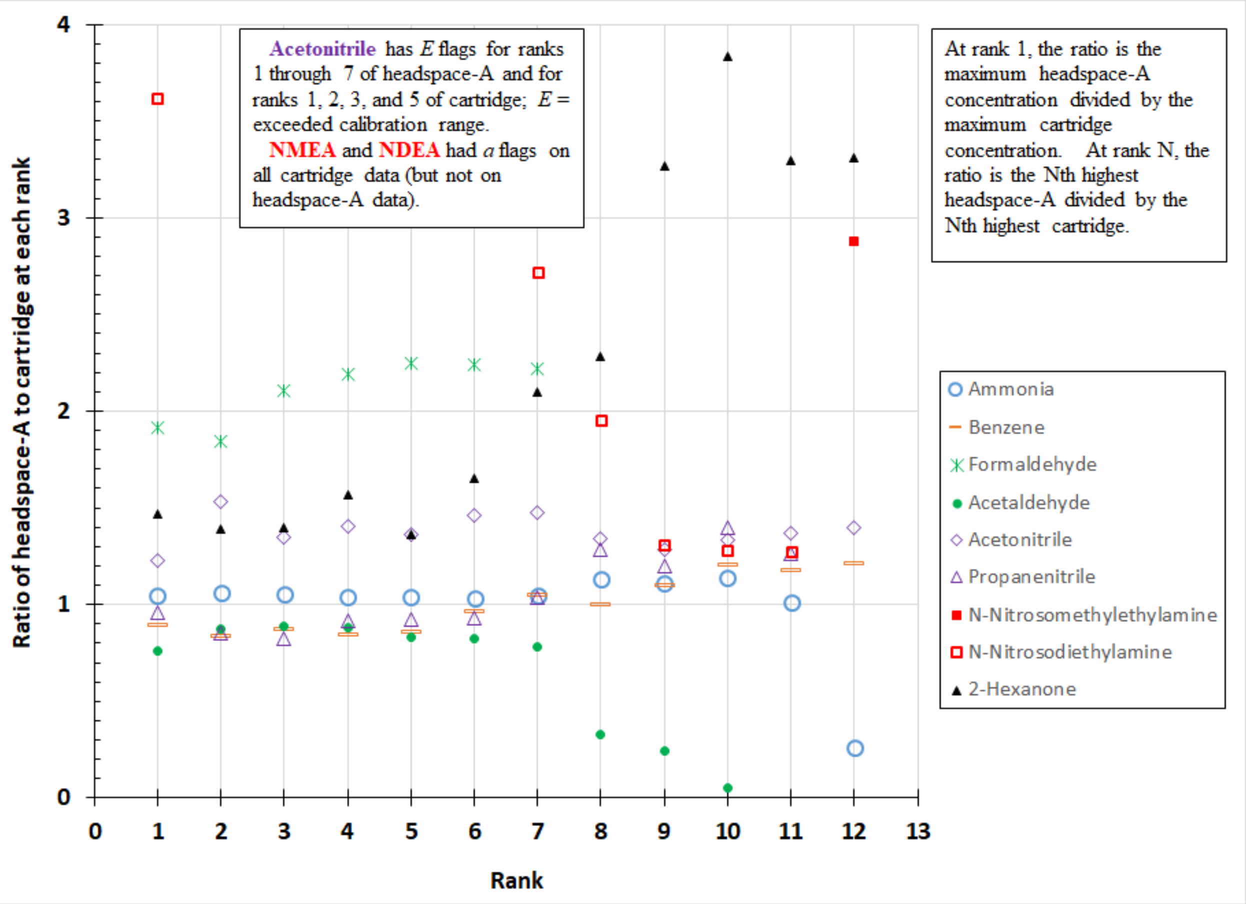


Figure D.15. Ratio of Headspace-A to Cartridge Concentration at Each Rank (including only non-censored COPC concentrations) for Ratios of 4.0 or Less.

These three figures were generated by ranking each data set, HS-A and CT, and then taking the ratio of HS to CT at each rank, with censored concentrations excluded. The ranks are given on the x axis, where maxima are ranked as 1 and the concentrations decrease toward the minima as the rank number increases. The only chemicals presented in the figures are COPCs for which there were six or more data points each in the HS-A and CT sets, and the number of data in each set was equal or nearly equal. Thus formaldehyde was included, with seven non-censored points in each set, as was acetaldehyde, with 10 non-censored points in the HS-A data and 12 in the CT data, but furan was excluded because it had 11 non-censored points in the HS-A data and only six in the CT data.

Figure D.14 shows the entire range of ranks (x axis) and rank-ratios (y axis). The two nitrosamines, NMEA and NDEA (colored red), stand out as having a variation in rank-ratio for different ranks that is unusually high, compared to other chemicals. Figure D.15 is a close-up that includes all ranks, for the same set of chemicals, but only shows the rank-ratios that were less than or equal to 4.0.

The variation in rank-ratios with ranks indicates the possibility of variation in bias, caused by scatter. If a small number of samples were taken in the future, using the CT sampling system, the bias could be different if the sample set came from one part of the scatter than from another.

D.9.4 Potential Bias from Sorbent Tubes

The sorbent tubes used for BY-110 comparison are given in Table D.13.

Table D.13. Properties of Tested Sorbent Tubes[57]

Analyte Category	Sorbent Media	Reference Analytical Method	Analytical Instrument Used	Batch No	Expiration Date	Mesh Size	Sorbent Weight	Media Sorption Capacity
Acetonitrile	Charcoal Tube, SKC-226-09	NIOSH 1606	GC–FID			20/40	200/400 mg	
Acetonitrile	Carbotrap 300 TDU Tube	EPA TO-17 Modified	GC/MS					
Furans	TDU Tenax TA	EPA TO-17 Modified	GC/MS					
Semi-Volatile Organic Compounds	Carbotrap 150 TDU Tube	EPA TO-17 Modified	GC/MS					
Volatile Organic Compounds	Carbotrap 300 TDU tube	EPA TO-17 Modified	GC/MS					
Mercury	Anasorb C300, SKC-226-17-1A	NIOSH-6009	CVAA			20/40	200 mg	
Methanol	Silica Gel, SKC-226-51	NIOSH-2000	GC–FID			20/40	50/100 mg	
Ammonia	Anasorb 747 (sulfuric acid), SKC-226-29	OSHA-ID-188	IC			20/40	250/500 mg	
1,3-butadiene	Charcoal, SKC-226-37, (Parts A and B)	NIOSH-1024	GC–FID			20/40	200/400 mg	
Aldehyde	DNPH Treated Silica Gel, SKC-226-119	EPA TO-11A	HPLC			20/40	150/300 mg	
Pyridine	Coconut Shell Charcoal, SKC-226-01	NIOSH-1613	GC–FID			20/40	50/100 mg	
Nitrosamines	Thermosorb/N	NIOSH-2522 Modified	GC–TEA					
Ethylamine	XAD-7 (NBD) Chloride), SKC 226-96	OSHA-ID-34, 36, 40,and 41	HPLC–UV			20/40	50/100 mg	

Various sorbent materials were used in different sorbent tubes tested. Sorbent materials include Charcoal, Carbotrap 300, Tenax TA (porous polymer resin based on 2.6-diphenylene oxide), Carbotrap 150, Anasorb C300, Silica Gel, Anasorb 747, DNPH Treated Silica Gel, Coconut Shell Charcoal, XAD-7 resin coated with 10% NBD chloride by weight. Of the sorbent tubes tested, Anasorb 747 is generally hydrophobic in nature and adsorbs less water than the carbon derived from coconut charcoal. Properties of the sorbent's tubes used are shown in Table D.13. All sorbent tubes used during BY-110 comparison test met NIOSH, OSHA, or EPA specifications. Manufacturer quality control ensured accurate sorbent weights for accurate and repeatable results with desorption efficiencies approaching 100%. For all the COPC's tested, new (or conditioned) sorbent tubes were used except for furans, VOA, and semi-volatile organic analytes. The new sorbent tubes (per manufacturer specifications) used have met or exceeded

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[57] Because data were not available at the time this report was prepared, data for Table D.13 are incomplete,.

NIOSH, OSHA or EPA requirements for sorbent purity, storage stability, sample retention and desorption efficiency described by the analytical methods. Mesh size, sorbent weight / density and sorption capacity of the sorbents play a critical role. Batch-to-batch sorbent quality may vary and may potentially have different sorption capacities, wherever possible, sorbent tubes from a single batch (Table D.13) were used during testing for reproducible recoveries.

All sorbent tubes were handled following the manufacturer's instructions. While testing, all sorbent tubes were used in vertical position preventing the possibility of channeling (responsible for under sampling). To ensure good sealing, both ends were capped immediately after sampling using the caps supplied. After collection, the tubes were stored in a refrigerator at 0°C. The tubes were stored for up to a week or more before the tubes were shipped to the analytical facilities for analysis.

Stringent criteria were followed during conditioning or regeneration of sorbent tubes before they were reused. After sorbent tubes were conditioned/regenerated, one TDU tube randomly selected from the preparation batch was analyzed before the remaining tubes were released for sample collection. The sorbent tube batch was certified for use if the selected tube met all of the following criteria:

1. No target analyte may be detected with a concentration equal to or greater than two times the MDL or equal to or greater than the RL whichever is the least amount.
2. Under certain circumstances it may be acceptable for the concentration of the following compounds to be greater than two times the MDL as long as the client is notified prior to use:
   - Methylene chloride
   - Hexane
   - Acetone
3. Artifact peaks, if present, shall not interfere with analysis of target compounds.
4. Tubes found to fail any of these criteria resulted in rejection of the entire batch.

Analytical Accuracy:

One source of bias could come from the accuracy of the analytical method. This includes the quality of the sorbent tubes used. Table D.14 shows the analytical accuracies of the main COPCs and several other compounds. Here, most of the compounds were analyzed via the VOC method with a stated accuracy of ±35%. Based on this information, it is difficult to see an accuracy as an observable cause of bias.

Table D.14. Analytical Accuracies

Compound	COPC?	Analytical Method	Accuracy of Method
Ammonia	Y	Ammonia	±10.9%
Benzene VOC	Y	VOC	±35%
2-Hexanone	Y	VOC	±35%
Formaldehyde	Y	Aldehydes	12.6 (RSD)
Acetaldehyde	Y	Aldehydes	16.5 (RSD)
Furan	Y	VOC	±35%
Acetonitrile	Y	VOC	±35%
Propanenitrile	Y	VOC	±35%
N-Nitrosodiethylamine	Y	Nitrosamines	Not Determined
N-Nitrosomethylethylamine	Y	Nitrosamines	Not Determined
1-Propanol	N	VOC	±35%
2-Butanone	N	VOC	±35%
3-Heptanone	N	VOC	±35%
4-Methyl-2-Pentanone	N	VOC	±35%
Cyclohexane	N	VOC	±35%
Ethanol	N	VOC	±35%
Hexane	N	VOC	±35%
n-Heptane	N	VOC	±35%
Toluene	N	VOC	±35%
Trichlorofluoromethane	N	VOC	±35%

D.10 References Cited in Appendix D

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