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AN-107 (C) Simulant Bench-Scale LAW Evaporation with Organic Regulatory Analysis

Westinghouse Savannah River Company
Savannah River Site
Aiken, SC 29808

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Contents

1.0 Summary

As part of a series of evaporation experiments, a Hanford Tank AN-107 Envelope C simulated waste was spiked with approximately 1 ppm of 14 target volatile, semi-volatile and pesticide compounds, and was concentrated from approximately 5.5 to 8.0 M Na to determine the fate of organic species entering the Low Activity Waste Melter Feed Evaporator. These studies were conducted in support of the Hanford River Protection Project Waste Treatment Plant (RPP-WTP). The information from these experiments will be used as input to the RPP-WTP environmental permits, risk assessments, and process flow sheet development. This experiment and an accompanying OLI model showed that: 1) volatile and light semi-volatile (1,2,4-trichlorobenzene, naphthalene) organic compounds largely exit the evaporator system through the condensor vent gas at individual species concentrations up to ~1000 ppm, 2) heavier semi-volatile organic and pesticide compounds tend to remain in the evaporator concentrate, 3) AN-107 simulant reaches a very sharp saturation point at about 10.1 M Na concentration, and 4) an OLI model can describe organics distribution over a wide molecular weight range from the evaporation of Hanford simulant, with a few exceptions. The final boildown experiment indicates the Envelope C simulant reaches saturation at 48.6 wt% (94.6 g total solids (TS)/100 g water, estimated 10.1 M Na), and that initial insoluble solids are sodium oxalate followed by sodium carbonate prior to precipitation of sodium nitrate. This work also showed that evaporation of the pretreated Envelope C simulated waste did not cause scaling, did not require an anti-foaming agent, and behaves as a Newtonian fluid. Lastly, a novel waste simulant spiking and storage system was developed for the creation of stable Hanford waste simulants spiked with organic compounds.

2.0 Introduction and Background

The Hanford River Protection Project Waste Treatment Plant (RPP-WTP) pretreatment and immobilization process will decontaminate Envelope A, B & C supernates using cesium and technetium ion exchange columns, after strontium and transuranics (Sr/TRU) are removed via a precipitation (Envelope C only) and filtration step. The decontaminated low activity waste (LAW) will be concentrated through the LAW Melter Feed Evaporator, a forced circulation evaporator. Glass formers will be added to the concentrated LAW and vitrified in a joule-heated, refractory-lined melter designed to operate at 1150°C (nominal). The design goal of the LAW Melter Feed Evaporator is to: 1) evaporate pretreated Envelope A, B, and C waste to 80% of bulk solubility thereby preventing the formation of solids[*], and 2) maximize the waste loading in the

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[*] Bulk solubility of a multi-electrolyte solution is defined here as the mass of total dissolved solids in solution, when one or more of the major salt constituents first begins to precipitate. Small quantities of solids should not challenge the design basis for the LAW melter feed lag storage vessels. The LAW melter feed lag storage vessels are each equipped with pulsed-jet mixing units that are capable of suspending small quantities of solids. The LAW melter feed will be transferred from the lag storage vessels to the LAW vitrification building using

melter feed by removing as much water as possible without over concentrating the slurry to the point that the material can not be transported to the melter, and to the point that inadequate distribution of the feed on the melt surface hinders melting.

The design of the Hanford RPP forced circulation evaporator is based upon the Hanford 242-A evaporator that is used to concentrate Hanford supernate wastes[1,2]. The Hanford 242-A evaporator is designed to operate at an absolute pressure of 40 to 80 torr[3]. During Part A of the Tank Waste Remediation System (TWRS) Privatization contract, Savannah River Technology Center (SRTC) evaporated the Hanford LAW melter feed in crucibles at atmospheric pressure. No attempt was made in Part A to demonstrate the LAW Melter Feed Evaporator unit operation. During Part B1, actual Hanford radioactive samples, pretreated to remove Cs and Tc, were batch evaporated under prototypical pressure and temperature. SRTC has also performed evaporation experiments on simulated Hanford wastes.

The overall objective of this work is to develop preliminary operating data including expected concentration endpoints using a C waste envelope simulant. The data is to be used for the preliminary Hanford RPP flow sheet development and LAW Melter Feed Evaporator design. A scoping study by Monson[4] and OLI model predictions were used as a basis to determine the maximum achievable concentration of Envelope C simulants without significant crystalline solids formation. A small bench scale evaporator (1 L) was fabricated and operated with simulated pretreated LAW solutions. Parameters that were monitored and /or measured included:

- foaming
- scaling
- heat flux, evaporator pressure and temperature,
- antifoam concentration (as required)
- air in-leakage
- entrainment
- distribution of select organics in the concentrate, condensate, and evaporator off gas
- composition of concentrate, condensate, and evaporator off gas
- physical properties of concentrate (e.g. viscosity)

Corrosion testing is covered under another experimental program and will be conducted using actual Hanford radioactive wastes. The data developed during the simulant evaporation experiments will be used to refine an OLI Environmental Simulation Program (ESP) evaporation

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centrifugal pumps which are to be designed to suspend solids and prevent settling in the underground pipeline. <u>System Description for the LAW Melter Feed Lag Storage System (LP-140)</u>, SD-W375LP-PR00001, revision 3, April 3, 2000, BNFL Inc., Richland Washington.

[1] M. Currey, “LAW Melter Feed Evaporator”, K0104_REP_013_PRC, BNFL Engineering Ltd, March 6, 1997.

[2] Verbal Conversation with M. E. Johnson concerning LAW Melter Feed Evaporator, January 19, 1999.

[3] M. D. Guthrie, “242-A Evaporator Campaign 97-1 Post Run Document”, HNF-SD-WM-PE-057, Waste Management Hanford, Richland WA 99352, August 15, 1997.

[4] Monson, P. R., “Envelopes A, B, and C Shaker/Bath Evaporation Saturation Studies”, BNF-003-98-0189, SRT-PTD-99-0062, Rev. 0, January 4, 2000.

model that is being developed by SRTC. This task, in addition to the small scale scoping studies, will define experimental parameters to be used in the active LAW evaporations.

This bench-scale evaporation with C-simulant (AN-107) spiked with several target organic compounds is one in a series of runs outlined in a Technical Task Plan (TTP) by Calloway and Lambert[5] examining evaporator operating parameters and evaporation endpoints for different Hanford RPP waste simulants under different feed conditions. The purpose of this experiment was to examine the regulatory off-gas emission impacts from the evaporation of a relatively organic-rich simulated waste containing a variety of volatile and semi-volatile organic compounds in addition to pesticides potentially present in actual Hanford RPP waste. An industrial-scale EPA (Environmental Protection Agency) SW-846 Methods 0010/0031 gas sampler was connected to the effluent of an operating bench-scale evaporator to collect and quantify emissions of regulated organic compounds as consistently as practically possible to the EPA SW-846 Methods. Based on the information gathered, evaporator off-gas permitting requirements will be determined.

Hence, the purpose of this work was to provide data as similar as possible to regulatory data on a bench-scale to serve as a guide for emissions permitting requirements for the actual industrial-scale evaporator to be installed at Hanford.

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[5] Calloway, T. B., Lambert, D. P., “Task Technical and Quality Assurance Plan for Bench Scale LAW Evaporation with Simulants”, BNF-003-98-0056, SRT-PTD-99-0018, Rev. 0, December 14, 1999.

3.0 Experimental

3.1 Equipment Description

The bench-scale evaporator used in the experiment is shown in Figure 1. The evaporator is mainly of glass and Teflon® construction to minimize potential organic absorption/adsorption during operation. Only very slight losses are expected to the stainless steel-sheathed thermocouples/RTD's (Resistance Temperature Detectors) used to monitor the evaporator (T2), condensor (T3) and condensate (T4) temperatures, and the Incoloy® heating rod (with internal thermocouple T1) used as the heating element in this natural circulation evaporator. Stainless steel Cajon® fittings mounted in Teflon® plugs were used on the lids of the evaporator and condensate chambers to secure temperature and pressure (pressure gauge PG) measurement devices and some material addition/removal ports. Again, minimal losses of organic are expected due to minimal surface area and exposure to the interior headspace rather than direct contact with the liquid. When feed, condensate, or concentrate was introduced or removed from the system, liquids were routed through Teflon® lines and valves (V1-V3). To also minimize

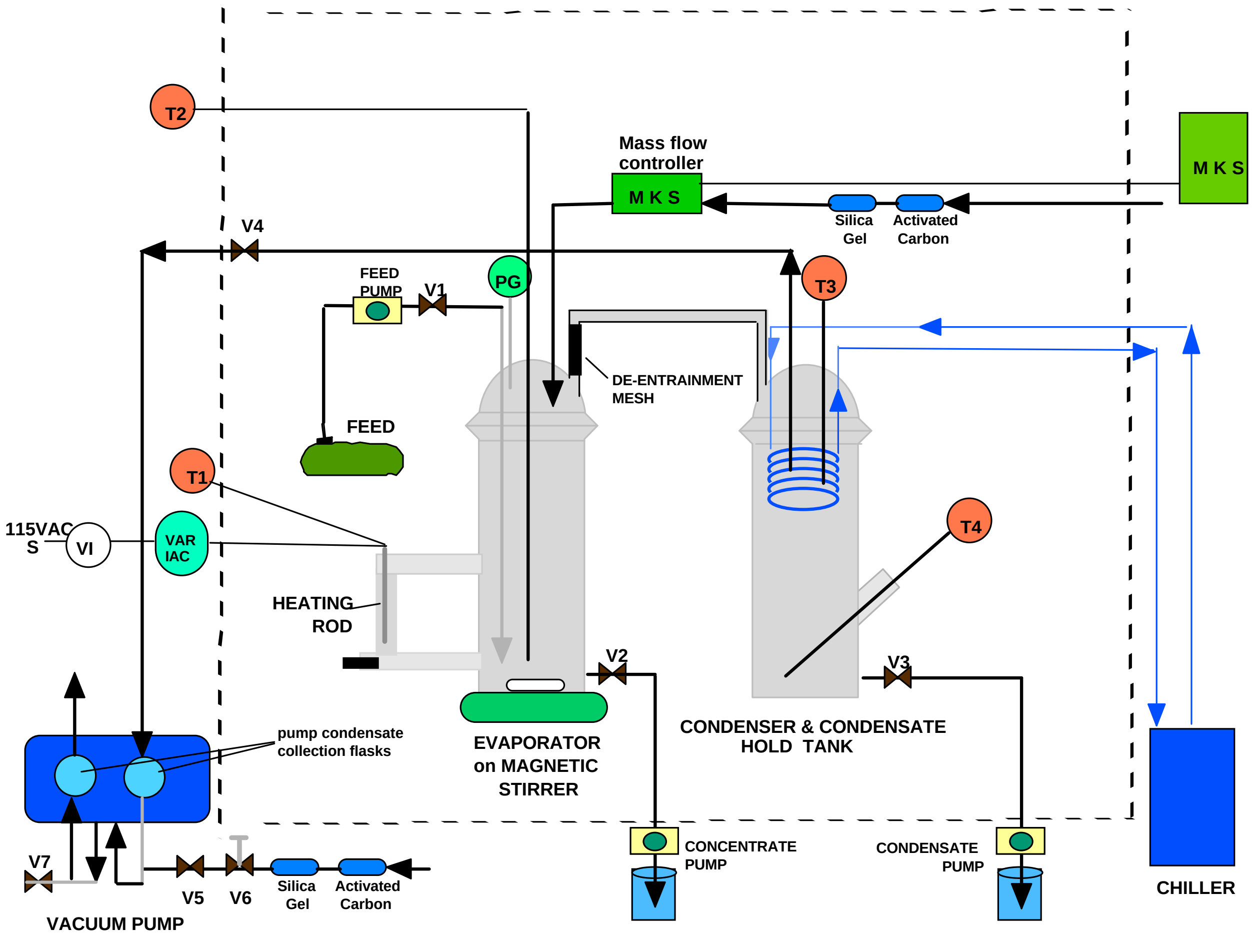


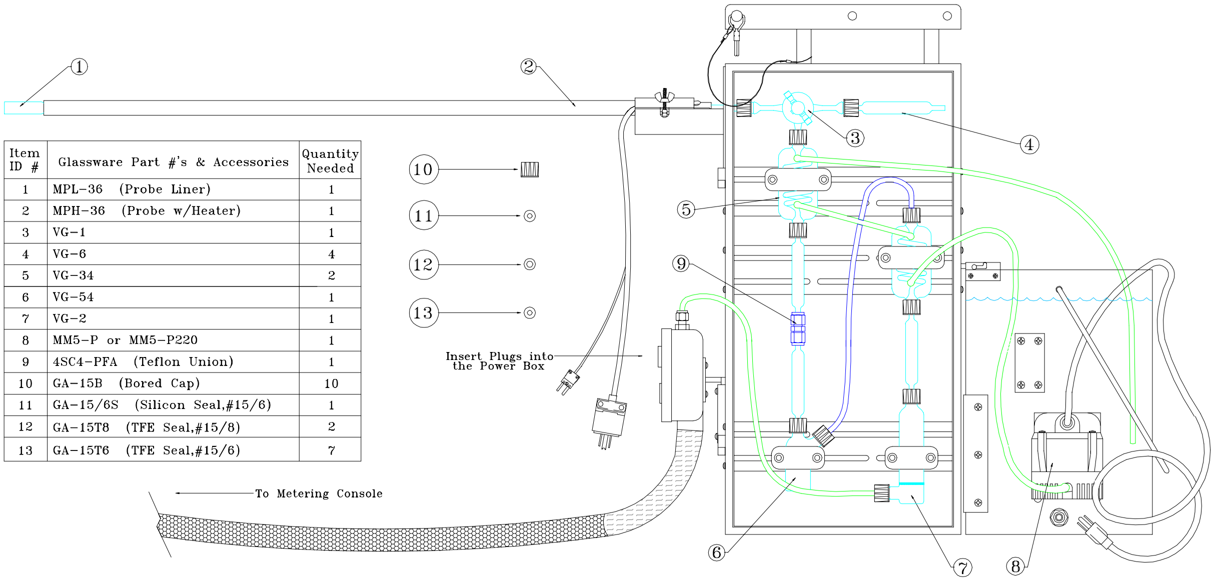
Figure 1. Evaporator System Schematic

organic losses and simulant contamination, the ground glass joints were sealed with Teflon® tape, a Viton O-ring, or a Teflon®-coated O-ring, rather than with conventional silicone vacuum grease. The internal volume of the evaporator was estimated to be approximately 5200 mL by filling the interior with water and measuring the water removed. The evaporator chamber and condensate hold tank are capable of holding nearly 2100 mL and 2000 mL, respectively, before liquid reaches the seam with the lid. Natural leak rates of as low as 0.2 mL/min (STP) were achieved with this system.

Continuous feed addition and concentrate removal was performed using Masterflex L/S® pumps equipped with a segment of size 15 Viton® tubing. The Viton® tubing was connected to the 1/8" OD teflon evaporator feed and concentrate lines by a Teflon® union and Teflon® 1/4" OD tubing secured with hose clamps. The condensate was removed in batches through 1/8" OD Teflon® tubing connected to a Masterflex L/S® rigid PTFE tubing pump head equipped with 6 mm OD tubing. Feed material was introduced from 1L Tedlar® (PVF, polyvinyl fluoride) bags to the feed line via size 14 Viton® Masterflex® tubing, for reasons to be discussed later.

A measured air in-leakage was input into the evaporator using an MKS mass-flow controller to supplement the natural air-inleakage rate. The sum of the these two air flows (total evaporator off-gas) were pulled out of top of the condensate tank through 1/4" Teflon® tubing using a two-stage Teflon® diaphragm pump (Vacuubrand, Inc., Model MZ-2C). To control the off-gas flow out of the evaporator, a bleed valve between the two pump stages was manually adjusted until a steady evaporator pressure was obtained. The measured evaporator in-leakage and pump bleed air were pretreated using moisture (silica gel) and carbon traps to minimize addition of target organics from the ambient air.

The total evaporator off-gas and pump bleed air were sent by Teflon® tubing to an Apex Inc. Model 602-V31 Super VOST (Volatile Organic Sampling Train) Sampling Kit (Figure 2)



Item ID #	Glassware Part #'s & Accessories	Quantity Needed
1	MPL-36 (Probe Liner)	1
2	MPH-36 (Probe w/Heater)	1
3	VG-1	1
4	VG-6	4
5	VG-34	2
6	VG-54	1
7	VG-2	1
8	MM5-P or MM5-P220	1
9	4SC4-PFA (Teflon Union)	1
10	GA-15B (Bored Cap)	10
11	GA-15/6S (Silicon Seal,#15/6)	1
12	GA-15T8 (TFE Seal,#15/8)	2
13	GA-15T6 (TFE Seal,#15/6)	7

Figure 2. Off-gas Sampling System (SuperVOST Sampling Kit, Apex Instruments, Inc.)

coupled with a Model 623 Metering Console. This sampling system is designed to withdraw from an emission source at an isokinetic sampling rate and collect target species in a multi-component sampling train that includes packed beds of porous polymeric adsorbent resin. The VOST system in Figure 2 is setup for EPA SW-846 Method 0031, where the sampled gas typically enters the sampling module through a glass-lined probe heated to 130°C ± 5°C. The gas stream is cooled to 20°C by passage through a water-cooled condenser and volatile organic compounds are collected on a set of three sorbent traps (Tenax®-GC/Tenax®-GC/Anasorb®-747). The first and second traps contain 1.6 g of Tenax®-GC each and the third trap (back trap) contains 5.0 g of Anasorb®-747. The sorbent tubes are glass tubes with approximate dimensions of 10 cm x 1.6 cm ID. The sampling module contains a condensate trap after the two Tenax®-GC tubes, a second condenser immediately upstream of the Anasorb®-747 tube, and silica gel to remove any moisture before entering the meter box. If required, traps may be analyzed separately to assess breakthrough or combined to improve detection limits.

For the capture of semi-volatile organic and pesticide compounds using Method 0010, the same sampling system was used where the Tenax and Anasorb sorbent tubes were replaced by a single XAD-2® tube. In typical application, a high-efficiency glass- or quartz-fiber filter is used to collect organic-laden particulate matter from the gas stream prior to sampling. The organic sampling module of the sampling train again consists of three sections, including a gas conditioning section, a sorbent trap, and a condensate knockout trap. In a typical Method 0010 stationary source emissions measurement application, the sorbent trap is sized to contain approximately 20 g of porous polymeric resin (Rohm and Haas XAD-2 or equivalent) and is jacketed to maintain the internal gas temperature not to exceed 20°C. However for this regulatory study, the XAD-2 sorbent trap was sized identical to the sorbent traps used to perform Method 0031 based on the expected quantity of target species to be captured and for equipment interchangability.

In this experiment, the condensers above each column of sorbent tubes was connected to a chiller to maintain a temperature of 10°C, rather than the ice bath shown at the right of Figure 2. The heated probe was also unnecessary as the entire pump gas effluent was sent directly into the gas sampler, and no in-line glass filter was used as no particulate matter in the off-gas was expected. The metering console was also equipped with a pump which maintained a slight vacuum (<51 mm Hg, or <2 in. Hg) on the gas sampling train to facilitate flow.

3.2 Air In-Leakage Determination

Gas flow in the evaporator was expected to be a major controlling variable influencing the rate of organic vapor transfer from the evaporator to the off-gas as well as the amount of liquid entrained from the evaporator to the condensate tank[6]. As the Hanford RPP tank waste supernatant liquids

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[6] A. S. Choi, Preliminary Modeling Results of Preterated LAW Evaporator, BNF-003-98-0080 Rev. 0, Westinghouse Savannah River Company, June 1, 1999.

are to be concentrated by vacuum evaporation, the primary contributor to gas flow would come from natural in-leakage of exterior ambient air into the vacuum evaporator system. To make this bench-scale experiment reflect an actual plant, a desired experimental air in-leakage rate into the bench-scale evaporator was determined by scaling down as a function of total internal volume from the expected full-scale system design. From a preliminary design, Ho and Washer[7] had determined a maximum air in-leakage rate of 37 lb/hr air for a recirculation evaporator vessel, condenser, and associated piping with a 3681.6 ft^3 internal volume operating in the 21-89 mm Hg pressure range. This translated to a 13.7 m^3 air (STP)/hr per 104.3 m^3 evaporator system internal volume at full-scale, or 11.5 mL/min air (STP) for this approximately 5200 mL internal volume bench-scale evaporator.

For actual implementation of the 11.5 mL/min air in-leakage rate, a natural leak rate for the evaporator was calculated from evaporator leak tests starting at evaporation operating pressure just prior to operation, and the remainder was made up using filtered/dehumidified air introduced through a calibrated mass flow controller.

3.3 Gas Sampling Time Determination

Evaporation run time was predominantly controlled by the minimum volume of condensate (3 L, in duplicate) required for regulatory analysis and the maximum evaporator condensate production rate (3 mL/min) obtained by equipment testing using de-ionized water. As 6 L condensate each was required for regulatory semi-volatiles and pesticide analysis with additional time for volatiles and in-house sample generation, a minimum required evaporation run time of 73.5 hours was determined. Consultation with the Analytical Chemistry Organization Sampling and Support Department at the Y-12 National Security Complex[8] indicated that Method 0031 was best suited for volatile organic compound (VOC) sampling and Method 0010 could be used for both semi-volatiles and pesticide sampling.

While Method 0030 was viewed as sufficient for the volatile organic compounds spiked into the Envelope C (AN-107) Hanford waste simulant, the other commonly-used Method 0031 was selected over Method 0030 for two reasons: 1) the regulatory C-simulant evaporation was a preparatory run for regulatory off-gas sampling from the evaporation of actual Envelope C (AN-102) Hanford waste immediately following, and 2) actual Hanford waste was suspected to contain VOC’s that are more volatile, polar, and difficult to collect than those for which Method 0030 was designed. Method 0010 was commonly used for the collection of semi-volatile organic compounds, with pesticides of interest in this study having similar molecular weights. EPA SW-846 Method 0031 calls for a withdrawal of a 20 L off-gas sample at a 1 L/min flow rate, and Method 0010 requires a minimum 3 dscm (dry standard cubic meters) or 3000 L (STP). With the

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[7] Ho, J., Washer, M., “RPP-WTP: Stage B – Air Inleakage into LAW Pretreatment Evaporation Systems”, BNFL Document CALC-W375PT-PR00011, Rev. 1, October 27, 1999.

[8] Gibson, Jr., Luther V., Burdette, Mark A., Sampling and Support Department, Analytical Chemistry Organization, Y-12 National Security Complex (BWXT Y-12, L.L.C.), personal communications, January – June, 2000.

total evaporator off-gas consisting of the 11.5 mL/min air in-leakage, the maximum amount of gas sampling time for each method was clearly needed, and the 73.5 hour run time was arbitrarily split into two equal off-gas sampling periods for each method. This long sampling time combined with the large expected pump air-bleed volumetric flow rate needed to maintain evaporator pressure further supported the use of Method 0031, which also employs an Anasorb-747 sorbent downstream of 2 Tenax-GC tubes which is known to be more "tenacious" in retaining organics than the Tenax and Tenax/charcoal combination used in Method 0030.

3.4 Evaporator Entrainment

Entrainment of evaporator tank liquids was undesirable due to potential artificially high condensate production rates, as well as high carry-over of metals and salts into the condensate and condenser vent (evaporator off-gas) stream. The bench-scale evaporator was built with basic anti-entrainment devices such as a "J"-shaped inlet port to the inverted U-tube connecting the evaporator and condensate tanks, and a small chamber between the "J"-shaped port and U-tube capable of holding a small amount of anti-entraiment mesh. With this initial arrangement, the evaporator was tested evaporating de-ionized water at 64 mm Hg (–27.4 in. Hg) and a nominal 40°C evaporator liquid temperature. In approximately 1.25 hours of steady state operation, approximately 39 mL of condensate formed in the traps of the Teflon® vacuum pump, translating to approximately 2.3 L of condensate in 73.5 hours. This was a potential problem for continuous operation as the pump traps can only hold about 1 L of condensate before pump operations would be forced to stop.

Assuming the pump trap condensates were due to entrainment, a calculation using the Souders-Brown expression[9] was done showing that experimental evaporator vapor head velocities were likely below the calculated typical maximum allowable vapor velocity (3.6 m/s), suggesting the vapor headspace in the experimental system may be small. Anti-entrainment using a stainless steel knitted mesh-packed inverted U-tube between the evaporator and condensate tank was chosen to counteract this possible effect. As anti-entrainment mesh performance improves with increasing vapor velocity, an attempt was made to match the expected upward vapor velocity in the evaporator vapor head in the preliminary Hanford RPP-WTP design to that in the inverted U-tube of the bench-scale apparatus. Preliminary RPP-WTP design specifications of 4.52 m^3/hr liquid condensate production from a 4.11 m (13.5 ft) diameter evaporator supplied by Washer[10] suggested that for an equivalent quantity of steam generated at 40°C and 50 mm Hg would create an upward vapor velocity of 2.04 m/s or 6.7 ft/s (air in-leakage rate was negligible) entering an anti-entrainment mesh screen mounted in a full-scale evaporator vapor headspace. This upward vapor velocity is sufficient for 99+% vapor-liquid separator efficiency for a knitted mesh

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[9] Standiford, F. C., "Evaporation", Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed., Vol. 16, J. Wiley and Sons, Inc., New York, 1995.

[10] Washer, M., electronic mail communication, BNFL, Inc., Richland, WA, March 9, 2000.

separator (1.42 m/s or 5 ft/s minimum[11]). A calculational error and structurally viable U-tube diameters led to the selection of a 11 mm ID U-tube, packed with approximately 15 cm vertical height of rolled knitted stainless steel mesh. For a gas stream that produces 3 mL/min liquid condensate and a saturated air stream at 40°C at 60 mm Hg based on 11.5 mL (STP) air in-leakage rate, corrected calculations show the vapor velocity entering the knitted stainless-steel anti-entrainment mesh was approximately 9.75 m/s (32 ft/s), more than sufficient to de-entrain the evaporator vapor stream. A subsequent de-ionized water evaporation test with the packed 11 mm ID U-tube and an uncooled impinger (equipped with an internal thermometer) between the evaporator condensate tank and the vacuum pump produced 5.2 g condensate in the impinger and no liquids in the pump trap after 1.5 hours steady state operation at 60 mm Hg (–27.6 in Hg) and 48°C nominal evaporator temperature. This amount was within 10% of the calculated quantity of water expected to condense from a 40°C water-saturated air stream after being cooled to the ambient room temperature (28.5°C, measured), and was consistent with ~255 mL pump trap liquid generation per 73.5 hours steady state operation.

3.5 AN-107 Envelope C Simulant History

The Hanford Tank AN-107 simulant used for this work is a product of the pilot-scale filtration study by Duignan[12] for concentration precipitated Envelope C waste. At SRTC's Thermal Fluids Laboratory, approximately 100 gallons of Envelope C simulant (107-AN) were synthesized using the recipe in Appendix A, including entrained solids at 0.5 wt% loading. This simulant was a non-toxic version that excluded addition of sodium chromate and lead nitrate. For Sr/TRU removal, the Hanford waste was diluted to 6 M Na before increasing free hydroxide concentration by 0.8 M with 19 M NaOH, strontium concentration by 0.075 M using 1 M $Sr(NO_3)_2$, and manganese concentration by 0.05 M with 1 M $NaMnO_4$ (recipe also in Appendix A). This precipitated AN-107 Envelope C simulant was then cross-flow filtered, producing a filtrate with a measured density of 1.276 g/mL and analyte concentrations summarized in Tables 12 and 13. Dark solids produced by post-filtration precipitation were observed when the filtrate was transferred from the Thermal Fluids Laboratory drum. As much as possible through settling, the observed dark solids were not introduced into the evaporator to minimize potential line pluggage.

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[11] Minton, P. E., Handbook of Evaporation Technology, pp. 153-7, Noyes Publications, Park Ridge, NJ, 1986.

[12] Duignan, M. R., "Final Report: Pilot-scale Cross-flow Ultrafiltration Test Using a Hanford Site Tank 241-AN-107 Waste Simulant – Envelope C + Entrained Solids + Strontium-Transuranic Precipitation," Savannah River Technology Center, BNF-003-98-0226, March 24, *2000*.

3.6 Target Organic Compound Selection

Of the original 20 organic Indicator Chemicals[13] listed in RPP-WTP's Screening Level Risk Assessment[14], SRTC recommended and the customer accepted removal of acrylonitrile, 1-chloroethene, 1,1-dichloroethene and dichloromethyl ether due to rapid chemical breakdown in caustic Hanford RPP waste or off-gas sampling/analysis capability issues. Experimental toxicity hazard concerns led to the selection of bis(2-ethylhexyl)phthalate (BEHP), a 2,3,7,8-TCDD toxicity equivalent, as the indicator for both PCB and dioxin/furan chemical groups based on thermal stability and vapor pressure criteria. Ultimately, the following 14 target organic compounds (Table 1) were selected to be representative compounds for volatile and semi-volatile organics and pesticides suspected to be present in Hanford RPP wastes:

Chemical	Formula	Molecular Weight	Chemical Group
Benzene	C_6H_6	78.11	Volatile Organic
Toluene	C_7H_8	92.13	Volatile Organic
4-methyl-2-pentanone (MIBK)	$C_6H_{12}O$	100.16	Volatile Organic
Chlorobenzene	C_6H_5Cl	112.56	Volatile Organic
1,2,3-trichloropropane	$C_3H_5Cl_3$	147.43	Volatile Organic
1,2-dibromoethane	$C_2H_4Br_2$	187.88	Volatile Organic
1,2,4-trichlorobenzene	$C_6H_3Cl_3$	181.46	Light Semi-volatile Organic
Naphthalene	$C_{10}H_8$	128.16	Light Semi-volatile Organic
Pyrene	$C_{16}H_{10}$	202.24	Semi-volatile Organic
Benzo(a)pyrene (BaP)	$C_{20}H12$	252.32	Semi-volatile Organic
Pentachlorophenol	C_6Cl_5OH	266.35	Semi-volatile Organic
Hexachlorobenzene	C_6Cl_6	284.8	Semi-volatile Organic
Bis(2-ethylhexyl)phthalate (BEHP)	$C_{24}H_{38}O_4$	390.54	PCB/Dioxin/Furan Equivalent (Semi-volatile)
Aldrin	$C_{12}H_8Cl_6$	364.93	Pesticide (Semi-volatile Organic)

Table 1. 14 Target Organic Compounds Spiked Into the Envelope C (AN-107) Simulant

3.7 Spike Solution/Evaporator Feed System Development

To feed the 14 target organic compounds with the AN-107 Envelope C simulant into an evaporator, two issues had to be overcome: 1) a method to "spike" or add the organics into the aqueous caustic solution, and 2) a storage and feeding mechanism to minimize volatile organic losses to headspace during the estimated 73.5 hour evaporator run. In addition, a realistic and practical target organic concentration also had to be determined. Based on the development descibed below, spiked feed solutions were made by injecting 1.3 mL of 1000 mg/L concentration (each target organic compound) spiking solution into pre-prepared Tedlar® (polyvinylfluoride, PVF) bags containing 1 L by mass (1262 g) Hanford RPP AN-107 Envelope C-simulant on the day prior to use in the evaporator run the following day. The spiked bags were

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[13] Johnson, M. E., "TWRS Privatization Contract No. DE-AC06-96RL13308 – Low Activity Waste Evaporator Modeling and Simulant Solution Evaporation", BNFL Letter No. 002709, BNFL Inc., 4/29/99

[14] Edwards, D. W., "Draft Work Plan for Screening Level Risk Assessment for the TWRS-P Facility", BNFL, Inc., RPT-W375-EN00001, Rev. C, May 7, 1999,

stored in a covered secondary container at ambient conditions on a benchtop until use, with every attempt made to use them within the 24-32 hour aging period. The bag of C-simulant with target organics was laid covered with dark cloth flat on the benchtop in the laboratory hood, and the contents were withdrawn by connecting Viton® Masterflex® tubing to the bag hose valve and controlling the withdrawal volumetric flowrate with the pump.

As the customer requested similar mass concentrations (ppm level) for each compound, solubility reference data indicated the need for a solvent as the 14 components could not be dissolved within each other to be directly introduced into the simulated Hanford waste. Joint work with Supelco, Inc. was performed to develop a 70% hexane/30% acetone mixture containing 1000 mg/L of each target organic compound. However discussions with BWXT Services, Inc. (of BWX Technologies, Inc.) indicated that large quantities of hexane would interfere with the volatiles analysis due to similar elution times to the target compounds. Other possibilities were considered weighing the following factors:

i) Maximize gas sample volumes for the target volatile organic compounds while minimizing total run time. This necessitated the need to produce one spiked C-simulant to allow regulatory liquid pesticide samples to be generated during volatiles gas sampling and intermittent volatiles liquid sampling. Semi-volatiles gas and liquid sampling would occur simultaneously afterward.

ii) Minimize solvent addition to the C-simulant. As the 14 target compounds were not expected to produce a single liquid sample without the use of a solvent, alternative solvents with high solubilities for all 14 target organics were few. Other solvents such as methanol, long-chain aliphatic alcohols and Tetraglyme® were considered but were eliminated due to solubility low limits or objectives i and iii.

iii) Avoid solvent interferences to the gas sample analyses. Long-chain alcohols and Tetraglyme® were thought to possibly allow for dissolution of all 14 target organic compounds, but were also expected to cause signal interference with the quantification of other target semi-volatiles.

iv) Avoid separate runs for volatiles and semi-volatiles/pesticide. This was not thought to be representative of actual RPP-WTP liquid wastes which would be encountered in the field. The required workload in order to develop and test two separate spiking solutions would double, and then run both for the requisite gas sampling times would conflict with objective i.

Ultimately, acetone was selected as the solvent through which to add the 14 target volatiles, semi-volatiles and pesticide organic compounds. The primary advantage of acetone was the high expected solubility of the resulting enolate formed in caustic solutions. BWXT Services, Inc. did express concern about detector overload and acetone contamination of their analytical equipment. However shutdown of the detector was determined to be the method to avoid detector overload.

With an SRTC Analytical Development Section (ADS) gas chromatograph connected to a purge and trap system, Young[15] showed that acetone contamination levels can be reduced to 15 μg/L acetone by subsequently running only 5 water blanks after initially injecting an aqueous solution containing 800,000 μg/L acetone. Young also felt that the Tekmar systems employed by BWXT Services, Inc. should purge acetone better than the SRTC ADS system. In the event that a long series of water blanks would not purge the BWXT equipment, a provision was made for analytical equipment refurbishing.

After determining the spiking solvent, testing of organic solubility in the C-simulant began. Based on dye experiments by Dworjanyn[16] examining the presence of benzene droplets in tetraphenylborate-treated SRS tank waste, a similar study was performed by adding 1 wt% Sudan Red 7B dissolved in acetone into the Hanford RPP simulant. 1.25 mL of the dye solution was added to 1 L simulant, a quantity of solution equivalent to spiking to 1 ppm using 1000 mg/L in acetone. The resulting solution of uniform color strongly indicated that the spiking solution containing 1000 mg/L of the 14 target organic compounds in acetone would be a viable method to introduce the chemicals of interest into the AN-107 Envelope C simulant.

Subsequently, batch spiking tests using acetone spike solutions were performed to target levels of 0.6, 1.0, and 3 ppm to find a predictable and consistent concentration for the target compounds. 0.8, 1.3, and 3.8 mL, respectively, were added to 1 L simulant in a 2 L Teflon® beaker for each test, and mixing was accomplished using a 2 3/8” OD Teflon® four-blade pitched-blade turbine mounted on a Lightnin LabMaster mixer set at 400 rpm. Mixing was done for 3 ½ minutes, except one 4 ¼ minute test, compared to a 3 second theoretical mixing time for three volume turnovers. Zero headspace samples were taken immediately after mixing for SRTC analysis (Table 2). The 1 ppm target levels were found experimentally to be readily generated with produced concentrations matching calculated/expected concentrations best, in comparison to batch-mixing tests also performed at 0.62 and 3.01 ppm target compound concentrations. The target concentration of 1 ppm was selected also as it was expected to represent regulated target organic compound concentrations encountered in actual Hanford Tank AN-107 liquid waste.

Target Compound	0.63 ppm target		1.03 ppm target		3.01 ppm target	
	Conc. (ppm)	Recovery (%)	Conc. (ppm)	Recovery (%)	Conc. (ppm)	Recovery (%)
benzene	0.301	48	0.533	52	***4.730***	157
4-methyl-2-pentanone (MIBK)	0.256	41	0.591	57	***3.653***	121
toluene	0.320	51	0.563	55	1.890	63
1,2-dibromoethane	***<0.04***	<6	***0.017***	2	***0.014***	0
chlorobenzene	0.311	49	0.537	52	1.987	66
1,2,3-trichloropropane	***0.079***	13	***0.095***	9	***0.117***	4
1,2,4-trichlorobenzene	0.135	21	0.515	50	1.983	66
hexachlorobenzene	0.397	63	0.777	75	2.617	87
naphthalene	0.127	20	0.508	49	1.903	63
aldrin	0.397	63	0.769	75	2.617	87
pyrene	0.428	68	0.793	77	2.696	90
bis(2-ethylhexyl)phthalate (BEHP)	***0.658***	104	***1.110***	108	***3.093***	103
benzo(a)pyrene (BaP)	0.420	67	0.872	85	2.934	97
pentachlorophenol	***<0.2 ppm***	<32	***<0.2 ppm***	<19	***<0.2 ppm***	<7

Table 2. Spiking Level Test Results: Target Organic Compound Concentrations in Envelope C (AN-107) Simulant

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[15] Young, J. E., unpublished results, March, 2000.

[16] Dworjanyn, L. O., “Benzene Release – Status Report”, WSRC-RP-97-903, Rev. 0, November 4, 1997.

Numbers that are italicized bold in Table 2 are deviations far from the expected. A literature review shows that the low levels of 1,2-dibromoethane and 1,2,3-trichloropropane (halogenated aliphatics) are likely due to hydrolysis with the caustic in the simulant, as indicated by a 16 day half-life for 1,2-dibromo-3-chloropropane at significantly milder conditions (pH=10 compared to pH=~13 of this simulant)[17]. Slightly low aldrin levels may also be due to slow hydrolysis[18]. Bis(2-ethylhexyl)phthalate losses were expected by saponification[19], but any loss appears to have been more than offset by leaching from the plastic pipettes used to extract the samples from the Teflon® beaker. Leaching is expected since bis(2-ethylhexyl)phthalate is used as an softening additive in plastics. Low pentachlorophenol concentrations are probably due to the loss of the phenolic hydrogen in the caustic solution, which would not permit liquid-liquid extraction into the organic methylene chloride phase used in the SRTC analytical method.

A related issue was the loss of analytes onto Viton® tubing mounted in the Masterflex® pumps used to feed material and remove concentrate. For the experiment, the target 1 ppm solution produced in the previous experiment was used after aging 10 days and storage in a polyethylene bottle with of order 50-100 mL headspace above the solution. A zero-headspace sample was taken before pumping three-fourths of the bottle contents into another 1 L polyethylene bottle at 10 mL/min, the projected feed flow rate, through approximately 3 feet (~1 m) of #16 Viton® Masterflex® hose. A second zero-headspace sample was taken by pipette immediately after pumping was stopped. The results (Table 3) indicate that large masses of volatiles were not lost, with the larger percentage losses for 1,2-dibromoethane, 1,2,3-trichloropropane, and chlorobenzene due to low initial concentrations. Semi-volatile mass losses were significant but relatively low at 17-25% in comparison to the SRTC analysis quoted 10% error. In the actual steady-state experiment, overall analyte losses were expected to be lower than in Table 3 since about half of the length of Viton tubing would be used, and sorption sites on the tubing would likely be occupied relatively early in the long run.

Target Compound	Before (ppm)	After (ppm)	Change (ppm)	% Loss
Benzene	0.068	0.054	0.014	21.3
4-Methyl-2-Pentanone (MIBK)	0.716	0.628	0.088	12.2
Toluene	0.014	0.013	0.001	7.0
1,2-dibromoethane	0.013	0.000	0.013	100.0
Chlorobenzene	0.019	0.013	0.006	32.8
1,2,3-trichloropropane	0.020	0.004	0.016	78.0
1,2,4-trichlorobenzene	0.000	0.000		
hexachlorobenzene	0.698	0.539	0.159	22.7
naphthalene	0.000	0.000		
aldrin	0.698	0.539	0.159	22.7
pyrene	0.650	0.492	0.158	24.4
bis(2-ethylhexyl)phthalate (BEHP)	1.348	1.110	0.238	17.6
benzo(a)pyrene (BaP)	0.785	0.571	0.214	27.3
pentachlorophenol	0.000	0.000		

Table 3. Target Organic Compound Concentrations in Envelope C (AN-107) Simulant before and after pumping through ~1 m Viton® tubing at 10 mL/min

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[17] Milano, J.C., Guibourg, A., Vernet, J.L., *Wat. Res.*, **22**, 1553, *1988*.
[18] Schuphan, I., Sajko, B., Ballschmiter, K.Z., *Naturforsch. B.*, **27**, 147, *1972*.
[19] Wolf, N.L., Steen, W.C., Burns, L.A., *Chemosphere*, **9**, 403, *1980*.

The last major issue was to find a preparation and storage method yielding stable concentrations of analytes. Using the 1 ppm target solution in the batch mixing and viton-tubing losses experiments, typical volatilization rates potentially encountered during the experiment and from actual waste in Hanford RPP tanks could be gauged. Again, headspace was of order 50-100 mL above the 1 L solution for the first 10 days, and was considered the "best case" scenario should continuous pumping of spiked batches of bottled feed be used. For the following twenty days, headspace increased to approximately 300-400 mL as only about 3/4 of the test solution was transferred in the Viton tubing loss study. The data in the last column of Table 4 was also corrected for mass losses to tubing during the Viton tubing test discussed above.

Target Compound	Concentrations (ppb)		
	Initial	10 days	30 days*
benzene	533	68	0
4-methyl-2-pentanone (MIBK)	591	716	0
toluene	563	14	0
1,2-dibromoethane	17	13	0
chlorobenzene	537	19	0
1,2,3-trichloropropane	95	20	0
1,2,4-trichlorobenzene	515	0	1
hexachlorobenzene	777	698	791
naphthalene	508	0	2
aldrin	769	698	795
pyrene	793	650	662
bis(2-ethylhexyl)phthalate (BEHP)	1110	1348	1887
benzo(a)pyrene (BaP)	872	785	1197
pentachlorophenol	0	0	0

* adjusted for Viton tubing losses at 10 days, and bottle only 3/4 full from 10-30 days

Table 4. Batch Storage Test Results: Target Organic Compound Concentrations in Envelope C (AN-107) Simulant from 0 to 30 days

The data (Table 4) shows that volatiles except 4-methyl-2-pentanone and the lighter semi-volatiles (naphthalene, 1,2,4-trichlorobenzene) are lost quickly, while semi-volatile concentrations generally remain unchanged. This trend is also expected in actual Hanford tank waste. Hence, a spiking and storage system without headspace was desirable for the experiment.

In-line mixing was thought to be a promising approach to avoid both headspace and storage of spiked feed solution before entry into the evaporator. Unspiked feed simulant exiting from a Masterflex pump contacting spiking solution fed from a syringe pump before entering an in-line static tube mixer and the evaporator feed line was the tested concept. A syringe pump was desired to eliminate volatiles loss from the spiking solution to headspace under vacuum conditions. During calibration of the syringe pump against a –27.6 in Hg vacuum, the Teflon® seal on the barrel of the Hamilton Gastight® syringe was not able to prevent ambient air from leaking in at a rate below 12.1 μL/min, the maximum spiking solution rate for 1 ppm loading at ~10 mL/min simulant feed rates. The 20 mL syringe pump of a TOA Electronics Ltd. Auto-Buret® (Model ABT-511) automatic dispenser was also tested against vacuum with the same result. Since the syringe barrel seals appear to work best against pressure, the in-line mixing method of spiking organics into the feed solution prior to injection into the evaporator was abandoned.

SRTC proposed and tested the use of 1 L Tedlar® bags, used for collection of EPA Method 1311 Toxicity Characteristic Leaching Procedure (TCLP) volatile extracts, as a means to store variable quantities of spiked feed material with almost zero-headspace. In the initial aging study, 1 L simulant by mass (1262 g) and 1.3 mL 1000 mg/L spiking solution were mixed using a Teflon® beaker and impeller, before being pumped into the Tedlar® bag by a Masterflex® pump using Viton® tubing. The Tedlar® bag was stored at ambient temperature on the benchtop, and zero-headspace samples withdrawn periodically by draining bags via the bag hose valve into teflon-lined cap glass sample vials. Sample analyses (Table 5) showed relatively uniform losses, suggesting there may be sorption losses to the bag interior surface, chemical degradation, or photolytic degradation. For the retention calculation, the bolded 7-day concentrations were replaced by the 3-day concentrations since the bolded values far exceeded the downward trend observed in the first 3 days of aging.

	Actual Detected Concentrations (ppb)					% Initial retained
Target Compound	Initial*	1 Day	2 Day	3 Day	7 Day	
benzene	212	**290**	172	196	161	76.3
4-methyl-2-pentanone (MIBK)	439	**556**	313	361	263	59.8
toluene	447	**784**	384	376	212	47.4
1,2-dibromoethane	0	**251**	0	0	0	
chlorobenzene	431	**768**	345	313	172	40.0
1,2,3-trichloropropane	0	0	0	0	0	
1,2,4-trichlorobenzene	234	257	176	109	102	43.6
hexachlorobenzene	746	583	562	*428*	**722**	*57.4*
naphthalene	192	**291**	178	124	89	46.5
aldrin	777	610	583	433	**679**	*55.7*
pyrene	861	697	583	460	**700**	*53.4*
bis(2-ethylhexyl)phthalate (BEHP)	**1619**	1328	1223	1127	**1530**	
benzo(a)pyrene (BaP)	904	766	674	566	**896**	*62.6*
pentachlorophenol	0	0	0	0	0	
*Low due to losses during transfer to bag **Questionably high values**						

Table 5. Tedlar Bag Aging Test Initial Results: Target Organic Compound Concentrations in Envelope C (AN-107) Simulant from storage up to 1 week (organics pre-mixed into solution in a separate container prior to being pumped into the Tedlar bag)

To determine the mechanism for analyte loss, the aging experiment was repeated for a period of three days where the spiked sample bag was protected from light by storage in a box on the laboratory benchtop. Additionally to maximize target organic compound concentrations, the solution was prepared by pumping in nearly 1 L by mass (1239 g) AN-107 simulant and injecting 1.3 mL spiking solution directly into the bag via the septum-lined syringe port. Compared to the initial test results in Table 5, Figures 3 and 4 show that the more volatile organic compound concentrations and percentage of initial retained are improved after 72 hours in all cases except toluene, and that volatiles concentrations are temperature dependent as shown by the significant drop after 32 hours when the laboratory warmed from ~22°C to 30°C. Hence, chemical degradation of the volatile target organic compounds appears to be the dominating factor for losses observed. Besides bis(2-ethylhexyl)phthalate (DEHP) concentrations being higher than theoretical likely due to extraction from the Tedlar® bag, the semi-volatiles concentrations (Figure 5) appear essentially constant over the experimental period despite significant scatter in the data, suggesting that semi-volatile photolytic degradation was the significant factor in the first experiment. Error bars in Figures 3-5 are standard deviations (one sigma) calculated from

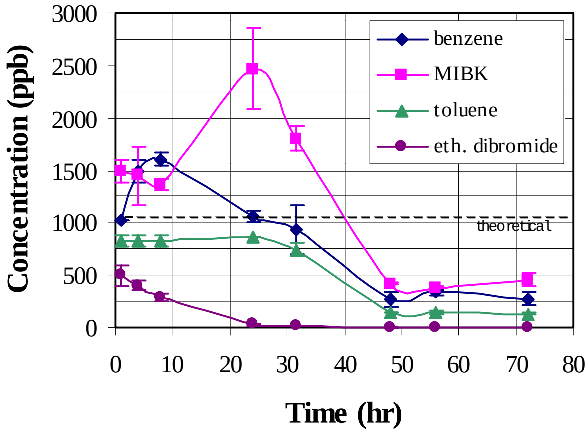

Figure 3. Tedlar Bag Aging Test Results: Volatile Organic Compound Concentrations vs. Time, stored at ambient conditions in box. (Organics spiked and mixed in pre-filled Tedlar bag)

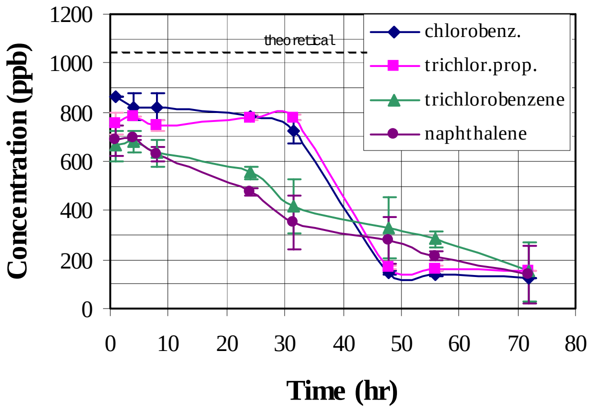

Figure 4. Tedlar Bag Aging Test Results: Volatile and Light Semi-volatile Organic Compound Concentrations vs. Time, stored at ambient conditions in box. (Organics spiked and mixed in pre-filled Tedlar bag)

analysis of duplicate samples, and higher than theoretical values are thought to be due to signal interferences.

Based on Figures 3-5, an aging period of 24-32 hours for a 1 L bag of simulant after spiking with 1.3 mL of spiking solution was selected as most of the compounds are largely retained in the C-simulant for up to 32 hours (relative changes of less than approximately 15%). Notable exceptions are 1,2-dibromoethane which mostly degrades to a low asymptotic value after 24 hours, and 1,2,3-trichloropropane and naphthalene which statistically may be equivalent at 24 and 32 hours aging time. Table 6, drawn from data in Figures 3-5, lists the concentrations at initial (1 hour aging to allow sufficient diffusion of spiking solution) and at 24-32 hours aging.

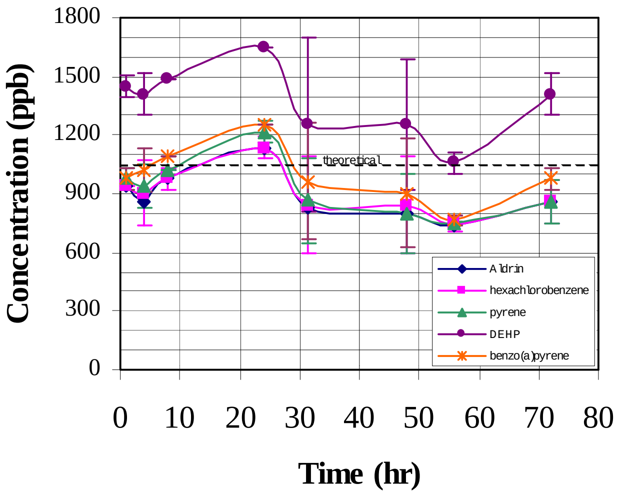

Figure 5. Tedlar Bag Aging Test Results: Semi-volatile Organic Compound Concentrations vs. Time, stored at ambient conditions in box. (Organics spiked and mixed in pre-filled Tedlar bag)

Based on this analysis, spiked feed solutions were made by injecting 1.3 mL of 1000 mg/L concentration (each target organic compound) spiking solution into pre-prepared Tedlar® bags containing 1 L by mass (1267 – 1287 g) Hanford RPP AN-107 Envelope C-simulant on the day prior to use in the evaporator run the following day. The spiked bags were stored in a covered secondary container at ambient conditions on a benchtop until use, with every attempt made to use them within the 24-32 hour aging period. The bag of C-simulant with target organics was laid covered with dark cloth flat on the benchtop in the laboratory hood, and the contents were withdrawn by connecting size 14 Viton® Masterflex® tubing to the bag hose valve and controlling the withdrawal volumetric flowrate with the pump.

Target Compound	Concentration (ppm)	
	After 1 hr.	After 24-32 hrs.
benzene	1.019	0.933-1.058
4-methyl-2-pentanone (MIBK)	1.489	1.803-2.469
toluene	0.823	0.741-0.862
1,2-dibromoethane	0.502	0.016-0.029
chlorobenzene	0.862	0.721-0.784
1,2,3-trichloropropane	0.752	0.776
1,2,4-trichlorobenzene	0.662	0.415-0.553
hexachlorobenzene	0.940	0.842-1.136
naphthalene	0.686	0.353-0.474
aldrin	0.940	0.831-1.136
pyrene	0.980	0.866-1.215
bis(2-ethylhexyl)phthalate (BEHP)	***1.450***	***1.254-1.646***
benzo(a)pyrene (BaP)	0.980	0.964-1.2544
pentachlorophenol	<0.2 ppm	<0.2 ppm

Table 6. Tedlar Bag Aging Test Results: Target Organic Compound Concentrations in Envelope C (AN-107) Simulant from 1 hour and 24-32 hours after spiking. Solution storage in box at ambient (~22°C) to 32 hours. (Organics spiked and mixed in pre-filled Tedlar bag)

Overall, the average aging times from spiking to the beginning and the end of bag use were 29.28 and 31.15 hours, respectively. Due to an unexpected delay at the start of operations, the first 10 bags for steady state operation did age significantly longer, 37-51 hours until start of use, but were refrigerated overnight and allowed to slowly warm to room temperature to mitigate the effects of the added aging. Analytical data of these feed samples shows no significant losses of the target organic compounds due to the additional aging and refrigeration. If these refrigerated samples are removed from the analysis, the average aging times from spiking to the beginning and end of bag use were reduced to 24.76 and 26.4 hours, respectively. Given that average aging times were within the specified 24-32 hour aging period, no significant deviations due to aging were expected or found.

The aging studies discussed above show that the SRTC analyses for these 14 volatile and semi-volatile organic species are generally consistent and reproducible to the cited 10% analytical random error, with a few potential considerations. Bis(ethylhexyl)phthalate concentrations will generally tend to be high due to extraction from the Tedlar® bag or polyethylene bottle. Similarly, 4-methyl-2-pentanone concentrations may possibly be affected due to its use as a solvent for applying protective films. Lastly, the results in Figure 5 indicate that the SRTC semi-volatile results can sometimes result in systematically high values for all species, likely due to organic solvent evaporation after liquid-liquid extraction of the target compounds prior to analysis.

3.8 SW-846 Method Parameter Selection/Exceptions

The customer requested that duplicate liquid samples be taken in all cases where possible. The EPA SW-846 Methods call for a 40 mL zero-headspace liquid sample for each volatiles analysis, and 3 x 1L samples each for liquid sample semi-volatiles and pesticide analysis (1 L each for sample, method spike, and method spike duplicate). Hence, regulatory analysis required for each the evaporator feed, condensate, and concentrate samples the following volumes in Table 7:

Organic Analysis Type	Sample Volume
Volatiles (VOA)	2 x 40 mL
Semi-volatiles (SVOA)	6 x 1 L
Pesticide	6 x 1 L

Table 7. Regulatory Analysis Liquid Sample Volumes per the EPA SW-846 Methods

All regulatory liquid samples and associated blanks were collected, stored, and shipped "as-is" in I-Chem® Certified Series 300 environmental sample amber glass bottles or clear vials that were laboratory-certified to meet US EPA analyte specifications. The only possible exceptions were a few volatiles analysis liquid samples whose volumes were insufficient due to the uncertainty in generation, such as pump trap liquids and off-gas sampler condensates, where samples were "topped off" with reagent water to create zero-headspace samples. In these cases, pre- and post-dilution masses were recorded, and the resulting higher detection limits from the analytical laboratory (BWXT Services, Inc.) were accepted.

Reagent blanks and trip blanks were poured in a separate "clean" laboratory to minimize effects of laboratory contamination, while field blanks were poured in the laboratory where the evaporator and off-gas sampling system were set up. All blank volumes were matched to required sample volumes (1 L for semi-volatiles and pesticide analysis, 40 mL for volatiles analysis), except a few cases where blank volumes were larger than regulatory sample volumes due to less than expected sample volumes. The water and 50% v/v methylene choride/methanol reagent blanks were samples of freshly prepared material taken just prior to experimentation. Trip blanks were only required for volatiles analysis, and water was chosen as the representative material since water was less likely to pick up material from the sample container (covered by field blank).

1 M NaOH solution was chosen as the field blank solution to represent the feed and concentrate samples since caustic and neutral solutions air contamination behavior could possibly be different, and caustic solution is more likely to leach any contamination from the sample containers. The 1 M concentration was chosen to represent the 0.56 M free OH^- and 1.41 M total OH^- concentrations found from duplicate feed analyses. The concentrate hydroxide concentrations were expected to be roughly 20-30% higher than the feed concentrations. 1 M NaOH solution was also used for the condensate sample field blanks as a "worst case", with the high alkalinity more likely to extract contaminants than a neutral pH solution, to minimize blank volume shipped. Feed field blanks were collected at the beginning of each off-gas sampling run again as a "worst case" just in case there was any air contact before introduction into the evaporator. Feed solution air contact was considered highly unlikely since the feed solution was

being fed directly from a Tedlar bag through hosing directly to the evaporator inlet without intentional exposure to ambient air. By contrast, concentrate samples were collected continuously and condensate samples semi-continuously into open narrow-neck bottles, and hence field blanks were taken in parallel to the extent possible to adequately capture any day-to-day atmospheric contamination variations.

AN-107 C-simulant spiked with acetone at a level comparable to that in the actual feed was selected to incorporate effects of any leaching of organic and inorganic components from the evaporator during the regulatory analysis run. Since caustic solutions were again thought to more likely leach components from the evaporator system, contact of the process blank liquid with only the evaporator tank was believed to be adequate. Hence, liquid process blanks were taken by simply filling the evaporator tank with acetone-spiked simulant at –27.6 in Hg and pumping the solution out through the concentrate line into the appropriate sample containers.

Single volatile and semi-volatile/pesticide off-gas samples were taken since SW-846 Method gas sample volume requirements were anticipated to be difficult to meet, as mentioned previously. Since a vacuum pump bleed air flow rate of ~400 mL/min was expected to enter the off-gas sampler with the 11.5 mL/min natural and set air in-leakage, a decision was made to collect 20 L of combined air in-leakage/bleed air as the process blank, and any detectable quantities of target analytes to be scaled by off-gas sample volume. To be representative of an actual evaporator run, the process blank off-gas sample was taken with an empty evaporator at –27.6 in Hg vacuum pressure. The volatile and semi-volatile/pesticide off-gas process blanks were taken before any other liquid such as the process blank liquids was introduced to the system to minimize potential contamination of the off-gas sampling sorbent tubes. Prior to assembly, the evaporator glassware was washed with dishwashing detergent and hot water, and dried. Subsequently, the evaporator interior was further cleaned through evaporator testing using de-ionized water and unspiked Envelope C simulant, before being drained for the regulatory run. The off-gas sampling glassware was cleaned and dried per the stricter EPA SW-846 Method 0010 for semi-volatiles.

Off-gas sample field blanks were taken according to their related EPA SW-846 Methods, Method 0031 and 0010, through pre-sampling leak checks. Method 0031 volatiles trip blanks were prepared by simply packaging for shipment stored tubes as received from the Southwest Research Institute (SWRI). As BWXT Services, Inc. did not have the sorbent tube conditioning capabilities, SWRI was asked to prepare and condition Tenax, Anasorb, and XAD-2 tubes used for this experiment. The sorbent tubes used in the off-gas sampling and as blanks were all employed within 14 days of conditioning.

All filled liquid samples and spent sorbent tubes were immediately sealed and stored in a 4°C refrigerator to cool before being packaged and shipped for analysis at BWXT Services, Inc. Tenax, Anasorb, and XAD-2 sorbent tubes sealed with endcaps were individually bagged, sealed with a signed custody seal, bagged again in batches, and shipped in coolers containing ice separate from the liquid samples. Liquid samples were sealed with a signed custody seal, individually bagged, and placed in 2 gallon cylindrical coolers separated by “bubble wrap” before ice was added. These 2 gallon coolers were then packaged in 10 gallon drums lined with shock absorbent material, before shipment. All samples were shipped from SRTC to BWXT Services, Inc. by Federal Express overnight delivery.

Method 0031, "Sampling Method for Volatile Organic Compounds (SMVOC)", is applicable to volatile organic compounds that have a boiling point between -15°C and 121°C. Method 0031 is generally not applicable to polar water-soluble and reactive volatile organic compounds, and requires support of laboratory data to demonstrate sampling and analysis method efficiencies for application to volatile organic compounds with boiling points less than 0°C. The method is applicable to the determination of volatile organic compounds in the gaseous effluent of stationary sources with an upper concentration limit of 1.5 parts per million (ppm), and is designed to be operated between 0.25 and 1 L/min. In a typical measurement application on a stationary source effluent, the traps are typically replaced every 20 min at an operating rate of 1 L/min, and, every 40 min at 0.5 L/min. In the application of Method 0031 in this regulatory study, the entire off-gas stream (approximately 0.4 L/min) was directed through the sampling module from a vacuum pump that had condensate beakers to remove some of the liquid that could condense within the vacuum pump and harm it. The liquid condensed upstream of the sampling module was collected and analyzed. Based on the anticipated mass loading of volatile organics on the traps, it was judged that the total volume of gas sample could be extended beyond the 20 L of a typical effluent measurement. It was also judged that Method 0031 was the best single method to quantify the wide range of volatile organics specified in this investigation.

Method 0010, "Modified Method 5 Sampling Train", is applicable to the determination of semivolatile (boiling point >100°C) Principal Organic Hazardous Organic Compounds (POHCs) from incineration systems. The gas sampling rate is typically 0.5-1.0 dry standard cubic feet per minute (dscfm) or 14-28 L/min, to collect a minimum 3 dry standard cubic meters (dscm) or 105.9 dscf. In the application of Method 0010 in this regulatory study, the lower flow rate of the entire off-gas stream (approximately 0.4 L/min) was thought to not affect sampling efficiency, and the XAD-2 sorbent trap was sized identical to the sorbent traps used to perform Method 0031 based on the total material expected to be captured during semi-volatiles/pesticide off-gas sampling. As the volume of gas to be sampled (of order 950 L) was less than the minimum specified sampling volume, sampling duration was again extended beyond that of a typical effluent measurement from a stationary emission source.

For the regulatory analyses, one major deviation widening the acceptable analyte recoveries to 20-130% was accepted and approved by the customer[20], based on input from BWXT Services, Inc. on expected low recoveries of certain species in the target list of compounds.

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[20] Ferrara, D., Groseclose, R., Ray, R., Crawford, C., Calloway, T. B.," Task Technical, Analytical Study, and Quality Assurance Plan in Support of BNFL Part B - "'Regulatory' Sample Analyses from A, B, C, and LC Studies at SRTC", BNF-003-98-0082, January, *1999*.

4.0 Results and Discussion

4.1 Initial Endpoint Determination

To determine the saturation point for the C-simulant spiked with the 14 target volatiles, semi-volatiles, and pesticide, an OLI model was formulated by Choi[21]. Inconsistencies between the C-simulant analytical data led to conflicts such as in balancing excess anions, and in resolving predicted initial solution density to total solids. Of particular concern was an analytically high fluoride concentration that could rapidly lead to formation of a sodium phosphate-fluoride double salt in the simulated waste. After repeating several analyses and using theoretical calculations to correct some analytical results, the "best" model inputs were determined to be 1.276 g/mL density (matches analytical data), 5.8 M Na (vs. 5.5 M Na by AA and ICP-ES), and 31 wt.% total solids (vs. 32.5 wt.% by oven method, 35% by microwave method).

Based on these "best" model inputs, a saturation point of over 11 M Na, 52.2 wt.% total solids, and 1.51 g/mL density was predicted. Trace quantities of precipitated sodium oxalate was also predicted. As this final sodium concentration was viewed to be high, 5.5 M Na C-simulant was boiled down in the laboratory where samples were taken after calculated concentration to 8.7 M Na, 9.4 M Na, and 10.3 M Na. After these concentrated C-simulant samples were cooled, white solids were observed in the first two samples and the last sample was mostly precipitated salt. As the original 5.5 M Na C-simulant was also opaque with white solids (approximately 0.8 wt.%), visual determination of the endpoint through back-addition of produced condensate to the concentrated samples generated was impossible. As the operation of the evaporator was thought to be unaffected by the suspended solids in the simulant up to 10 M Na and due to the undetermined end-point, concentrating to the current Hanford RPP-WTP design flowsheet specification of 8.0 M Na was determined as the best basis.

By assuming 80% saturation (25°C) at 8 M Na, the evaporator feed will be concentrated from 32.5 to 41.9 wt.% solids as determined experimentally by back-addition of condensate to the 9.4 M Na sample produced during the boildown study. Choi's OLI model[22] run concentrating to 8 M Na predicted 40.6% total solids. Required water removal per liter of feed was estimated by two methods: simple arithmetic (assuming ideal mixing behavior) and based on experimental total solids quantities above.

Simple arithmetic suggests that the following quantity of condensate must be generated (or water removed from the feed) per liter of 5.5 M Na C-simulant fed to the evaporator to produce an 8 M Na concentrate:

$$\begin{aligned} 1\text{ L feed }(1 - 5.5\text{ M Na}/8\text{ M Na}) &= 0.3125\text{ L condensate} \\ &= 312.5\text{ mL condensate (per liter feed)} \end{aligned}$$

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[21] Choi, A. S., forthcoming report for Hanford Tank AN-107 Envelope C-simulant evaporation OLI modeling, *2001*.
[22] Choi, A. S., *ibid*.

The ideal mixing assumption indicates generation of a 1.40 g/mL and 43 wt.% total solids in the 8.0 M Na concentrate.

Using the experimentally measured 5.5 M Na simulant density and the experimentally determined total wt.% solids results obtained (the 8.0 M Na total solids was obtained from the drying of a solution produced from somewhat approximate boildown and condensate back-addition experiments), the following condensate production was determined as necessary per liter of feed:

Water removal (per liter feed) based on experimental data	
5.5 M Na: Density (g/mL)	1.276
5.5 M Na: Tot. wt.% solids	32.5
Total salt per liter feed (g)	414.7
Total water per liter feed (g)	861.3
8.0 M Na: Total wt.% solids	41.9
Resulting 8.0 M Na solution mass (g)	989.7
Water remaining (g)	575.0
Required water removal (g)	286.3

Table 8. Required water removal per liter 5.5 M Na feed based on initial boildown experiment

The similarity of the two calculated quantities suggest the C-simulant may exhibit ideal mixing behavior. The initial calculated number to which the experimental run schedule was made (312.5 mL condensate produced per 1 L simulant) was selected for use in this experiment, given the somewhat rough nature of the calculated water removal based on the boildown/condensate back-addition work and the uncertain nature of the true saturation point.

The difference between the OLI model prediction of saturation at 11.4 M Na concentration and the experimental boildown result of approximately 10.3 M Na based on the volume of condensate produced at saturation strongly indicates the necessity of a second final boildown experiment (Section 4.5) to confirm this result and to produce samples of larger quantities for further analysis (density, total solids, etc.).

4.2 Execution of Experiment

Approximately 100 gallons of simulated Envelope C (107-AN) supernate with entrained solids were synthesized using the recipe in Appendix A, precipitated with NaOH/$Sr(NO_3)_2$/$NaMnO_4$, and cross-flow filtered in the Thermal Fluids Laboratory. As noted, this simulant was a non-toxic version that excluded addition of sodium chromate and lead nitrate. The resulting filtrate had a density of 1.276 g/mL. Using a Masterflex® pump with Viton® tubing operating at 50-100 mL/min, 60 L of simulant was pumped into 60 1 L Tedlar® bags a few days prior to use in the evaporator. A notable difficulty was that post-precipitation solids often encountered in AN-107 simulants restricted flow into the hose valves on the 1 L bags. This problem was eliminated by initially mixing the simulant, and allowing the post-precipitation solids to settle for 30-60 minutes prior to pumping simulant from near the top of the liquid. Bags were spiked with the target organic compounds 24-32 hours prior to anticipated use, with schedules being continually adjusted for any operational difficulties.

On the first day (June 4, 2000), semi-volatile and volatiles off-gas process blanks were taken before the liquid process blank samples taken. Due to air flow control difficulty, an empty evaporator operating at 82 mm Hg (–26.7 in. Hg) steady-state vacuum was run for approximately 50 and 43 minutes, respectively, to collect 20 L of treated laboratory air as a basis to reflect any effect of laboratory air leaking or introduced into the evaporator. Air flow for the process blanks was controlled through a needle valve before entering a silica gel and a carbon trap (to remove water and trace organics) and subsequently entering the evaporator through the evaporator feed line to maximize air contact within the apparatus interior. In both cases, no condensate was generated in the off-gas sampler, and only a small quantity of pump trap liquids (~1 mL) was generated in the outlet pump flask, the latter of the two pump trap bulbs. The leak rate for the volatiles off-gas field blank was approximately 5% higher than the Method 0031 specification, but only resulted in detection of slight quantities of toluene (374 ng), 1,2,4-trichlorobenzene (22 ng), and naphthalene (45 ng).

Beginning the second day of experiments (June 5, 2000), an evaporator leak check was performed for 1 hour and 40 minutes, yielding a natural leak rate of 0.35 mL/min. A simulant spiked with 800 ppm acetone was prepared in a carboy and then pulled into the –27.8 in. Hg evaporator tank through the feed line in 1600 mL batches. Some initial difficulties starting and priming the concentrate pump were solved by temporarily raising evaporator pressure to –12 in. Hg, and some bubbling of air through the process blank solution did result. After concentrate pump flow and –27.6 in. Hg evaporator pressure were established, the requisite volume (~6.5 L) of process blank samples were generated within 5 ½ hours of solution generation. The pump priming difficulties resulted in detectable quantities of benzene, 4-methyl-2-pentanone, hexachlorobenzene, pentachlorophenol, and bis(ethylhexyl)phthalate in the volatile and first semi-volatile process blank samples. However, these quantities were deemed negligible since the quantities were less than the minimum reportable quantity, except bis(ethylhexyl)phthalate which was only 6 ppb above the 10 ppb minimimum reportable quantity. Additionally, the quantities of semi-volatiles fell below detectable in the following two process blank samples. In preparation for the steady-state experiment, the evaporator was emptied using the concentrate pump leaving a 50-75 mL heel of the process blank solution at the base of the evaporator tank.

Feed from prepared Tedlar bags #8, #7, and #9 (bags #1 to #6 were used for feed samples) were added to the evaporator during the 6 ½ hour initial boildown of the evaporator tank to a target 8.0 M Na from the initial 5.5 M Na. Feed was added in batches until approximately 2100 mL (not including concentrate samples) was boiled down to the steady state level of 1450 mL. Assuming ideal mixing behavior, the approximate 710 mL condensate produced from nearly 2150 mL feed material produced a calculated 8.2 M Na solution. The initial boildown mass balance was closed to within 6.5% based on volume of spiked feed material fed (1.276 g/ml measured density), volume of condensate produced (1 g/ml density assumed), evaporator tank level (1.42 g/ml density assumed based on OLI model results), and mass of concentrate samples removed. Evaporator operation targets for both boildown and steady state operation are shown in Table 9:

Operation Parameter	Operational Target	Typical Operational Range
Evaporator tank level	1450 ± 150 mL	1450 ± 150 mL
Vacuum pressure	60 ± 8 mm Hg (P) –27.6 ± 0.3 in Hg	60 ± 8 mm Hg (P) –27.6 ± 0.3 in Hg
Evaporator tank temperatures	50 ± 3°C (T1)	60 ± 2°C (T1) 50 ± 2°C (T2)
Condenser temperature	40 ± 1°C (T3)	40 ± 1°C (T3)

Table 9. Evaporator Operational Targets and Typical Ranges.

Higher than target evaporator tank (T2) and heating rod temperatures (T1) were required to maintain a 3 mL/min condensate production rate necessary for a 74.5 hour steady state run time. After completing the initial boildown, the evaporator operation was immediately converted to steady state by turning on both the feed (9.6 mL/min target) and concentrate (6.6 mL/min target) pumps to pre-determined settings obtained by pumping deionized water to and from the evaporator system at 59 mm Hg (–27.6 in. Hg). Soon afterwards, the vacuum pump effluent (evaporator air in-leakage and pump bleed air) was directed to the Apex off-gas sampler setup for volatiles off-gas sampling. Regulatory samples and samples for in-house (SRTC) analysis were scheduled to be taken according to the timeline in Figure 6. Arrows signify volatiles zero-headspace samples and “H”-shape symbols represent the expected time to fill 1 L IChem bottles. In-house samples are labeled as such in the Figure. Semi-volatiles and pesticide regulatory feed samples were not included on this figure as these were scheduled to be taken prior to the beginning of each off-gas sampling period. Off-gas sampler regulatory samples and field blanks were also not included in this Figure. Refer to the Run Plan[23] (BNF-003-98-0234, Rev. 0) for spreadsheets tabulating the sample schedule and sample details.

As pump flows can vary with time, the evaporator was run at steady state successfully maintaining reasonably constant evaporator tank volumes for the first 20 hours until solids were observed, indicating that the simulant in the evaporator was becoming too concentrated. The concentrate line was backflushed to dislodge accumulated solids by naturally pulling in previously produced concentrate product. The concentrate withdrawal rate was increased to reduce tank levels sufficiently before the feed flow rate was increased and concentrate removal was reduced to dilute the evaporator tank contents. This strategy was pursued for 12 hours until a concentrate density measurement was taken and the 1.35 g/mL result indicated a dilute concentrate, compared to the 1.40 g/mL density of a sample taken 14 hours previous (a spot check at 28 hours steady-state operation showed 1.41 g/mL). The concentrate and feed pumps were then shutoff and the evaporator tank contents were boiled down again for approximately 80 minutes until a concentrate density of 1.40 g/mL was obtained by pycnometer. Steady state evaporation was resumed and pump flow rates re-calibrated for the final 4 hours of volatiles off-

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[23] Saito, H., Calloway, T. B., “Bench Scale LAW Evaporation of Simulants With Target Organic Indicators – Run 7E Run Plan – Rev. 0”, BNF-003-98-0234, Rev. 0, June 4, 2000.

gas sampling which was done for a total of 37 hours 37 minutes collecting sample from 928.5 L of evaporator condenser vent gas (11.5 mL/min) and pump bleed air (400 mL/min). The mass balance for liquids was closed to within 4.5% (Table 10) for the total volatiles off-gas sampling period of steady-state evaporator operation. No condensate in the volatiles off-gas sampling train was recovered, although the chilled condensate collection flask did have an unrecoverable thin film of condensed vapor on the walls. Vacuum pump trap liquid volume for this portion of the run (236.9 g) was thought to be atypically high since the silica gel trap used to clean pump bleed air was found to have settled at the end of the run, leaving a void space for inefficiently treated air to enter the pump flasks and condense moisture.

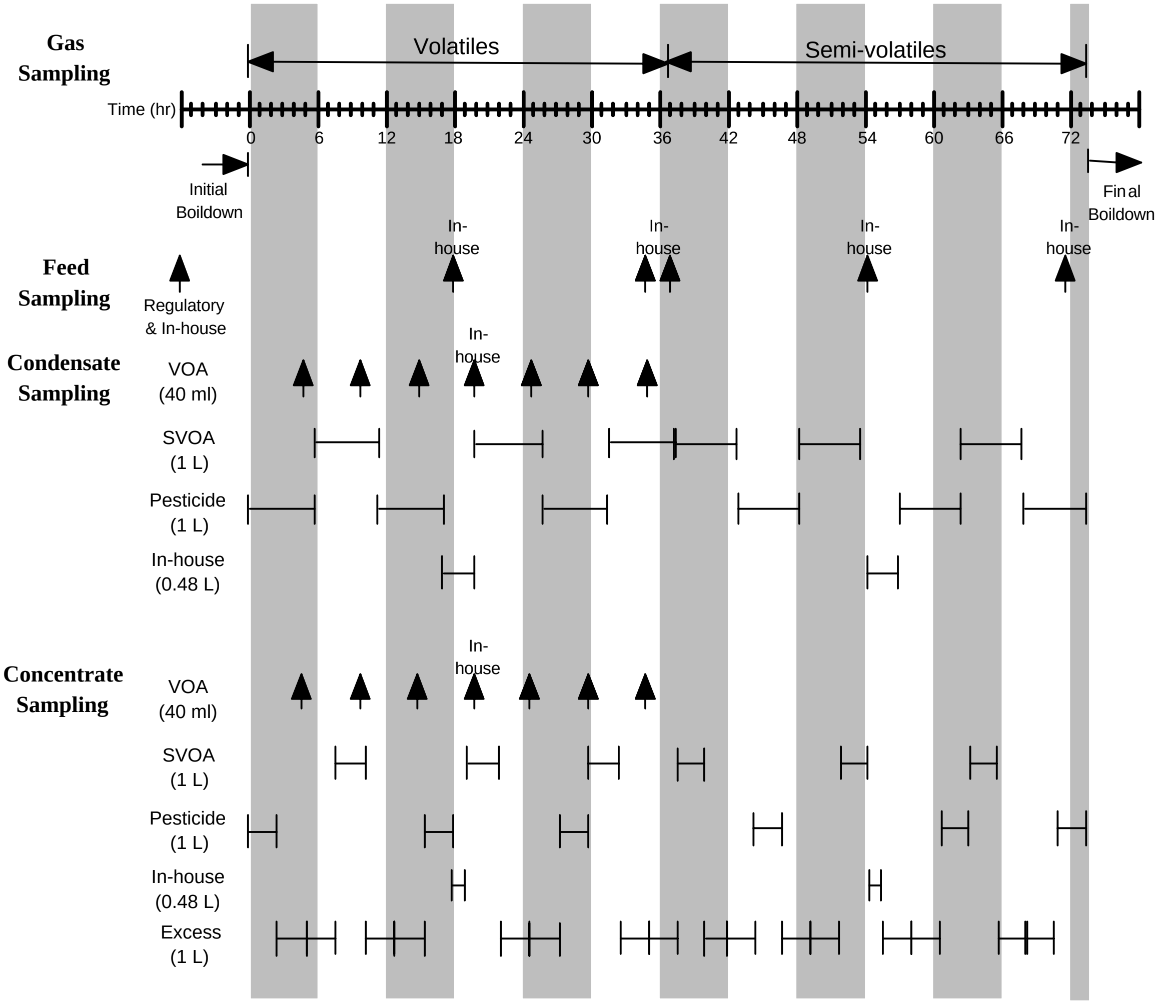

Figure 6. Regulatory sample and in-house analysis sample withdrawal schedule.

To minimize run time and to remove any potential effects from evaporation shutdown and restart, an "on-the-fly" transition from volatiles off-gas sampling (Method 0031) to semi-volatiles/pesticide off-gas sampling (Method 0010) was attempted and accomplished in less than 35 minutes on June 7, 2000. During this period, the evaporator outlet was valved off from the vacuum pump and the off-gas sampling operation was stopped. As the transition was initially expected to be shorter, evaporator heating, air-inleakage, and the concentrate pump operation continued while feed introduction was stopped. The vacuum pump was stopped, pump trap bulbs replaced, and the silica gel trap for the pump bleed air emptied and refilled with fresh dessicant. Simultaneously, pump trap liquid volatiles were poured to create zero-headspace samples for regulatory analysis, and a preprepared and leak-checked semi-volatiles gas sampling train was attached to the pump outlet line. The vacuum pump was then restarted to lower the pressure which had crept up due to the continuing air-inleakage, and the feed pump turned on with the concentrate pump turned off to regain a sufficient volume in the evaporator tank. Once evaporator operating conditions were stabilized, the vacuum effluent was valved to the semi-volatiles off-gas sampling train, and Method 0010 sampling was began when off-gas sampler operations were stabilized.

By comparison to the evaporator operation during Method 0031 execution, steady-state was more easily achieved during Method 0010 semi-volatiles/pesticide off-gas sampling due to the more frequent concentrate density checks performed by pycnometer. Target steady-state operation was maintained for 12 hours before the evaporator began running a bit dilute with a concentrate density of 1.38 g/mL. Feed pump flow rates were gradually reduced due to increasing evaporator tank levels, and the concentrate density rose to 1.39 g/mL over the next 5 hours. Various in-house condensate and concentrate samples were collected before another concentrate spot-check showed a drop in density to 1.38 g/mL due to rising evaporator tank levels 3 hours later. The feed and concentrate pumps were turned off, and a 25-minute boildown was performed to concentrate from a calculated 7.2 M Na concentration. After the target 1.40 g/mL concentrate density was recovered, both pumps were restarted and reset to target flow rates. Another 9 hours later, a last concentrate density check and very stable evaporator operation suggested continued desired steady-state evaporator operation. A 1.38 g/mL density of the final boildown starting material suggests that the evaporator ran somewhat dilute towards the end of the last 6 hours of Method 0010 sampling. Ending in the early morning of June 9, 2000, semi-volatiles/pesticide off-gas sampling was done for a total of 34 hours 50 minutes collecting sample from 953.9 L of evaporator condenser vent gas (11.5 mL/min) and pump bleed air (445 mL/min). The mass balance for liquids was closed to within 1.7% (Table 10) for the total volatiles and semi-volatiles/pesticide off-gas sampling periods of steady-state evaporator operation.

A small amount of condensate (1.25 g) in the semi-volatiles/pesticide off-gas sampling train was recovered for analysis. Vacuum pump trap liquid volume for this portion of the run (72.9 g) was lower than for the volatiles run (236.9 g), as expected, due to a more efficiently packed silica gel trap to treat the pump bleed air. The mid-run in-house condensate and concentrate samples were taken at slight dilution (1.39 g/mL concentrate density) from target steady state operating conditions.

Review of the regulatory process, field, trip and reagent blank data shows that contamination was a minor issue in 22 of the approximately 72 blanks (Appendix B, A. Raw Data), with most detected analytes being only slightly above detection limits or at levels far below those detected in associated samples. The remainder did not show detectable quantities. Many of these “positive” results never impacted results since “positive” trip blanks were discounted due to non-detectable levels in associated field blanks, and one case was a water reagent blank for dilution that was never needed. As a result, only about 10 sample results had to be adjusted slightly as a result of detected contamination. Sample results that were adjusted are identified in a subsequent section (Appendix B, B. Validated and Corrected Data).

While preparations were made to add Dow US-1520 anti-foam in the case of evaporator tank liquid foaming during evaporation, anti-foam use was not necessary as foaming was not encountered either during the nearly 75 hour steady-state operation or during the final boildown experiment.

4.3 Overall and Target Organics Mass Balance

Mass and volume balances for the volatiles and semi-volatiles/pesticide sampling portions of the run were completed and are summarized in Table 10. Mass of spiked feed material fed into the evaporator and mass of concentrate and condensate extracted were recorded throughout the experiment. Remaining condensate and concentrate in the evaporator were estimated by multiplying estimated volumes determined from equipment graduations and assumed densities such as 1 g/mL for condensate and the most recent concentrate density measurement. By this method, a mass balance was maintained throughout the experiment. Based on the mass balance results, a volume balance was performed using the assumed densities listed at the bottom of Table 10.

Sampling Period/Event	Mass Fed (g)	Condensate Generated (g)	Concentrate Generated (g)	Mass Balance Closure (%)
Volatiles Off-gas	24704	6475	19343	4.5
Semi-volatiles/Pesticide Off-gas	24881	6107	18531	1.0
Total	49585	12582	37874	1.7

Sampling Period/Event	Volume Fed (mL)	Condensate Generated (mL)	Concentrate Generated (mL)	Volume Balance Closure (%)
Volatiles Off-gas	19361	6475	13816	4.8
Semi-volatiles/Pesticide Off-gas	19499	6107	13236	0.8
Total	38860	12582	27052	2.0
Assumed density	1.276	1	1.4	----

Table 10. Experiment Mass and Volume Balance Results: Overall and by Sampling Event.

The material for each sampling period was accounted for to within 5% of the mass fed. The densities assumed for the volume balances are from experimental measurements of the feed before experiments and of the concentrate during the experiment. As mentioned earlier, a concentrate density of 1.40 g/mL was the target, but deviations in the actual concentrate densities will affect the volume balance only slightly.

When occasionally necessary, the raw regulatory analytical data obtained from BWXT Services, Inc. was corrected for the almost negligible contamination as quantified in the trip, field, and process blanks generated in parallel to the regulatory samples. The SRTC Quality Assurance-approved regulatory raw analytical data and corrected quantities are tabulated in Appendix B (refer to BWXT Services, Inc. report numbers 0006015 VOC AQUEOUS, VOC SOLID, SVOC, and PEST in reference [24] for the raw data package). The corrected regulatory analytical data was then combined with the experimental mass balance data to understand the fate of the 14 target organic compounds fed into the evaporator. Table 11 lists the calculated quantity and standard deviation of each target organic compound entering or leaving through each evaporator stream for the overall experiment (See Appendix C for calculations).

Given the 20-130% acceptable analyte recoveries specified for this work, acceptable mass balances (-30 to 80% mass closure) were obtained for all species except for 1,2-dibromoethane, 1,2,3-trichloropropane and pentachlorophenol whose quantities are small (likely due to hydrolysis) and large analytical errors are expected. Similar material balances were performed individually for both the volatiles and semi-volatiles/pesticide off-gas sampling periods and were not found to change the results or trends significantly.

	Chemical	Mass Fed (ug)	Condensate	Concentrate	Sorbent Tube	Pump Traps	Off-gas Line Rinse	TOTAL	Mass Closure (%)
Volatiles	Benzene	55550	405	174*	*49896*	15*	0	*50491*	*9.11*
	Std. Dev	2748		111				111	4.50
	4-methyl-2-pentanone (MIBK)	*99928*	2063*	1833*	*66401*	373*	0	*70670*	*29.28*
	Std. Dev	*9068*	1644	1099				1977	6.72
	Toluene	41386	326	235*	*22736*	10*	0	*23307*	*43.68*
	Std. Dev	2473		83				83	3.37
	1,2-dibromoethane	*2821*	523	55*	*9335*	24*	0	*9938*	*-252.25*
	Std. Dev	*346*		50				50	43.27
	Chlorobenzene	45660	554	166*	*17811*	11*	0	*18542*	*59.39*
	Std. Dev	5770		27				27	5.13
	1,2,3-trichloropropane	*38471*	2139*	6222*	*0*	34*	0	*8395*	*78.18*
	Std. Dev		448	3085				3117	8.10
Semi-volatiles	1,2,4-trichlorobenzene	22927*	1000	1508*	19599	130	0	22238	3.01
	Std. Dev		476	443		35		651	2.84
	Naphthalene	22021*	3712	683*	17024	448	0	21867	0.69
	Std. Dev	1365	1623	461		47		1688	9.83
	Hexachlorobenzene	31574	*22*	22522*	0	0*	940	23483	25.62
	Std. Dev	10443	*26*	3847				3847	27.45
	Pentachlorophenol	*2332*	0	4058	0	0*	0	4058	-74.04
	Std. Dev	*1124*		716				716	89.36
	Pyrene	36140*	1699	20425*	0	28*	719	22870	36.72
	Std. Dev	0	417	2353				2390	6.61
	Bis(ethylhexyl)phthalate (BEHP)	40220	*38*	24618*	0	0	0	24656	38.70
	Std. Dev	275	*75*	2231				2232	5.57
	Benzo[a]pyrene (BaP)	56735*	0	31449*	0	0*	0	31449	44.57
	Std. Dev	7859		4975				4975	11.66
Pest-icide	Aldrin	40285*	315	31449*	*0*	18*	*0*	31782	21.11
	Std. Dev	809	142	4975				4977	12.46
	Theoretical (each)	50518							

*from SRTC Analytical Result

Table 11. Overall Experiment Mass Balance for Each Target Organic Compound

Table 11 shows that the target organic volatiles and the more volatile semi-volatiles (1,2,4-trichlorobenzene and naphthalene) largely exit the evaporator through the evaporator off-gas, generally leaving small quantities in the concentrate and slightly greater quantities in the

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[24] Ferrara, D. M., "Data Package for AN-107 Env. C-simulant Regulatory Evaporation", WSRC-TR-2000-00528, SRT-RPP-2000-00062, *2001*.

produced condensate. The remaining semi-volatiles were found to predominantly remain in the evaporator concentrate with slight quantities being captured in the condensate. No significant quantities of the less-volatile semi-volatiles were detected in the off-gas sampling train, although a few percent of the fed hexachlorobenzene and pyrene were found to have condensed in the evaporator off-gas line.

The yellow/italic cells in Table 11 signify that there is analytical uncertainty (lack of accuracy) in the values due to data qualification by BWXT Services, Inc. or by SRTC Quality Assurance Department. Regulatory feed analyses for 4-methyl-2-pentanone (methyl iso-butyl ketone, MIBK), 1,2-dibromoethane, and pentachlorophenol were qualified as inaccurate, which could explain the discrepancies in the material balances observed. The same is true for hexachlorobenzene in the condensate. The quantity of 1,2,3-trichloropropane fed into the evaporator during the experiment is a calculated quantity based on the aging studies discussed earlier. The actual quantity is expected to be between the 800 μg/L minimum detection limit cited by BWXT Services from their sample analysis, and 140 μg/L obtained by belated analysis of an in-house sample. BWXT Services also expects that the lack of recovery of 1,2,3-trichloropropane in the off-gas sampling tubes is due to chemical degradation on the sorbent material or during extraction. Pesticide numbers colored yellow were deemed uncertain as insufficient sample was set aside for these analyses. MIBK totals are thought to be higher than the theoretical input due to extraction of this compound, often used for plastic coatings, from the Tedlar bags.

The regulatory data from BWXT Services, Inc. were used to the maximum extent possible. But analytical problems and issues required that some of the data be replaced by analytical results from SRTC in-house analysis of identical samples, or that regulatory data be used that were qualified as inaccurate or “uncertain” by the Quality Assurance Department at either SRTC or the vendor laboratory. Regulatory semi-volatiles and pesticide analytical results for both feed and concentrate samples were replaced by SRTC in-house analytical results. The EPA SW-846 Methods require that semi-volatiles and pesticide samples be acidified to pH=2 prior to analysis. However the vendor laboratory noted that the samples bubbled on acidification and that lower than expected target semi-volatile organic compound concentrations were obtained. It is believed that the added acid is reacting with the abundant nitrite in the Hanford AN-107 simulated waste to form the highly reactive nitrous acid which is oxidizing and consuming the target organics. As the SRTC analytical method concentrates the analytes through the use of liquid-liquid extraction with methylene chloride, the in-house results for both feed and concentrate semi-volatiles and pesticides were deemed more accurate and were used in the analysis, except pentachlorophenol. It is believed that sample acidification helps reprotonate the deprotonated phenolic group for quantification, while a deprotonated pentachlorophenol in the caustic simulated waste would not be extractable by methylene chloride.

The volatiles off-gas numbers were deemed uncertain for two primary reasons. First, low surrogate recoveries, average 8% for Anasorb sorbent tubes and an acceptable but low 34% average for Tenax sample tubes, were initially reported. A regulatory sample Tenax and the Anasorb tube had to be methanol-extracted since the quantities of target components on the first thermally-desorbed Tenax tube overloaded the analytical equipment detector. As the low quantities of spike material (50 μg each component) combined with permananent sorption losses onto the sorbent material were thought to be causing the reported low recoveries, recovery testing using the maximum quantity of analyte observed on each regulatory sample tube (3000 μg on Tenax, 30000 μg on Anasorb) was performed by BWXT Services, Inc. The recoveries obtained with these larger spiked quantities improved to 15% for Anasorb and 88% for Tenax (refer to BWXT Services, Inc. Report No. 0011102 VOC TENAX AND ANASORB[25] for raw data package). The low average surrogate recovery for Anasorb are due to <11% recoveries of benzene, toluene, and chlorobenzene by methanol extraction. The recovered quantities of volatiles cited in Table 11 were not adjusted for reported recoveries, as is standard practice[26]. Second, due to the sorbent tube analysis difficulties, the obtained analytical volatiles quantities for one volatiles Tenax sample tube is known to be approximate and low due to detector overload. As a result, all sorbent tube recovered quantities were deemed approximate, although reasonable material balances were obtained and the target organic compound distribution trends appear unaffected.

An important note from BWXT Services, Inc. was that all Anasorb and one sample Tenax tube were solvent extracted to yield the analytical results. Hence, the process, field, and trip blank Tenax tube results were thermally desorbed for analysis and those results (where significant) were not affected by the aforementioned difficulties.

4.4 Product Chemical Analysis Results

Tables 12 and 13 show the analytical results from SRTC analysis of the feed and evaporation products. Density was obtained by pycnometer, total solids by staged oven drying at 90, 105, 120, 135, and 150°C (if needed due to large sample size), and insoluble solids by vacuum filtration using a 0.22 μm pore-size cellulose filter followed by staged drying with the total solids analysis samples. Metals concentrations were obtained by induced coupled plasma-emission spectroscopy (ICP-ES), with Cs, K, and Na analyzed by atomic absorption (AA) or by induced coupled plasma-mass spectrometry (ICP-MS). Anion concentrations were obtained by ion chromatography (IC-Anion), total and free hydroxide wet chemical analysis, and total inorganic carbon/total organic carbon (TIC/TOC) analysis. The concentrate data presented below are thought to be slightly dilute compared to the overall run average concentrations as the evaporator concentrate density at the time of sampling was 1.38 g/mL compared to the experimental target 1.40 g/mL specified by the OLI model.

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[25] Ferrara, D. M., *op. cit.*, WSRC-TR-2000-00528, SRT-RPP-2000-00062, *2001*.

[26] Gibson, Jr., L.V., Sampling and Support Department, Analytical Chemistry Organization, Y-12 National Security Complex (BWXT Y-12, L.L.C.), electronic mail, October 16, *2000*.

Property/Analyte	Feed		Condensate	Calculated DF	Concentrate
Density	1.276				1.382
Total Solids (wt.%)	32.5				42.9*
Insoluble Solids (wt.%)	~0.3				0.39*
Ag (mg/L)			*<0.056*		*<0.28*
Al (mg/L)	236	223	*<0.048*	>4800	328
B (mg/L)	23	22	*<0.042*	>540	28.7
Ba (mg/L)	*<0.1*		*<0.004*		*<0.2*
Ca (mg/L)	160	143	*<0.008*	>18900	202
Cd (mg/L)		*<0.14*	*<0.004*		*<0.2*
Co (mg/L)			*<0.01*		*<0.5*
Cr (mg/L)	0.5	*<0.74*	*<0.01*	>62	*<0.5*
Cs (mg/L)	9.24 (AA)		0.000019 (ICP-MS)	486000	
Cu (mg/L)	13	13	*<0.01*	>1300	17.5
Fe (mg/L)	34	35	*<0.01*	>3450	47.0
K (mg/L, AA)	2563	1119			
La (mg/L)	1.5				
Li (mg/L)			*<0.02*		*<1*
Mg (mg/L)	*<0.1*	*<0.084*	*<0.018*		*<0.9*
Mn (mg/L)	11	24	*<0.002*	>8750	22.4
Mo (mg/L)		20	*<0.02*	>1000	30.2
Na (mg/L)	125258	131057	*<2*	>64100	184200
Na (mg/L, AA)	121043	128128			
Nb (mg/L)			*<0.1*		*<5*
Ni (mg/L)	315	283	*<0.014*	>21400	427
P (mg/L)	280	299	*<0.14*	>2070	376
Pb (mg/L)	*<1*	*<2*	*<0.14*		*<7*
Si (mg/L)	8	9.2	0.09	96	19.8
Sn (mg/L)			*<0.052*		*<2.6*
Sr (mg/L)	80	73	*<0.0004*	>191000	106
Ti (mg/L)			*<0.028*		*<1.4*
V (mg/L)			*<0.026*		*<1.3*
Zn (mg/L)	18	17	*<0.074*	>236	24.8
Zr (mg/L)	2	1.7	*<0.01*	>185	1.9
Na (M)	5.45	5.70	<0.00009		8.01
Na (M) - predicted	5.58 (basis)				7.89
Tot. Solids (wt%)–pred.	32.5 (basis)				42.5
* from Final Boildown data for similar solution density					

Table 12. Bulk property and cationic concentration (ICP-ES, unless otherwise specified) data with calculated DF for Envelope C simulant feed and evaporation products.

Calculation of decontamination factors (DF) using Table 12 and 13 data, where DF = feed concentration/condensate concentration, allows for evaluation of evaporator operation during the experiment. In addition to the below detection limit condensate ICP-ES and IC-Anion analyte concentrations, the high decontamination factors for Cs, OH^- and Sr show that de-entrainment of droplets from the evaporator tank to the condensate tank by the packed stainless steel mesh was excellent. Minimum calculated DF's were calculated using analytical feed data and the minimum detection limits cited for the condensate data. Low feed concentrations and relatively high minimum detection limits are likely responsible for the low DF's calculated for Cr, Zn, Zr, formate, oxalate and phosphate, and to a lesser degree for other species with calculated DF's in the 800-10000 range. However, the low DF for Si suggests that individual species verification is necessary and that high DF may not occur for all species.

Analyte	Feed		Condensate	Calculated DF	Concentrate
Chloride (mg/L)	1308	2477	<2	>946	1559
Fluoride (mg/L)	2864	2455	<2	>1330	3177
Formate (mg/L)	7179	6636	<10	>691	10105
Nitrate (mg/L)	145186	137961	<10	>14200	188331
Nitrite (mg/L)	38751	36145	<10	>3750	42364
Oxalate (mg/L)	1578	1306	<10	>144	1647
Phosphate (mg/L)	1529	2349	<10	>194	2148
Sulfate (mg/L)	5273	5297	<5	>1060	5913
Total OH$^-$ (M)	1.395	1.421			2.059
Free OH$^-$ (M)	0.553	0.561	2.51 x 10^{-6} (pH=8.4)	222000	0.987
Total Inorganic C (mg/L)	17512				15046
Total Organic C (mg/L)	11070				17328

Table 13. IC-Anion, Total/Free Hydroxide and TIC/TOC analytical results with calculated DF for Envelope C simulant feed and evaporation products.

Property/Analyte	Measured Feed (basis)		Measured Concentrate	Volume Additivity Concentrate Prediction	% Difference vs. Measured
Al (mg/L)	236	223	328	325	0.9
B (mg/L)	23	22	28.7	31.9	11.0
Ca (mg/L)	160	143	202	215	6.2
Cu (mg/L)	13	13	17.5	18.4	5.2
Fe (mg/L)	34	35	47.0	48.8	3.9
Mn (mg/L)	11	24	22.4	24.8	10.6
Mo (mg/L)		20	30.2	28.3	6.2
Na (mg/L)	125258	131057	184200	181460	1.5
Si (mg/L)	8	9.2	19.8	12.2	38.5
Sr (mg/L)	80	73	106	108	2.2
Zn (mg/L)	18	17	24.8	24.8	0.1
Zr (mg/L)	2	1.7	1.9	2.6	37.9
Na (M)	5.58		8.01	7.90	1.5
Tot. Solids (wt%)	32.5		42.9	42.5	0.9
Total Mass Processed (g)	49585		37874	*Conc. Factor*	
Total Volume Processed (mL)	38860		27445	***1.42***	
Assumed Density (g/mL)	1.276		1.38	-----	

Table 14. Actual concentrate metal concentrations versus prediction by volume additivity (ideal mixing behavior), and percent difference from measured.

The overall mass balance data (Table 10) indicate that the feed was concentrated by a factor of 1.42 (bottom of Table 14), assuming ideal mixing and that the condensate is pure water. Combining this concentration factor with evaporator feed data in Tables 12 and 13 also allows for a comparison of the predicted species concentrations in the concentrate assuming ideal mixing behavior with analytical concentrate data for the Hanford Tank AN-107 Envelope C-simulant salt solution. Given the estimated 10% random error in the analytical data, the actual and predicted concentrate metals and total solids concentrations (Table 14) match very well, being within 12% for the majority of analytes except Si and Zr, and suggests the Envelope C simulant behaves similarly to an ideal mixture in this concentration range.

By the same calculation method, the predicted anion concentrations (Table 15) were not found to compare as well, with the majority of analyzed species being overpredicted by at least 20% except fluoride, formate, nitrate, total hydroxide and total organic carbon. As verified by comparing feed analytical data to the simulant recipes, the SRTC method used for IC-Anion analysis was not specific ion selective and signal interferences were found to lead to high estimates for chloride, fluoride, and phosphate due to co-elution with formate, acetate, gluconate and other organic compounds present in the Envelope C simulant. Oxalate predictions are possibly high due to the precipitation of sodium oxalate as detected in the Final Boildown initial concentrate insoluble solids (see **Final Boildown** section), although the small quantities of insoluble solids are expected to have been included in the sample used for IC-Anion analysis.

Analyte	Feed		Concentrate	Concentrate Prediction	% Difference
Chloride (mg/L)	1308	2477	1559	2680	71.9
Fluoride (mg/L)	2864	2455	3177	3766	18.5
Formate (mg/L)	7179	6636	10105	9780	3.2
Nitrate (mg/L)	145186	137961	188331	200456	6.4
Nitrite (mg/L)	38751	36145	42364	53023	25.2
Oxalate (mg/L)	1578	1306	1647	2042	24.0
Phosphate (mg/L)	1529	2349	2148	2745	27.8
Sulfate (mg/L)	5273	5297	5913	7483	26.6
Total OH^- (M)	1.395	1.421	2.059	1.994	3.2
Free OH^- (M)	0.553	0.561	0.987	0.789	20.1
Total Inorganic C (mg/L)	17512		15046	24795	64.8
Total Organic C (mg/L)	11070		17328	15674	9.5

Table 15. Actual concentrate anion concentrations versus prediction by volume additivity (ideal mixing behavior).

The good comparisons for major and/or highly soluble species such as nitrate, total hydroxide, formate and total organic carbon suggest analytical error which could account for up to 20% of the difference is not a major factor, although error in nitrite indicates the contrary. The unaccounted for sulfate (1570 mg/L) is sufficient to add 0.1 wt% insoluble solids that was not detected by X-ray diffraction of insoluble solids.

Tables 16 and 17 compare the simulant analytical data to the analytical data obtained for actual Hanford Tank AN-107 waste that has been pre-treated to the completion of Tc-99 removal by ion exchange (Fiskum[27]) to assess simulant quality. The first column in Tables 16 and 17 are the analytical data from Table 3.5 of Fiskum's report which is at a sodium concentration consistent with post-ion exchange solutions. The following two columns are calculated concentrations for each species in the Hanford waste at the concentrations used for the simulant steady state evaporator, assuming ideal mixing and that no species are lost to the condensate.

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[27] Fiskum, S. K., Kurath, D. E., Rapko, B. M., "Development and Demonstration of a Sulfate Precipitation Process for Hanford Waste Tank 241-AN-107", PNWD-3050, BNFL-RPT-029, Rev. 0, Battelle, Pacific Northwest Division, Richland, WA, August, *2000*.

	Concentration in mg/L					
	Actual AN-107 Post Tc IX Material				AN-107 Simulant	
	Fiskum Data		5.58 M Na Feed	8.01 M Na Conc.	5.58 M Na Feed	8.01 M Na Conc.
Al	2340		2704	3882	230	328
B	19		22	32	23	28.7
Ca	172		199	285	152	202
Cd	27		31	45	<0.14	<0.2
Cr	43.0		50	71	0.5	<0.5
Cu	13		15	22	13	17.5
Fe	8.6		10	14	35	47
Mn	1.4		1.6	2.3	18	22.4
Mo	16.0		18	27	20	30.2
Na	111000		128283	184148	128158	184200
Ni	210		243	348	299	427
P	302.0		349	501	290	376
Pb	58		67	96	<2	<7
Si	32		37	53	8.6	19.8
Sr	130		150	216	77	106
Zn	7.6		8.8	13	18	24.8
Zr	2.9		3.4	5	1.9	1.9

Table 16. Expected metals concentrations in Hanford AN-107 waste versus observed metals concentrations in the AN-107 simulant.

	Concentration in mg/L					
	Actual AN-107 Post Tc IX Material				AN-107 Simulant (Averaged values)	
	Fiskum Data		5.6 M Na Feed	8.01 M Na Conc.	5.6 M Na Feed	8.01 M Na Conc.
Na (M)	4.83		5.58	8.01	5.58	8.01
Fluoride	3500		4045	5806	2660	3177
Nitrate	112000		129439	185807	141574	188331
Nitrite	28800		33284	47779	37448	42364
Phosphate	1400		1618	2323	1939	2148
Sulfate	4020		4646	6639	5285	5913
Oxalate	1400		1618	2323	1442	1647

Table 17. Expected anion concentrations in Hanford AN-107 waste versus observed anion concentrations in the AN-107 simulant.

The low cadmium, chromium and lead in the AN-107 simulant is because these components were not added to this “non-toxic” version. Good matches are found for boron, copper, molybdenum, nitrate and nitrite, with less favorable matches found for phosphate and sulfate. The Hanford waste is higher in aluminum, calcium, phosphorous, silicon, strontium, zirconium, fluoride and oxalate. The higher concentrations of iron, manganese, nickel, and zinc in the simulant suggest some dissolution of stainless steel components used during processing.

Material		Viscosity (cP)	
		25°C	50°C
Simulated AN-107	Feed (5.6 M Na)	4.6	1.9
	Concentrate (8.0 M Na)	8.3	3.9
Hanford AN-107	6 M Na	8	4
	8 M Na	12	7

Table 18. Comparison of AN-107 simulant feed and concentrate viscosity and

actual Hanford AN-107 waste at 25 and 50°C.

Other data obtained relevant for evaporator operation is evaporator feed (5.6 M Na) and concentrate (8.0 M Na) viscosity shown in Table 18 at the ambient feed and the evaporator concentrate effluent temperatures. Viscosity, measured by a RV20 Haake rheometer (M5 measuring head with NV sensor), was found to decrease with temperature as expected, with the slightly greater percentage drop in the feed material likely due to increased dissolution of insoluble solids in the less concentrated salt solution. The increase in the viscosity with salt concentration may be due to slightly increased insoluble solids likely present in the concentrate, although this was not verifiable experimentally due to relatively high scatter in the insoluble solids determinations. The simulant at 5.6 and 8.0 M Na was found to be a Newtonian fluid, as was the actual Hanford waste at similar concentrations[28]. Although insoluble solids (IS) concentrations are not reported, the higher viscosities for the Hanford waste samples may be due to slightly greater IS content than in the simulant as evidenced by 60% by volume insoluble solids observed in the 9.7 M Na actual waste sample compared to 40% by volume (5.0 wt%) insoluble solids content in 10 M Na simulated waste.

4.5 Final Boildown

Five days following the completion of the 75 hour steady-state evaporation, the remaining evaporator tank contents were boiled down to find the maximum Na concentration of the C-simulant concentrate before flow characteristics significantly deteriorate. The evaporator was again operated at –27.6 in Hg vacuum with a total natural and calibrated air-inleakage of 11.5 mL/min. From an initial 1630 mL evaporator tank volume, 30 mL concentrate samples were taken every 15 minutes, or every 48 mL of condensate produced at 3.2 mL/min production rate, until the concentrate could not be pumped out through the 1/8” Teflon® concentrate line during the withdrawal of the fifth sample. Exhibiting a sharp transition, the evaporator concentrate within a 1-2 minute period went from a green semi-translucent liquid to a very viscous greenish-white gel. The top picture

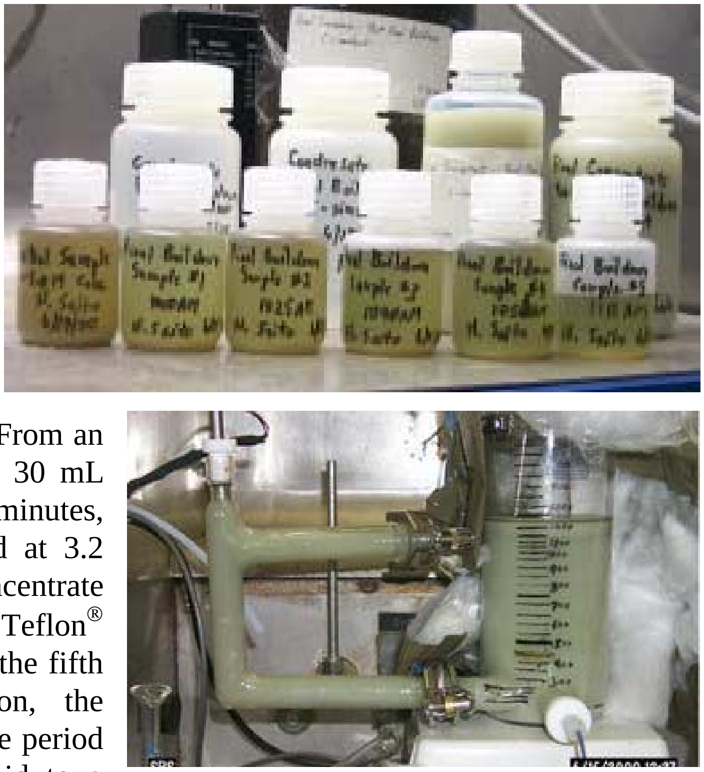

Figure 7. Boildown concentrate samples, first to last, with final concentrate in rear; final concentrate in evaporator.

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[28] Bredt, P. R., Swoboda, R. G., “Rheological Studies on Pretreated Feed and Melter Feed from AW-101 and AN-107”, BNFL-RPT-034, PNWD-3034, Rev. 0, Battelle, Pacific Northwest Division, Richalnd, WA, April, *2000*.

in Figure 7 shows the contrast between samples obtained prior to bulk saturation (front row, left to right, initial ~8.0 M Na concentrate sample to progressively more concentrated) and the "near saturated" samples obtained (back row, right two bottles), and the bottom picture shows more clearly the color of the saturated solution in the evaporator. The stir bar in the evaporator tank was apparently only mixing the lower fourth of the tank contents after bulk saturation, and no recirculation was observed in the evaporator arm containing the heating rod. The final evaporator tank volume was ~1250 mL after evaporator heating was discontinued, with 350 mL condensate produced. As in the steady-state operation, no antifoam was used in this experiment.

To obtain a sample of this bulk saturated concentrate that was removeable by pump, 36 g condensate was back-added by suction through the concentrate line to dilute the concentrate slightly, and agitation was increased to the maximum. However, viscosity of the gel-like concentrate limited dilution to the lower fourth of the evaporator, leaving the slurry in the heating arm and the bulk of the evaporator unaffected. Using the vacuum in the evaporator, mixing was accomplished by additionally sparging laboratory air in through the concentrate and feed lines as well as from the seal around the heating rod eventually creating a "pumpable" slurry. The final evaporator volume was ~1290 mL, and sparging had reduced the vacuum to –23.4 in Hg. The vacuum was then released, and the near-saturated concentrate was pumped out of the evaporator system.

Selected samples from the final boildown experiment were sent for total and insoluble solids, density, ICP-ES and XRD (X-ray diffraction) analysis (Table 19). The total solids analytical results indicates that the AN-107 Envelope C simulated waste reaches bulk saturation at 48.6 wt%, which is equivalent to 94.6 g total salt (TS) per 100 g water at an estimated 10.1 M Na (50°C). This extent of concentration before "first" solids formation is slightly exceeded by that for AN-105 Envelope A simulant[29] (99 g TS/100 g water, 7.5 M Na at 50°C), and is slightly higher than for AZ-101 Envelope B simulant[30] (88-90 g TS/100 g water, 9.9-10.1 M Na at 50°C). The insoluble solids data and second experiment confirmed the sharp change in salt solution characteristics upon reaching bulk saturation, with measured insoluble solids content increasing approximately by a factor of 10 over a very slight change (calculated ~0.1 M Na) in salt concentration. X-ray diffraction data indicates that initial insoluble solids at 5.5 M Na are largely sodium oxalate, with sodium carbonate decahydrate appearing by 9.6 M Na before the bulk salt, sodium nitrate, precipitates at the saturation point near 10.1 M Na. Sodium nitrate and nitrite detected below saturation is a result of dried simulant that was the interstitial liquid in the insoluble solids filter cake.

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[29] Calloway, Jr., T.B., "Evaporation of Hanford Envelope A Simulant (AN-105)", WSRC-TR-2000-00300, SRT-RPP-2000-00010, Rev. 0, August, *2000*.

[30] Calloway, Jr., T.B., Choi, A.S., Monson, P.R., "Evaporation of Hanford Envelope B Simulant (AZ-101) Preliminary Report", BNF-003-98-0166, Rev. 1, January 6, *2000*.

Property/Analyte	Initial Sample		Sample #2	Sample #4		Sample #5	Near-saturation Sample	
Density	1.380			1.427			1.437	
Total Solids (wt.%)	42.9		45.4	46.8		48.6	48.6	
Insoluble Solids (wt.%) (std. dev.)			0.39 (0.26)			0.43 (0.02)	4.99 (0.15)	
XRD-Identified Insoluble Salts	Sodium Oxalate Sodium Nitrate			Sodium Oxalate Sodium Carbonate Sodium Nitrite Sodium Nitrate			Sodium Oxalate Sodium Carbonate Sodium Nitrite Sodium Nitrate	
ICP-ES Data								
Al (mg/L)	328	317		364	364		385	390
B (mg/L)	32	32		36	36		38	38
Ba (mg/L)	*<0.12*	*<0.12*		*<0.12*	*<0.12*		*<0.12*	*<0.12*
Ca (mg/L)	202	199		228	227		241	242
Cd (mg/L)	*<0.14*	*<0.14*		*<0.14*	*<0.14*		*<0.14*	*<0.14*
Cr (mg/L)	*<1*	*<1*		*<1*	*<1*		*<1*	*<1*
Cu (mg/L)	17	16		19	18		19	19
Fe (mg/L)	36	35		42	41		46	45
La (mg/L)	1	1		2	2		2	2
Li (mg/L)	*<1*	*<1*		*<1*	*<1*		*<1*	*<1*
Mg (mg/L)	*<0.84*	*<0.84*		*<0.84*	*<0.84*		*<0.84*	*<0.84*
Mn (mg/L)	2	2		2	2		3	3
Mo (mg/L)	30	30		35	33		37	36
Na (mg/L)	192591	191150		222691	221667		207326	216559
Ni (mg/L)	424	414		473	474		501	507
P (mg/L)	405	396		463	447		440	451
Pb (mg/L)	*<6.8*	*<6.8*		*<6.8*	*<6.8*		*<6.8*	*<6.8*
Si (mg/L)	23	22		29	28		32	31
Sn (mg/L)	*<1.3*	*<1.3*		*<1.3*	*<1.3*		*<1.3*	*<1.3*
Sr (mg/L)	110	109		125	124		130	130
Ti (mg/L)	0.2	*<0.02*		*<0.02*	0.1		*<0.02*	*<0.02*
V (mg/L)	*<1.4*	*<1.4*		*<1.4*	*<1.4*		*<1.4*	*<1.4*
Zn (mg/L)	24	24		27	26		29	29
Zr (mg/L)	*<3.7*	*<3.7*		*<3.7*	*<3.7*		*<3.7*	*<3.7*
K (mg/L)	1740	1700		1943	1952		2074	2103
S (mg/L)	2279	2237		2539	2457		2688	2654
Ag (mg/L)	*<5*	*<5*		*<5*	*<5*		*<5*	*<5*
Na (M)	8.38	8.31		9.69	9.64		(9.22)	
Na (M) - predicted	8.35 (basis)		8.92	9.65		10.08	10.16	
Tot. Solids (wt%)–pred.	42.9 (basis)		45.0	47.6		49.0	49.2	

Table 19. Final Boildown Sample Analytical Results.

Predicted values for Na concentration and total solids were calculated based on condensate production data using as a basis: 1) SRTC data for Na obtained by ICP-ES, 2) total solids obtained by oven-drying for an initial boildown sample taken before evaporator heat input, 3) assuming volumes are additive (ideal mixing), and 4) assuming condensate produced is pure water. Predicted and average actual Na concentrations were within 0.2% for Sample #4, but did not match well for the near saturation sample due to sampling error. The 9.2 M Na average value obtained for the near saturation sample is low because only the filtrate of the sample, known to precipitate solids after filtration, was analyzed. A repeat analysis of the near saturation sample was attempted omitting filtration and using a heated sample to dissolve insoluble solids prior to drawing an aliquot for analysis, but nearly identical sodium concentrations (207861 and 215038 mg/L) were obtained likely because of solids recrystallization inside the sampling pipette. Given the uncertainties in the initial values used in the calculations due to sample splattering described below and the measured condensate volumes, the predicted and actual total solids also compared well (less than 0.6 wt% difference), with the predicted value initially lower before tending high.

The insoluble solids results reflect the observation that the change to bulk saturation (between Sample #5 and "Near Saturation" sample) is very sudden, occurring within ~10-20 mL of condensate produced. Despite the uncertainty in the duplicate measurements, the quantity of settled insoluble solids visually observed in Figure 7 combined with the data for select samples in Table 19 indicate that the measured insoluble solids content is very possibly already above the target evaporation endpoint of 0.1 wt% insoluble solids simply from steady state concentration to 8.3 M Na. If this is true, this work has demonstrated that evaporation operations were not significantly impacted due to higher than 0.1 wt% insoluble solids.

Insoluble solids measurements were obtained by vacuum filtration of a known mass of sample through a pre-weighed 0.22 μm cellulose filter, and oven drying the filter cake. Insoluble solids analytical results for the initial sample and sample #4 are not listed in Table 19 due to wide scatter caused by an overly aggressive drying procedure initially used, which led to splattering of neighboring total solids samples onto the insoluble solids samples as well as possible splattering of the insoluble samples themselves. The initial approach, using sample 4 with the initial and near saturation samples, was based on earlier sample analysis completed on the same simulant at similar concentrations, where a three-day schedule of heating at 105, 120, and 145°C for 24 hours each was found to be sufficient. Probably due to smaller simulant quantities used in the second attempt, the near saturated concentrate samples showed the most significant splatter visually, yielding a measured total solids content of only 42.6 wt% similar to the initial sample. This suggests that voilent boiling of a viscous near-saturated concentrate caused the sample loss, suggesting that the total solids for sample 4 and initial sample results may be affected but to a lesser degree. However this splattering led to wide scatter in the insoluble solids results whose tests could not be repeated due to limited sample. Hence, samples 2 and 5 were selected as surrogates for the initial sample and sample 4, and the analysis was repeated for the near saturation sample. For this second attempt, a very conservative approach was used within initial heating to dryness at 90°C for 24 hours, followed by 24 hours at 105°C, 31 hours at 120°C, and drying to constant weight at 135°C (46 hours). The insoluble solids samples were dried with the total solids samples, with some samples requiring an additional 48-60 hours of additional drying at 135°C. This latter approach yielded more consistent data.

Another detail embedded in the insoluble solids data is a correction for solids produced from the drying of interstitial liquids in the filter cake as well as in filter paper used to capture the sample. A procedure was devised at SRTC by Charles Coleman, where a correction for the interstitial liquids could be estimated by wetting pre-weighed filter paper with the filtrate produced from insoluble solids filtration. The dried filtrate on the wetted paper mass could be used to subtract from the dried insoluble solids filter cake on filter paper. However when executing this procedure with the highly concentrated salt solutions generated during the final boildown, the filtrate was found to precipitate solids continually with time yielding a scatter of several fold sometimes yielding a correction larger than the sample mass itself. As a result, an average of three reasonable correction masses from the most dilute samples, initial sample and sample 2, was used as a correction for the interstitial liquid contribution in all cases. It is recognized that interstitial liquid contributions are likely to rise with increasing insoluble solids content, but insufficient data was available to account for this effect.

Table 20 compares the observed near-saturation concentrate anion concentration and predictions calculated by assuming ideal mixing and a pure water condensate produced from concentrating the 5.6 M Na feed. Similar to the 8.0 M Na data for the concentrate produced during steady state evaporation (Table 15), 1) agreement was good for the very soluble species nitrate and formate, and 2) other observed concentrations are 25-82% low compared to predictions. As Table 12 and 13 showed, no significant amount of the measured species were carried over into the condensate indicating that SRTC IC-Anion measurements tend to underestimate anion quantities in Hanford simulants significantly as the salt concentration increases beyond 8.0 M Na.

Analyte	Feed		Concentrate Prediction	Concentrate		Average % Difference
Na (M)	5.58		10.16	10.16 (estimated)		
Chloride (mg/L)	1308	2477	3446	1724	1740	50
Fluoride (mg/L)	2864	2455	4842	3561	3599	26
Formate (mg/L)	7179	6636	12577	11020	11412	11
Nitrate (mg/L)	145186	137961	257775	236007	236839	8
Nitrite (mg/L)	38751	36145	68185	51839	53619	23
Oxalate (mg/L)	1578	1306	2626	509	455	82
Phosphate (mg/L)	1529	2349	3531	1118	1271	66

Table 20. Actual concentrate anion concentrations versus prediction by volume additivity (ideal mixing behavior).

Despite these limitations in the data, Table 19 does indicate that the assumptions of volume additivity (ideal mixing) and pure water condensate can predict reasonably well basic bulk solution properties for AN-107 simulant evaporation.

4.6 OLI Model Comparison

After resolving the model input charge balance to simulant analytical data, Choi[31] initially employed OLI models to predict the endpoint where total insoluble solids would exceed 0.2 wt%. The constructed model predicted saturation at over 11 M Na where sodium nitrate would precipitate, matching reasonably well with the experimental 10.1 M Na final boildown concentration where the simulated waste suddenly transformed into a viscous gel-like slurry.

Choi subsequently added into the model the 14 target organic compounds to predict their distribution between the produced condensate, concentrate and off-gas during steady state evaporation from 5.8 M Na to 8.0 M Na (See Appendix C for summary of model output). Table 21 provides a comparison of the experimental values and the OLI model predicted values for

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[31] Choi, A. S., forthcoming report for Hanford Tank AN-107 Envelope C-simulant evaporation OLI modeling, *2001*.

distribution of the 14 target organic compounds between the condensate, concentrate, and off-gas phases.

		% of total feed						Condensor Vent (ug/g)
		EXPERIMENTAL DATA			OLI Model Prediction			
	Target Organic	Condensate	Concentrate	Off-gas	Condensate	Concentrate	Off-gas	
Volatile	Benzene	0.7	0.3*	*89.8*	0.4	0.0	99.5	*723*
	4-methyl-2-pentanone (MIBK)	2.1*	1.8*	*66.8*	11.9	0.2	87.9	*963*
	Toluene	0.8	0.6*	*55.0*	0.4	0.0	99.6	*330*
	1,2-dibromoethane	18.6	2.0*	*331.7*	3.5	0.1	96.4	*135*
	Chlorobenzene	1.2	0.4*	*39.0*	0.9	0.0	99.1	*258*
	1,2,3-trichloropropane	5.6*	16.2*	*0.1*	4.9	0.1	95.1	*0*
Semi-volatile	1,2,4-trichlorobenzene	4.4	6.6*	86.1	0.9	0.0	99.0	315
	Naphthalene	16.9	3.1*	79.3	2.8	0.0	97.2	274
	Hexachlorobenzene	*0.1*	71.3*	3.0	0.0	100.0	0.0	0
	Pentachlorophenol	0.0	174.0	0.0	77.8	19.4	2.8	0
	Pyrene	4.7	56.5*	2.1	88.3	6.0	5.6	0
	Bis(ethylhexyl)phthalate (BEHP)	*0.1*	61.2*	0.0	12.6	87.4	0.0	0
	Benzo(a)pyrene	0.0	55.4*	0.0	0.0	100.0	0.0	0
Pesticide	Aldrin	0.8	78.1*	*0.0*	67.7	31.3	1.0	0

* from SRTC Analytical Result

Table 21. Experimental and OLI model predicted organics distribution as a percentage of each species fed, with calculated evaporator condensor vent species concentrations.

Despite Quality Assurance qualification of some experimental values (in yellow/italic), the OLI model generally correctly predicted the relative partitioning of each target organic between condensate, concentrate and off-gas, with all volatiles and light semivolatiles (1,2,4-trichlorobenzene and naphthalene) exiting the evaporator system through the off-gas and the heavier semi-volatiles examined remaining predominantly in the evaporator concentrate. The notable exceptions were pentachlorophenol, pyrene and Aldrin where the model predicted would mostly accumulate in the evaporator condensate. This is likely due to the model predicting a separate organic phase in all aqueous streams, and possibly not accounting for secondary interactions between water and acetone to assist in the dissolution of the heavier organic compounds into the Hanford waste simulant. The organic phase in the feed was predicted to consist mainly of aldrin, BEHP, pyrene, naphthalene, and 1,2,4-trichlorobenzene. The majority of the aldrin, pyrene, and some BEHP would evaporate to form the organic layer in the condensate, while pentachlorophenol was deposited in the condensate aqueous phase. Benzo[a]pyrene was predicted to not dissolve significantly, and flowed through the model evaporator mostly in the solid phase.

The experimentally determined quantity of 1,2,3-trichloropropane in the off-gas is again expected to be low as BWXT Services, Inc. expected chemical degradation on the sorbent material or during extraction from the sorbent material.

Another notable difference between OLI model predictions and experimental data is the quantity of BEHP in the condensate. As discussed earlier, regulatory data was used to the greatest extent possible when valid data existed, with the BWXT Services regulatory results not detecting BEHP in the condensate in 5 samples and slightly (12 μg/L) in 1 sample. However, in-house SRTC analysis of four other condensate samples taken throughout the experiment all showed significant BEHP concentrations (320-360 μg/L). If the in-house analytical results for condensate BEHP were used instead, the percentage of feed BEHP exiting the evaporator dissolved in the condensate would rise to approximately 10.2%, similar to the 12.6% OLI model prediction. Unsuccessful attempts were made to identify potential causes for the discrepancy, such as sample preparation, sample storage containers, and analytical sample preparation. The only significant difference was that the in-house sample was refrigerated a few weeks longer than the regulatory sample prior to analysis, but BEHP contamination into a refrigerated sealed zero-headspace sample is not considered likely. As a result, both results are reported here.

Lastly for evaporator design purposes, total quantities of volatilized species detected in the off-gas samplers were divided by the total mass of air in-leaked at 11.5 mL/min for their respective sampling event to estimate the concentration of each target organic compound present in the evaporator condensor vent stream. The volatiles and light semi-volatile condensor vent concentrations are high due to the high input of these target organic compounds through the feed, the high degree of volatilization, and the low volume of air-inleakage.

5.0 Conclusion/Summary

The following was found from the regulatory off-gas sampling from the evaporation of Hanford RPP Tank AN-107 (Envelope C) simulated waste spiked with 14 (1.03 ppm theoretical concentration) volatiles, semi-volatiles, and pesticide target compounds:

- Steady state evaporation
    - Volatiles and light semi-volatiles (1,2,4-trichlorobenzene and naphthalene) almost completely exit the evaporator system in the off-gas.
    - Maximum target organic compound concentrations in the condensor vent gas were calculated to be approximately 130-970 ppm for lighter volatile compounds such as benzene and methyl iso-butyl ketone (MIBK).
    - Heavier semi-volatiles appear to remain in the evaporator concentrate, with slight quantities observed in the condensate and non-detection in the off-gas sampling
    - Pesticides appear to behave as a heavier semi-volatile organic compound

- Final boildown
    - At saturation, the bulk solubility of the waste was found to be approximately 94.6 g total salt (TS) per 100 g water at an estimated 10.1 M Na, or equivalently 48.6 wt% total solids.

  - Insoluble solids increase only slightly during concentration from approximately 8.3 M Na.
  - Sodium oxalate is the initial insoluble solid, and is followed by sodium carbonate decahydrate formation during concentration before saturation.
  - A very sharp transition to saturation at approximately 10.1 M Na concentrate concentration was observed, suggesting a major salt such as nitrate precipitated.

- OLI Modeling Results
  - An OLI model used to simulate evaporation predicted the saturation endpoint reasonably and predicted solution behavior at saturation well.
  - An OLI model incorporating the 14 target organic compounds predicted trends in the volatiles and semi-volatiles well, except pentachlorophenol, pyrene and aldrin. The model predicted a separate organic phase for all aqueous streams and non-dissolution of benzo[a]pyrene into the simulated waste, possibly accounting for the prediction discrepancies.
- The ICP-ES analytical results from both steady-state evaporation and final boildown suggest Hanford RPP Tank AN-107 Envelope C waste simulant appears to behave as an ideal mixture. IC-Anion data for soluble species such as nitrate and formate appears to support this, but other species do not possibly due to precipitation of small quantities of solids.
- No anti-foaming agent was needed for the evaporation or boildown of the AN-107 waste simulant.
- No evaporator scaling was observed, and the salt solution behaved as a Newtonian fluid.
- A novel method was developed to produce and stably store a Hanford caustic waste simulant spiked with volatile and semi-volatile organic compounds.

6.0 Quality Assurance

This work was carried out in accordance to the Task Technical and Quality Assurance Plan for Bench Scale LAW Evaporation with Simulants, T. B. Calloway, D. P. Lambert, BNF-003-99-0056, January 4, *2000*. Other QA and QC programs applied to the testing described in this technical report include SRTC procedures for control of measurement and testing equipment (M&TE), control of laboratory notebooks, and routine ADS QA and QC[32,33,34]. The QA program applied by SRTC for preparation and analysis of the AN-107 simulant evaporation samples complies with the requirements of NQA-1.

Analytic standards were required for all analyses performed for this study. Use of these standards is part of routine ADS QA and QC and are part of the procedures in Manual L16.1 for the operating the analytical instrument.

All M&TE used to perform the evaporation and vitrification experiments was used within the specified calibration period. Calibrations were verified as required for each mass balance instrument. A record of the calibration was routinely maintained in the logbook designated for that piece of equipment.

All laboratory data obtained in the tasks described in this technical report are included as permanent record in Hiroshi Saito's WSRC laboratory notebook WSRC-NB-2000-00043. Regulatory analytical data received from BWXT Services, Inc. is kept as permanent record in the three-ring binders labeled as**:** Data Package for AN-107 Envelope C-Simulant Regulatory Evaporation, D. M. Ferrara, WSRC-TR-2000-00528, SRT-RPP-2000-00062, December, *2000*. SRTC QC validation of the regulatory analytical data is recorded in Report of Analytical Data Validation of Regulatory Analyses for SRTC Contract WFO-98-003: Envelope C Simulant Samples; Rev. 0, Kubilius, W., ESH-EMS-2000761, August 24, *2000***.** SRTC QA also performed a surveillance of sample preparation and sample packaging of the Envelope C simulant samples for regulatory analysis at BWXT Services, Inc. (BNFL Envelope C Simulant Sample Preparation and Packaging (U), S. A. Martin, L. D. Prince, 2000-SUR-11-00015, June 22, *2000*). No deviations from the Run Plan or Task Technical and Quality Assurance Plans were found.

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[32] Westinghouse Savannah River Company, "WSRC 1Q Quality Assurance Manual", Manual 1Q, current revision.

[33] Westinghouse Savannah River Company, "WSRC L1 Savannah River Technology Center Procedures Manual", current revision.

[34] Westinghouse Savannah River Company, "WSRC L16.1 Analytical Development Section Analytical Operating Procedures Manual", current revision.

7.0 Acknowledgments

The results presented in this report are the product of the efforts of a task team made up of over twenty individuals at the Savannah River Site, BWX Technologies, Inc. (BWXT) Y-12, L.L.C., BWXT Services, Inc. and the Southwest Research Institute (SWRI). The success of this program was only possible because of the exceptional teamwork of these individuals. The authors would like to thank: Frances Williams and Nick Odom (Immobilization Technology Section, ITS) for extraordinary efforts to obtain and organize critical resources and supplies; Mary Moss, Vicki Williams, Sammie King, John Duvall, Tony Burkhalter (ITS) for valuable help in executing the experiments and packaging samples for shipment; Bill Stagg and Paul Macek (BWXT Services, Inc.) for their critical help coordinating regulatory sample shipping and analysis, and resolving analytical issues; Chee-Kai Tan (SWRI) for his timely help preparing sorbent tubes; John Young and Steve Crump (Analytical Development Section) for valuable technical input for organic spike development and timely chemical analyses; Alfred "Boots" Camp and Susan Jergensen for their help resolving Hazardous Materials Transport issues; Gary Dobos and Curt Sexton (SRS Glass Shop) for valuable input enhancing glassware design and for supplying critical parts; and Brad Stinnett (BWXT Y-12) for assistance with the off-gas sampling.

Appendices

Appendix A – Envelope C (AN-107) Simulant Recipe

A. Supernate recipe

Complete Envelope C Supernate Recipe at 7 Molar Na+

(valid as of 6/22/99)

Volume of Feed			Need, g
1000	mL	Fill the container with water	200

Transition Metals and Complexing agents

Compounds	Formula	Conc., PPM	M	Need Mass, g
Calcium Nitrate	Ca(NO3)2.4H2O	2083	1.18E-02	2.779
Cerium Nitrate	Ce(NO3)3.6H2O	98	3.01E-04	0.131
Cesium Nitrate	CsNO3	14	9.58E-05	0.019
Copper Nitrate	Cu(NO3)2.2.5H2O	66	3.78E-04	0.088
Ferric Nitrate	Fe(NO3)3.9H2O	7315	2.42E-02	9.758
Lanthanum Nitrate	La(NO3)3.6H2O	85	2.61E-04	0.113
Lead nitrate	Pb(NO3)2	0	0.00E+00	0.000
Magnesium Nitrate	Mg(NO3)2.6H2O	158	8.21E-04	0.211
Manganous Chloride	MnCl2.4H2O	1213	8.18E-03	1.619
Neodymium Nitrate	Nd(NO3)3.6H2O	174	5.31E-04	0.233
Nickel Nitrate	Ni(NO3)2.6H2O	1571	7.21E-03	2.096
Potassium Nitrate	KNO3	2755	3.64E-02	3.675
Strontium Nitrate	Sr(NO3)2	8	5.16E-05	0.011
Zinc Nitrate	Zn(NO3)2.6H2O	123	5.53E-04	0.165
Zirconyl Nitrate		114	6.13E-04	0.153
EDTA*	Na2EDTA	4343	1.56E-02	5.794
HEDTA*	HEDTA	1294	6.21E-03	1.727
Sodium Gluconate		2349	1.44E-02	3.134
Glycolic Acid		16112	1.98E-01	21.494
Citric Acid		5648	3.59E-02	7.535
Nitrilotriacetic Acid		341	2.38E-03	0.455
Iminodiacetic Acid		3613	3.62E-02	4.820
Boric acid	H3BO3	120	2.58E-03	0.160
Sodium Chloride	NaCl	1088	2.48E-02	1.452
Sodium Fluoride	NaF	176	5.59E-03	0.235
Sodium Chromate	Na2CrO4	0	0.00E+00	0.000
Sodium Sulfate	Na2SO4	7299	6.86E-02	9.737
Potassium Molybdate	K2MoO4	53	2.98E-04	0.071

		Need, g
In separate container mix the following:	Fill the container with water	200

Add	Formula	Conc., PPM	M	Need, g
Sodium Hydroxide	NaOH	15047	5.02E-01	20.073
Aluminum Nitrate	Al(NO3)3.9H2O	3211	1.14E-02	4.284
Sodium Phosphate	Na3PO4.12H2O	2658	9.33E-03	3.546
Sodium Formate	NaHCOO	9401	1.84E-01	12.541
Sodium Acetate	NaCH3COO.3H2O	1418	1.39E-02	1.891
Sodium Oxalate	Na2C2O4	752	7.49E-03	1.004

*(EDTA=Ethylenediaminetetraacetic Acid Disodium Salt Dihydrate)

*(HETDA=N-(2-Hydroxyethyl)ethylenediaminetriacetic Acid))

Mix thoroughly. Then add this solution to the container. Then

Add	Formula	Conc., PPM	M	Need, g
Sodium Carbonate	Na2CO3	88703	1.12E+00	118.330

Mix thoroughly. Then

Add	Formula	Conc., PPM	M	Need, g
Sodium Nitrate	NaNO3	178069	2.79E+00	237.544
Sodium Nitrite	NaNO2	54741	1.06E+00	73.024

Mix thoroughly and dilute to the mark.

The final addition of water would be = 385.02 grams
(grams based upon a density of 1.334 g/mL)

Final Weight, grams	1334.00	(2.93 lbs.)

B. Entrained solids recipe

Envelope C Entrained Solids

Approximate Supernate Volume	1000.0 mL

Approximate Supernate Density	1.334 g/mL
Approximate Supernate Mass	1334.0 grams

At 0.5 wt% solids loading	6.70 grams

Total Mass Supernate + Solids	1340.7 grams

Compound	Compound	Concentration	Needed
Name	Formula	g/100g solids	grams
Alumina	Al2O3	5.10%	0.34
Calcium Phosphate, tribasic	Ca3(PO4)2	0.10%	0.01
Chromium Oxide	Cr2O3	0.40%	0.03
Ferric Oxide	Fe3O2: 1-2 micron	2.40%	0.16
Ferric Oxide	Fe3O2: 5-10 micron	2.40%	0.16
Manganese Oxide	MnO2: 1-2 micron	1.55%	0.10
Manganese Oxide	MnO2: 5-10 micon	1.55%	0.10
Sodium Aluminosilicate	Na2OAl2O3(SiO2).2.5H2O	1.60%	0.11
Sodium Oxalate	Na2C2O4	34.20%	2.29
Sodium Carbonate Monohydrate	Na2CO3.H2O	32.30%	2.17
Sodium Fluoride	NaF	5.00%	0.34
Sodium Sulfate Decahydrate	Na2SO4.10H2O	4.10%	0.27
Sodium Phosphate Dodecahydrate	Na3PO4.12H2O	9.30%	0.62

Total	100.00%	6.70

C. Sr/TRU precipitation recipe

1. In a container, place a fixed volume of 7 M Na Envelope C supernate with entrained solids, agitate, and raise solution temperature to 50 ± 5°C.

2. Add 166.7 mL de-ionized and filtered water per liter of 7 M Na supernate to dilute solution to 6 M Na. Allow solution to mix 10-15 minutes.

3. Slowly add 55.6 mL 19 M NaOH solution per liter of 6 M Na supernate solution, and allow solution to mix 10-15 minutes.

4. Slowly add 90.5 mL 1 M $Sr(NO_3)_2$ solution per liter of 6 M Na supernate solution, and allow solution to mix 10-15 minutes.

5. Slowly add 60.3 mL 1 M $NaMnO_4$ solution per liter of 6 M Na supernate solution.

6. Continue agitation and maintain 50 ± 5°C temperature for 4 hours.

7. Allow mixture to cool.

Appendix B – Regulatory Analysis Raw Data Summary

This section contains the regulatory data from this study in two forms:

- Summary of raw data as received from BWXT Services, Inc. contained in reference:

  Ferrara, D. M., "Data Package for AN-107 Env. C-simulant Regulatory Evaporation", WSRC-TR-2000-00528, SRT-RPP-2000-00062, *2000*.

- Data after validation by Savannah River Technology Center (SRTC) Quality Assurance and Quality Control (QA/QC) documented in reference:

  Kubilius, W., "Report of Analytical Data Validation of Regulatory Analyses for SRTC Contract WFO-98-003: Envelope C Simulant Samples; Rev. 0", Internal memorandum, ESH-EMS-2000761, August 24, *2000*.

  and correction by process, field, trip, and reagent blank data.

A. Raw Data

BWXT VOA Raw Data by Stream

24-Aug-00
Hiroshi Saito

Liquid Concentration (ug/L)

Feed

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAfd1	VOA Feed Sample #1 (6/6/00, 2300)	**1480**		**2740**		**1110**		*78.9*	J	**1280**		800	U	**1170**		**1580**	
RGNEVPVAfd2	VOA Feed Sample #2 (6/6/00, 2300)	**1380**		**2410**		**1020**		*66.3*	J	**1070**		800	U	*529*	J	**1080**	
300145159	pre-run feed sample (7E-15, 6/5/00, late PM)	**200**		**260**		**170**		**0**		**120**		**130**					
300145160	mid-VOST feed sample (6/7/00, 0300, 24 hr)	**220**		**270**		**150**		**1.4**		**110**		**150**					
300145161	mid-SVOST feed sample (6/7/00, 2210, 7 hr)	**210**		**280**		**160**		**0**		**120**		**130**					

Liquid Concentration (ug/L)

Concentrate

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAcc1	VOA Concentrate Sample #1 (6/6/00, 1600)	*20.9*	J	*54.5*	J	*11.8*	J	400	U	*13.2*	J	400	U	*19.1*	J	*21.6*	J
RGNEVPVAcc2	VOA Concentrate Sample #2 (6/6/00, 2230)	400	U	400	U	400	U	400	U	*13*	J	400	U	*7.1*	J	*17.3*	J
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**12**		**77**		**8.2**		**0**		**7.6**		**170**					
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**2.2**		**48**		**11**		**1.9**		**5.8**		**160**					
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**5.3**		**26**		**11**		**1.8**		**5.4**		**190**					
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**6.3**		**120**		**4.5**		**4.5**		**5.7**		**400**					

Liquid Concentration (ug/L)

Condensate

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAcd1	VOA Condensate Sample #1 (6/6/00, 1625)	**32.7**		*712*	E	**25.9**		**41.6**		**44**		10	U	**60.8**		*257*	E
RGNEVPVAcd1DL	Above, with 10 dilution factor	*26.8*	DJ	*688*	D	*18.3*	DJ	*36.2*	DJ	*31*	DJ	100	U	*40.6*	DJ	**200**	D
RGNEVPVAcd2	VOA Condensate Sample #2 (6/6/00, 2230)	*12.9*	J	*479*	E	*10.9*	J	*18.1*	J	*17.5*	J	20	U	**25.5**		**151**	
RGNEVPVAcd2MS	Method spike	93.4		484	E	89.7		17.8	J	98.8		62.1		22.1		139	
RGNEVPVAcd2MSD	Method spike duplicate	93.5		495	E	90.3		19	J	101		62.4		25.5		152	
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**7.2**		**130**		**26**		**2.8**		**5.5**		**120**					
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**1.2**		**160**		**4.1**		**2.2**		**6.6**		**170**					
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr	**5.3**		**26**		**11**		**1.8**		**5.4**		**190**					
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**25**		**340**		**18**		**19**		**28**		**200**					

Liquid Concentration (ug/L)

Pump Trap Liquids

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene		
RGNEVPVATrap1	Sample Pump Liquids Sample #1 (6/7/00, 1500)	*1460*	E	*28400*	E	*1200*	E	*2920*	E	*272*	E	10	U	*483*	E	*832*	E	toluene-d8 recovery high so diluted; split total liquid with two below
RGNEVPVATrap1DL	Above, with 100 dilution factor	*164*	DJ	*7250*	D	*115*	DJ	*339*	DJ	*212*	DJ	1000	U	*445*	DJ	**2260**	D	
RGNEVPVATrap2	Sample Pump Liqu. Samp. #2, 100X dil. (6/7,150	*226*	J	7760		*176*	J	*392*	J	*309*	J	1000	U	*678*	J	**2820**		toluene & benzene recoveries slightly low; split with above and below
RGNEVPVATrap2MS	Method spike	4820		8010		4750		*378*	J	4920		1000	U	*573*	J	2590		toluene & benzene recoveries in MS's okay, so RPD's a bit high
RGNEVPVATrap2MSD	Method spike duplicate	3940		7280		3870		*336*	J	4160		1000	U	*482*	J	2350		
300145170	in-house sample, no headspace (6/7/00, 1500)	**49**		**1200**		**33**		**76**		**35**		**110**						

Solid Content (ng)

Sorbent Tubes

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene		
RGNEVPVATenax1	Sample Tenax Tube #1 (6/7/00, 1500)	5000000	U	*1160000*	J	*1140000*	J	5000000	U	*3000000*	J	5000000	U	**48800000**		**55900000**		40% recoveries, ~100000 factor dilution needed
RGNEVPVATenax2	Sample Tenax Tube #2 (6/7/00, 1500)	11900	E	230000	E	25300	E	21700	E	658000	E	50	U	**434**		2090	E	Thermal desorption result, where quantities overblew detector
RGNEVPVAAnasorb1	Sample Anasorb Tube (6/7/00, 1500)	**24700000**		**31500000**		**10100000**		**4600000**		**5160000**		4500000	U	4500000	U	4500000	U	20% recoveries, ~100000 factor dilution needed

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
J = estimated value (e.g., quantity between MDL and MRL)
U = Undetected analyte (searched for)
E = Quantity exceeds upper level of calibration range
R = SRTC QA rejected result

Data Guide

🟨 *Italic text/Yellow box = qualified data*
🟩 **Bold text/Green box = Significant/good data**
🟥 Bold box/red box = corrected data

										Liquid Concentration (ug/L)								
Gas Sampler Condensate				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVACond1	Sampler Condensate Sample #1 (6/7/00, 1500)	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced
RGNEVPVACond2	Sampler Condensate Sample #2 (6/7/00, 1500)	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced
	in-house sample, no headspace	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced

										Liquid Concentration (ug/L)								
Process Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVP1	Process Blank Liquid Sample	*0.5*	J	*3.5*	J	20	U	20	U	20	U	20	U	*0.27*	J	*1.2*	J	Bottle 1 of 1, Simulant + ca. 800 ppm acetone, no headspace
										Solid Content (ng)								
RGNEVPVPTenax1	Proc. Blank Tenax Tube #1																	
RGNEVPVPTenax2	Proc. Blank Tenax Tube #2	**202**		**434**		**549**		50	U	50	U	50	U	**75.2**		**251**		
RGNEVPVPAnasorb1	Proc. Blank Anasorb Tube	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	
										Liquid Concentration (ug/L)								
RGNEVPVPCond	Proc. Blank Gas Sampler Condensate	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced
RGNEVPVPTrap	Proc. Blank Pump Trap Liquids	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	No headspace, fill with reagent water

										Liquid Concentration (ug/L)								
Field Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVF1	Equipment Field Blank (6/4/00, 1715)	20	U	20	U	20	U	20	U	20	U	20	U	20	U	20	U	Equipment Field Blank, NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF2	Day #2 for Feed Sample #2 (6/5/00, 2200)	20	U	20	U	20	U	20	U	20	U	20	U	20	U	20	U	Day #2 for Feed Sample #2, NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF3	Day #2 for Feed Sample #1 (6/5/00, 2200)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Day #2 for Feed Sample #1, NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF4	Day #2 for Cond/Conc (1of 2) (6/5/00, 2200)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Day #2 for Cond/Conc (1of 2), NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF5	Day #3 for Cond/Conc (2 of 2) (6/7/00, 1115)	20	U	20	U	20	U	20	U	20	U	20	U	20	U	20	U	Day #3 for Cond/Conc (2 of 2), NaOH solution bottle-to-bottle pour, no headspace
										Solid Content (ng)								
RGNEVPVFTenax1	Field blank associated with Process Blank																	Tube 1 of 4, Field blank associated with Process Blank
RGNEVPVFTenax2	Field blank associated with Process Blank	50	U	50	U	**374**		50	U	50	U	50	U	*22.3*	J	*45.4*	J	Tube 2 of 4, Field blank associated with Process Blank
RGNEVPVFAnasorb1	Field blank associated with Process Blank	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	Tube 1 of 2, Field blank associated with Process Blank
RGNEVPVFTenax3	Per Method 0031																	Tube 3 of 4, Per Method 0031
RGNEVPVFTenax4	Per Method 0031	50	U	50	U	**388**		50	U	50	U	50	U	*7.5*	J	*20.3*	J	Tube 4 of 4, Per Method 0031
RGNEVPVFAnasorb2	Per Method 0031	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	Tube 2 of 2, Per Method 0031
RGNEVPVF1	Field blank for Proc. Blank Condensate	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced

										Liquid Concentration (ug/L)								
Trip Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVT1	Day #1-Proc. Blanks, Reagent H2O (6/4, 1945)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/6/00
	(6/6/00, 0300)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/7/00
RGNEVPVT2	Day #2-1st half VOST run, Reag. H2O (6/6, 0300	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/7/00
	(6/7/00, 1800)	10	U	10	U	*1.4*	J	10	U	10	U	10	U	10	U	10	U	Received 6/9/00, Extra, IGNORE
RGNEVPVT3	Day #3-2nd half VOST run, Reag. H2O (6/7, 011	10	U	10	U	*1.3*	J	10	U	10	U	10	U	10	U	10	U	
										Solid Content (ng)								
RGNEVPVTTenax1	Trip blanks, Day #1 (Process Blanks)	-----		-----		-----		-----		-----		-----		-----		-----		
RGNEVPVTTenax2		-----		-----		-----		-----		-----		-----		-----		-----		
RGNEVPVTTenax3	Trip blanks, Day #2 (Field Blanks)																	
RGNEVPVTTenax4		50	U	**156**		**154**		50	U	50	U	50	U	**174**		**736**		
RGNEVPVTTenax5	Trip blanks, Day #3 (with Sample Tube)																	
RGNEVPVTTenax6		50	U	50	U	**561**		50	U	50	U	50	U	*33.2*	J	**151**		
RGNEVPVTAnasorb1	Trip blanks, Day #1 (Process Blanks)	-----		-----		-----		-----		-----		-----		-----		-----		
RGNEVPVTAnasorb2	Trip blanks, Day #2 (Field Blanks)	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	
RGNEVPVTAnasorb3	Trip blanks, Day #3 (with Sample Tube)	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	25000	U	

										Liquid Concentration (ug/L)								
Reagent Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVRH2O1	VOA Reagent Water Blank	10	U	10	U	**19.3**		10	U	10	U	10	U	10	U	10	U	DI H2O used to remove headspace, no headspace
RGNEVPVRH2O2	VOA Reagent Water Blank	10	U	10	U	*7.8*	J	10	U	10	U	10	U	10	U	10	U	DI H2O used to remove headspace, no headspace

BWXT SVOA Raw Data by Stream

24-Aug-00
Hiroshi Saito

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
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Data Guide

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Concentration (ug/L)

Feed Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAfd1	Feed Sample #1 (6/6/00, 2300)	500	U	500	U	*410*	J	500	U	500	U	200	J	500	U
RGNEVPSAfd2	Feed Sample #2 (6/6/00, 2300)	*17*	J	100	U	**430**		*27*	J	100	U	15000	E	100	U
RGNEVPSAfd3	Feed Sample #3 (6/6/00, 2300)	*41*	J	*15*	J	**820**		*81*	J	100	U	98000	E	100	U
RGNEVPSAfd4	Feed Sample #4 (6/7/00, 2130)	*55*	J	300	U	**1000**		*72*	J	300	U	**2800**		300	U
RGNEVPSAfd4MS	Method Spike	210	J	311	U	1000		300	U	300	U	2800		300	U
RGNEVPSAfd4MSD	Method Spike Duplicate	210	J	55	J	1100		330	U	330	U	2900		330	U
RGNEVPSAfd5	Feed Sample #5 (6/7/00, 2130)	1000	U	1000	U	**1000**		1000	U	1000	U	**2900**		1000	U
RGNEVPSAfd6	Feed Sample #6 (6/7/00, 2130)	2000	U	2000	U	*850*	J	2000	U	2000	U	2000	U	2000	U
300145159	pre-run feed sample (7E-15, 6/5/00, late PM)	**610**		**570**		**1110**		**0**		**930**		**1040**		**1310**	
300145160	mid-VOST feed sample (6/7/00, 0300, 24 hr)	**580**		**600**		**1070**		**0**		**930**		**1030**		**1380**	
300145161	mid-SVOST feed sample (6/7/00, 2210, 7 hr)	**580**		**530**		**950**		**0**		**930**		10		**1690**	

Concentration (ug/L)

Concentrate Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAcc1	Concentrate Sample #1 (6/6/00, 1357)	30	U	30	U	13	J	**180**		30	U	**39**		30	U
RGNEVPSAcc1MS	Method Spike	90		30	U	39		150		30	U	120		30	U
RGNEVPSAcc1MSD	Method Spike Duplicate	95		31	U	8	J	230		31	U	35		31	U
RGNEVPSAcc2	Concentrate Sample #2 (6/6/00, 2310)	21	U	21	U	**210**		**130**		**84**		**230**		21	U
RGNEVPSAcc3	Concentrate Sample #3 (6/7/00, 0350)	51	U	51	U	**360**		**140**		51	U	**340**		51	U
RGNEVPSAcc4	Concentrate Sample #4 (6/7/00, 1800)	100	U	100	U	**330**		100	U	100	U	**280**		100	U
RGNEVPSAcc5	Concentrate Sample #5 (6/8/00, 1152)	30	U	30	U	**470**		**130**		30	U	68000	E	30	U
RGNEVPSAcc6	Concentrate Sample #6 (6/8/00, 2045)	2000	U	2000	U	1200	J	2000	U	2000	U	2000		2000	U
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**57**		**36**		**720**		**0**		**690**		**920**		**950**	
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**75**		**35**		**940**		**0**		**830**		**920**		**1290**	
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**35**		**0**		**700**		**0**		**670**		**800**		**1070**	
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**56**		**30**		**970**		**0**		**830**		**1000**		**1340**	

Concentration (ug/L)

Condensate Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAcd1	Condensate Sample #1 (6/6/00, 1302)	**45**		**160**		*3*	J	10	U	**130**		**12**		10	U
RGNEVPSAcd2	Condensate Sample #2 (6/6/00, 2132)	**32**		**140**		*4*	J	20	U	**180**		20	U	20	U
RGNEVPSAcd3	Condensate Sample #3 (6/7/00, 1321)	**110**		**380**		50	U	50	U	**140**		50	U	50	U
RGNEVPSAcd4	Condensate Sample #4 (6/7/00, 1923)	**45**		*190*	E	11	U	11	U	**83**		11	U	11	U
RGNEVPSAcd5	Condensate Sample #5 (6/8/00, 0705)	**66**		**240**		20	U	20	U	**110**		20	U	20	U
RGNEVPSAcd6	Condensate Sample #1 (6/8/00, 2045)	**110**		**420**		50	U	50	U	**110**		50	U	50	U
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**0**		**100**		**0**		**0**		**200**		**360**		**0**	
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**0**		**100**		**0**		**0**		**190**		**330**		**0**	
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr)	**90**		**390**		**0**		**0**		**270**		**320**		**0**	
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**120**		**490**		**0**		**0**		**210**		**320**		**0**	

Concentration (ug/L)

Pump Trap Liquids Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
RGNEVPSATrap1	Pump Trap Sample #1 (6/9/00, 0300)	**340**		**1600**		230	U	230	U	*38*	J	230	U	230	U	Split with two below
RGNEVPSATrap2	Pump Trap Sample #2 (6/9/00, 0300)	*270*	J	1300		280	U	280	U	*35*	J	280	U	280	U	Split with above and below
300145170	in-house VOST sample, no SVOST (6/7/00, 1500)	**500**		**1430**		**0**		**0**		**91**		**3300**		**0**		
RGNEVPSAExLinRinse	post-SVOST run MeOH/MeCl2 rinse of line to pump	3300	U	3300	U	**34000**		3300	U	26000		3300	U	3300	U	

Mass (ug)

Sorbent Tubes Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
RGNEVPSAXad	Off-gas Sampling Tube (6/9/00, 0300)	**9900**		**8600**		1000	U	1000	U	1000	U	1000	U	1000	U	Diluted by 100

Concentration (ug/L)

Gas Sampler Condensate		1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
Sample Name	Sample Description															
RGNEVPSACond1	Off-gas Sampler Condensate #1 (6/9/00, 0300)	1000	U	1000	U	1000	U	1000	U	1000	U	1000	U	1000	U	Usually split with below
RGNEVPSACond2	Off-gas Sampler Condensate #2 (6/9/00, 0300)	-----		-----		-----		-----		-----		-----		-----		Not generated due to low volume
	in-house sample															

Concentration (ug/L)

Gas Sampler Rinse		1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
Sample Name	Sample Description															
RGNEVPSARinse	Off-gas Sampler Glassware Rinse (6/9/00, 0300)	960	U	960	U	960	U	960	U	960	U	960	U	960	U	Liquid used to rinse sampling system after sampling

Concentration (ug/L)

Process Blanks	(6/4/00)	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
Sample Name	Sample Description															
RGNEVPSP1	Bottle 1 of 3, Simulant + ca. 800 ppm acetone	10	U	10	U	*5*	J	*3*	J	10	U	**16**		10	U	Bottle 1 of 3, Simulant + ca. 800 ppm acetone
RGNEVPSP1Ri	????	10	U	10	U	*8*	J	*3*	J	10	U	**30**		10	U	
RGNEVPSP2	Bottle 2 of 3, Simulant + ca. 800 ppm acetone	150	U	150	U	150	U	150	U	150	U	150	U	150	U	Bottle 2 of 3, Simulant + ca. 800 ppm acetone
RGNEVPSP2MS	Method Spike	64	J	150	U	150	U	150	U	150	U	150	U	150	U	
RGNEVPSP2MSD	Method Spike Duplicate	84	J	150	U	150	U	150	U	150	U	110	J	150	U	
RGNEVPSP3	Bottle 3 of 3, Simulant + ca. 800 ppm acetone	10	U	10	U	10	U	10	U	10	U	**12**		10	U	Bottle 3 of 3, Simulant + ca. 800 ppm acetone
								Mass (ug)								
RGNEVPSPXad		10	U	10	U	10	U	10	U	10	U	10	U	10	U	Went dry during extraction
								Concentration (ug/L)								
RGNEVPSPTrap	For any pump trap liquid from process blank	3300	U	3300	U	3300	U	3300	U	3300	U	3300	U	3300	U	
RGNEVPSPCond	For any condensate from process blank	-----		-----		-----		-----		-----		-----		-----		
RGNEVPSPRinse	1:1 (v/v) Methanol/Methylene Chloride Wash Liquid	120	U	120	U	120	U	120	U	120	U	120	U	120	U	

Concentration (ug/L)

Field Blanks		1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
Sample Name	Sample Description															
RGNEVPSF1	Day #1, Bottle 1 of 3 (6/4/00, 1715)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF2	Day #1, Bottle 2 of 3 (6/4/00, 1715)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF3	Day #1, Bottle 3 of 3 (6/4/00, 1715)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF4	Day #2, for Feed Sample, Bottle 1 of 3 (6/5/00, 2200	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF5	Day #2, for Feed Sample, Bottle 2 of 3 (6/5/00, 2200	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF6	Day #2, for Feed Sample, Bottle 3 of 3 (6/5/00, 2200	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF7	For Cond/Conc, Bottle 1 (Day 2) of 3 (6/5/00, 2200)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF8	For Cond/Conc, Bottle 2 (Day 3) of 3 (6/6/00, 1000)	10	U	10	U	10	U	10	U	*1*	J	10	U	10	U	Received 6/8
	(6/7/00, 2130)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/9
RGNEVPSF9	For Cond/Conc, Bottle 3 (Day 3) of 3 (6/7/00, 2130)	10	U	10	U	10	U	10	U	10	U	*0.3*	J	10	U	
RGNEVPSF10	Day #3, for Feed Sample, Bottle 1 of 3 (6/7/00, 2130	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF11	Day #3, for Feed Sample, Bottle 2 of 3 (6/8/00, 2100	10	U	10	U	10	U	10	U	*6*	J	10	U	10	U	
RGNEVPSF12	Day #3, for Feed Sample, Bottle 3 of 3 (6/8/00, 2100	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF13	For Cond/Conc, Bottle 1 (Day 4) of 3 (6/7/00, 1830)	10	U	10	U	10	U	10	U	*1*	J	10	U	10	U	
RGNEVPSF13DL	Above, with 5.0 dilution factor	150	U	150	U	520	D	150	U	150	U	*600*	D	150	U	
RGNEVPSF13MS	Method Spike	110		33	U	760	E	250		120		86000	E	33	U	
RGNEVPSF13MSD	Method Spike Duplicate	100		33	U	710	E	200		410		120000	E	33	U	
RGNEVPSF14	For Cond/Conc, Bottle 2 (Day 4) of 3 (6/7/00, 1830)	10	U	10	U	10	U	10	U	10	U	*0.3*	J	10	U	
RGNEVPSF15	For Cond/Conc, Bottle 3 (Day 5) of 3															
								Mass (ug)								
RGNEVPSFXad1	Field blank associated with process blank	-----		-----		-----		-----		-----		-----		-----		Went dry during extraction, and then lost during concentration step
RGNEVPSFXad2	Per Method 0010	*4*	J	*4*	J	10	U	10	U	10	U	10	U	10	U	Went dry during extraction
								Concentration (ug/L)								
RGNEVPSFRinse1	Field blank associated with process blank	130	U	130	U	130	U	130	U	130	U	130	U	130	U	
RGNEVPSFRinse2	Per Method 0010	570	U	570	U	570	U	570	U	570	U	*64*	J	570	U	
RGNEVPSFCond	Reagent water	-----		-----		-----		-----		-----		-----		-----		

Concentration (ug/L)

Reagent Blanks		1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
Sample Name	Sample Description															
RGNEVPSRMeth	Fresh 1:1 (v/v) MeOH/MeCl2 Wash Liquid	85	U	85	U	85	U	85	U	85	U	85	U	85	U	

BWXT Aldrin Raw Data by Stream

24-Aug-00
Hiroshi Saito

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
J = estimated value (e.g., quantity between MDL and MRL)
U = Undetected analyte (searched for)
E = Quantity exceeds upper level of calibration range
R = SRTC QA rejected result
P = High scatter in duplicate data, lower value reported

Data Guide

Italic text/Yellow box = qualified data
Bold text/Green box = Significant/good data
Bold box/red box = corrected data

Feed

Sample Name	Sample Description	Result		Units	
RGNEVPPAfd1	Feed Sample #1 (6/6/00, 2300)	0.160		ug/L	
RGNEVPPAfd1MS	Method Spike	0.180		ug/L	
RGNEVPPAfd1MSD	Method Spike Duplicate	0.190	P	ug/L	
RGNEVPPAfd2	Feed Sample #2 (6/6/00, 2300)	*0.089*	P	ug/L	
RGNEVPPAfd3	Feed Sample #3 (6/6/00, 2300)	*0.079*	P	ug/L	caustic recoveries bad??
RGNEVPPAfd4	Feed Sample #4 (6/7/00, 2130)	0.100	U	ug/L	
RGNEVPPAfd5	Feed Sample #5 (6/7/00, 2130)	*0.790*	P	ug/L	
RGNEVPPAfd6	Feed Sample #6 (6/7/00, 2130)	0.100	U	ug/L	
300145159	pre-run feed sample (7E-15, 6/5/00, late PM)	**1060**		ug/L	
300145160	mid-VOST feed sample (6/7/00, 0300, 24 hr)	**1030**		ug/L	
300145161	mid-SVOST feed sample (6/7/00, 2210, 7 hr)	**1020**		ug/L	

Concentrate

Sample Name	Sample Description	Result		Units	
RGNEVPPAcc1	Concentrate Sample #1 (6/6/00, 0420)	*54*	EP	ug/L	
RGNEVPPAcc1DL	Above, with 100 dilution factor	*82*	DP	ug/L	
RGNEVPPAcc1MS	Method Spike	13	EP	ug/L	
RGNEVPPAcc1MSD	Method Spike Duplicate	0.29		ug/L	
RGNEVPPAcc2	Concentrate Sample #2 (6/7/00, 0120)	*320*	E	ug/L	
RGNEVPPAcc3	Concentrate Sample #3 (6/7/00, 0450)	*0.74*	P	ug/L	
RGNEVPPAcc4	Concentrate Sample #4 (6/8/00, 0140)	*0.11*	P	ug/L	caustic recoveries bad??
RGNEVPPAcc5	Concentrate Sample #5 (6/8/00, 1650)	**0.37**		ug/L	
RGNEVPPAcc6	Concentrate Sample #6 (6/9/00, 0030)	*8*	P	ug/L	
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**430**		ug/L	
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**580**		ug/L	
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**340**		ug/L	
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**5300**		ug/L	

Condensate

Sample Name	Sample Description	Result		Units
RGNEVPPAcd1	Condensate Sample #1 (6/6/00, 0857)	*28*	P	ug/L
RGNEVPPAcd2	Condensate Sample #2 (6/7/00, 0240)	**17**		ug/L
RGNEVPPAcd3	Condensate Sample #3 (6/7/00, 0800)	*28*	P	ug/L
RGNEVPPAcd4	Condensate Sample #4 (6/8/00, 0125)	*22*	P	ug/L
RGNEVPPAcd5	Condensate Sample #5 (6/8/00, 1438)	**33**		ug/L
RGNEVPPAcd6	Condensate Sample #6 (6/9/00, 0220)	*24*	EP	ug/L
RGNEVPPAcd6DL	Above, with 50 dilution factor	*24*	DP	ug/L
RGNEVPPAcd6MS	Method Spike	16	EP	ug/L
RGNEVPPAcd6MSD	Method Spike Duplicate	16	EP	ug/L
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**0**		ug/L
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**0**		ug/L
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr)	**51**		ug/L
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**60**		ug/L

Pump Trap Liquids

Sample Name	Sample Description	Result		Units	
RGNEVPSATrap1	Pump Trap Sample #1 (6/9/00, 0300)				Split with two below
RGNEVPSATrap2	Pump Trap Sample #2 (6/9/00, 0300)				Split with above and below
300145170	in-house VOST sample, no SVOST (6/7/00, 1500)	**58**		ug/L	

Sorbent Tubes

Sample Name	Sample Description	Result		Units		
RGNEVPSAXad	Off-gas Sampling Tube (6/9/00, 0300)	-----				Went dry during extraction, then lost during concentration

Gas Sampler Condensate

Sample Name	Sample Description	Result		Units		
RGNEVPSACond1	Off-gas Sampler Condensate #1 (6/9/00, 0300)					Split with two below
RGNEVPSACond2	Off-gas Sampler Condensate #2 (6/9/00, 0300)	-----				Split with above and below
	in-house sample					

Gas Sampler Rinse

Sample Name	Sample Description	Result		Units		
RGNEVPSARinse	Off-gas Sampler Glassware Rinse (6/9/00, 0300)					Liquid used to rinse sampling system after sampling

Process Blanks (6/5/00)

Sample Name	Sample Description	Result		Units		
RGNEVPPP1	Bottle 1 of 3, Simulant + ca. 800 ppm acetone	0.050	U	ug/L		Bottle 1 of 3, Simulant + ca. 800 ppm acetone
RGNEVPPP2	Bottle 2 of 3, Simulant + ca. 800 ppm acetone	0.050	U	ug/L		Bottle 2 of 3, Simulant + ca. 800 ppm acetone
RGNEVPPP3	Bottle 3 of 3, Simulant + ca. 800 ppm acetone	0.050	U	ug/L		Bottle 3 of 3, Simulant + ca. 800 ppm acetone
RGNEVPSPXad						
RGNEVPSPTrap	For any pump trap liquid from process blank					
RGNEVPSPCond	For any condensate from process blank	-----				
RGNEVPSPRinse	1:1 (v/v) Methanol/Methylene Chloride Wash Liquid					

Field Blanks

Sample Name	Sample Description	Result		Units		
RGNEVPPF1	Day #1, Bottle 1 of 3 (6/4/00, 1715)	0.050	U	ug/L		
RGNEVPPF2	Day #1, Bottle 2 of 3 (6/4/00, 1715)					
RGNEVPPF3	Day #1, Bottle 3 of 3 (6/4/00, 1715)	0.050	U	ug/L		
RGNEVPPF4	Day #2, for Feed Sample, Bottle 1 of 3 (6/5, 2200)	0.050	U	ug/L		
RGNEVPPF5	Day #2, for Feed Sample, Bottle 2 of 3 (6/5, 2200)	0.050	U	ug/L		
RGNEVPPF6	Day #2, for Feed Sample, Bottle 3 of 3 (6/5, 2200)	0.050	U	ug/L		
RGNEVPPF7	For Cond/Conc, Bottle 1 (Day 2) of 3 (6/5/00, 2200)	0.050	U	ug/L		
RGNEVPPF8	For Cond/Conc, Bottle 2 (Day 3) of 3 (6/6/00, 1500)	**0.092**		ug/L	received 6/8/00	
	(6/7/00, 2130)	0.050	U	ug/L	received 6/9/00	
RGNEVPPF9	For Cond/Conc, Bottle 3 (Day 3) of 3 (6/7/00, 2130)	0.050	U	ug/L		
RGNEVPPF10	Day #3, for Feed Sample, Bottle 1 of 3 (6/7, 2130)	0.050	U	ug/L		
RGNEVPPF11	Day #3, for Feed Sample, Bottle 2 of 3					
RGNEVPPF12	Day #3, for Feed Sample, Bottle 3 of 3 (6/7, 1830)	0.050	U	ug/L		
RGNEVPPF13	For Cond/Conc, Bottle 1 (Day 4) of 3 (6/7, 1830)	0.050	U	ug/L		
RGNEVPPF14	For Cond/Conc, Bottle 2 (Day 5) of 3	0.050	U	ug/L		
RGNEVPPF15	For Cond/Conc, Bottle 3 (Day 5) of 3	0.050	U	ug/L		
RGNEVPSFXad1	Field blank associated with process blank					
RGNEVPSFXad2	Per Method 0010					
RGNEVPSFRinse1	Field blank associated with process blank					
RGNEVPSFRinse2	Per Method 0010					
RGNEVPSFCond	Reagent water	-----				

Reagent Blanks

Sample Name	Sample Description	Result		Units		
RGNEVPSRMeth	Fresh 1:1 (v/v) MeOH/MeCl2 Wash Liquid					

B. Validated and Corrected Data

VOA Data by Stream

1-Dec-00
Hiroshi Saito

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
J = estimated value (e.g., quantity between MDL and MRL)
U = Undetected analyte (searched for)
E = Quantity exceeds upper level of calibration range
R = SRTC QA rejected result

Data Guide

Italic text/Yellow box = qualified data
Bold text/Green box = Significant/good data
Bold box/red box = corrected data

BWXT Data Validated by WSRC QA

Liquid Concentration (ug/L)

Feed

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAfd1	VOA Feed Sample #1 (6/6/00, 2300)	**1480**		*2740*	J	**1110**		*78.9*	J	**1280**		800	U	**1170**		**1580**	
RGNEVPVAfd2	VOA Feed Sample #2 (6/6/00, 2300)	**1380**		*2410*	J	**1020**		*66.3*	J	**1070**		800	U	*529*	J	**1080**	
300145159	pre-run feed sample (7E-15, 6/5/00, late PM)	**200**		**260**		**170**		**0**		**120**		**130**					
300145160	mid-VOST feed sample (6/7/00, 0300, 24 hr)	**220**		**270**		**150**		**1.4**		**110**		**150**					
300145161	mid-SVOST feed sample (6/7/00, 2210, 7 hr)	**210**		**280**		**160**		**0**		**120**		**130**					

Liquid Concentration (ug/L)

Concentrate

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAcc1	VOA Concentrate Sample #1 (6/6/00, 1600)	*20.9*	J	*54.5*	J	*11.8*	J	400	U	*13.2*	J	400	U	*19.1*	J	*21.6*	J
RGNEVPVAcc2	VOA Concentrate Sample #2 (6/6/00, 2230)	400	U	400	U	400	U	400	U	*13*	J	400	U	*7.1*	J	*17.3*	J
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**12**		**77**		**8.2**		**0**		**7.6**		**170**					
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**2.2**		**48**		**11**		**1.9**		**5.8**		**160**					
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**5.3**		**26**		**11**		**1.8**		**5.4**		**190**					
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**6.3**		**120**		**4.5**		**4.5**		**5.7**		**400**					

Liquid Concentration (ug/L)

Condensate

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAcd1	VOA Condensate Sample #1 (6/6/00, 1625)	**32.7**		*712*	E	**25.9**		**41.6**		**44**		10	U	**60.8**		257	E
RGNEVPVAcd1DL	Above, with 10 dilution factor	*26.8*	DJ	*688*	J	*18.3*	DJ	*36.2*	DJ	*31*	DJ	100	U	*40.6*	DJ	200	D
RGNEVPVAcd2	VOA Condensate Sample #2 (6/6/00, 2230)	*12.9*	J	479	E	*10.9*	J	*18.1*	J	*17.5*	J	20	U	**25.5**		**151**	
RGNEVPVAcd2MS	Method spike	93.4		484	E	89.7		17.8	J	98.8		62.1		22.1		139	
RGNEVPVAcd2MSD	Method spike duplicate	93.5		495	E	90.3		19	J	101		62.4		25.5		152	
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**7.2**		**130**		**26**		**2.8**		**5.5**		**120**					
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**1.2**		**160**		**4.1**		**2.2**		**6.6**		**170**					
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr	**5.3**		**26**		**11**		**1.8**		**5.4**		**190**					
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**25**		**340**		**18**		**19**		**28**		**200**					

Liquid Concentration (ug/L)

Pump Trap Liquids

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene		
RGNEVPVATrap1	Sample Pump Liquids Sample #1 (6/7/00, 1500)	*1460*	J	*28400*	J	*1200*	J	*2920*	J	*272*	J	10	U	*483*	J	*832*	J	toluene-d8 recovery high so diluted; split total liquid with two below
RGNEVPVATrap1DL	Above, with 100 dilution factor	*164*	DJ	*7250*	J	*115*	DJ	*339*	DJ	*212*	DJ	1000	U	*445*	DJ	*2260*	D	
RGNEVPVATrap2	Sample Pump Liqu. Samp. #2, 100X dil. (6/7,150	*226*	J	*7760*	J	*176*	J	*392*	J	*309*	J	1000	U	*678*	J	**2820**		toluene & benzene recoveries slightly low; split with above and below
RGNEVPVATrap2MS	Method spike	4820		8010		4750		378	J	4920		1000	U	573	J	2590		toluene & benzene recoveries in MS's okay, so RPD's a bit high
RGNEVPVATrap2MSD	Method spike duplicate	3940		7280		3870		336	J	4160		1000	U	482	J	2350		
300145170	in-house sample, no headspace (6/7/00, 1500)	**49**		**1200**		**33**		**76**		**35**		**110**						

Mass (ng)

Sorbent Tubes

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene		
RGNEVPVATenax1	Sample Tenax Tube #1 (6/7/00, 1500)	5000000	UJ	*1160000*	J	*1140000*	J	5000000	UJ	*3000000*	J	5000000	UJ	*48800000*	J	*55900000*	J	40% recoveries, ~100000 factor dilution needed
RGNEVPVATenax2	Sample Tenax Tube #2 (6/7/00, 1500)	*11900*	E	*230000*	E	*25300*	E	*21700*	E	*658000*	E	50	U	**434**		*2090*	E	Thermal desorption result, where quantities overblew detector
RGNEVPVAAnasorb1	Sample Anasorb Tube (6/7/00, 1500)	*24700000*	J	*31500000*	J	*10100000*	J	*4600000*	J	*5160000*	J	4500000	UJ	4500000	UJ	4500000	UJ	20% recoveries, ~100000 factor dilution needed

										Liquid Concentration (ug/L)								
Gas Sampler Condensate				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVACond1	Sampler Condensate Sample #1 (6/7/00, 1500)	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced
RGNEVPVACond2	Sampler Condensate Sample #2 (6/7/00, 1500)	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced
	in-house sample, no headspace	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced

										Liquid Concentration (ug/L)								
Process Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVP1	Process Blank Liquid Sample	*0.5*	J	*3.5*	J	20	U	20	U	20	U	20	U	*0.27*	J	*1.2*	J	Bottle 1 of 1, Simulant + ca. 800 ppm acetone, no headspace
										Solid Content (ng)								
RGNEVPVPTenax1	Proc. Blank Tenax Tube #1																	
RGNEVPVPTenax2	Proc. Blank Tenax Tube #2	**202**		**434**		**549**		50	U	50	U	50	U	**75.2**		**251**		
RGNEVPVPAnasorb1	Proc. Blank Anasorb Tube	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	
										Liquid Concentration (ug/L)								
RGNEVPVPCond	Proc. Blank Gas Sampler Condensate	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced
RGNEVPVPTrap	Proc. Blank Pump Trap Liquids	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	No headspace, fill with reagent water

										Liquid Concentration (ug/L)								
Field Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVF1	Equipment Field Blank (6/4/00, 1715)	20	U	20	U	20	U	20	U	20	U	20	U	20	U	20	U	Equipment Field Blank, NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF2	Day #2 for Feed Sample #2 (6/5/00, 2200)	20	U	20	U	20	U	20	U	20	U	20	U	20	U	20	U	Day #2 for Feed Sample #2, NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF3	Day #2 for Feed Sample #1 (6/5/00, 2200)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Day #2 for Feed Sample #1, NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF4	Day #2 for Cond/Conc (1of 2) (6/5/00, 2200)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Day #2 for Cond/Conc (1of 2), NaOH solution bottle-to-bottle pour, no headspace
RGNEVPVF5	Day #3 for Cond/Conc (2 of 2) (6/7/00, 1115)	20	U	20	U	20	U	20	U	20	U	20	U	20	U	20	U	Day #3 for Cond/Conc (2 of 2), NaOH solution bottle-to-bottle pour, no headspace
										Solid Content (ng)								
RGNEVPVFTenax1	Field blank associated with Process Blank																	Tube 1 of 4, Field blank associated with Process Blank
RGNEVPVFTenax2	Field blank associated with Process Blank	50	U	50	U	**374**		50	U	50	U	50	U	*22.3*	J	*45.4*	J	Tube 2 of 4, Field blank associated with Process Blank
RGNEVPVFAnasorb1	Field blank associated with Process Blank	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	Tube 1 of 2, Field blank associated with Process Blank
RGNEVPVFTenax3	Per Method 0031																	Tube 3 of 4, Per Method 0031
RGNEVPVFTenax4	Per Method 0031	50	U	50	U	**388**		50	U	50	U	50	U	*7.5*	J	*20.3*	J	Tube 4 of 4, Per Method 0031
RGNEVPVFAnasorb2	Per Method 0031	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	Tube 2 of 2, Per Method 0031
RGNEVPVF1	Field blank for Proc. Blank Condensate	-----		-----		-----		-----		-----		-----		-----		-----		No condensate produced

										Liquid Concentration (ug/L)								
Trip Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVT1	Day #1-Proc. Blanks, Reagent H2O (6/4, 1945)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/6/00
	(6/6/00, 0300)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/7/00
RGNEVPVT2	Day #2-1st half VOST run, Reag. H2O (6/6, 0300	10	U	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/7/00
	(6/7/00, 1800)	10	U	10	U	*1.4*	J	10	U	10	U	10	U	10	U	10	U	Received 6/9/00, Extra, IGNORE
RGNEVPVT3	Day #3-2nd half VOST run, Reag. H2O (6/7, 011	10	U	10	U	*1.3*	J	10	U	10	U	10	U	10	U	10	U	
										Solid Content (ng)								
RGNEVPVTTenax1	Trip blanks, Day #1 (Process Blanks)	-----		-----		-----		-----		-----		-----		-----		-----		
RGNEVPVTTenax2		-----		-----		-----		-----		-----		-----		-----		-----		
RGNEVPVTTenax3	Trip blanks, Day #2 (Field Blanks)																	
RGNEVPVTTenax4		50	U	**156**		164	U	50	U	50	U	50	U	*174*	J	*736*	J	
RGNEVPVTTenax5	Trip blanks, Day #3 (with Sample Tube)																	
RGNEVPVTTenax6		50	U	50	U	**561**		50	U	50	U	50	U	*33.2*	J	**151**		
RGNEVPVTAnasorb1	Trip blanks, Day #1 (Process Blanks)	-----		-----		-----		-----		-----		-----		-----		-----		
RGNEVPVTAnasorb2	Trip blanks, Day #2 (Field Blanks)	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	
RGNEVPVTAnasorb3	Trip blanks, Day #3 (with Sample Tube)	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	25000	UJ	

										Liquid Concentration (ug/L)								
Reagent Blanks				4-methyl-2-				1,2-dibromo		chloro		1,2,3-tri		1,2,4-tri				
Sample Name	Sample Description	benzene		pentanone		toluene		ethane		benzene		chloropropane		chlorobenzene		naphthalene		
RGNEVPVRH2O1	VOA Reagent Water Blank	10	U	10	U	**19.3**		10	U	10	U	10	U	10	U	10	U	DI H2O used to remove headspace, no headspace
RGNEVPVRH2O2	VOA Reagent Water Blank	10	U	10	U	*7.8*	J	10	U	10	U	10	U	10	U	10	U	DI H2O used to remove headspace, no headspace

Corrected Validated VOA Data

2-Dec-00
Hiroshi Saito

Feed

Liquid Concentration (ug/L)

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAfd1	VOA Feed Sample #1 (6/6/00, 2300)	**1479.5**		*2736.5*	J	**1110**		*78.9*	J	**1280**		800	U	**1169.73**		**1578.8**	
RGNEVPVAfd2	VOA Feed Sample #2 (6/6/00, 2300)	**1379.5**		*2406.5*	J	**1020**		*66.3*	J	**1070**		800	U	*528.73*	J	**1078.8**	

Concentrate

Liquid Concentration (ug/L)

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAcc1	VOA Concentrate Sample #1 (6/6/00, 1600)	*20.4*	J	*51*	J	*11.8*	J	400	U	*13.2*	J	400	U	*18.83*	J	*20.4*	J
RGNEVPVAcc2	VOA Concentrate Sample #2 (6/6/00, 2230)	399.5	U	396.5	U	400	U	400	U	*13*	J	400	U	*6.83*	J	*16.1*	J
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**12**		**77**		**8.2**		**0**		**7.6**		**170**					
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**2.2**		**48**		**11**		**1.9**		**5.8**		**160**					
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**5.3**		**26**		**11**		**1.8**		**5.4**		**190**					
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**6.3**		**120**		**4.5**		**4.5**		**5.7**		**400**					

Condensate

Liquid Concentration (ug/L)

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVAcd1	VOA Condensate Sample #1 (6/6/00, 1625)	**32.2**		*708.5*	E	**25.9**		**41.6**		**44**		10	U	**60.53**		*255.8*	E
RGNEVPVAcd1DL	Above, with 10 dilution factor	*26.3*	DJ	*684.5*	J	*18.3*	DJ	*36.2*	DJ	*31*	DJ	100	U	*40.33*	DJ	*198.8*	D
RGNEVPVAcd2	VOA Condensate Sample #2 (6/6/00, 2230)	*12.4*	J	*475.5*	E	*10.9*	J	*18.1*	J	*17.5*	J	20	U	**25.23**		**149.8**	
RGNEVPVAcd2MS	Method spike	93.4		484	E	89.7		17.8	J	98.8		62.1		22.1		139	
RGNEVPVAcd2MSD	Method spike duplicate	93.5		495	E	90.3		19	J	101		62.4		25.5		152	
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**7.2**		**130**		**26**		**2.8**		**5.5**		**120**					
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**1.2**		**160**		**4.1**		**2.2**		**6.6**		**170**					
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr)	**5.3**		**26**		**11**		**1.8**		**5.4**		**190**					
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**25**		**340**		**18**		**19**		**28**		**200**					

Pump Trap Liquids

Liquid Concentration (ug/L)

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVATrap1	Sample Pump Liquids Sample #1 (6/7/00, 1500)	*1460*	J	*28400*	J	*1200*	J	*2920*	J	*272*	J	10	U	*483*	J	*832*	J
RGNEVPVATrap1DL	Above, with 100 dilution factor	*164*	DJ	*7250*	J	*115*	DJ	*339*	DJ	*212*	DJ	1000	U	*445*	DJ	*2260*	D
RGNEVPVATrap2	Sample Pump Liqu. Samp. #2, 100X dil. (6/7,1500)	*226*	J	*7760*	J	*176*	J	*392*	J	*309*	J	1000	U	*678*	J	**2820**	
RGNEVPVATrap2MS	Method spike	4820		8010		4750		378	J	4920		1000	U	573	J	2590	
RGNEVPVATrap2MSD	Method spike duplicate	3940		7280		3870		336	J	4160		1000	U	482	J	2350	
300145170	in-house sample, no headspace (6/7/00, 1500)	**49**		**1200**		**33**		**76**		**35**		**110**					

Sorbent Tubes

Mass (ng)

Sample Name	Sample Description	benzene		4-methyl-2-pentanone		toluene		1,2-dibromoethane		chlorobenzene		1,2,3-trichloropropane		1,2,4-trichlorobenzene		naphthalene	
RGNEVPVATenax1/2	Sample Tenax Tube #1/2 (6/7/00, 1500)	*2519.558*	E	*1373468*	J	*1156224*	J	*21700*	E	*3658000*	J	5000000	UJ	*48800400.8*	J	*55901939*	J
RGNEVPVAAnasorb1	Sample Anasorb Tube (6/7/00, 1500)	*24700000*	J	*31500000*	J	*10100000*	J	*4600000*	J	*5160000*	J	4500000	UJ	4500000	UJ	4500000	UJ

			Room conditions	
928.486	liters gas sampled		1002	mbar
1.036	Y factor		295.15	K
944.9718	standard liters gas			

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
J = estimated value (e.g., quantity between MDL and MRL)
U = Undetected analyte (searched for)
E = Quantity exceeds upper level of calibration range
R = SRTC QA rejected result

Data Guide

Italic text/Yellow box = qualified data
Bold text/Green box = Significant/good data
Bold box/red box = corrected data

Blank Corrections														
					Liquid Concentration (ug/L)									
			4-methyl-2-		1,2-dibromo	chloro	1,2,3-tri	1,2,4-tri						
		benzene	pentanone	toluene	ethane	benzene	chloropropane	chlorobenzene	naphthalene					
Day #0	Process Blank - Liquid Sample	*0.5*	*3.5*					*0.27*	*1.2*					
	Field Blank - Liquid Sample													
Day #1	Field Blank - Liquid Sample													
	Trip Blank - Liquid Sample													
Day #2	Field Blank - Liquid Sample													
	Trip Blank - Liquid Sample			0						Reagent contam. > trip blank contam.				
Day #3	Field Blank - Liquid Sample													
	Trip Blank - Liquid Sample			0						Reagent contam. > trip blank contam.				
	Reagent Blank - Liquid			*13.6*										
						Mass (ng)								
	Trip Blank for Sample - Tenax			561				*33.2*	151					
	Field Blank for Sample - Tenax		0	388				0	0					
	Trip Blank for Sample Field Blank- Tenax		156					*174*	*736*					
													Room conditions	
	Process Blank - Tenax	202	356	175				0	0	Corrected by field blank & trip blank	20.008	liters gas sampled	1004.7	mbar
	Field Blank for Process Blank- Tenax			93.5				*22.3*	*45.4*	Corrected by trip blank	1.036	Y factor	296.15	K
	Trip Blank for Process Blank- Tenax (Day 1)		78	280.5				*103.6*	*443.5*	Average of Days 2 and 3	20.34918	standard liters gas		
	Tenax tube corrections are for pairs of tubes													
	Anasorb tube field and trip blanks all nondetectable													

SVOA Data by Stream

2-Dec-00
Hiroshi Saito

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
J = estimated value (e.g., quantity between MDL and MRL)
U = Undetected analyte (searched for)
E = Quantity exceeds upper level of calibration range
R = SRTC QA rejected result

Data Guide
Italic text/Yellow box = qualified data
Bold text/Green box = Significant/good data
Bold box/red box = corrected data

BWXT Data Validated by WSRC QA

Concentration (ug/L)

Feed Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAfd1	Feed Sample #1 (6/6/00, 2300)	500	U	500	U	410	J	500	U	500	UJ	*200*	J	500	UJ
RGNEVPSAfd2	Feed Sample #2 (6/6/00, 2300)	*17*	J	100	U	**430**		*27*	J	100	UJ	*15000*	J	100	UJ
RGNEVPSAfd3	Feed Sample #3 (6/6/00, 2300)	*41*	J	*15*	J	**820**		*81*	J	100	U	98000	J	100	UJ
RGNEVPSAfd4	Feed Sample #4 (6/7/00, 2130)	*55*	J	300	UJ	**1000**		*72*	J	300	U	**2800**		300	UJ
RGNEVPSAfd4MS	Method Spike	210	J	311	U	1000		300	U	300	U	2800		300	U
RGNEVPSAfd4MSD	Method Spike Duplicate	210	J	55	J	1100		330	U	330	U	2900		330	U
RGNEVPSAfd5	Feed Sample #5 (6/7/00, 2130)	1000	U	1000	U	**1000**		1000	U	1000	U	**2900**		1000	UJ
RGNEVPSAfd6	Feed Sample #6 (6/7/00, 2130)	2000	U	2000	U	*850*	J	2000	U	2000	U	2000	U	2000	UJ
300145159	pre-run feed sample (7E-15, 6/5/00, late PM)	**610**		**570**		**1110**		**0**		**930**		**1040**		**1310**	
300145160	mid-VOST feed sample (6/7/00, 0300, 24 hr)	**580**		**600**		**1070**		**0**		**930**		**1030**		**1380**	
300145161	mid-SVOST feed sample (6/7/00, 2210, 7 hr)	**580**		**530**		**950**		**0**		**930**		**10**		**1690**	

Concentration (ug/L)

Concentrate Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAcc1	Concentrate Sample #1 (6/6/00, 1357)	30	U	30	U	*13*	J	**180**		30	U	**39**		30	UJ
RGNEVPSAcc1MS	Method Spike	90		30	U	39		150		30	U	120		30	U
RGNEVPSAcc1MSD	Method Spike Duplicate	95		31	U	8	J	230		31	U	35		31	U
RGNEVPSAcc2	Concentrate Sample #2 (6/6/00, 2310)	21	U	21	U	**210**		**130**		**84**		**230**		21	UJ
RGNEVPSAcc3	Concentrate Sample #3 (6/7/00, 0350)	51	U	51	U	**360**		**140**		51	U	**340**		51	UJ
RGNEVPSAcc4	Concentrate Sample #4 (6/7/00, 1800)	100	U	100	U	**330**		100	U	100	U	**280**		100	UJ
RGNEVPSAcc5	Concentrate Sample #5 (6/8/00, 1152)	30	R	30	R	*470*	J	*130*	J	30	R	*68000*	J	30	R
RGNEVPSAcc6	Concentrate Sample #6 (6/8/00, 2045)	2000	U	2000	U	*1200*	J	2000	U	2000	U	**2000**		2000	UJ
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**57**		**36**		**720**		**0**		**690**		**920**		**950**	
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**75**		**35**		**940**		**0**		**830**		**920**		**1290**	
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**35**		**0**		**700**		**0**		**670**		**800**		**1070**	
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**56**		**30**		**970**		**0**		**830**		**1000**		**1340**	

Concentration (ug/L)

Condensate Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAcd1	Condensate Sample #1 (6/6/00, 1302)	*45*	J	*160*	J	*3*	J	10	U	**130**	J	*12*	J	10	U
RGNEVPSAcd2	Condensate Sample #2 (6/6/00, 2132)	**32**		**140**		*4*	J	20	U	**180**		20	U	20	U
RGNEVPSAcd3	Condensate Sample #3 (6/7/00, 1321)	**110**		**380**		50	U	50	U	**140**		50	U	50	U
RGNEVPSAcd4	Condensate Sample #4 (6/7/00, 1923)	*45*	J	*190*	J	11	UJ	11	UJ	*83*	J	11	UJ	11	UJ
RGNEVPSAcd5	Condensate Sample #5 (6/8/00, 0705)	**66**		**240**		20	U	20	U	**110**		20	U	20	U
RGNEVPSAcd6	Condensate Sample #6 (6/8/00, 2045)	**110**		**420**		50	U	50	U	**110**		50	U	50	UJ
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**0**		**100**		**0**		**0**		**200**		**360**		**0**	
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**0**		**100**		**0**		**0**		**190**		**330**		**0**	
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr)	**90**		**390**		**0**		**0**		**270**		**320**		**0**	
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**120**		**490**		**0**		**0**		**210**		**320**		**0**	

Concentration (ug/L)

Pump Trap Liquids Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
RGNEVPSATrap1	Pump Trap Sample #1 (6/9/00, 0300)	**340**		**1600**		230	U	230	U	*38*	J	230	U	230	U	Split with two below
RGNEVPSATrap2	Pump Trap Sample #2 (6/9/00, 0300)	*270*	J	**1300**		280	U	280	U	*35*	J	280	U	280	U	Split with above and below
300145170	in-house VOST sample, no SVOST (6/7/00, 1500)	**500**		**1430**		**0**		**0**		**91**		**3300**		**0**		
RGNEVPSAExLinRinse	post-SVOST run MeOH/MeCl2 rinse of line to pump	3300	U	3300	U	**34000**		3300	U	**26000**		3300	U	3300	U	

Mass (ug)

Sorbent Tubes Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
RGNEVPSAXad	Off-gas Sampling Tube (6/9/00, 0300)	**9900**		**8600**		1000	U	1000	U	1000	U	1000	U	1000	U	Diluted by 100

								Concentration (ug/L)								
Gas Sampler Condensate		1,2,4-trichloro				Hexachloro		Pentachloro								
Sample Name	Sample Description	benzene		Naphthalene		benzene		phenol		pyrene		BEHP		BaP		
RGNEVPSACond1	Off-gas Sampler Condensate #1 (6/9/00, 0300)	1000	UJ	1000	UJ	1000	UJ	1000	UJ	1000	UJ	1000	UJ	1000	UJ	Usually split with below
RGNEVPSACond2	Off-gas Sampler Condensate #2 (6/9/00, 0300)	-----		-----		-----		-----		-----		-----		-----		Not generated due to low volume
	in-house sample															
								Concentration (ug/L)								
Gas Sampler Rinse		1,2,4-trichloro				Hexachloro		Pentachloro								
Sample Name	Sample Description	benzene		Naphthalene		benzene		phenol		pyrene		BEHP		BaP		
RGNEVPSARinse	Off-gas Sampler Glassware Rinse (6/9/00, 0300)	960	U	960	U	960	U	960	U	960	U	960	U	960	U	Liquid used to rinse sampling system after sampling
								Concentration (ug/L)								
Process Blanks	(6/4/00)	1,2,4-trichloro				Hexachloro		Pentachloro								
Sample Name	Sample Description	benzene		Naphthalene		benzene		phenol		pyrene		BEHP		BaP		
RGNEVPSP1	Bottle 1 of 3, Simulant + ca. 800 ppm acetone	10	U	10	U	*5*	J	*3*	J	10	U	**16**		10	UJ	Bottle 1 of 3, Simulant + ca. 800 ppm acetone
RGNEVPSP1Ri	????	10	U	10	U	*8*	J	*3*	J	10	U	**30**		10	UJ	
RGNEVPSP2	Bottle 2 of 3, Simulant + ca. 800 ppm acetone	150	UJ	150	UJ	150	UJ	150	UJ	150	UJ	150	UJ	150	UJ	Bottle 2 of 3, Simulant + ca. 800 ppm acetone
RGNEVPSP2MS	Method Spike	64	J	150	U	150	U	150	U	150	U	150	U	150	U	
RGNEVPSP2MSD	Method Spike Duplicate	84	J	150	U	150	U	150	U	150	U	110	J	150	U	
RGNEVPSP3	Bottle 3 of 3, Simulant + ca. 800 ppm acetone	10	UJ	10	UJ	10	UJ	10	UJ	10	UJ	*12*	J	10	UJ	Bottle 3 of 3, Simulant + ca. 800 ppm acetone
								Mass (ug)								
RGNEVPSPXad		10	U	10	U	10	U	10	U	10	U	10	U	10	U	Went dry during extraction
								Concentration (ug/L)								
RGNEVPSPTrap	For any pump trap liquid from process blank	3300	U	3300	U	3300	U	3300	U	3300	U	3300	U	3300	U	
RGNEVPSPCond	For any condensate from process blank	-----		-----		-----		-----		-----		-----		-----		
RGNEVPSPRinse	1:1 (v/v) Methanol/Methylene Chloride Wash Liquid	120	U	120	U	120	U	120	U	120	U	120	U	120	U	
								Concentration (ug/L)								
Field Blanks		1,2,4-trichloro				Hexachloro		Pentachloro								
Sample Name	Sample Description	benzene		Naphthalene		benzene		phenol		pyrene		BEHP		BaP		
RGNEVPSF1	Day #1, Bottle 1 of 3 (6/4/00, 1715)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF2	Day #1, Bottle 2 of 3 (6/4/00, 1715)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF3	Day #1, Bottle 3 of 3 (6/4/00, 1715)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF4	Day #2, for Feed Sample, Bottle 1 of 3 (6/5/00, 2200	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF5	Day #2, for Feed Sample, Bottle 2 of 3 (6/5/00, 2200	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF6	Day #2, for Feed Sample, Bottle 3 of 3 (6/5/00, 2200	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF7	For Cond/Conc, Bottle 1 (Day 2) of 3 (6/5/00, 2200)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF8	For Cond/Conc, Bottle 2 (Day 3) of 3 (6/6/00, 1000)	10	U	10	U	10	U	10	U	*1*	J	10	U	10	U	Received 6/8
	(6/7/00, 2130)	10	U	10	U	10	U	10	U	10	U	10	U	10	U	Received 6/9
RGNEVPSF9	For Cond/Conc, Bottle 3 (Day 3) of 3 (6/7/00, 2130)	10	U	10	U	10	U	10	U	10	U	*0.3*	J	10	U	
RGNEVPSF10	Day #3, for Feed Sample, Bottle 1 of 3 (6/7/00, 2130	10	U	10	U	10	U	10	U	10	U	10	U	10	U	
RGNEVPSF11	Day #3, for Feed Sample, Bottle 2 of 3 (6/8/00, 2100	10	U	10	U	10	U	10	U	*6*	J	10	U	10	U	
RGNEVPSF12	Day #3, for Feed Sample, Bottle 3 of 3 (6/8/00, 2100	10	UJ	10	UJ	10	UJ	10	UJ	10	UJ	10	UJ	10	UJ	
RGNEVPSF13	For Cond/Conc, Bottle 1 (Day 4) of 3 (6/7/00, 1830)	10	U	10	U	10	U	10	U	*1*	J	10	U	10	U	
RGNEVPSF13DL	Above, with 5.0 dilution factor	150	U	150	U	*520*	D	150	U	150	U	*600*	D	150	UJ	
RGNEVPSF13MS	Method Spike	110		33	U	760	E	250		120		86000	E	33	U	
RGNEVPSF13MSD	Method Spike Duplicate	100		33	U	710	E	200		410		120000	E	33	U	
RGNEVPSF14	For Cond/Conc, Bottle 2 (Day 4) of 3 (6/7/00, 1830)	10	U	10	U	10	U	10	U	10	U	*0.3*	J	10	U	
RGNEVPSF15	For Cond/Conc, Bottle 3 (Day 5) of 3															
								Mass (ug)								
RGNEVPSFXad1	Field blank associated with process blank	-----		-----		-----		-----		-----		-----		-----		Went dry during extraction, and then lost during concentration step
RGNEVPSFXad2	Per Method 0010	*4*	J	*4*	J	10	U	10	U	10	U	10	U	10	U	Went dry during extraction
								Concentration (ug/L)								
RGNEVPSFRinse1	Field blank associated with process blank	130	U	130	U	130	U	130	U	130	U	130	U	130	U	
RGNEVPSFRinse2	Per Method 0010	570	U	570	U	570	U	570	U	570	U	*64*	J	570	U	
RGNEVPSFCond	Reagent water	-----		-----		-----		-----		-----		-----		-----		
								Concentration (ug/L)								
Reagent Blanks		1,2,4-trichloro				Hexachloro		Pentachloro								
Sample Name	Sample Description	benzene		Naphthalene		benzene		phenol		pyrene		BEHP		BaP		
RGNEVPSRMeth	Fresh 1:1 (v/v) MeOH/MeCl2 Wash Liquid	85	U	85	U	85	U	85	U	85	U	85	U	85	U	

Corrected Validated SVOA Data

4-Dec-00
Hiroshi Saito

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
J = estimated value (e.g., quantity between MDL and MRL)
U = Undetected analyte (searched for)
E = Quantity exceeds upper level of calibration range
R = SRTC QA rejected result

Data Guide
Italic text/Yellow box = qualified data
Bold text/Green box = Significant/good data
Bold box/red box = corrected data

Concentration (ug/L)

Feed

Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAfd1	Feed Sample #1 (6/6/00, 2300)	500	U	500	U	410	J	500	U	500	UJ	*200*	J	500	UJ
RGNEVPSAfd2	Feed Sample #2 (6/6/00, 2300)	*17*	J	100	U	**430**		*27*	J	100	UJ	*15000*	J	100	UJ
RGNEVPSAfd3	Feed Sample #3 (6/6/00, 2300)	*41*	J	*15*	J	**820**		*81*	J	100	U	98000	J	100	UJ
RGNEVPSAfd4	Feed Sample #4 (6/7/00, 2130)	*55*	J	300	UJ	**1000**		*72*	J	300	U	**2800**		300	UJ
RGNEVPSAfd4MS	Method Spike	210	J	311	U	1000		300	U	300	U	2800		300	U
RGNEVPSAfd4MSD	Method Spike Duplicate	210	J	55	J	1100		330	U	330	U	2900		330	U
RGNEVPSAfd5	Feed Sample #5 (6/7/00, 2130)	1000	U	1000	U	**1000**		1000	U	1000	U	**2900**		1000	UJ
RGNEVPSAfd6	Feed Sample #6 (6/7/00, 2130)	2000	U	2000	U	*850*	J	2000	U	2000	U	2000	U	2000	UJ
300145159	pre-run feed sample (7E-15, 6/5/00, late PM)	**610**		**570**		**1110**		**0**		**930**		**1040**		**1310**	
300145160	mid-VOST feed sample (6/7/00, 0300, 24 hr)	**580**		**600**		**1070**		**0**		**930**		**1030**		**1380**	
300145161	mid-SVOST feed sample (6/7/00, 2210, 7 hr)	**580**		**530**		**950**		**0**		**930**		**10**		**1690**	

Concentration (ug/L)

Concentrate

Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAcc1	Concentrate Sample #1 (6/6/00, 1357)	30	U	30	U	*13*	J	**180**		30	U	**39**		30	UJ
RGNEVPSAcc1MS	Method Spike	90		30	U	39		150		30	U	120		30	U
RGNEVPSAcc1MSD	Method Spike Duplicate	95		31	U	8	J	230		31	U	35		31	U
RGNEVPSAcc2	Concentrate Sample #2 (6/6/00, 2310)	21	U	21	U	**210**		**130**		**84**		**230**		21	UJ
RGNEVPSAcc3	Concentrate Sample #3 (6/7/00, 0350)	51	U	51	U	**360**		**140**		51	U	**340**		51	UJ
RGNEVPSAcc4	Concentrate Sample #4 (6/7/00, 1800)	100	U	100	U	**330**		100	U	100	U	**280**		100	UJ
RGNEVPSAcc5	Concentrate Sample #5 (6/8/00, 1152)	30	R	30	R	*470*	J	*130*	J	30	R	*68000*	J	30	R
RGNEVPSAcc6	Concentrate Sample #6 (6/8/00, 2045)	2000	U	2000	U	*1200*	J	2000	U	2000	U	**2000**		2000	UJ
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**57**		**36**		**720**		**0**		**690**		**920**		**950**	
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**75**		**35**		**940**		**0**		**830**		**920**		**1290**	
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**35**		**0**		**700**		**0**		**670**		**800**		**1070**	
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**56**		**30**		**970**		**0**		**830**		**1000**		**1340**	

Concentration (ug/L)

Condensate

Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP	
RGNEVPSAcd1	Condensate Sample #1 (6/6/00, 1302)	*45*	J	*160*	J	*3*	J	10	U	*130*	J	*12*	J	10	U
RGNEVPSAcd2	Condensate Sample #2 (6/6/00, 2132)	**32**		**140**		*4*	J	20	U	**180**		20	U	20	U
RGNEVPSAcd3	Condensate Sample #3 (6/7/00, 1321)	**110**		**380**		50	U	50	U	**140**		50	U	50	U
RGNEVPSAcd4	Condensate Sample #4 (6/7/00, 1923)	*45*	J	*190*	J	11	UJ	11	UJ	*83*	J	11	UJ	11	UJ
RGNEVPSAcd5	Condensate Sample #5 (6/8/00, 0705)	**66**		**240**		20	U	20	U	**110**		20	U	20	U
RGNEVPSAcd6	Condensate Sample #6 (6/8/00, 2045)	**110**		**420**		50	U	50	U	**110**		50	U	50	UJ
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**0**		**100**		**0**		**0**		**200**		**360**		**0**	
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**0**		**100**		**0**		**0**		**190**		**330**		**0**	
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr)	**90**		**390**		**0**		**0**		**270**		**320**		**0**	
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**120**		**490**		**0**		**0**		**210**		**320**		**0**	

Concentration (ug/L)

Pump Trap Liquids

Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
RGNEVPSATrap1	Pump Trap Sample #1 (6/9/00, 0300)	**340**		**1600**		230	U	230	U	*38*	J	230	U	230	U	Split with two below
RGNEVPSATrap2	Pump Trap Sample #2 (6/9/00, 0300)	*270*	J	**1300**		280	U	280	U	*35*	J	280	U	280	U	Split with above and below
300145170	in-house VOST sample, no SVOST (6/7/00, 1500)	**500**		**1430**		**0**		**0**		**91**		**3300**		**0**		
RGNEVPSAExLinRinse	post-SVOST run MeOH/MeCl2 rinse of line to pump	3300	U	3300	U	**34000**		3300	U	**26000**		3300	U	3300	U	

29.19 g 50% CH2Cl2/MeOH line rinse sample
1.05605 g/ml assumed density
0.027641 L 50% CH2Cl2/MeOH

Mass (ug)

Sorbent Tubes

Sample Name	Sample Description	1,2,4-trichloro benzene		Naphthalene		Hexachloro benzene		Pentachloro phenol		pyrene		BEHP		BaP		
RGNEVPSAXad	Off-gas Sampling Tube (6/9/00, 0300)	**9896**		**8596**		1000	U	1000	U	1000	U	1000	U	1000	U	Diluted by 100

		Room conditions	
953.946	liters gas sampled	1011.5	mbar
1.036	Y factor	300.15	K
963.7622	standard liters gas		

Blank Corrections									
					Concentration (ug/L)				
		1,2,4-trichloro benzene	Naphthalene	Hexachloro benzene	Pentachloro phenol	pyrene	BEHP	BaP	
Day #3	Field Blank - Feed Liquid Sample					*2*			
Day #4-5	Field Blank - Liquid Sample								
					Mass (ug)				
	Field Blank for Sample - XAD-2	*4*	*4*						Low? - sample dried during extraction
	Process Blank - XAD-2								No data - sample dried during extraction
	Field Blank for Process Blank- XAD-2								No data - sample dried during extraction

Aldrin Data by Stream

24-Aug-00
Hiroshi Saito

BWXT Data Validated by WSRC QA and Corrected Values

Data Qualifier Key

D = Sample reanalyzed by dilution. Caution for dilution error
J = estimated value (e.g., quantity between MDL and MRL)
U = Undetected analyte (searched for)
E = Quantity exceeds upper level of calibration range
R = SRTC QA rejected result
P = High scatter in duplicate data, lower value reported

Feed

Sample Name	Sample Description	Result		Units	
RGNEVPPAfd1	Feed Sample #1 (6/6/00, 2300)	*0.160*	J	ug/L	
RGNEVPPAfd1MS	Method Spike	0.180		ug/L	
RGNEVPPAfd1MSD	Method Spike Duplicate	0.190	P	ug/L	
RGNEVPPAfd2	Feed Sample #2 (6/6/00, 2300)	*0.089*	J	ug/L	
RGNEVPPAfd3	Feed Sample #3 (6/6/00, 2300)	*0.079*	J	ug/L	caustic recoveries bad??
RGNEVPPAfd4	Feed Sample #4 (6/7/00, 2130)	0.100	R	ug/L	
RGNEVPPAfd5	Feed Sample #5 (6/7/00, 2130)	*0.790*	J	ug/L	
RGNEVPPAfd6	Feed Sample #6 (6/7/00, 2130)	0.100	R	ug/L	
300145159	pre-run feed sample (7E-15, 6/5/00, late PM)	**1060**		ug/L	
300145160	mid-VOST feed sample (6/7/00, 0300, 24 hr)	**1030**		ug/L	
300145161	mid-SVOST feed sample (6/7/00, 2210, 7 hr)	**1020**		ug/L	

Data Guide

Italic text/Yellow box = qualified data
Bold text/Green box = Significant/good data
Bold box/red box = corrected data

Concentrate

Sample Name	Sample Description	Result		Units	
RGNEVPPAcc1	Concentrate Sample #1 (6/6/00, 0420)	*54*	EP	ug/L	
RGNEVPPAcc1DL	Above, with 100 dilution factor	*82*	DP	ug/L	
RGNEVPPAcc1MS	Method Spike	13	EP	ug/L	
RGNEVPPAcc1MSD	Method Spike Duplicate	0.29		ug/L	
RGNEVPPAcc2	Concentrate Sample #2 (6/7/00, 0120)	*320*	J	ug/L	
RGNEVPPAcc3	Concentrate Sample #3 (6/7/00, 0450)	*0.74*	J	ug/L	
RGNEVPPAcc4	Concentrate Sample #4 (6/8/00, 0140)	*0.11*	J	ug/L	caustic recoveries bad??
RGNEVPPAcc5	Concentrate Sample #5 (6/8/00, 1650)	*0.37*	J	ug/L	
RGNEVPPAcc6	Concentrate Sample #6 (6/9/00, 0030)	*8*	J	ug/L	
300145166	6-hr. VOST concentrate sample (6/6/00, 0907)	**430**		ug/L	
300145167	mid-run VOST conc. sample (6/6, 2230, 20 hr)	**580**		ug/L	
300145168	end-run VOST conc. Sample (6/7, 1443, 35.5 hr)	**340**		ug/L	
300145169	mid-run. SVOST conc. Sample (6/8, 0927, 18 hr)	**5300**		ug/L	

Condensate

Sample Name	Sample Description	Result		Units	Corrected
RGNEVPPAcd1	Condensate Sample #1 (6/6/00, 0857)	*28*	P	ug/L	*28.0*
RGNEVPPAcd2	Condensate Sample #2 (6/7/00, 0240)	**17**		ug/L	**17.0**
RGNEVPPAcd3	Condensate Sample #3 (6/7/00, 0800)	*28*	P	ug/L	*28.0*
RGNEVPPAcd4	Condensate Sample #4 (6/8/00, 0125)	*22*	P	ug/L	
RGNEVPPAcd5	Condensate Sample #5 (6/8/00, 1438)	**33**		ug/L	
RGNEVPPAcd6	Condensate Sample #6 (6/9/00, 0220)	*24*	J	ug/L	
RGNEVPPAcd6DL	Above, with 50 dilution factor	*24*	J	ug/L	
RGNEVPPAcd6MS	Method Spike	16	EP	ug/L	
RGNEVPPAcd6MSD	Method Spike Duplicate	16	EP	ug/L	
300145162	5.5-hr. VOST condensate sample (6/6/00, 0842)	**0**		ug/L	
300145163	mid-run VOA cond. Sample (6/6, 2330, 20 hr)	**0**		ug/L	
300145164	end-run. VOST cond. Sample (6/7, 1443, 35.5 hr)	**51**		ug/L	
300145165	mid-run SVOST cond. Sample (6/8, 0840, 17 hr)	**60**		ug/L	

Pump Trap Liquids

Sample Name	Sample Description	Result		Units	
RGNEVPSATrap1	Pump Trap Sample #1 (6/9/00, 0300)				Split with two below
RGNEVPSATrap2	Pump Trap Sample #2 (6/9/00, 0300)				Split with above and below
300145170	in-house VOST sample, no SVOST (6/7/00, 1500)	**58**		ug/L	

Sorbent Tubes							
Sample Name	Sample Description	Result		Units			
RGNEVPSAXad	Off-gas Sampling Tube (6/9/00, 0300)	-----				Went dry during extraction, then lost during concentration	
Gas Sampler Condensate							
Sample Name	Sample Description	Result		Units			
RGNEVPSACond1	Off-gas Sampler Condensate #1 (6/9/00, 0300)					Split with two below	
RGNEVPSACond2	Off-gas Sampler Condensate #2 (6/9/00, 0300)	-----				Split with above and below	
	in-house sample						
Gas Sampler Rinse							
Sample Name	Sample Description	Result		Units			
RGNEVPSARinse	Off-gas Sampler Glassware Rinse (6/9/00, 0300)					Liquid used to rinse sampling system after sampling	
Process Blanks	(6/5/00)						
Sample Name	Sample Description	Result		Units			
RGNEVPPP1	Bottle 1 of 3, Simulant + ca. 800 ppm acetone	0.050	U	ug/L		Bottle 1 of 3, Simulant + ca. 800 ppm acetone	
RGNEVPPP2	Bottle 2 of 3, Simulant + ca. 800 ppm acetone	0.050	U	ug/L		Bottle 2 of 3, Simulant + ca. 800 ppm acetone	
RGNEVPPP3	Bottle 3 of 3, Simulant + ca. 800 ppm acetone	0.050	U	ug/L		Bottle 3 of 3, Simulant + ca. 800 ppm acetone	
RGNEVPSPXad							
RGNEVPSPTrap	For any pump trap liquid from process blank						
RGNEVPSPCond	For any condensate from process blank	-----					
RGNEVPSPRinse	1:1 (v/v) Methanol/Methylene Chloride Wash Liquid						
Field Blanks							
Sample Name	Sample Description	Result		Units			
RGNEVPPF1	Day #1, Bottle 1 of 3 (6/4/00, 1715)	0.050	U	ug/L			
RGNEVPPF2	Day #1, Bottle 2 of 3 (6/4/00, 1715)						
RGNEVPPF3	Day #1, Bottle 3 of 3 (6/4/00, 1715)	0.050	U	ug/L			
RGNEVPPF4	Day #2, for Feed Sample, Bottle 1 of 3 (6/5, 2200)	0.050	U	ug/L			
RGNEVPPF5	Day #2, for Feed Sample, Bottle 2 of 3 (6/5, 2200)	0.050	U	ug/L			
RGNEVPPF6	Day #2, for Feed Sample, Bottle 3 of 3 (6/5, 2200)	0.050	U	ug/L			
RGNEVPPF7	For Cond/Conc, Bottle 1 (Day 2) of 3 (6/5/00, 2200)	0.050	U	ug/L			Correction
RGNEVPPF8	For Cond/Conc, Bottle 2 (Day 3) of 3 (6/6/00, 1500)	**0.092**		ug/L	received 6/8/00		**0.031**
	(6/7/00, 2130)	0.050	U	ug/L	received 6/9/00		
RGNEVPPF9	For Cond/Conc, Bottle 3 (Day 3) of 3 (6/7/00, 2130)	0.050	R	ug/L			
RGNEVPPF10	Day #3, for Feed Sample, Bottle 1 of 3 (6/7, 2130)	0.050	U	ug/L			
RGNEVPPF11	Day #3, for Feed Sample, Bottle 2 of 3						
RGNEVPPF12	Day #3, for Feed Sample, Bottle 3 of 3 (6/7, 1830)	0.050	U	ug/L			
RGNEVPPF13	For Cond/Conc, Bottle 1 (Day 4) of 3 (6/7, 1830)	0.050	U	ug/L			
RGNEVPPF14	For Cond/Conc, Bottle 2 (Day 5) of 3	0.050	UJ	ug/L			
RGNEVPPF15	For Cond/Conc, Bottle 3 (Day 5) of 3	0.050	UJ	ug/L			
RGNEVPSFXad1	Field blank associated with process blank						
RGNEVPSFXad2	Per Method 0010						
RGNEVPSFRinse1	Field blank associated with process blank						
RGNEVPSFRinse2	Per Method 0010						
RGNEVPSFCond	Reagent water	-----					
Reagent Blanks							
Sample Name	Sample Description	Result		Units			
RGNEVPSRMeth	Fresh 1:1 (v/v) MeOH/MeCl2 Wash Liquid						

Appendix C – Target Organic Compound Mass Balances

This section presents mass balance information in four ways:

- Overall for the entire experiment, using volatiles off-gas sampling data to estimate volatiles emissions during semi-volatiles/pesticide off-gas sampling, and vice-versa.
- Using data obtained only during volatiles off-gas sampling (Method 0031)
- Using data obtained only during semi-volatiles off-gas sampling (Method 0010)
- OLI model results for predicting organics distribution among evaporator streams when concentrating from 5.8 to 8.0 M Na

A. Overall Mass Balance

Overall Mass Balance/Material Distribution

Hiroshi Saito
12/5/00

Data Qualifier Key
J = estimated value (e.g., quantity between MDL and MRL)

Data Guide
Italic text/Yellow box = qualified data

Feed Data

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	B&W		1479.5	1379.5			1429.5	71	
	4-methyl-2-pentanone	B&W	J	2736.5	2406.5			2571.5	233	
	toluene	B&W		1110	1020			1065	64	
	1,2-dibromoethane	B&W	J	78.9	66.3			72.6	9	
	chlorobenzene	B&W		1280	1070			1175	148	
	1,2,3-trichloropropane	Predicted		990				990		B&W nondetects (800 ug/L det. limit)
Semi-volatiles	1,2,4-trichlorobenzene	SRTC*		610	580	580		590		B&W SVOA nondetects (500 ug/L) or low (17, 41, 55, J=uncertain)
	naphthalene	SRTC*		570	600	530		567	35	B&W SVOA nondetects (100 ug/L) or low (15, J=uncertain)
	Hexachlorobenzene	B&W		430	820	1000	1000	813	269	*B&W VOA high due to signal interference? (1,2,4TCB=1169.7,naph=1578.8, 1078.8)
	Pentachlorophenol	B&W	J	27	81	72		60	29	
	pyrene	SRTC		930	930	930		930	0	B&W SVOA nondetects (100 ug/L)
	BEHP	SRTC		1040	1030			1035	7	B&W results too high (2800, 2900 ug/L)
	BaP	SRTC		1310	1380	1690		1460	202	B&W SVOA nondetects (100 ug/L)
Pesticide	Aldrin	SRTC		1060	1030	1020		1037	21	B&W Pest. low (0.079 - 0.79 ug/L, J=uncertain)
	VOST Feed	24704		19361						
	SVOST Feed	24881		19499						
		g		ml						
		density =		1.276						

Condensate Data

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	B&W		32.2				32.2		
	4-methyl-2-pentanone	SRTC		130	160	26	340	164	131	B&W high (712, 479, E=too conc., 688, J=uncertain)
	toluene	B&W		25.9				25.9		
	1,2-dibromoethane	B&W		41.6				41.6		
	chlorobenzene	B&W		44				44		
	1,2,3-trichloropropane	SRTC		120	170	190	200	170	36	B&W nondetect (<10 ug/L det. Limit)
Semi-volatiles	1,2,4-trichlorobenzene	B&W		32	110	66	110	80	38	
	naphthalene	B&W		140	380	240	420	295	129	
	Hexachlorobenzene	B&W	J	3	4	0	0	1.8	2	SRTC < 1 ppb, B&W < 11 ug/L
	Pentachlorophenol	B&W/SRTC		0				0		SRTC < 1 ppb, B&W < 10 ug/L
	pyrene	B&W		180	140	110	110	135	33	
	BEHP	B&W	J	12	0	0	0	3	6	SRTC values high (360, 330, 320, 320)
	BaP	B&W/SRTC		0				0		SRTC < 1 ppb, B&W < 10 ug/L
Pesticide	Aldrin	B&W		17	33			25	11	SRTC data (0, 0, 51, 60)
	VOST Product	6475		6475						
	SVOST Product	6107		6107						
		g		ml						
		density =		1						

Concentrate Data										
	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	SRTC		12	2.2	5.3	6.3	6.5	4	B&W (20.9, J = uncertain)
	4-methyl-2-pentanone	SRTC		77	48	26	120	68	41	B&W (54.5, J = uncertain)
	toluene	SRTC		8.2	11	11	4.5	8.7	3	B&W (11.8, J = uncertain)
	1,2-dibromoethane	SRTC		0	1.9	1.8	4.5	2.1	2	0 means <1 ppb
	chlorobenzene	SRTC		7.6	5.8	5.4	5.7	6.1	1	B&W (13, 13.2, J = uncertain)
	1,2,3-trichloropropane	SRTC		170	160	190	400	230	114	B&W det. Limit = 400
Semi-volatiles	1,2,4-trichlorobenzene	SRTC		57	75	35	56	56	16	B&W VOA (19.1, 7.1, J = uncertain), B&W SVOA non-detect
	naphthalene	SRTC		36	35	0	30	25	17	B&W VOA (21.6, 17.3, J = uncertain), B&W SVOA non-detect
	Hexachlorobenzene	SRTC		720	940	700	970	833	142	B&W values low (210, 360, 330)
	Pentachlorophenol	B&W		180	130	140		150	26	SRTC values < 1 ug/L
	pyrene	SRTC		690	830	670	830	755	87	B&W low (84) or nondetect (30 ug/L det. Limit)
	BEHP	SRTC		920	920	800	1000	910	82	B&W values high scatter (30, 230, 340, 280, 2000)
	BaP	SRTC		950	1290	1070	1340	1163	184	B&W nondetects (<30 ug/L det.limit)
Pesticide	Aldrin	SRTC		430	340	580		450	121	B&W data (wide scatter on uncertain values)
	VOST Product	19343		13816						
	SVOST Product	18531		13236						
		g		ml						
			density =	1.4						

Sorbent Tube Data										
									Condensor	
				Mass (ug)					Vent	
	Chemical	Data Source		Tenax #1	Tenax #2	Anasorb	XAD-2	TOTAL	(ug/g)	
Volatiles	benzene	B&W	J	2.5		24700		24703	723	Tenax #1 recovery= ~<40%, data orginally in ng
	4-methyl-2-pentanone	B&W	J	1373		31500		32873	963	Tenax #2 recovery unknown (high losses with thermal desorption)
	toluene	B&W	J	1156		10100		11256	330	Anasorb recovery = ~<20%
	1,2-dibromoethane	B&W	J	21.7		4600		4622	135	VOA 5000 ug detection limit
	chlorobenzene	B&W	J	3658		5160		8818	258	
	1,2,3-trichloropropane	B&W	J	0		0		0	0	
Semi-volatiles	1,2,4-trichlorobenzene	B&W		48800		0	9896	9896	315	XAD-2 data QA qualified, Tenax/Anasorb uncertain (J)
	naphthalene	B&W		55902		0	8596	8596	274	
	Hexachlorobenzene	B&W					0	0	0	SVOA 1000 ug detection limit
	Pentachlorophenol	B&W					0	0	0	
	pyrene	B&W					0	0	0	
	BEHP	B&W					0	0	0	
	BaP	B&W					0	0	0	
Pesticide	Aldrin	B&W								No data
	Liters air sampled (STP)				945.0		963.8			
	Total Off-gas flow (ml/min)				411.4		456.4			
	Air in-leakage				11.5		11.5			

Pump Trap Liquids										VOST	SVOST	
	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	Mass (ug)	Mass (ug)	
Volatiles	benzene	SRTC		49				49		12	4	B&W data: 164, 226 (uncertain)
	4-methyl-2-pentanone	SRTC		1200				1200		284	88	B&W data: 7250, 7760 (uncertain)
	toluene	SRTC		33				33		8	2	B&W data: 115, 176 (uncertain)
	1,2-dibromoethane	SRTC		76				76		18	6	B&W data: 339, 392 (uncertain)
	chlorobenzene	SRTC		35				35		8	3	B&W data: 309, 212 (uncertain)
	1,2,3-trichloropropane	SRTC		110				110		26	8	B&W nondetect (<1000 ug/L)
Semi-volatiles	1,2,4-trichlorobenzene	B&W/SRTC		340	500			420	113	99	31	
	naphthalene	B&W/SRTC		1600	1300	1430		1443	150	342	106	
	Hexachlorobenzene	SRTC		0				0				B&W nondetect (<230 ug/L)
	Pentachlorophenol	SRTC		0				0				B&W nondetect (<230 ug/L)
	pyrene	SRTC		91				91		22	7	B&W data: 38, 35 (uncertain)
	BEHP	B&W		0				0				
	BaP	SRTC		0				0				B&W nondetect (<230 ug/L)
Pesticide	Aldrin	SRTC		58				58		14	4	
	VOST Production	236.9		237		Pump trap liquids appear to have reached equilibrium with vapor						
	SVOST Product	73.7		74		Semivolatiles concentrations same for both VOST and SVOST						
		g		ml			pump trap liquids					
			density =	1								

Pump Line Rinse

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	Mass (ug)
Semi-volatiles	1,2,4-trichlorobenzene	B&W		0				0	
	naphthalene	B&W		0				0	
	Hexachlorobenzene	B&W		34000				34000	940
	Pentachlorophenol	B&W		0				0	
	pyrene	B&W		26000				26000	719
	BEHP	B&W		0				0	
	BaP	B&W		0				0	
Pesticide	Aldrin	No data							
		29.19	g 50% CH2Cl2/MeOH line rinse sample						
		1.056	g/ml assumed density						
		0.0276	L 50% CH2Cl2/MeOH						

Overall Mass Balance Data

					Sorbent	Pump	Off-gas		Mass	% of total feed						Condensor
										EXPERIMENTAL DATA			OLI Model Prediction			Vent
	Chemical	Mass Fed (ug)	Condensate	Concentrate	Tube	Traps	Line Rinse	TOTAL	Closure (%)	Condensate	Concentrate	Off-gas	Condensate	Concentrate	Off-gas	(ug/g)
Volatiles	benzene	55550	405	174	49896	15	0	50491	9.11	0.7	0.3	89.8	0.4	0.0	99.5	723
	Std. Dev	2748		111				111	4.50		0.2					
	4-methyl-2-pentanone	99928	2063	1833	66401	373	0	70670	29.28	2.1	1.8	66.8	11.9	0.2	87.9	963
	Std. Dev	9068	1644	1099				1977	6.72	1.6	1.1					
	toluene	41386	326	235	22736	10	0	23307	43.68	0.8	0.6	55.0	0.4	0.0	99.6	330
	Std. Dev	2473		83				83	3.37		0.2					
	1,2-dibromoethane	2821	523	55	9335	24	0	9938	-252.25	18.6	2.0	331.7	3.5	0.1	96.4	135
	Std. Dev	346		50				50	43.27		1.8					
	chlorobenzene	45660	554	166	17811	11	0	18542	59.39	1.2	0.4	39.0	0.9	0.0	99.1	258
	Std. Dev	5770		27				27	5.13		0.1					
	1,2,3-trichloropropane	38471	2139	6222	0	34	0	8395	78.18	5.6	16.2	0.1	4.9	0.1	95.1	0
	Std. Dev		448	3085				3117	8.10	1.2	8.0					
Semi-volatiles	1,2,4-trichlorobenzene	22927	1000	1508	19599	130	0	22238	3.01	4.4	6.6	86.1	0.9	0.0	99.0	315
	Std. Dev		476	443		35		651	2.84	2.1	1.9	0.2				
	naphthalene	22021	3712	683	17024	448	0	21867	0.69	16.9	3.1	79.3	2.8	0.0	97.2	274
	Std. Dev	1365	1623	461		47		1688	9.83	7.4	2.1	0.2				
	Hexachlorobenzene	31574	22	22522	0	0	940	23483	25.62	0.1	71.3	3.0	0.0	100.0	0.0	0
	Std. Dev	10443	26	3847				3847	27.45	0.08	12.2					
	Pentachlorophenol	2332	0	4058	0	0	0	4058	-74.04	0.0	174.0	0.0	77.8	19.4	2.8	0
	Std. Dev	1124		716				716	89.36		30.7					
	pyrene	36140	1699	20425	0	28	719	22870	36.72	4.7	56.5	2.1	88.3	6.0	5.6	0
	Std. Dev	0	417	2353				2390	6.61	1.2	6.5					
	BEHP	40220	38	24618	0	0	0	24656	38.70	0.1	61.2	0.0	12.6	87.4	0.0	0
	Std. Dev	275	75	2231				2232	5.57	0.2	5.5					
	BaP	56735	0	31449	0	0	0	31449	44.57	0.0	55.4	0.0	0.0	100.0	0.0	0
	Std. Dev	7859		4975				4975	11.66		8.8					
Pesticide	Aldrin	40285	315	31449	0	18	0	31782	21.11	0.8	78.1	0.0	67.7	31.3	1.0	0
	Std. Dev	809	142	4975				4977	12.46	0.4	12.4					
	Theoretical (each)	50518														

					Sorbent	Pump	Off-gas		Mass	% of total feed						Condensor
										EXPERIMENTAL DATA			OLI Model Prediction			Vent
	Chemical	Mass Fed (ug)	Condensate	Concentrate	Tube	Traps	Line Rinse	TOTAL	Closure (%)	Condensate	Concentrate	Off-gas	Condensate	Concentrate	Off-gas	(ug/g)
Volatiles	benzene	55550	405	174	49896	15	0	50476	9.13	0.7	0.3	89.8	0.4	0.0	99.5	723
	4-methyl-2-pentanone	99928	2063	1833	66401	373	0	70297	29.65	2.1	1.8	66.8	11.9	0.2	87.9	963
	toluene	41386	326	235	22736	10	0	23297	43.71	0.8	0.6	55.0	0.4	0.0	99.6	330
	1,2-dibromoethane	2821	523	55	9335	24	0	9914	-251.41	18.6	2.0	331.7	3.5	0.1	96.4	135
	chlorobenzene	45660	554	166	17811	11	0	18531	59.42	1.2	0.4	39.0	0.9	0.0	99.1	258
	1,2,3-trichloropropane	38471	2139	6222	0	34	0	8361	78.27	5.6	16.2	0.1	4.9	0.1	95.1	0
Semi-volatiles	1,2,4-trichlorobenzene	22927	1000	1508	19599	130	0	22108	3.58	4.4	6.6	86.1	0.9	0.0	99.0	315
	naphthalene	22021	3712	683	17024	448	0	21419	2.73	16.9	3.1	79.3	2.8	0.0	97.2	274
	Hexachlorobenzene	31574	22	22522	0	0	940	22544	28.60	0.1	71.3	3.0	0.0	100.0	0.0	0
	Pentachlorophenol	2332	0	4058	0	0	0	4058	-74.04	0.0	174.0	0.0	77.8	19.4	2.8	0
	pyrene	36140	1699	20425	0	28	719	22123	38.78	4.7	56.5	2.1	88.3	6.0	5.6	0
	BEHP	40220	38	24618	0	0	0	24656	38.70	0.1	61.2	0.0	12.6	87.4	0.0	0
	BaP	56735	0	31449	0	0	0	31449	44.57	0.0	55.4	0.0	0.0	100.0	0.0	0
Pesticide	Aldrin	40285	315	31449	0	18	0	31763	21.15	0.8	78.1	0.0	67.7	31.3	1.0	0
	Theoretical (each)	50518														

1.3 ml spike solution/liter feed

Spike solution conc. = 1000 ug/ml per compound

B. Volatiles Off-gas Sampling Mass Balance (VOST)

VOST Sampling Mass Balance/Material Distribution

Hiroshi Saito
12/5/00

Data Qualifier Key
J = estimated value (e.g., quantity between MDL and MRL)

Data Guide
Italic text/Yellow box = qualified data

Feed Data

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	B&W		1479.5	1379.5			1429.5	71	
	4-methyl-2-pentanone	B&W	J	*2736.5*	*2406.5*			*2571.5*	*233*	
	toluene	B&W		1110	1020			1065	64	
	1,2-dibromoethane	B&W	J	*78.9*	*66.3*			*72.6*	*9*	
	chlorobenzene	B&W		1280	1070			1175	148	
	1,2,3-trichloropropane	Predicted		*990*				*990*		B&W nondetects (800 ug/L det. limit)
Semi-volatiles	1,2,4-trichlorobenzene	SRTC*		610	580	580		590		B&W SVOA nondetects (500 ug/L) or low (17, 41, 55, J=uncertain)
	naphthalene	SRTC*		570	600	530		567	35	B&W SVOA nondetects (100 ug/L) or low (15, J=uncertain)
	Hexachlorobenzene	B&W		430	820			625	276	*B&W VOA high due to signal interference? (1,2,4TCB=1169.7,naph=1578.8, 1078.8)
	Pentachlorophenol	B&W	J	*27*	*81*			*54*	*38*	
	pyrene	SRTC		930	930			930	0	B&W SVOA nondetects (100 ug/L)
	BEHP	B&W		1040	1030			1035	7	B&W results too high (2800, 2900 ug/L)
	BaP	SRTC		1310	1380			1345	49	B&W SVOA nondetects (100 ug/L)
Pesticide	Aldrin	SRTC		1060	1030			1045	21	B&W Pest. low (0.079 - 0.79 ug/L, J=uncertain)
	VOST Feed	24704		19361						
	SVOST Feed									
		g		ml						
		density =		1.276						

Condensate Data

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	B&W		32.2				32.2		
	4-methyl-2-pentanone	SRTC		130	160	26		105	70	B&W high (712, 479, E=too conc., 688, J=uncertain)
	toluene	B&W		25.9				25.9		
	1,2-dibromoethane	B&W		41.6				41.6		
	chlorobenzene	B&W		44				44		
	1,2,3-trichloropropane	SRTC		120	170	190		160	36	B&W nondetect (<10 ug/L det. Limit)
Semi-volatiles	1,2,4-trichlorobenzene	B&W		32	110			71	55	
	naphthalene	B&W		140	380			260	170	
	Hexachlorobenzene	B&W	J	*3*	*4*	0		*2.3*	*2*	SRTC < 1 ppb, B&W < 11 ug/L
	Pentachlorophenol	B&W/SRTC		0				0		SRTC < 1 ppb, B&W < 10 ug/L
	pyrene	B&W		180	140			160	28	
	BEHP	B&W	J	*12*	0	0		*4*	*7*	SRTC values high (360, 330, 320, 320)
	BaP	B&W/SRTC		0				0		SRTC < 1 ppb, B&W < 10 ug/L
Pesticide	Aldrin	B&W		17				17		SRTC data (0, 0, 51, 60)
	VOST Product	6475		6475						
	SVOST Product									
		g		ml						
		density =		1						

Concentrate Data										
	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	SRTC		12	2.2	5.3		6.5	5	B&W (20.9, J = uncertain)
	4-methyl-2-pentanone	SRTC		77	48	26		50	26	B&W (54.5, J = uncertain)
	toluene	SRTC		8.2	11	11		10.1	2	B&W (11.8, J = uncertain)
	1,2-dibromoethane	SRTC		0	1.9	1.8		1.2	1	0 means <1 ppb
	chlorobenzene	SRTC		7.6	5.8	5.4		6.3	1	B&W (13, 13.2, J = uncertain)
	1,2,3-trichloropropane	SRTC		170	160	190		173	15	B&W det. Limit = 400
Semi-volatiles	1,2,4-trichlorobenzene	SRTC		57	75	35		56	20	B&W VOA (19.1, 7.1, J = uncertain), B&W SVOA non-detect
	naphthalene	SRTC		36	35	0		24	21	B&W VOA (21.6, 17.3, J = uncertain), B&W SVOA non-detect
	Hexachlorobenzene	SRTC		720	940	700		787	133	B&W values low (210, 360, 330)
	Pentachlorophenol	B&W		180	130	140		150	26	SRTC values < 1 ug/L
	pyrene	SRTC		690	830	670		730	87	B&W low (84) or nondetect (30 ug/L det. Limit)
	BEHP	SRTC		920	920	800		880	69	B&W values high scatter (30, 230, 340, 280, 2000)
	BaP	SRTC		950	1290	1070		1103	172	B&W nondetects (<30 ug/L det.limit)
Pesticide	Aldrin	SRTC		430	340	580		450	121	B&W data (wide scatter on uncertain values)
	VOST Product	19343		13816						
	SVOST Product									
		g		ml						
		density =		1.4						

Sorbent Tube Data									Condensor	
				Mass (ug)					Vent	
	Chemical	Data Source		Tenax #1	Tenax #2	Anasorb	XAD-2	TOTAL	(ug/g)	
Volatiles	benzene	B&W	J	2.5		24700		24703	723	Tenax #1 recovery= ~<40%, data orginally in ng
	4-methyl-2-pentanone	B&W	J	1373		31500		32873	963	Tenax #2 recovery unknown (high losses with thermal desorption)
	toluene	B&W	J	1156		10100		11256	330	Anasorb recovery = ~<20%
	1,2-dibromoethane	B&W	J	21.7		4600		4622	135	VOA 5000 ug detection limit
	chlorobenzene	B&W	J	3658		5160		8818	258	
	1,2,3-trichloropropane	B&W	J	0		0		0	0	
Semi-volatiles	1,2,4-trichlorobenzene	B&W		48800		0	9896	9703	315	XAD-2 data QA qualified, Tenax/Anasorb uncertain (J)
	naphthalene	B&W		55902		0	8596	8428	274	
	Hexachlorobenzene	B&W					0	0	0	SVOA 1000 ug detection limit
	Pentachlorophenol	B&W					0	0	0	
	pyrene	B&W					0	0	0	
	BEHP	B&W					0	0	0	
	BaP	B&W					0	0	0	
Pesticide	Aldrin	B&W								No data
	Liters air sampled (STP)			945.0			963.8	SVOA mass scaled by volume		
	Total Off-gas flow (ml/min)				411.4		456.4			
	Air in-leakage				11.5		11.5			

Pump Trap Liquids									VOST	SVOST	
	Chemical	Data Source	Concentration Data (ug/L)				AVERAGE	STD. DEV.	Mass (ug)	Mass (ug)	
Volatiles	benzene	SRTC	49				49		12		B&W data: 164, 226 (uncertain)
	4-methyl-2-pentanone	SRTC	1200				1200		284		B&W data: 7250, 7760 (uncertain)
	toluene	SRTC	33				33		8		B&W data: 115, 176 (uncertain)
	1,2-dibromoethane	SRTC	76				76		18		B&W data: 339, 392 (uncertain)
	chlorobenzene	SRTC	35				35		8		B&W data: 309, 212 (uncertain)
	1,2,3-trichloropropane	SRTC	110				110		26		B&W nondetect (<1000 ug/L)
Semi-volatiles	1,2,4-trichlorobenzene	B&W/SRTC	340	500			420	113	99		
	naphthalene	B&W/SRTC	1600	1300	1430		1443	150	342		
	Hexachlorobenzene	SRTC	0				0				B&W nondetect (<230 ug/L)
	Pentachlorophenol	SRTC	0				0				B&W nondetect (<230 ug/L)
	pyrene	SRTC	91				91		22		B&W data: 38, 35 (uncertain)
	BEHP	B&W	0				0				
	BaP	SRTC	0				0				B&W nondetect (<230 ug/L)
Pesticide	Aldrin	SRTC	58				58		14		
	VOST Production	236.9	237		Pump trap liquids appear to have reached equilibrium with vapor						
	SVOST Product	73.7	74		Semivolatiles concentrations same for both VOST and SVOST						
		g	ml			pump trap liquids					
		density =	1								

Pump Line Rinse									
	Chemical	Data Source	Concentration Data (ug/L)				AVERAGE	Mass (ug)	
Semi-volatiles	1,2,4-trichlorobenzene	B&W	0				0		
	naphthalene	B&W	0				0		
	Hexachlorobenzene	B&W	34000				34000	465	Scaled by volume
	Pentachlorophenol	B&W	0				0		
	pyrene	B&W	26000				26000	356	Scaled by volume
	BEHP	B&W	0				0		
	BaP	B&W	0				0		
Pesticide	Aldrin	No data							
		29.19	g 50% CH2Cl2/MeOH line rinse sample						
		1.056	g/ml assumed density						
		0.0276	L 50% CH2Cl2/MeOH						

VOST Mass Balance Data

					Sorbent	Pump	Off-gas		Mass	% of total feed						Condensor
										EXPERIMENTAL DATA			OLI Model Prediction			Vent
	Chemical	Mass In (ug)	Condensate	Concentrate	Tube	Traps	Line Rinse	TOTAL	Closure (%)	Condensate	Concentrate	Off-gas	Condensate	Concentrate	Off-gas	(ug/g)
Volatiles	benzene	27676	208	90	24703	12	0	25012	9.62	0.8	0.3	89.3	0.4	0.0	99.5	723
	Std. Dev	1369		69				69	4.48		0.3					
	4-methyl-2-pentanone	49786	682	695	32873	284	0	34535	30.63	1.4	1.4	66.6	11.9	0.2	87.9	963
	Std. Dev	4518	455	353				576	6.40	0.9	0.7					
	toluene	20619	168	139	11256	8	0	11571	43.88	0.8	0.7	54.6	0.4	0.0	99.6	330
	Std. Dev	1232		22				22	3.36		0.1					
	1,2-dibromoethane	1406	269	17	4622	18	0	4926	-250.47	19.2	1.2	330.1	3.5	0.1	96.4	135
	Std. Dev	172		15				15	43.02		1.1					
	chlorobenzene	22749	285	87	8818	8	0	9198	59.57	1.3	0.4	38.8	0.9	0.0	99.1	258
	Std. Dev	2875		16				16	5.11		0.1					
	1,2,3-trichloropropane	19167	1036	2395	0	26	0	3457	81.96	5.4	12.5	0.1	4.9	0.1	95.1	0
	Std. Dev		233	211				315	1.64	1.2	1.1					
Semi-volatiles	1,2,4-trichlorobenzene	11423	460	769	9703	99	0	11031	3.43	4.0	6.7	85.8	0.9	0.0	99.0	315
	Std. Dev		357	277		35		453	3.97	3.1	2.4	0.3				
	naphthalene	10971	1684	327	8428	342	0	10781	1.73	15.3	3.0	79.9	2.8	0.0	97.2	274
	Std. Dev	680	1099	283		47		1136	12.01	10.0	2.6	0.4				
	Hexachlorobenzene	12100	15	10869	0	0	465	11349	6.21	0.1	89.8	3.8	0.0	100.0	0.0	0
	Std. Dev	5339	13	1840				1840	44.09	0.11	15.2					
	Pentachlorophenol	1045	0	2072	0	0	0	2072	-98.23	0.0	198.2	0.0	77.8	19.4	2.8	0
	Std. Dev	739		366				366	144.47		35.0					
	pyrene	18005	1036	10086	0	22	356	11499	36.13	5.8	56.0	2.1	88.3	6.0	5.6	0
	Std. Dev	0	183	1204				1218	6.77	1.0	6.7					
	BEHP	20038	26	12158	0	0	0	12184	39.19	0.1	60.7	0.0	12.6	87.4	0.0	0
	Std. Dev	137	45	957				958	4.80	0.2	4.8					
	BaP	26040	0	15244	0	0	0	15244	41.46	0.0	58.5	0.0	0.0	100.0	0.0	0
	Std. Dev	958		2382				2382	9.40		9.1					
Pesticide	Aldrin	20232	110	15244	0	14	0	15368	24.04	0.5	75.3	0.1	67.7	31.3	1.0	0
	Std. Dev	411	0	2382				2382	11.88	0.0	11.8					

					Sorbent	Pump	Off-gas		Mass	% of total feed						Condensor
										EXPERIMENTAL DATA			OLI Model Prediction			Vent
	Chemical	Mass In (ug)	Condensate	Concentrate	Tube	Traps	Line Rinse	TOTAL	Closure (%)	Condensate	Concentrate	Off-gas	Condensate	Concentrate	Off-gas	(ug/g)
Volatiles	benzene	27676	208	90	24703	12	0	25001	9.67	0.8	0.3	89.3	0.4	0.0	99.5	723
	4-methyl-2-pentanone	49786	682	695	32873	284	0	34251	31.20	1.4	1.4	66.6	11.9	0.2	87.9	963
	toluene	20619	168	139	11256	8	0	11563	43.92	0.8	0.7	54.6	0.4	0.0	99.6	330
	1,2-dibromoethane	1406	269	17	4622	18	0	4908	-249.19	19.2	1.2	330.1	3.5	0.1	96.4	135
	chlorobenzene	22749	285	87	8818	8	0	9189	59.60	1.3	0.4	38.8	0.9	0.0	99.1	258
	1,2,3-trichloropropane	19167	1036	2395	0	26	0	3431	82.10	5.4	12.5	0.1	4.9	0.1	95.1	0
Semi-volatiles	1,2,4-trichlorobenzene	11423	460	769	9703	99	0	10932	4.30	4.0	6.7	85.8	0.9	0.0	99.0	315
	naphthalene	10971	1684	327	8428	342	0	10439	4.85	15.3	3.0	79.9	2.8	0.0	97.2	274
	Hexachlorobenzene	12100	15	10869	0	0	465	10884	10.05	0.1	89.8	3.8	0.0	100.0	0.0	0
	Pentachlorophenol	1045	0	2072	0	0	0	2072	-98.23	0.0	198.2	0.0	77.8	19.4	2.8	0
	pyrene	18005	1036	10086	0	22	356	11122	38.23	5.8	56.0	2.1	88.3	6.0	5.6	0
	BEHP	20038	26	12158	0	0	0	12184	39.19	0.1	60.7	0.0	12.6	87.4	0.0	0
	BaP	26040	0	15244	0	0	0	15244	41.46	0.0	58.5	0.0	0.0	100.0	0.0	0
Pesticide	Aldrin	20232	110	15244		14		15354	24.11	0.5	75.3	0.1	67.7	31.3	1.0	0
	Theoretical (each)	25169														

1.3 ml spike solution/liter feed

Spike solution conc. = 1000 ug/ml per compound

C. Semi-volatiles Off-gas Sampling Mass Balance (SVOST)

SVOST Sampling Mass Balance/Material Distribution

Hiroshi Saito
12/5/00

Data Qualifier Key
J = estimated value (e.g., quantity between MDL and MRL)

Data Guide
Italic text/Yellow box = qualified data

Feed Data

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	B&W		1479.5	1379.5			1429.5	71	Use VOST data for all volatiles,as no suitable SVOST data
	4-methyl-2-pentanone	B&W	J	2736.5	2406.5			2571.5	233	
	toluene	B&W		1110	1020			1065	64	
	1,2-dibromoethane	B&W	J	78.9	66.3			72.6	9	
	chlorobenzene	B&W		1280	1070			1175	148	
	1,2,3-trichloropropane	Predicted		990				990		B&W nondetects (800 ug/L det. limit)
Semi-volatiles	1,2,4-trichlorobenzene	SRTC*				580		580		B&W SVOA nondetects (500 ug/L) or low (17, 41, 55, J=uncertain)
	naphthalene	SRTC*				530		530		B&W SVOA nondetects (100 ug/L) or low (15, J=uncertain)
	Hexachlorobenzene	B&W				1000	1000	1000	0	*B&W VOA high due to signal interference? (1,2,4TCB=1169.7,naph=1578.8, 1078.8)
	Pentachlorophenol	B&W	J			72		72		
	pyrene	SRTC				930		930		B&W SVOA nondetects (100 ug/L)
	BEHP	SRTC		1040	1030			1035	7	B&W results too high (2800, 2900 ug/L), using VOST results
	BaP	SRTC				1690		1690		B&W SVOA nondetects (100 ug/L)
Pesticide	Aldrin	SRTC				1020		1020		B&W Pest. low (0.079 - 0.79 ug/L, J=uncertain)
	VOST Feed									
	SVOST Feed	24881		19499						
		g		ml						
		density =		1.276						

Condensate Data

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	B&W		32.2				32.2		Using VOST data as no suitable SVOST data
	4-methyl-2-pentanone	SRTC					340	340		B&W high (712, 479, E=too conc., 688, J=uncertain)
	toluene	B&W		25.9				25.9		Using VOST data as no suitable SVOST data
	1,2-dibromoethane	B&W		41.6				41.6		Using VOST data as no suitable SVOST data
	chlorobenzene	B&W		44				44		Using VOST data as no suitable SVOST data
	1,2,3-trichloropropane	SRTC					200	200		B&W nondetect (<10 ug/L det. Limit)
Semi-volatiles	1,2,4-trichlorobenzene	B&W				66	110	88	31	
	naphthalene	B&W				240	420	330	127	
	Hexachlorobenzene	B&W		0	0	0		0	0	
	Pentachlorophenol	B&W/SRTC		0				0		SRTC < 1 ppb, B&W < 10 ug/L
	pyrene	B&W				110	110	110	0	
	BEHP	B&W		0	0	0		0	0	SRTC values high (360, 330, 320, 320)
	BaP	B&W/SRTC		0				0		SRTC < 1 ppb, B&W < 10 ug/L
Pesticide	Aldrin	B&W			33			33		SRTC data (0, 0, 51, 60)
	VOST Product									
	SVOST Product	6107		6107						
		g		ml						
		density =		1						

Concentrate Data

	Chemical	Data Source		Concentration Data (ug/L)				AVERAGE	STD. DEV.	
Volatiles	benzene	SRTC					6.3	6.3		B&W (20.9, J = uncertain)
	4-methyl-2-pentanone	SRTC					120	120		B&W (54.5, J = uncertain)
	toluene	SRTC					4.5	4.5		B&W (11.8, J = uncertain)
	1,2-dibromoethane	SRTC					4.5	4.5		0 means <1 ppb
	chlorobenzene	SRTC					5.7	5.7		B&W (13, 13.2, J = uncertain)
	1,2,3-trichloropropane	SRTC					400	400		B&W det. Limit = 400
Semi-volatiles	1,2,4-trichlorobenzene	SRTC					56	56		B&W VOA (19.1, 7.1, J = uncertain), B&W SVOA non-detect
	naphthalene	SRTC					30	30		B&W VOA (21.6, 17.3, J = uncertain), B&W SVOA non-detect
	Hexachlorobenzene	SRTC					970	970		B&W values low (210, 360, 330)
	Pentachlorophenol	B&W		180	130	140		150	26	SRTC values < 1 ug/L, using VOST data as no suitable SVOST data
	pyrene	SRTC					830	830		B&W low (84) or nondetect (30 ug/L det. Limit)
	BEHP	SRTC					1000	1000		B&W values high scatter (30, 230, 340, 280, 2000)
	BaP	SRTC					1340	1340		B&W nondetects (<30 ug/L det.limit)
Pesticide	Aldrin	SRTC		430	340	580		450	121	B&W data (wide scatter on uncertain values), using VOST data as no suitable SVOST data
	VOST Product									
	SVOST Product	18531		13236						
		g		ml						
			density =	1.4						

Sorbent Tube Data

				Mass (ug)					Condensor Vent (ug/g)	
	Chemical	Data Source		Tenax #1	Tenax #2	Anasorb	XAD-2	TOTAL		
Volatiles	benzene	B&W	J	2.5		24700		25194	723	Tenax #1 recovery= ~<40%, data orginally in ng
	4-methyl-2-pentanone	B&W	J	1373		31500		33527	963	Tenax #2 recovery unknown (high losses with thermal desorption)
	toluene	B&W	J	1156		10100		11480	330	Anasorb recovery = ~<20%
	1,2-dibromoethane	B&W	J	21.7		4600		4714	135	VOA 5000 ug detection limit
	chlorobenzene	B&W	J	3658		5160		8993	258	
	1,2,3-trichloropropane	B&W	J	0		0		0	0	
Semi-volatiles	1,2,4-trichlorobenzene	B&W		48800		0	9896	9896	315	XAD-2 data QA qualified, Tenax/Anasorb uncertain (J)
	naphthalene	B&W		55902		0	8596	8596	274	
	Hexachlorobenzene	B&W					0	0	0	SVOA 1000 ug detection limit
	Pentachlorophenol	B&W					0	0	0	
	pyrene	B&W					0	0	0	
	BEHP	B&W					0	0	0	
	BaP	B&W					0	0	0	
Pesticide	Aldrin	B&W								No data
	Liters air sampled (STP)			945.0			963.8			
	Total Off-gas flow (ml/min)			411.4			456.4			
	Air in-leakage			11.5			11.5			

Pump Trap Liquids									VOST	SVOST	
	Chemical	Data Source	Concentration Data (ug/L)				AVERAGE	STD. DEV.	Mass (ug)	Mass (ug)	
Volatiles	benzene	SRTC	49				49			4	B&W data: 164, 226 (uncertain)
	4-methyl-2-pentanone	SRTC	1200				1200			88	B&W data: 7250, 7760 (uncertain)
	toluene	SRTC	33				33			2	B&W data: 115, 176 (uncertain)
	1,2-dibromoethane	SRTC	76				76			6	B&W data: 339, 392 (uncertain)
	chlorobenzene	SRTC	35				35			3	B&W data: 309, 212 (uncertain)
	1,2,3-trichloropropane	SRTC	110				110			8	B&W nondetect (<1000 ug/L)
Semi-volatiles	1,2,4-trichlorobenzene	B&W/SRTC	340	500			420	113		31	
	naphthalene	B&W/SRTC	1600	1300	1430		1443	150		106	
	Hexachlorobenzene	SRTC	0				0				B&W nondetect (<230 ug/L)
	Pentachlorophenol	SRTC	0				0				B&W nondetect (<230 ug/L)
	pyrene	SRTC	91				91			7	B&W data: 38, 35 (uncertain)
	BEHP	B&W	0				0				
	BaP	SRTC	0				0				B&W nondetect (<230 ug/L)
Pesticide	Aldrin	SRTC	58				58			4	
	VOST Production	236.9	237		Pump trap liquids appear to have reached equilibrium with vapor						
	SVOST Product	73.7	74		Semivolatiles concentrations same for both VOST and SVOST						
		g	ml			pump trap liquids					
		density =	1								

Pump Line Rinse								
	Chemical	Data Source	Concentration Data (ug/L)				AVERAGE	Mass (ug)
Semi-volatiles	1,2,4-trichlorobenzene	B&W	0				0	
	naphthalene	B&W	0				0	
	Hexachlorobenzene	B&W	34000				34000	475
	Pentachlorophenol	B&W	0				0	
	pyrene	B&W	26000				26000	363
	BEHP	B&W	0				0	
	BaP	B&W	0				0	
Pesticide	Aldrin	No data						
		29.19	g 50% CH_2Cl_2/MeOH line rinse sample					
		1.056	g/ml assumed density					
		0.0276	L 50% CH_2Cl_2/MeOH					

SVOST Mass Balance Data

										% of total feed						Condensor
					Sorbent	Pump	Off-gas		Mass	EXPERIMENTAL DATA			OLI Model Prediction			Vent
	Chemical	Mass In (ug)	Condensate	Concentrate	Tube	Traps	Line Rinse	TOTAL	Closure (%)	Condensate	Concentrate	Off-gas	Condensate	Concentrate	Off-gas	(ug/g)
Volatiles	benzene	27874	197	83	25194	4	0	25477	8.60	0.7	0.3	90.4	0.4	0.0	99.5	723
	Std. Dev	1379							4.52							
	4-methyl-2-pentanone	50142	2076	1588	33527	88	0	37280	25.65	4.1	3.2	67.0	11.9	0.2	87.9	963
	Std. Dev	4550							6.75							
	toluene	20767	158	60	11480	2	0	11700	43.66	0.8	0.3	55.3	0.4	0.0	99.6	330
	Std. Dev	1241							3.37							
	1,2-dibromoethane	1416	254	60	4714	6	0	5033	-255.51	17.9	4.2	333.4	3.5	0.1	96.4	135
	Std. Dev	174							43.63							
	chlorobenzene	22912	269	75	8993	3	0	9340	59.23	1.2	0.3	39.3	0.9	0.0	99.1	258
	Std. Dev	2895		0				0	5.15							
	1,2,3-trichloropropane	19304	1221	5295	0	8	0	6524	66.20	6.3	27.4	0.0	4.9	0.1	95.1	0
	Std. Dev															
Semi-volatiles	1,2,4-trichlorobenzene	11310	537	741	9896	31	0	11206	0.92	4.8	6.6	87.8	0.9	0.0	99.0	315
	Std. Dev		190			35		193	1.71	1.7		0.3				
	naphthalene	10335	2015	397	8596	106	0	11115	-7.55	19.5	3.8	84.2	2.8	0.0	97.2	274
	Std. Dev		777			47		779	7.53	7.5		0.5				
	Hexachlorobenzene	19499	0	12839	0	0	475	13314	31.72	0.0	65.8	2.4	0.0	100.0	0.0	0
	Std. Dev		0					0	0.00	0.00						
	Pentachlorophenol	1404	0	1985	0	0	0	1985	-41.42	0.0	141.4	0.0	77.8	19.4	2.8	0
	Std. Dev			350				350	24.94		24.9					
	pyrene	18134	672	10986	0	7	363	12028	33.67	3.7	60.6	2.0	88.3	6.0	5.6	0
	Std. Dev															
	BEHP	20182	0	13236	0	0	0	13236	34.41	0.0	65.6	0.0	12.6	87.4	0.0	0
	Std. Dev	138							0.45							
	BaP	32954	0	17737	0	0	0	17737	46.18	0.0	53.8	0.0	0.0	100.0	0.0	0
	Std. Dev															
Pesticide	Aldrin	19889	202	17737	0	4	0	17943	9.79	1.0	89.2	0.0	67.7	31.3	1.0	0
	Std. Dev															

										% of total feed						Condensor
					Sorbent	Pump	Off-gas		Mass	EXPERIMENTAL DATA			OLI Model Prediction			Vent
	Chemical	Mass In (ug)	Condensate	Concentrate	Tube	Traps	Line Rinse	TOTAL	Closure (%)	Condensate	Concentrate	Off-gas	Condensate	Concentrate	Off-gas	(ug/g)
Volatiles	benzene	27874	197	83	25194	4	0	25474	8.61	0.7	0.3	90.4	0.4	0.0	99.5	723
	4-methyl-2-pentanone	50142	2076	1588	33527	88	0	37192	25.83	4.1	3.2	67.0	11.9	0.2	87.9	963
	toluene	20767	158	60	11480	2	0	11698	43.67	0.8	0.3	55.3	0.4	0.0	99.6	330
	1,2-dibromoethane	1416	254	60	4714	6	0	5027	-255.12	17.9	4.2	333.4	3.5	0.1	96.4	135
	chlorobenzene	22912	269	75	8993	3	0	9337	59.25	1.2	0.3	39.3	0.9	0.0	99.1	258
	1,2,3-trichloropropane	19304	1221	5295	0	8	0	6516	66.25	6.3	27.4	0.0	4.9	0.1	95.1	0
Semi-volatiles	1,2,4-trichlorobenzene	11310	537	741	9896	31	0	11175	1.19	4.8	6.6	87.8	0.9	0.0	99.0	315
	naphthalene	10335	2015	397	8596	106	0	11008	-6.52	19.5	3.8	84.2	2.8	0.0	97.2	274
	Hexachlorobenzene	19499	0	12839	0	0	475	12839	34.15	0.0	65.8	2.4	0.0	100.0	0.0	0
	Pentachlorophenol	1404	0	1985	0	0	0	1985	-41.42	0.0	141.4	0.0	77.8	19.4	2.8	0
	pyrene	18134	672	10986	0	7	363	11658	35.71	3.7	60.6	2.0	88.3	6.0	5.6	0
	BEHP	20182	0	13236	0	0	0	13236	34.41	0.0	65.6	0.0	12.6	87.4	0.0	0
	BaP	32954	0	17737	0	0	0	17737	46.18	0.0	53.8	0.0	0.0	100.0	0.0	0
Pesticide	Aldrin	19889	202	17737		4		17938	9.81	1.0	89.2	0.0	67.7	31.3	1.0	0
	Theoretical (each)	25349														

1.3 ml spike solution/liter feed

Spike solution conc. = 1000 ug/ml per compound

D. OLI Model Prediction – Concentration from 5.8 to 8.0 M Na

OLI Model Predictions (5.8 M to 8.0 M Na Evaporation)

A. S. Choi
5/18/00

									Percentage out as		
	Chemical	Amt. In (mole)	Condensate	Concentrate	Sorbent Tube	TOTAL	Mass Closure (%)		Condensate	Concentrate	Off-gas
Volatiles	benzene	0.019185	0.000085	0.000001	0.019098	0.019185	0.00		0.4	0.0	99.5
	4-methyl-2-pentanone	0.014962	0.001778	0.000025	0.013159	0.014962	0.00		11.9	0.2	87.9
	toluene	0.016264	0.000063	0.000001	0.016200	0.016264	0.00		0.4	0.0	99.6
	1,2-dibromoethane	0.007977	0.000280	0.000004	0.007693	0.007977	0.00		3.5	0.1	96.4
	chlorobenzene	0.013314	0.000115	0.000002	0.013197	0.013314	0.00		0.9	0.0	99.1
	1,2,3-trichloropropane	0.010165	0.000496	0.000007	0.009662	0.010165	0.00		4.9	0.1	95.1
Semi-volatiles	1,2,4-trichlorobenzene	0.008259	0.000078	0.000001	0.008180	0.008259	0.00		0.9	0.0	99.0
	naphthalene	0.011692	0.000323	0.000005	0.011364	0.011692	0.00		2.8	0.0	97.2
	Hexachlorobenzene	0.005262	0	0.005261	0	0.005261	0.02		0.0	100.0	0.0
	Pentachlorophenol	0.005627	0.004380	0.001091	0.000155	0.005627	0.00		77.8	19.4	2.8
	pyrene	0.007409	0.006540	0.000447	0.000412	0.007399	0.15		88.3	6.0	5.6
	BEHP	0.003837	0.000483	0.003353	0.000001	0.003836	0.02		12.6	87.4	0.0
	BaP	0.005939	0	0.005938	0	0.005938	0.02		0.0	100.0	0.0
Pesticide	Aldrin	0.004107	0.002780	0.001284	0.000042	0.004106	0.01		67.7	31.3	1.0