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Modeling Unsteady-State VOC Transport in Simulated Waste Drums

Kevin J. Liekhus
Garold L. Gresham
Eric S. Peterson
Cathy Rae
Norman J. Hotz
Mike J. Connolly

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Idaho National Engineering Laboratory
EG&G Idaho, Inc.
Idaho Falls, Idaho 83415

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DISCLAIMER

ABSTRACT

This report is a revision of an EG&G Idaho informal report originally titled *Modeling VOC Transport in Simulated Waste Drums*. A volatile organic compound (VOC) transport model has been developed to describe unsteady-state VOC permeation and diffusion within a waste drum. Model equations account for three primary mechanisms for VOC transport from a void volume within the drum. These mechanisms are VOC permeation across a polymer boundary, VOC diffusion across an opening in a volume boundary, and VOC solubilization in a polymer boundary. A series of lab-scale experiments was performed in which the VOC concentration was measured in simulated waste drums under different conditions. A lab-scale simulated waste drum consisted of a sized-down 55-gal metal drum containing a modified rigid polyethylene drum liner. Four polyethylene bags were sealed inside a large polyethylene bag, supported by a wire cage, and placed inside the drum liner. The small bags were filled with VOC-air gas mixture and the VOC concentration was measured throughout the drum over a period of time. Test variables included the type of VOC-air gas mixtures introduced into the small bags, the small bag closure type, and the presence or absence of a variable external heat source.

Model results were calculated for those trials where the VOC permeability had been measured. Permeabilities for five VOCs [methylene chloride, 1,1,1-trichloroethane, carbon tetrachloride, trichloroethylene, and 1,1,2-trichloro-1,2,2-trifluoroethane (Freon-113)] were measured across a polyethylene bag. Comparison of model and experimental results of VOC concentration as a function of time indicate that model accurately accounts for significant VOC transport mechanisms in a lab-scale waste drum.

EXECUTIVE SUMMARY

Pretest waste characterization of waste drums for the bin-scale tests at the Waste Isolation Pilot Plant (WIPP) includes sampling for volatile organic compounds (VOCs) from three areas within drums (drum headspace, the 55-gal poly bag headspace, and the innermost layers of confinement headspace) of transuranic waste. A test program has been initiated at the Idaho National Engineering Laboratory to demonstrate that a VOC concentration in the void space of each layer of confinement can be estimated without extensive sampling of the waste by using a model incorporating theoretical diffusive and permeative transport principles and limited waste drum sampling data. A model incorporating these fundamental transport principles was used to describe unsteady-state VOC transport from lab-scale simulated waste drums. An accurate model of VOC transport in a lab-scale simulated waste drum will serve as the foundation for model development for VOC transport in an actual waste drum. A model capable of characterizing the VOC concentration in a real waste drum will be used to assist in defining drum headspace representativeness and may more quickly eliminate the need for sampling of inner layers of confinement resulting in lower worker radiation exposure, decreased bin loading times, and significant cost savings over the life of the WIPP test phase and operational phase.

The VOC transport model consisted of a series of material balance equations describing unsteady-state VOC transport between each void volume. Model equations accounted for three primary mechanisms for VOC transport from a void volume. These mechanisms were VOC permeation across a polymer boundary, VOC diffusion across an opening in volume boundary, and VOC accumulation in a polymer due to VOC solubility. In order to test the model, experiments were performed to measure VOC concentration throughout a lab-scale simulated waste drum. Each waste drum consisted of a sized-down 55-gal metal drum containing a modified 90-mil high-density rigid polyethylene drum liner. Four small polyethylene bags were sealed inside a large polyethylene bag, supported by a wire cage and placed inside the drum liner. The small bags were each filled with four liters of a VOC-air mixture and the concentration within the waste drum was measured over the 3-week test period. Measurements of the VOC concentrations were taken from six locations inside a simulated waste drum: each small bag headspace, large bag headspace, and drum headspace. Sixteen trials were performed based on a two-level three-variable experimental design with two replications. Test variables included the initial VOC gas mixtures placed in the small bags, the type of small bag closure, and the presence or absence of a variable external heat source.

In addition, permeability measurements were made for VOCs in a gas mixture across the polyethylene bags. Permeabilities for five VOCs (methylene chloride, 1,1,1-trichloroethane, 1,1,2-trichloro-1,2,2-trifluoroethane (Freon-113), carbon tetrachloride, and trichloroethylene) in one gas mixture were measured. Permeability measurements for the VOCs in the other gas mixture (methanol, cyclohexane, 1,1,1-trichloroethane, toluene, p-xylene) used in the lab-scale waste drums experiments were not completed due to system limitations in handling high boiling-point VOCs (toluene and p-xylene).

Most model parameters were measured or estimated from available process information. Other parameters not measured directly were estimated using the VOC transport model and lab-scale waste drum data from a single trial. Model parameters determined in this fashion were used in all other model calculations. Model results were calculated for those trials where the

VOC permeability had been measured. The mean absolute relative deviation (MARD) defining the mean absolute difference between model predictions and experimental values for a given trial were calculated for small bag, large bag, and drum headspace void volumes. In most trials, the small-bag MARD for each high-permeability VOC was less than 2% of the initial VOC concentration introduced in the small bags. The average MARD value for the low-permeability VOC (Freon-113) was greater than for the high-permeability VOCs as the result of less accurate model estimates. The model assumption of well-mixed volumes may be inappropriate where large concentrations of low-permeability VOCs are present. The large bag MARD followed the same trends as observed for the small bags. The MARD for the drum headspace void volume in drums maintained at room temperature was less than 2% for a majority of the trials. The MARD for the drum headspace void volume in waste drums maintained under a variable-temperature environment were between 2% and 4%. The increase in the deviation between the model and experimental results in the heated drums was attributed to the failure of the model to account for increased VOC solubility in the polyethylene drum liner at higher temperatures.

Experimental results demonstrated that VOC transport from waste drums exposed to a variable external heat source was greater than drums maintained at a constant temperature. The difference was attributed to an increase of VOC solubility in the polyethylene liner at higher temperatures and an increased rate of aspiration due to fluctuating drum temperature. The model does predict lower drum headspace VOC concentrations in a waste drum exposed to thermal cycling instead of being maintained at room temperature but currently does not account for the temperature dependence of VOC solubility in the polymer drum liner. The effect of the small bag closure type on VOC transport in the lab-scale drum could not be determined from a direct comparison of measured VOC concentration in small bags. Since the model had been demonstrated to accurately follow the small bag VOC concentration over the course of the test period, the model was used to estimate the relative importance of VOC transport through a small bag horsetail compared to VOC permeation across the bag wall in the lab-scale experiments. For the case of a low-permeability VOC, the rate of VOC transport via permeation was estimated to be over 500 times greater than the VOC transport rate across the horsetail.

Future work includes obtaining VOC permeability and solubility data for VOCs in the other gas mixture used in the lab experiments and further examining the capability of the VOC transport model of predicting the VOC concentration throughout the lab-scale waste drum. In addition, the rate of VOC transport out of polymer bottles will be analyzed. Measurement of VOC permeabilities as a function of temperature and over a wider range of VOC concentrations will be made. A major feature of these VOC transport experiments was the transient nature of the VOC gas phase concentration as the result of having no VOC source in the waste drum. The presence of VOC-containing waste, such as a waste sludge, would replenish VOC molecules that had permeated and diffused out of the void volume. The presence of a VOC source in the lab-scale waste drums should more closely simulate real waste. Future simulated waste drum experiments will place VOC-contaminated simulated waste in waste drums and measure VOC concentration over a relatively long period of time. The applicability of the current model to predict the VOC concentration throughout a simulated waste drum containing VOC-contaminated waste will be investigated. Finally, a model that predicts VOC concentration throughout an actual waste drum based on process knowledge and the measured VOC concentration in the drum headspace will be developed and tested.

FOREWORD

This report is a revision of an EG&G Idaho informal report originally titled *Modeling VOC Transport in Simulated Waste Drums*. The new title more accurately reflects the content of the report. In addition, experimental data and model results incorrectly attributed to methylene chloride and 1,1,2-trichloro-1,2,2-trifluoroethane (Freon-113) were placed in their proper tables or replaced. The conclusions of the original report remain the same in this revised report.

CONTENTS

FIGURES

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ACRONYMS

CCS	continuing calibration standards
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
FID	flame ionization detector
GC	gas chromatograph
INEL	Idaho National Engineering Laboratory
MARD	mean absolute relative deviation
MC	methylene chloride
STP	standard temperature and pressure
TCA	1,1,1-trichloroethane
TCD	thermal conductivity detectors
TCE	trichloroethylene
VOC	volatile organic compound
WIPP	Waste Isolation Pilot Plant

Modeling Unsteady-State VOC Transport in Simulated Waste Drums

1. INTRODUCTION

Pretest waste characterization of waste drums for the bin-scale tests at the Waste Isolation Pilot Plant (WIPP) includes sampling for volatile organic compounds (VOCs) from three areas within drums (drum headspace, the 55-gal poly bag headspace, and the innermost layers of confinement headspace) of transuranic waste.[1] The Department of Energy (DOE) must demonstrate to the Environmental Protection Agency (EPA) that a drum headspace sample is representative of the VOCs within the entire void space of the waste container in order to demonstrate compliance in the future when drums could be directly emplaced in the WIPP. It is specified in the WIPP No-Migration Determination (55 FR 44700) that the EPA expects all layers of confinement in a container will have to be sampled until DOE can demonstrate, based on data collected, that sampling of all layers is either unnecessary or can be safely reduced.

A test program has been initiated at the Idaho National Engineering Laboratory to demonstrate that the VOC concentration in the void space of each layer of confinement can be estimated using a model incorporating theoretical diffusive and permeative transport principles and limited waste drum sampling data. This approach will be used to model unsteady state and quasi-steady state VOC transport from simulated waste drums. An accurate model of VOC transport in a simulated waste drum will serve as the foundation for model development for VOC transport in an actual waste drum. Finally, the accuracy of a VOC transport model to estimate VOC concentration within actual waste drums will be investigated. A model capable of characterizing the VOC concentration in an actual waste drum will be used to assist in defining drum headspace representativeness and may more quickly eliminate the need for sampling of inner layers of confinement, resulting in lower worker radiation exposure, decreased bin loading times, and significant cost savings over the life of the WIPP test phase and operational phase.

In this report, the development and application of a VOC transport model to predict the VOC concentration within simulated waste drums under unsteady-state conditions is described. Development of the VOC transport model for a simulated waste drum is presented in Section 2. Section 3 contains a description of the experimental for the VOC transport experiments and permeability measurements. The results of these experiments are presented and discussed in Section 4. Model results are presented and discussed in Section 5. Conclusions of VOC transport model applicability to other waste drum configurations are summarized in Section 6.

2. VOC TRANSPORT MODEL

A VOC transport model is developed to estimate the transient VOC gas-phase concentration throughout a simulated waste drum. A simulated waste drum is a scaled-down vented metal drum containing a rigid polymer drum liner that holds a large polyethylene bag with four smaller bags initially filled with a VOC-containing gas mixture. A small hole is punctured in the drum liner lid. The small bags, large bag, drum liner and drum headspace are distinct and separate void volumes. The model consists of a series of material balance equations describing unsteady-state VOC transport between each void volume. The small bags are referred to as the first, or innermost, void volume. The large poly bag, drum liner and drum are the second, third, and fourth void volumes, respectively.

2.1 Model Equations

The rate of VOC permeation across a polymer film is defined by

$$Q_{P,i} = \wp A_{P,i} \frac{\Delta p}{\Delta x_{P,i}} \tag{1}$$

where

$Q_{P,i}$ = rate of VOC permeation from i^{th} void volume at standard temperature and pressure, cm^3 (STP) s^{-1}

$\wp$ = VOC permeability coefficient, cm^3 (STP) cm cm^{-2} (cm Hg)$^{-1}$ s^{-1}

$A_{P,i}$ = surface area across which VOC permeates from i^{th} void volume, cm^2

Δp = VOC partial pressure difference across polymer boundary, cm Hg

$\Delta x_{P,i}$ = thickness of polymer boundary surrounding i^{th} void volume, cm.

The rate of VOC diffusion in air across an opening, such as a punctured hole or bag horsetail is defined by

$$Q_{D,i} = DA_{D,i} \frac{\Delta y}{\Delta x_{D,i}} \tag{2}$$

where

$Q_{D,i}$ = rate of VOC diffusion from i^{th} void volume, cm^3 s^{-1}

D = VOC diffusivity in air, cm^2 s^{-1}

$A_{D,i}$ = cross-sectional area of diffusional path across i^{th} void volume, cm^2

Δy = VOC mole fraction difference across opening, (cm^3 VOC) cm^{-3}

$\Delta x_{D,i}$ = diffusional path length between void volumes, cm.

Soluble VOCs will accumulate within a polymer film until an equilibrium concentration is reached. The rate of accumulation is estimated to be

$$P\frac{ds_i}{dt} = \eta P[s_{\infty,i} - s_i] \tag{3}$$

where

s_i = average VOC solubility in i^{th} polymer volume, [cm^3 (STP) VOC] (cm^{-3} polymer) (cm Hg^{-1})

$s_{\infty,i}$ = VOC equilibrium solubility in i^{th} polymer volume, [cm^3 (STP) VOC] (cm^{-3} polymer) (cm Hg^{-1})

dt = differential time interval, s

η = transfer coefficient, sec^{-1}

P = absolute pressure, cm Hg

The total rate of VOC transport from each small polymer bag is defined by summing the contribution of each transport mechanism defined by Equations (1)–(3)

$$V_{1,j}\frac{dy_{1,j}}{dt} = (\alpha\phi + \beta)_{1,j}\,[y_2 - y_{1,j}] - \gamma_{1,j}\phi\,\frac{ds_{1,j}}{dt} \tag{4}$$

where

$V_{1,j}$ = void volume within j^{th} small bag, cm^3

$y_{1,j}$ = VOC mole fraction in $V_{1,j}$, mol cm^{-3}

Δy = $y_2 - y_{1,j}$, (cm^3 VOC) cm^{-3}

$f_{1,j}$ = $y_{1,j}V_{1,j}/[y_{1,j}V_{1,j} + y_2V_2]$

$V_{p,1,j}$ = polymer volume of j^{th} small bag, cm^3 polymer.

$\alpha_{1,j}$ = $(\rho A_pP/\Delta x_p)_{1,j}$

$\beta_{1,j}$ = $(DA_D/\Delta x_D)_{1,j}$

$\gamma_{1,j}$ = $(fV_pP)_{1,j}$.

$\phi_{1,j}$ = $76\ T_1/(273.15\ P)$

T_i = temperature in i^{th} void volume, K.

In defining the coefficient f, it was assumed that the number of moles sorbed on a polymer film from a void volume is proportional to the total number of moles available in all void volumes adjacent to the film.

The VOCs exiting the small bags enter the void space within the large bag. The equation for the rate of change in the large bag is defined as

$$V_2 \frac{dy_2}{dt} = \left[\sum_{j=1}^{4} -(\alpha\phi+\beta)_{1,j} [y_2 - y_{1,j}] \right] + (\alpha\phi+\beta)_2 [y_3 - y_2] - \phi g(s_1, s_2) \tag{5}$$

where, in general

$$g(s_k, s_m) = (1-\gamma_k)\frac{ds_k}{dt} + \gamma_m \frac{ds_m}{dt} \ . \tag{6}$$

In the liner and drum lids there are relatively large openings through which VOCs exit by diffusion and convective flow resulting from changes in temperature. In the case of increasing temperature, the rate of change in the liner headspace is defined as

$$V_3 \frac{dy_3}{dt} = \left[\sum_{i=2}^{3} (-1)^{3-i} (\alpha\phi+\beta)_i [y_{i+1} - y_i] \right] - \phi g(s_2, s_3) - \frac{V_3 y_3}{T_3}\frac{dT_3}{dt} \ , \tag{7}$$

and in the drum headspace the rate of change is defined as

$$V_4 \frac{dy_4}{dt} = -(\alpha\phi+\beta)_3 [y_4 - y_3] - \frac{D^*}{C_o} y_4 \frac{T_4}{T_o} - \phi g(s_3, s_4) + V_4 y_4 \left[\frac{T_4}{T_3^2}\frac{dT_3}{dt} + \frac{1}{T_4}\frac{dT_4}{dt} \right] \tag{8}$$

where

D^* = VOC-filter diffusion characteristic, mol s^{-1} (mol fraction)$^{-1}$

C_o = total gas concentration in drum = P/RT_o, mol cm^{-3}

T_o = gas temperature during filling of small bags, K.

In the case of decreasing temperature, the rate of change in the liner headspace is defined as

$$V_3 \frac{dy_3}{dt} = \left[\sum_{i=2}^{3} (-1)^{3-i} (\alpha\phi + \beta)_i \, [y_{i+1} - y_i] \right] - \phi g(s_2, s_3) - \frac{V_3 y_4}{T_3} \frac{dT_3}{dt} \quad , \tag{9}$$

and in the drum headspace is defined as

$$V_4 \frac{dy_4}{dt} = -(\alpha\phi + \beta)_3 [y_4 - y_3] - \frac{D^*}{C_o} y_4 \frac{T_4}{T_o} - \phi g(s_3, s_4) + \frac{V_4 y_4}{T_3} \frac{dT_3}{dt} \quad . \tag{10}$$

2.2 Model Assumptions

The following assumptions were made in deriving model equations:

- All void volumes are well-mixed and the VOC concentration is identical throughout.
- The diffusion pathway length between two void volumes is:
  - Across a horsetail, the length of the horsetail.
  - Across a puncture or hole, the sum of the polymer boundary thickness and the mean hole diameter.
- Pressure differential across puncture hole in the liner lid and drum filter is negligible.
- VOC molecules that exit the drum through the filter are not drawn back into the drum.
- All surface areas, void volumes, and diffusion path lengths specified for a given system remain constant during the entire test period.

2.3 Model Parameters

2.3.1 VOC-Polymer Permeability

The sorption, diffusion, and permeation of several organic vapors in polyethylenes of different densities over a wide range of vapor activity and concentrations has been investigated[2]. In general, VOC permeability is an exponential function of vapor activity (VOC partial pressure/VOC vapor pressure). As the vapor activity approaches zero, VOC permeability approaches a constant nonzero value.

The transmission rate of a number of organic liquids through low-density polyethylene at different temperatures has been reported.[3,4] A semi-empirical equation has been used to estimate the VOC transmission rate, Q, in polyethylene and related polymers:[3]

where

$$\log_{10} Q = K - c\pi \tag{11}$$

c = constant

π = function of VOC molecular structure.[3]

For low-density polyethylene[3]

$$K = 16.55 - \frac{3700}{T} \quad . \tag{12}$$

The transmission rate is often used to estimate VOC permeability when the saturated vapor pressure of the permeant at a specified temperature is applied across a film.[4] Thus,

$$\rho \propto \frac{Q}{P_{vap}} \tag{13}$$

where P_{vap} is the saturated vapor pressure at temperature T. Temperature dependence of the VOC vapor pressure is estimated using the Antoine Equation:[5]

$$\log_{10} P_{vap} = A - \frac{B}{C + T} \tag{14}$$

where A, B, and C are equation constants. The effect of temperature on VOC vapor permeability in low-density polyethylene is estimated by combining Equations (11)–(14):

$$\log_{10}\left[\frac{\rho(T_1)}{\rho(T_2)}\right] = B\left[\frac{1}{C + T_1} - \frac{1}{C + T_2}\right] - 3700\left[\frac{1}{T_1} - \frac{1}{T_2}\right] \quad . \tag{15}$$

2.3.2 VOC-Air Diffusivity

The VOC-air diffusivity can be estimated at low pressures using an equation developed from a combination of kinetic theory and corresponding-states arguments:[6]

$$D_{AB} = 2.745 \times 10^{-4} \; \frac{T^{1.823}}{P} \; \left[p_{cA}\, p_{cB}\right]^{1/3} \; \left[T_{cA}\, T_{cB}\right]^{-0.495} \; \left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2} \tag{16}$$

where

D_{AB} = mass diffusivity for VOC(A)-air(B) system, $cm^2\ s^{-1}$

p_{ci} = critical pressure of species i, atm

T_{ci}	=	critical temperature of species i, K
M_i	=	molecular weight of species i.

The VOC diffusion characteristic across a carbon-composite filter is estimated from the knowledge of the hydrogen (H_2) diffusion characteristic across the same filter and the ratio of VOC-to-H_2 diffusivity

$$D^*_{voc} = \left[\frac{D_{voc-air}}{D_{H_2-air}}\right] D^*_{H_2} \quad . \tag{17}$$

The diffusivity ratio has been estimated by the square root of the inverse ratio of molecular weights of the VOC and H_2.[7]

2.3.3 VOC Solubility in Polymer

Henry's law provides a good approximation of VOC vapor solubility in a polymer at very low vapor concentrations:[8]

$$x = y/H \tag{18}$$

where

x	=	VOC mole fraction in polymer ($\ll 1$)
y	=	VOC mole fraction in gas phase
H	=	Henry's constant.

3. EXPERIMENTAL

3.1 VOC Transport Experiments

3.1.1 Experimental Design

A two-level, three-variable, four-block experimental design with two replications was constructed to investigate VOC transport within lab-scale simulated waste drums. Test variables were the initial VOC gas mixtures placed in the small inner bags, the presence or absence of horsetail ties on the small bags, and the presence or absence of a variable external heat source. The experimental design is summarized in Table 1.

A two-level two-variable experiment was designed to investigate VOC transport from polyethylene bottles. Test variables were the size of the bottle lid and the presence or absence of seal across the bottle lid. The experimental design is summarized in Table 2.

3.1.2 Automated VOC Transport Experimental Configuration

The automated VOC transport experimental configuration, shown in Figure 1, consisted of four simulated waste drums, four polyethylene bottles, a heated environmental chamber, an automated gas sampling system which included a high and low level gas sampling manifold, a gas chromatograph (GC) with flame ionization detector (FID), a GC data station, a 10-port gas sampling valve, a mechanical vacuum pump, a Pirani micro controller, and a process controller.

3.1.2.1 Gas Chromatograph and GC Data System. A Hewlett Packard (HP) 5890 series II GC with FID configured with a Restek RT-35 analytical column (30 meters × 1.0μm df × 0.32 ID) was used to analyze the headspace samples. The column head pressure was set to 5 psi with a split flow of 35.5 cm^3/min. Splitless injections were made with a purge time of 1.0 min using a straight 2.0 mm ID inlet sleeve. An initial oven temperature of 50°C was held for 4.5 min and then ramped at 20°C/min to 150°C, with a final hold time of 1.25 min. Total GC run time was 10.75 min. An HP Vectra QS/20 personal computer with HP 3365 series II Chemstation (DOS) software, Version B.01.02 was used to control the GC and store all GC data files. The daily sampling sequences were loaded on to the GC data system to configure the 10-port sampling valve and select the correct sample loop for each sample run.

3.1.2.2 Simulated Lab-Scale Waste Drums. Each simulated waste drum consisted of a modified 55-gal metal drum containing a modified 90-mil, high-density, rigid polyethylene drum liner. Four small 4-liter polyethylene bags were sealed inside a large polyethylene bag, supported by a wire cage and placed inside the drum liner. A schematic of a lab-scale simulated waste drum is shown in Figure 2.

Each simulated waste drum was a scaled-down version of a DOT 17C 55-gal drum. A 21.75 in. center section of the drum was removed and the two end pieces welded together. The internal weld was smoothed so that no gross burrs were present and then spray painted. The modified drum had an internal diameter of 22.4 in. and an outside drum height of 14.25 in. A

Table 1. Experimental design for simulated waste drum VOC transport experiments.

Test period	Drum number	Trial number	Standard gas mixture[a]	Small bag closure	Variable heat source
I	1	1.1	A	Horsetail	Yes
	2	1.2	B	Heat sealed	Yes
	3	1.3	A	Heat sealed	No
	4	1.4	B	Horse tail	No
II	1	2.1	A	Heat sealed	Yes
	2	2.2	B	Horse tail	Yes
	3	2.3	A	Horse tail	No
	4	2.4	B	Heat sealed	No
III	1	3.1	A	Horse tail	Yes
	2	3.2	B	Heat sealed	Yes
	3	3.3	B	Horse tail	No
	4	3.4	A	Heat sealed	No
IV	1	4.1	A	Heat sealed	Yes
	2	4.2	B	Horse tail	Yes
	3	4.3	A	Horse tail	No
	4	4.4	B	Heat sealed	No

a. Standard gas mixture A (high-level) contains approximately 1,000 parts per million by volume (ppmv) 1,1,1-trichloroethane, 1,000 ppmv methylene chloride, 1,000 ppmv 1,1,2-trichloro-1,2,2-trifluoroethane (Freon-113), 300 ppmv carbon tetrachloride, and 300 ppmv trichloroethylene.

Standard gas mixture B (high-level) contains approximately 1,000 ppmv trichloroethane, 1,000 ppmv methanol, 750 ppmv cyclohexane, 400 ppmv toluene, and 100 ppmv para-xylene.

Table 2. Experimental design for polyethylene bottles VOC transport experiments.

Bottle number	Type of bottle lid	Lid seal
1	Large mouth	Yes
2	Large mouth	No
3	Small mouth	Yes
4	Small mouth	No

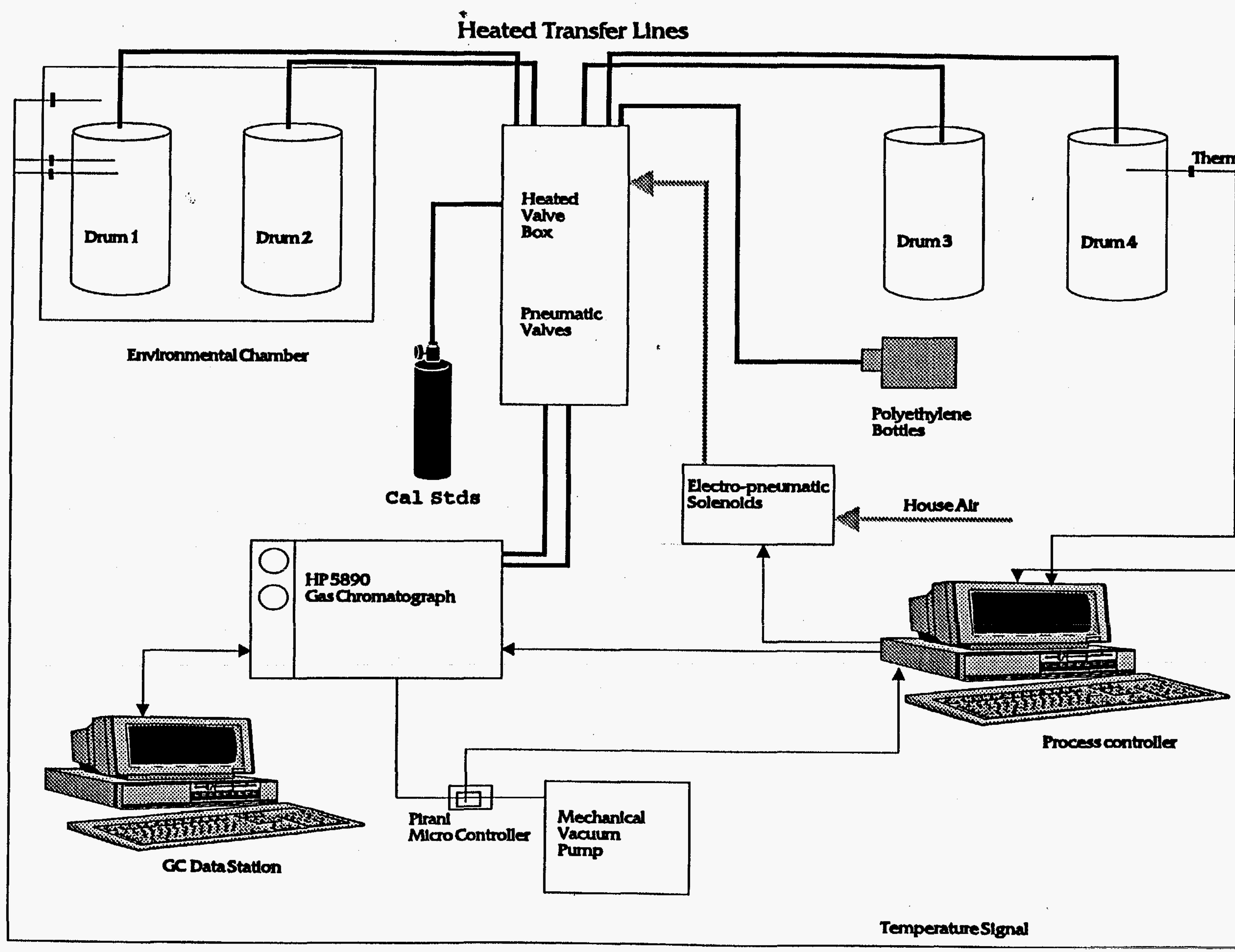

Figure 1. Automated VOC transport experimental configuration.

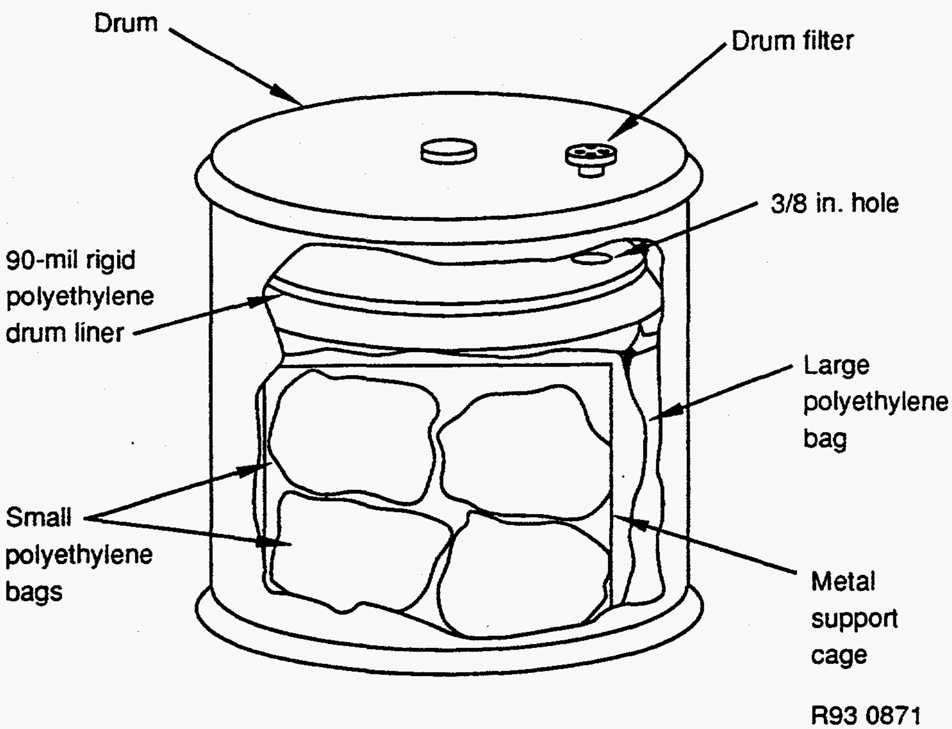

Figure 2. Simulated lab-scale waste drum.

0.375-in. hole was drilled in the drum lid approximate 4.3 in. from the outside edge and a NFT-020 (Nuclear Filter Technology Corp.) carbon-composite filter, shown in Figure 3, was screwed securely in the hole.

The drum liner was a scaled-down version of a Type III liner. The rigid 90-mil liner had a removable lid with a metal closure ring with bolt and gasket. A 21 in. center section of the liner was removed and the two end sections heat welded together. The modified Type III liner had an outside base diameter of 22.0 in., an inside lid diameter of 22.5 in., and outside height (with lid) of 11.5 in. The nominal wall thickness of the liner was 0.090 in. A 0.375 in. hole was drilled in the lid below the carbon composite filter in the drum lid.

Two sizes of yellow polyethylene bags were used in the experiment. Both sizes are used by the INEL for the disposal of radiologically contaminated waste. The original dimensions of the large bag were 33.0 in. in width and 40.0 in. in length and a wall thickness of 0.004 in. The original dimensions of the small bags were 18.0 in. in width and 24.0 in. in length and a wall thickness of 0.004 in. The length of the small bags were reduced to 18.5 in. before being sealed with a horsetail and reduced to 12.0 in. before being heat sealed.

Modified bulkhead feedthroughs were constructed to isolate each layer of confinement. The feedthroughs for the small bags, shown in Figure 4, were fabricated from modified 0.0625-in. brass Swagelock bulkhead unions with two backing washer, two teflon sealing washers, and an n-butyl O-ring. The outer sealing washer was machined to allow the O-ring to seat between the sealing washer and the polyethylene bag. The outer backing washer and outer teflon sealing washer were epoxied, using MasterMend E-POX-E epoxy (Loctite Corp.), to the body of the bulkhead union. The 0.0625-in. teflon ferrules were used to seal the 0.0625-in. sample transfer lines. The feedthroughs for the large bags, shown in Figure 5, were fabricated from 0.375-in. brass Swagelock bulkhead unions with a backing washer and two teflon sealing washers. Teflon coated silica septa (Supelco, Inc., 2-244) were pre-drilled to allow feedthrough of the five sample transfer lines. Feedthroughs for the drum, shown in Figure 6, were fabricated from 0.625-in. stainless steel Swagelock SAE/MS male connectors with two teflon sealing washers and backing nuts. Teflon coated silica septa were pre-drilled to allow feedthrough of the six sample transfer lines. Five holes of 0.060-in. diameter were drilled in the 90-mil liner lid to allow feedthrough of the sample transfer lines. Swagelock thermocouple connectors were place in the sides of drum #1 and drum #4 with 0.125-in. teflon ferrules to seal the thermocouple probes.

3.1.2.3 Polyethylene Bottles. Both large and small mouth polyethylene bottles were used to investigate the VOC transport from sealed bottles. The nominal volume of each bottle was 4,000 cm^3. The large-mouth bottles were made of high-density polyethylene with lids made of polypropylene (Nalge Labware, 2120-0010). The inside diameter of the bottle mouth was 3.5 in. and the nominal wall thickness of the bottle was 0.080 in. The small-mouth bottles were made of low-density polyethylene with lids made of polypropylene (Nalge Labware, 2202-0010). The inside diameter of the bottle mouth was 1.0 in. and the nominal wall thickness of the bottle was 0.100 in. Modified 0.0625-in. brass Swagelock bulkhead unions were tapped and epoxied into the caps of the bottles to allow feedthrough of the sample transfer lines. Teflon ferrules were used to seal 0.0625-in. sample transfer lines. The 0.125-in. brass Swagelock toggle valves were tapped and epoxied in the bottom center of the bottles to allow purging of the bottles during the initial filling

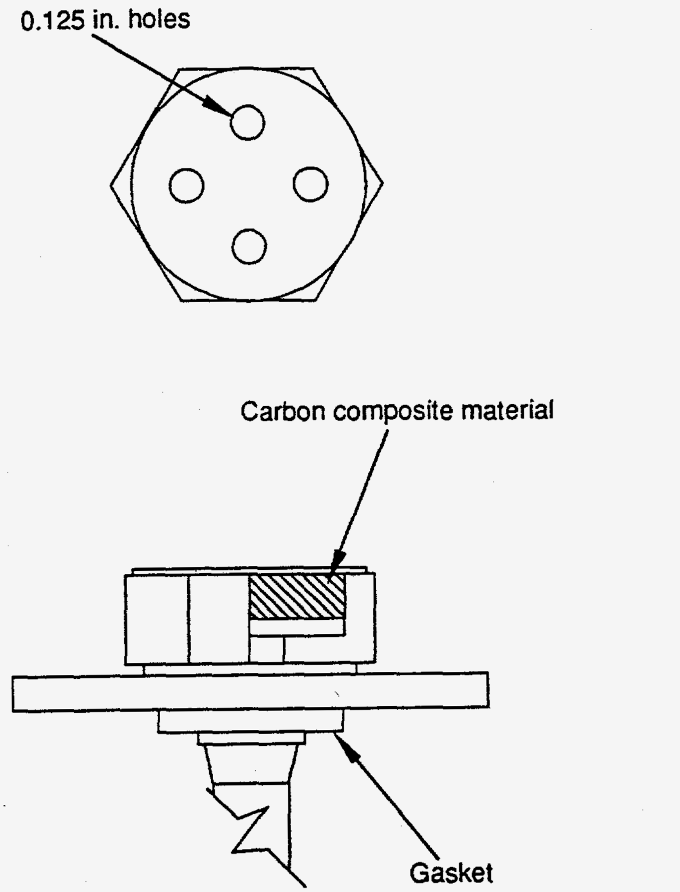

Figure 3. NFT-020 carbon-composite filter.

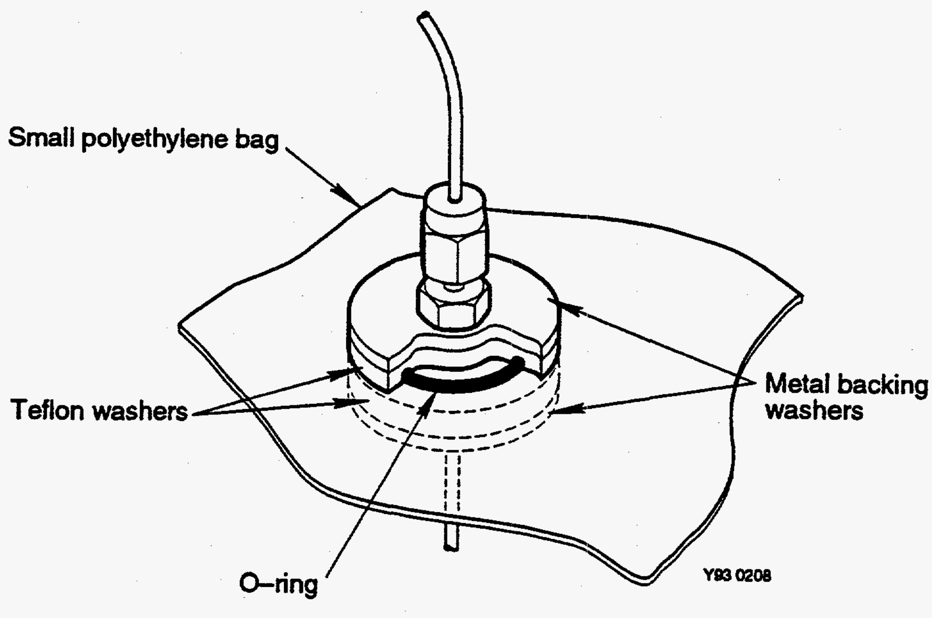

Figure 4. Feedthrough for small polyethylene bags.

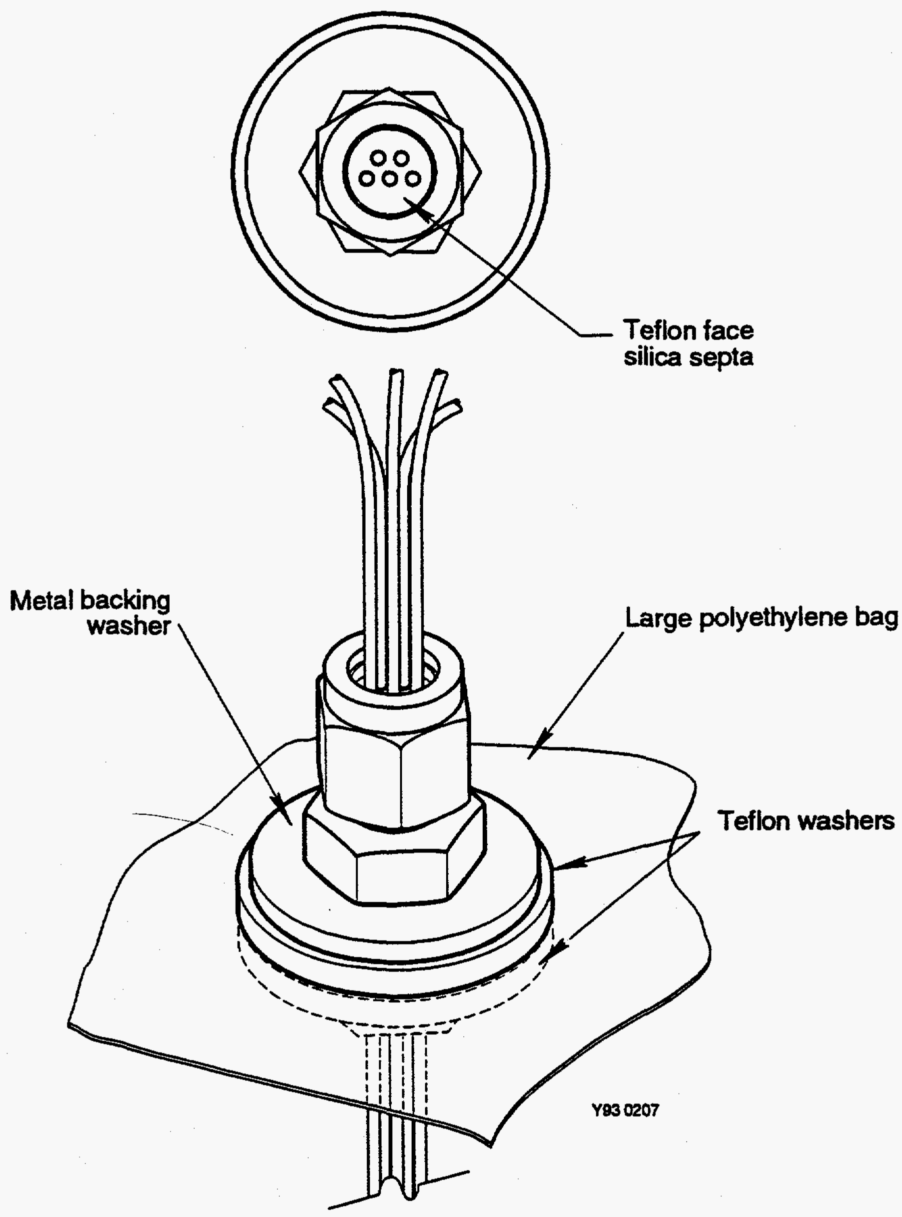

Figure 5. Feedthroughs for large polyethylene bags.

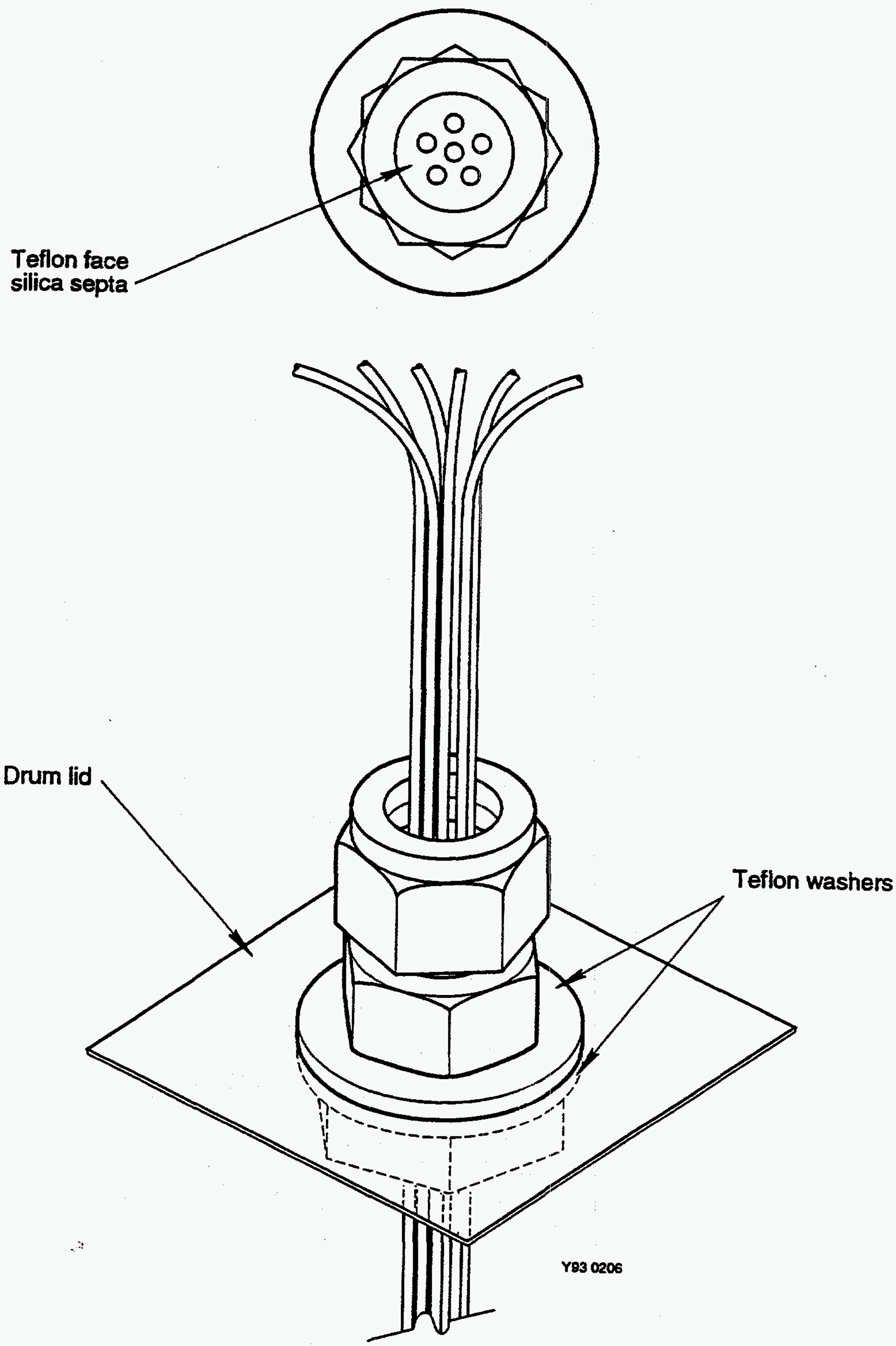

Figure 6. Feedthroughs for drum lid.

process. One large-mouth and one small-mouth bottle were sealed using an aluminum foil gasket place at the mouth of the bottle. A large-mouth polyethylene bottle adapted for these experiments is shown in Figure 7.

3.1.2.4 Environmental Chamber. An environmental chamber was constructed to expose two of the four simulated lab-scale waste drums to a variable heat source to determine the effect of temperature variation on VOC transport from the waste drum. The environmental chamber, shown in Figure 8, was constructed of 0.0625-in. aluminum sheet metal with overall dimensions of 58.0 in. in length, 32.0 in. in height, and 28.0 in. in depth. The lid and four walls of the chamber were insulated with 0.5-in. rigid Firestone polyiso insulation. Two simulated waste drums were set on a raised platform 9.0 in. above the chamber floor and centered in the environmental chamber to allow air to circulate around the drums. A 4.0-in. fan circulated air inside the sealed chamber. Six 100-watt light bulbs controlled by an Omega temperature controller (6102-J-0/300) coupled to a J-type thermocouple were used as a heat source. A Micronto programmable timer was used to turn the temperature controller on for 4 hours each day during each test period. The upper working temperature of the environmental chamber was set to 40°C. Temperature measurements were taken every 15 minutes throughout each test period. J-type Omega stainless steel 12-in. thermocouples (JQSS-18G-12) were used for all temperature measurements.

3.1.2.5 Automated Gas Sampling System. A schematic of the automatic gas sampling system is shown in Figure 9. Headspace samples were collected by evacuating the manifold system to a vacuum of 10 millitorr then back-filling the gas sampling loops. The gas sample flowed into the selected sampling loop until the pressure equilibrated to ambient pressure. Between samples, the automated gas sampling system evacuated both high and low sampling manifolds and both gas sampling loops. Pressurized standard gas mixtures were used to establish the initial calibration curves for the nine analytes of interest and also used on a daily basis as the continuing calibration standards (CCS). Initial calibration samples and CCS samples were collected by purging the manifold system and then allowing the standard gas mixture to equilibrate to ambient pressure. Between samples, the automated gas sampling system evacuated the high and low sampling manifolds and gas sampling loops. The system automatically monitored the pressure of the manifolds and 10-port gas sampling valve and sequenced the pneumatic valves in response to the sequence files downloaded to the process controller. Samples were transferred from the gas sampling loop to the GC injector and analyzed by GC-FID. A two-level (high and low level) sampling system was developed to quantitate VOC headspace samples with sample concentrations varying from less than 1.0 ppmv to greater than 1,000 ppmv.

The gas sampling system utilized a low- and a high-level sampling manifold configured to a 10-port gas sampling valve with 5.0 and 2.0 cm^3 sampling loops. The configuration of the 10-port gas sampling valve is shown in Figure 10. The 24.0 in. manifold headers were fabricated by Scientific Instrument Services from 0.25-in. OD stainless steel tubing (0.095-in. wall thickness) with 0.0625-in. stainless steel sampling ports. Pneumatic needle valves (Scientific Glass Engineering, #MOVP-1-100) were used for the manifold isolation valves, vacuum valve, purge valve, and sample isolation valves. Silcosteel 0.0625-in. silica lined stainless steel tubing (0.020 in. ID) was used for the gas sampling lines and manifold transfer lines. The valve box, all transfer lines, and 10-port gas sampling valve were heated to 145°C to prevent cold trapping of VOCs. For drums 1 and 2, 9-in. sections of the sample transfer lines were unheated inside the

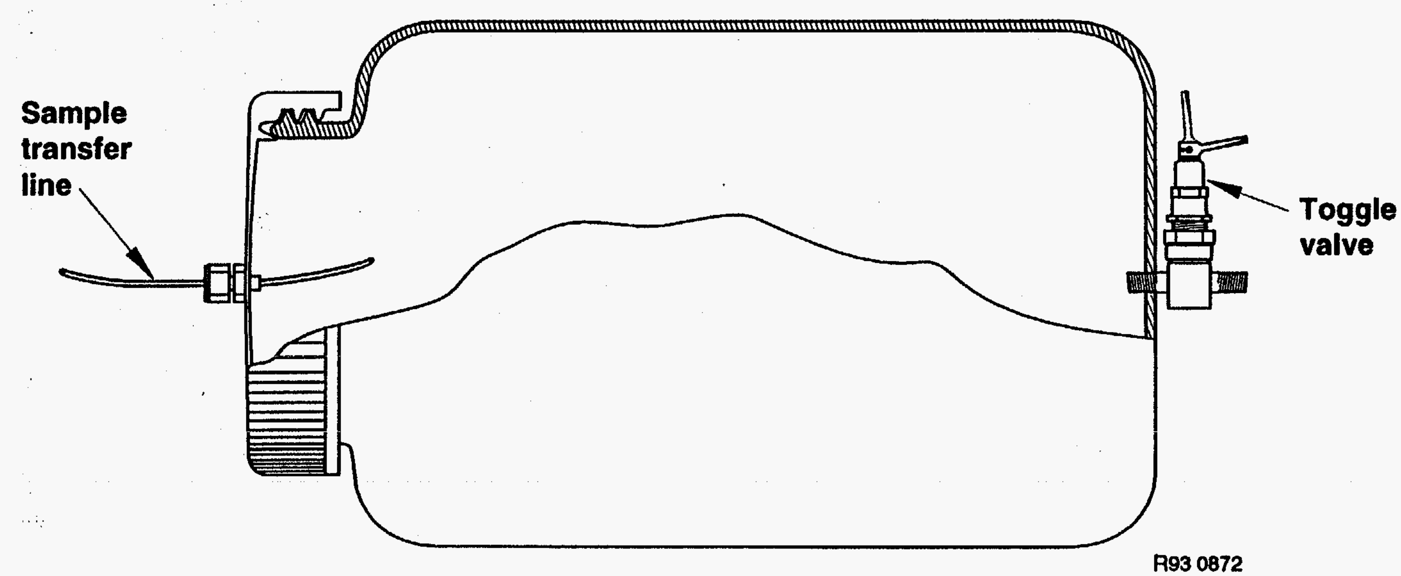

Figure 7. Large-mouth polyethylene bottle configuration.

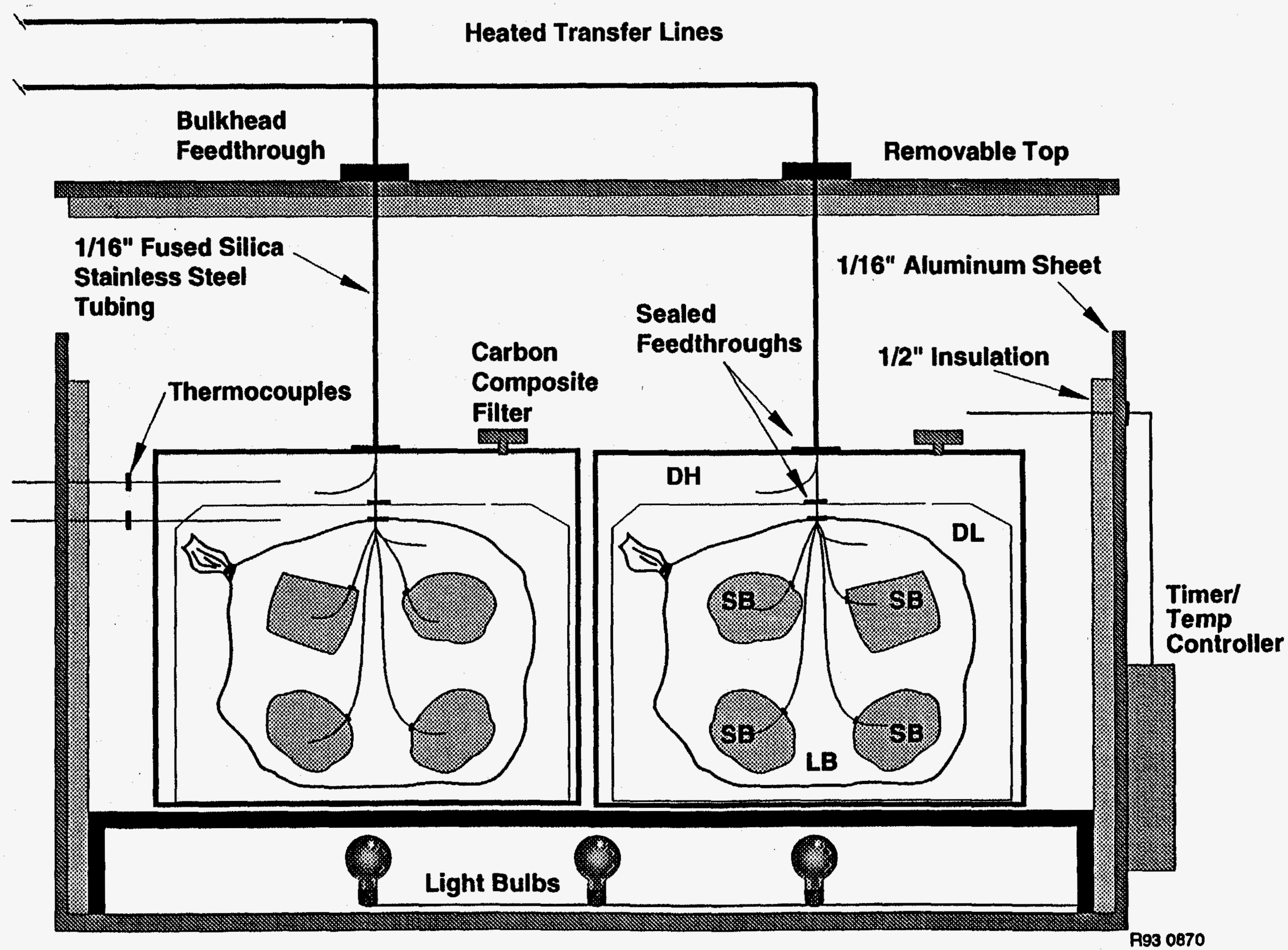

Figure 8. Environmental chamber.

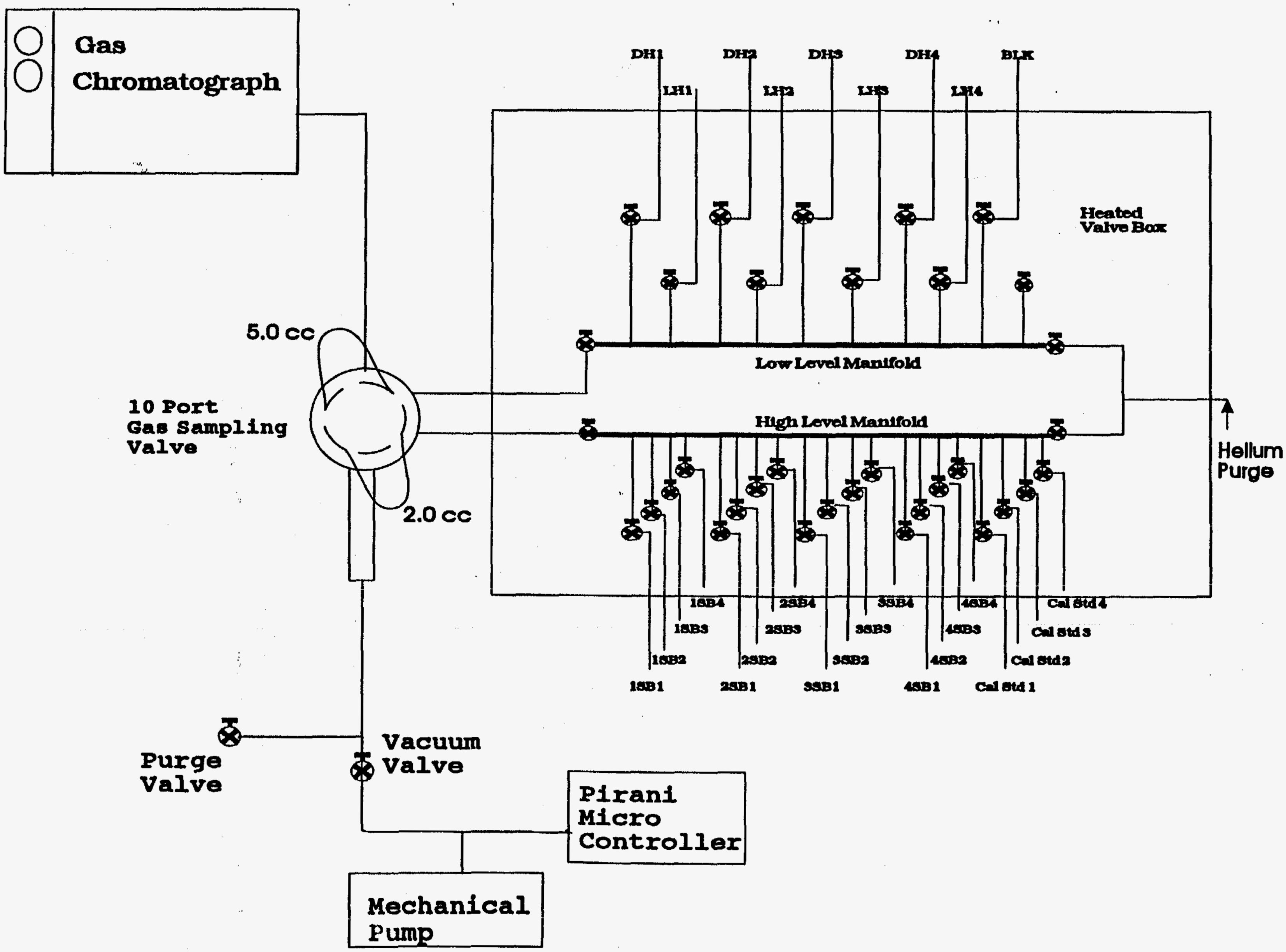

Figure 9. Automated gas sampling system.

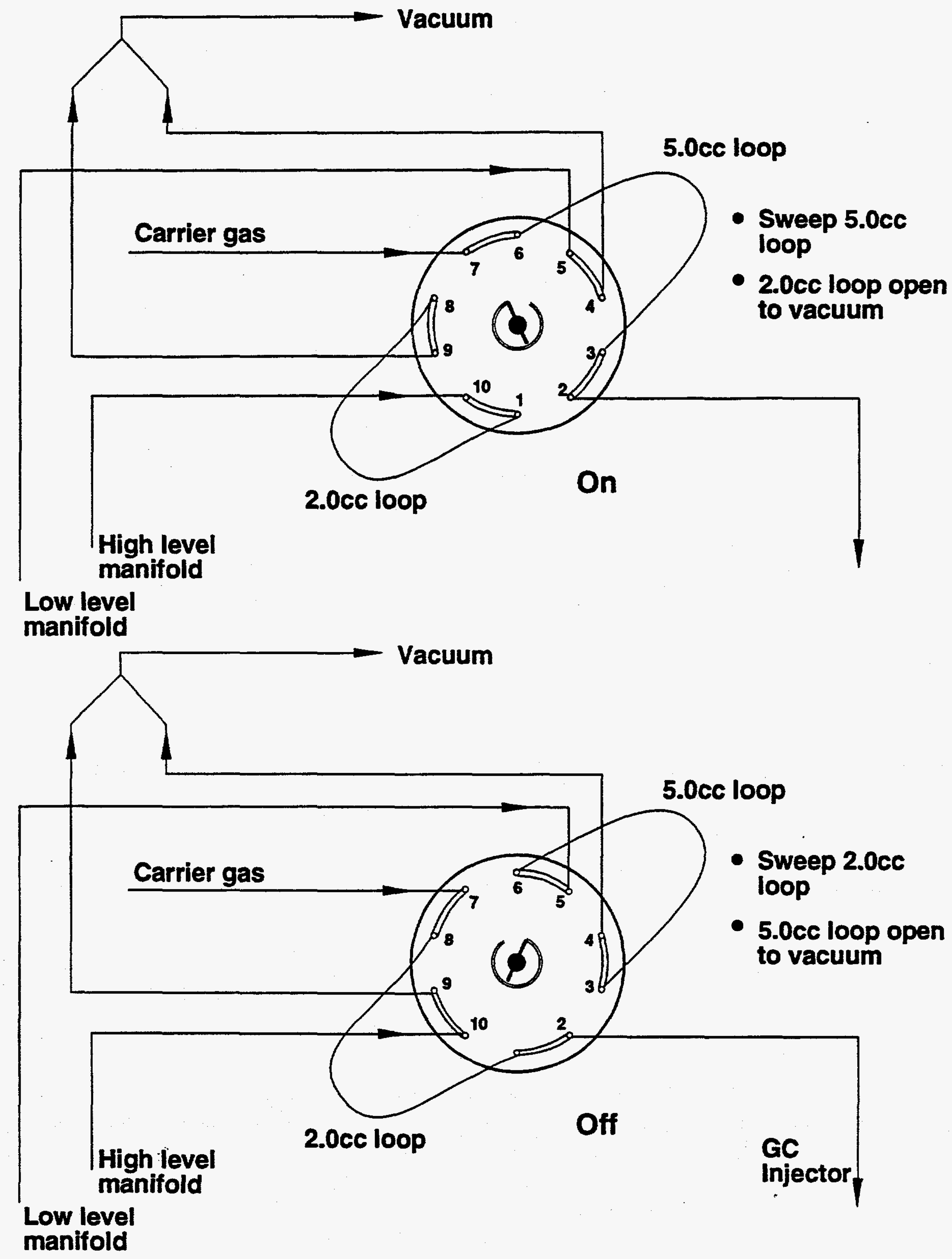

Figure 10. Configuration of 10-port gas sampling valve.

environmental chamber between the drum lid and top to the chamber. The pneumatic needle valves were actuated by electro-pneumatic Clippard solenoids (#ETO-3-24) controlled by the process control unit. The process control unit utilized a dedicated IBM AT personal computer operating with LabTech Notebook software, Version 7.0.0. The 16-channel multiplex temperature board (LabTech, #CIO-EXP16) was used to provide temperature data. A 48-channel system control module (LabTech, #CIO-DIO96) provided selection of the electro-pneumatic solenoids controlling the pneumatic needle valves. Remote start signals from the Pirani micro controller (MKS Instruments, Model 315) initiated the sampling sequence of the process control unit and began the GC run.

3.1.2.6 Standard Gas Mixtures. The gas standard mixtures used in this experiment were prepared by Alphagaz, Division of Liquid Air Corporation and Scott Specialty Gas, Incorporated with a specified analytical accuracy of ±2.0%. Three concentration levels of standard mixture A and B were prepared by Alphagaz, as shown in Table 3. Because of the limitations of analytes condensing out of the vapor phase at higher pressures, two low pressure cylinders of standard gas mix B-I were obtained from Alphagaz. Additional standard gas be prepared to meet experimental needs and were obtained from Scott Specialty Gas. During test period I, II, III standard gas mixtures A-I_a and B-I_{a1} were used to fill the small bags. Standard gas mixtures A-I_a, A-$II_{a,}$, and A-III_a and standard gas mixtures B-I_{a1}, B-$II_{a,}$, and B-III_a were used to establish the initial calibration curves. During test period IV standard gas mixtures A-I_s and B-I_s were used to fill the small poly bags. Standard gas mixtures A-I_s, A-$II_{a,}$, and A-III_a and standard gas mixtures B-I_s, B-$II_{a,}$, and B-III_a were used to establish the initial calibration curves. Standard gas mixture B-I_{a1} was used to purge and fill the polyethylene bottles.

3.1.3 Experimental Procedures

3.1.3.1 Bag Preparation and Filling Procedures. The small polyethylene bags configured with 0.0625-in. bulkhead feedthroughs were prepared and leak-tested before being placed into the simulated waste drums at the beginning of each test period. The heat-sealed polyethylene bags were cut to size (12 in. in height and 18 in. in width, with the bulkhead feedthrough 3 in. from the bottom of the bag) and heat-sealed. The horsetail polyethylene bags were heat-sealed before being cut down to their final size (18.5 in. in height and 18 in. in width, with the bulkhead feedthrough 3 in. from the bottom of the bag). The feedthroughs were sealed with an appropriate sized septa and each bag was filled with one to two liters of air. The entire bag and feedthrough were submerged under water and firm pressure placed on the bag. If any bubbles were observed indicating a leak, the feedthroughs were removed and the bag discarded.

Each small bag sealed by the horsetail method was cut to size and sealed before being placed in the waste drum. The horsetail was formed by bunching the bag together in one hand with 6-in. of the open end of the bag protruding. The 6-in. section of bag was twisted 360° once and an 8-in. piece of tape was wrapped over the entire length of the twist. The end of the horsetail was folded over and a 3-in. piece of tape was placed over the fold. As much air as possible was expelled from the small bags before being connected to gas sampling lines. After the small bags were placed inside the large poly bag along with the metal support cage, the same horsetail sealing procedure was used to seal the large bags.

Table 3. Gas standard mixtures.[a]

Analyte	A-I$_a$	A-II$_a$	A-III$_a$	A-I$_s$	B-I$_{a1}$	B-I$_{a2}$	B-II$_a$	B-III$_a$	B-I$_s$
Methylene chloride	1,012	475	95.2	1,010	—	—	—	—	—
Freon-113	903	451	91.0	1,010	—	—	—	—	—
Carbon tetrachloride	305	149	33.9	301	—	—	—	—	—
Trichloroethylene	310	153	35.3	297	—	—	—	—	—
1,1,1-trichloroethane	977	496	101	1,020	1,054	1,020	508	94.6	980
Methanol	—	—	—	—	987	1,002	499	103	764
Cyclohexane	—	—	—	—	787	777	377	71.4	746
Toluene	—	—	—	—	425	421	211	39.3	398
P-xylene	—	—	—	—	99.2	120	69	12.7	99

a. A-I$_a$ - Alphagaz high-level standard
A-II$_a$ - Alphagaz mid-level standard
A-III$_a$ - Alphagaz low-level standard
A-I$_s$ - Scott Specialty high-level standard
B-I$_{a1}$ - Alphagaz high-level standard bottle #1
B-I$_{a2}$ - Alphagaz high-level standard bottle #2
B-II$_a$ - Alphagaz mid-level standard
B-III$_a$ - Alphagaz low-level standard
B-I$_s$ - Scott Specialty Gas high level standard

Analytical accuracy ± 2%
Balance hydrocarbon free air
All gas concentrations in ppmv.

3.1.3.2 Introduction of Gas Mixture into Bags and Bottles. After each small bag was placed inside the drum; and the liner, and drum lids clamped into place, 4,000 cm^3 of a standard gas mixture were introduced into the small bags by back-filling through the sampling manifold using a MKS mass flow controller. The capacity of the small bags was slightly larger than 4,000 cm^3 so as not to generate a pressure differential across the bags. Each small bag was filled separately and all bags using the same standard gas mixture were filled sequentially.

The polyethylene bottles, which lay on their sides during the experiment, were purged and filled with standard gas mixture B-I_{a1} using the toggle valve as the purge vent. The bottles were sequentially purged with 4,000 cm^3 of the standard gas mixture at a rate of 1,000 cm^3/min for 4 min. The toggle valves were closed after flow was stopped so as not to generate a pressure differential across the bottles. The bottles were allowed to equilibrate for 1 hour and then purged with an additional 15,000 cm^3 liters of the standard gas mixture before being sealed off for the duration of the experiment.

3.1.3.3 Automated Sampling Sequence. The sequence for the initial calibration standards and CCS, summarized in the flow diagram in Figure 11, was initiated with the GC ready signal. The GC sequence specified the ON position for the 10-port gas sampling valve with the 2.0 cm^3 loop open to the high level manifold. This was coordinated with the sampling sequence file loaded onto the process controller. At the beginning of each sequence all valves were closed. At time 0 min the vacuum valve and the high manifold valve were opened to evacuate the manifold system. When pressure set point #1 was reached (1.1×10^{-2} torr) and 1.5 min had elapsed, the vacuum valve closed and the calibration gas and vent valves were opened simultaneously. After the vacuum valve closed, pressure set point #2 ($5.2 - 5.6 \times 10^{-3}$ torr) was reached within 2 seconds starting the GC. The calibration gas valve was opened for approximately 16 seconds, while the vent valve remained open to atmosphere for an additional 20 seconds to allow the system pressure to equalize. The 10-port gas sampling valve was switched to the OFF position 30 seconds into the GC run and the 2.0 cm^3 sample loop was swept to the injector. At 45 seconds all valves were closed. At 3.75 min, the vacuum valve and the high and low manifold valves were opened to evacuate the manifold system and eliminate any sample carryover. At 10.5 min into the GC run, the 10-port gas sampling valve switched to the ON position to prepare for the next calibration sample. Total cycle time was approximately 15 min.

The sequence for headspace sampling, summarized in the flow diagram in Figure 12, was initiated with a GC ready signal. The GC sequence specified the position of the 10-port gas sampling valve and which loop was opened to the manifold. This was coordinated with the sampling sequence file loaded in the process controller. At the beginning of each sequence all valves were closed. At time 0 min, the vacuum valve and the selected manifold valve were opened to evacuate the manifold system. When pressure set point #1 was reached (1.1×10^{-2} torr) and 1.5 min had elapsed, the vacuum valve closed and the selected sample valve was opened. After the vacuum valve closed, pressure set point #2 ($5.2 - 5.6 \times 10^{-3}$ torr) was reached within 2 seconds starting the GC. The 10-port gas sampling valve was switched 30 seconds into the GC run and the sample loop was swept to the injector. At 45 seconds all valves were closed. At 2.75 min, the vacuum valve and the high and low manifold valves were opened to evacuate the system and eliminate any sample carryover. At 10.5 min into the GC run, the 10-port gas

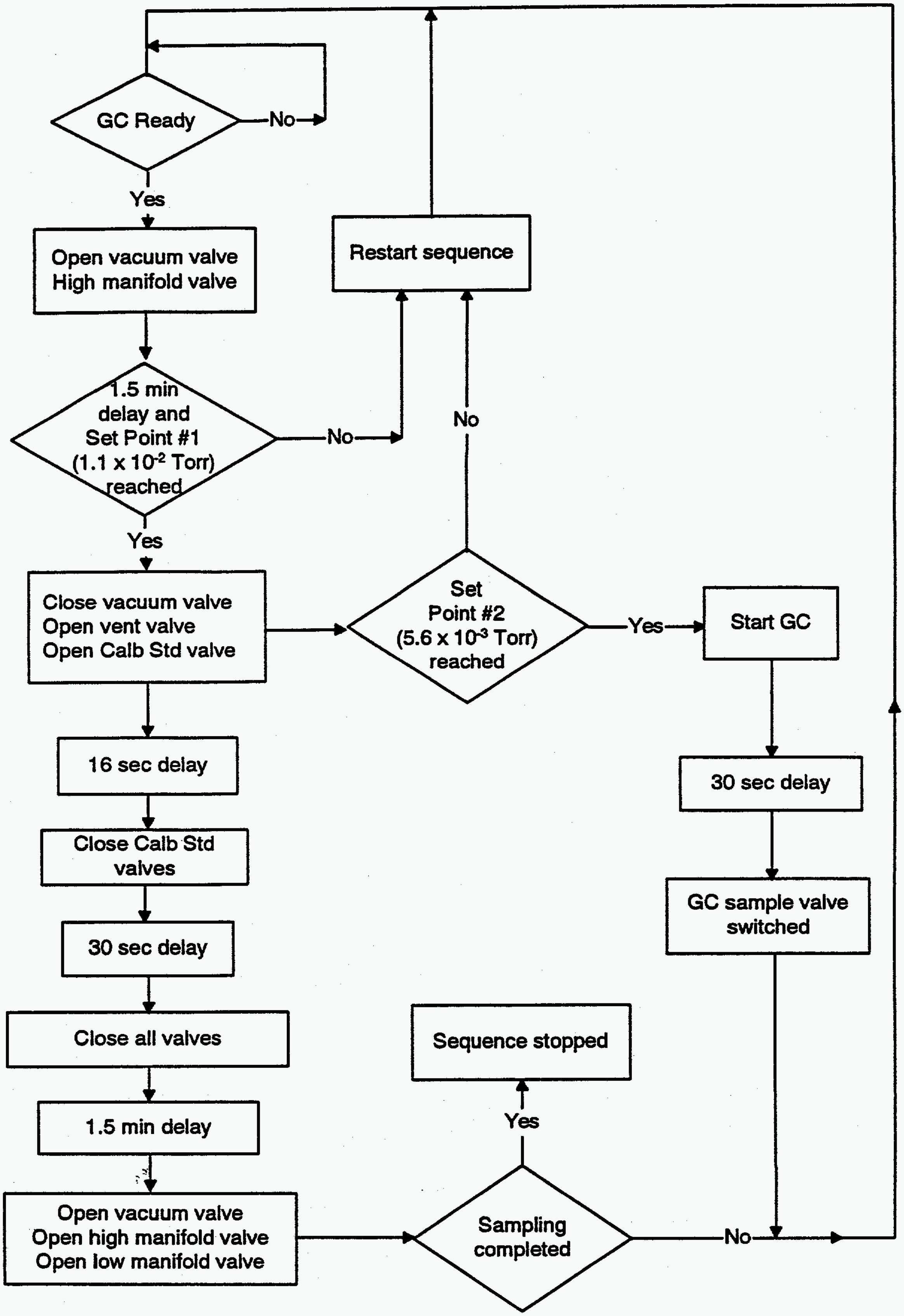

Figure 11. Automated calibration sequence.

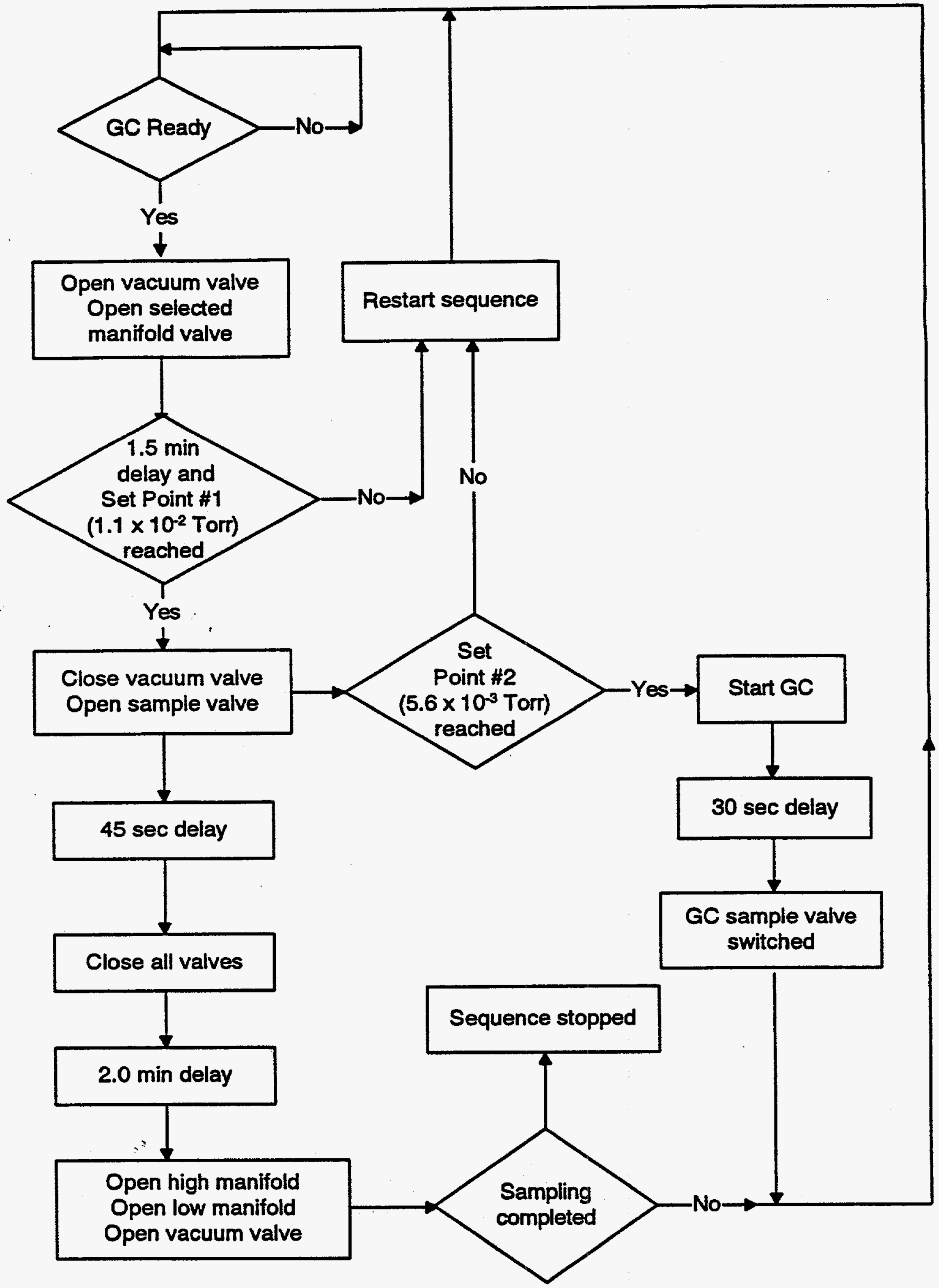

Figure 12. Automated sampling sequence.

sampling valve switched to the sequence selected position to prepare for the next headspace sample. Total cycle time was approximately 15 min.

3.1.3.4 Analytical Sampling Scheme. Measurements of the VOC concentrations were taken from six locations inside each simulated waste drum: the four small poly bags, the large bag headspace, and the drum headspace. Measurements of the drum headspace and liner headspace temperature in drum #1 and the drum headspace temperature in drum #4 were made during the entire duration of each test period. Ambient laboratory temperature was also measured. Barometric pressure measurements were made on each sampling day.

Samples were first collected from all small bags approximately 24 hrs after the bags were filled. During a 3-week period, gas samples were collected from two small bags, the large bag headspace, and drum headspace. Samples were collected every two to four days. At the end of the 3-week period, all four small bags were sampled again. The sampling scheme for the simulated waste drums is listed in Table 4. The sample identification numbers were defined by the following nomenclature. The identification number (i.e. 312-2SB1D) included the test period number (3), the sampling day (12), the drum number (2), the sampling location (DH = drum headspace, LB = large bag headspace, SB1 = small bag #1), and the duplicate (D). A 3-point initial standard calibration was established prior to each test period. Continuing calibration standards were analyzed and evaluated against the initial calibration curve prior to samples analysis. A sample blank from the low level manifold was analyzed at the beginning of the sample sequence to determine if there were any interference or residual VOCs in the sampling system. One sample duplicate of a small poly bag was randomly selected and analyzed on each sampling day. The polyethylene bottles were filled at the beginning of test period I and sampled immediately after the final filling to establish the time zero concentrations. Each bottle was sampled on day 1, day 21, day 50, day 81 and day 124 of the experiment.

3.1.4 Quality Control

This section defines the quality control procedures and components that were used in the performance of the VOC transfer experiments.

3.1.4.1 Quality Control Samples. Initial calibration curves, continuing calibration standards, system blanks, and sample duplicates were part of the quality control procedures used to ensure the quality of the experimental data. An initial calibration curve is defined as a curve which plots concentration of known analyte standards versus the instrument response (area counts) to the analyte. Three-point five-replicate external calibration curves were prepared for every target compound prior to the start of each test period. Continuing calibration standards are defined as analyte standards used to validate the initial calibration curve and verify system performance (retention time shifts, peak shape, etc.). The CCS analyses were performed at the beginning of each sampling day prior to sample analysis using the mid-level standard gas mixtures

Table 4. Sampling scheme for simulated waste drums.

Sample days			
Test periods I, II, IV	Test period III	Drum number	Headspace sample identification number[a]
2	2	1	X02-1SB1, X02-1SB2, X02-1SB3, X02-1SB4
		2	X02-2SB1, X02-2SB2, X02-2SB3, X02-2SB4
		3	X02-3SB1, X02-3SB2, X02-3SB3, X02-3SB4
		4	X02-4SB1, X02-4SB2, X02-4SB3, X02-4SB4
3	5	1	X05-1DH, X05-1LB, X05-1SB1, X05-1SB3
		2	X05-2DH, X05-2LB, X05-2SB1, X05-2SB2
		3	X05-3DH, X05-3LB, X05-3SB2, X05-3SB4
		4	X05-4DH, X05-4LB, X05-4SB2, X05-4SB3
5	7	1	X07-1DH, X07-1LB, X07-1SB2, X07-1SB4
		2	X07-2DH, X07-2LB, X07-2SB2, X07-2SB4
		3	X07-3DH, X07-3LB, X07-3SB3, X07-3SB4
		4	X07-4DH, X07-4LB, X07-4SB1, X07-4SB4
8	9	1	X09-1DH, X09-1LB, X09-1SB2, X09-1SB4
		2	X09-2DH, X09-2LB, X09-2SB1, X09-2SB2
		3	X09-3DH, X09-3LB, X09-3SB1, X09-3SB3
		4	X09-4DH, X09-4LB, X09-4SB1, X09-4SB4
10	12	1	X12-1DH, X12-1LB, X12-1SB1, X12-1SB2
		2	X12-2DH, X12-2LB, X12-2SB1, X12-2SB4
		3	X12-3DH, X12-3LB, X12-3SB1, X12-3SB4
		4	X12-4DH, X12-4LB, X12-4SB1, X12-4SB2
12	14	1	X14-1DH, X14-1LB, X14-1SB2, X14-1SB4
		2	X14-2DH, X14-2LB, X14-2SB2, X14-2SB3
		3	X14-3DH, X14-3LB, X14-3SB2, X14-3SB3
		4	X14-4DH, X14-4LB, X14-4SB1, X14-4SB4

a. Sample identification number (example 105-3SB2)

1—Test period number; 05—Sample day; 3—Drum number

SB2—Small bag #2 (DH—Drum head space; LB—Large bag).

Table 4. (continued).

Sample days			
Test periods I, II, IV	Test period III	Drum number	Headspace sample identification number[a]
16	16	1	X16-1DH, X16-1LB, X16-1SB3, X16-1SB4
		2	X16-2DH, X16-2LB, X16-2SB3, X16-2SB4
		3	X16-3DH, X16-3LB, X16-3SB1, X16-3SB3
		4	X16-4DH, X16-4LB, X16-4SB3, X16-4SB4
19	19	1	X19-1DH, X19-1LB, X19-1SB1, X19-1SB3
		2	X19-2DH, X19-2LB, X19-2SB1, X19-2SB3
		3	X19-3DH, X19-3LB, X19-3SB1, X19-3SB2
		4	X19-4DH, X19-4LB, X19-4SB2, X19-4SB3
22	22	1	X22-1SB1, X22-1SB2, X22-1SB3, X22-1SB4
		2	X22-2SB1, X22-2SB2, X22-2SB3, X22-2SB4
		3	X22-3SB1, X22-3SB2, X22-3SB3, X22-3SB4
		4	X22-4SB1, X22-4SB2, X22-4SB3, X22-4SB4

a. Sample identification number (example 105-3SB2)

1—Test period number; 05—Sample day; 3—Drum number

SB2—Small bag #2 (DH—Drum head space; LB—Large bag).

($A\text{-}II_a$ and $B\text{-}II_a$). The validity of the initial calibration curve was checked by calculating the percent recovery and the relative percent error for each target analyte

$$\%Rec = \frac{C_c}{C_k} \times 100 \tag{19}$$

$$\%RE = \left(\frac{C_c}{C_k} - 1\right) \times 100 \tag{20}$$

where

%Rec	=	percent recovery
%RE	=	relative percent error
C_C	=	calculated concentration
C_K	=	known concentration.

The data were corrected for bias based on the relative percent error.

For the VOC transport experiments, a clean small polyethylene bag filled with filtered house air was attached to the low level manifold and used as a system blank. One sample duplicate of a small bag was performed each sampling day. Relative percent differences for the sample duplicate were calculated to evaluate the precision of the automated sampling and analytical system.

The relative percent difference is defined as

$$RPD = \frac{C_s - C_D}{C_s + C_D} \times 200 \tag{21}$$

where

RPD	=	relative percent difference
C_s	=	sample concentration
C_D	=	duplicate concentration.

3.1.4.2 Other Quality Control Components. Additional baseline checks were performed to ensure that the system performed as designed.

- The process controller block configuration controlling the Clippard pneumatic solenoids was checked to verify that when a valve was actuated the valve did open and close as specified.

- Sequential timing was verified to allow quantitative sample transfer prior to any sample analysis.

- The maximum attainable vacuum for the vacuums and open manifold system were determined. Pressure set points #1 and #2 were based on those determinations and were modified slightly as needed to ensure the correct sequencing.

- The leak rate of the manifold system was determined and found to be within experimental parameters.

- The temperature thermocouples were standardized using a calibrated thermocouple and Fluke 52 K/J thermometer. At the beginning of each test period and randomly throughout the experiments the temperatures of the heated transfer lines and manifold valve box were checked.

- Before filling the bottles and small poly bags, the mass flow controller was calibrated using digital and bubbles flow meters.

- The small bag and bulkhead feedthroughs were prepared and leak-tested prior to being placed in the simulated waste drum. The same procedures were used for testing the large bag feedthroughs.

3.2 VOC-Polymer Permeability Measurements

Two methods were used for the measuring gas permeabilities. The single-component pressure change method was used to determine VOC solubility in the polyethylene bag. The mixed-component chromatography detection method was used to determine individual VOC permeability across polyethylene bag.

3.2.1 Single-Component Pressure Change Method

A schematic of the single-component pressure change experimental configuration is shown in Figure 13. A fully automated membrane cell and gas valving system with pressure transducers was used to pressurize a gas mixture on one side of a polymer film while measuring the resultant pressure increase (at constant volume) on the evacuated side of the film.[11] The experimental sequence of events during data acquisition was as follows:

- Both sides of the film were evacuated to less than 10 um-Hg to de-gas the system and the polymer film.

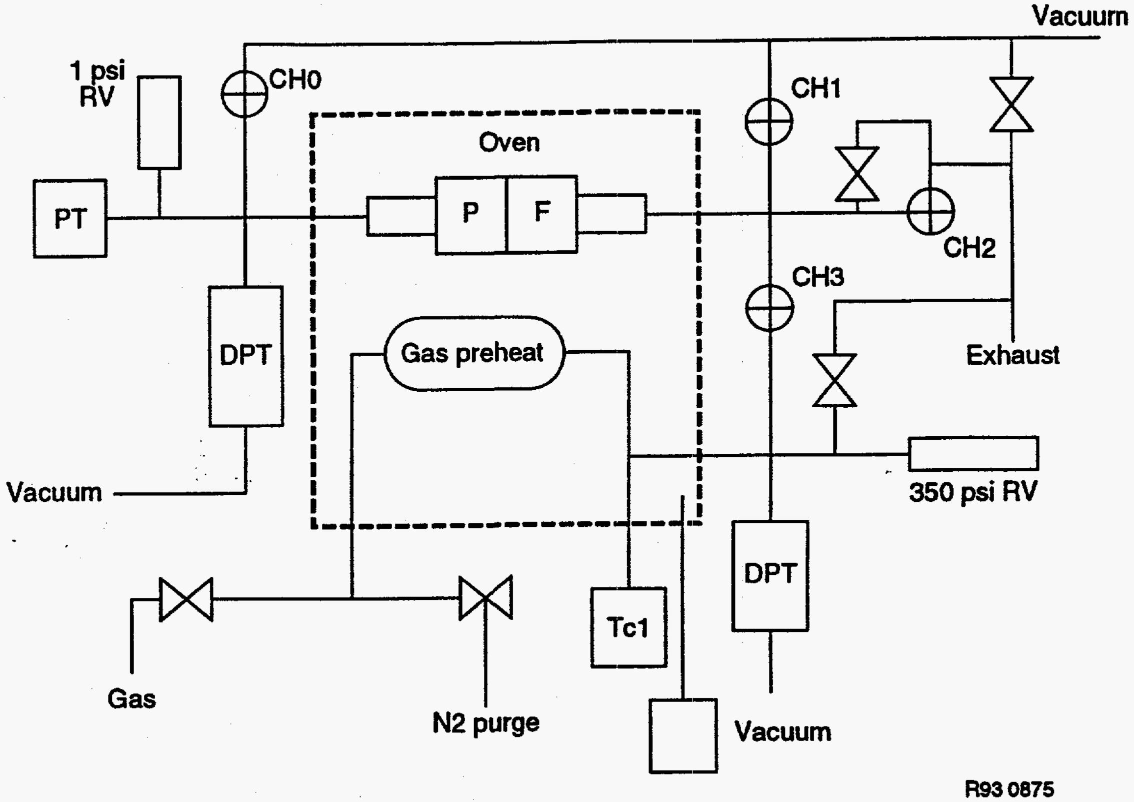

Figure 13. Single-component pressure change experimental configuration.

- Baseline pressure measurements on both sides of the membrane were taken to account for potential atmospheric diffusion (via small leaks) into the system.

- The feed gas side of the film was pressurized while the other side was still essentially evacuated. Data collection occurred as the permeate transducer detected the increasing pressure due to gas permeation. Another transducer monitored the feed pressure.

- Repeat sequence 1 through 3 for the next test.

The transducers for data collection and operational valving were facilitated via an in-house PASCAL program run from an IBM AT computer. Raw data and determined values for permeability, diffusivity, and solubility were stored on a hard disk at the end of each test. A number of standard test gases (oxygen, nitrogen, argon, helium, carbon dioxide, and propane) were used on polyethylene for comparison to literature values and calibration of the instrument.

3.2.2 Mixed-Component Chromatographic Detection Method

A schematic of the experimental configuration used for the mixed-component chromatographic detection method is shown in Figure 14. The system consisted of two subsystems. The first subsystem involved the metered delivery of an inert sweep gas and a feed gas to opposite sides of a cell containing the membrane material. The purpose of the sweep gas was to carry permeating vapors from the permeate side of the cell to the detection system. The feed gas was operated at a differential pressure of 17 to 18 psi above the sweep side and at twice the sweep flow to provide ample permeate potential. Typical flow rates were 1.5 cm^3/min for the sweep gas and 3.0 cm^3/min for the feed gas. The detection system consisted of two Hewlett Packard 5800 series gas chromatographs. The first chromatograph in the series, an HP 5890 series II, contained two Restek 10454, (30 meter, 0.32 mm id., 1.0 um df) columns with flame ionization detectors (FID) to determine the concentrations of the feed and permeating gases. The second chromatograph in the series, an HP 5890a, contained two CHROMPACK 007551, 25 meter, 0.32 mm id., Poraplot Q coated columns with thermal conductivity detectors (TCD) to monitor the components of the compressed air.

The following single VOC-air mixtures were tested on 0.004-in. (0.01-cm) polyethylene membranes: Methylene chloride at 1,006 ppmv, Freon-113 at 1,010 ppmv, 1,1,1-trichloroethane at 994 ppmv, and trichloroethylene at 300 ppmv. In addition, gas standards A-I_a, A-III_a, and B-I_{1a} were used to determine VOC permeability across the polyethylene bags in VOC mixture.

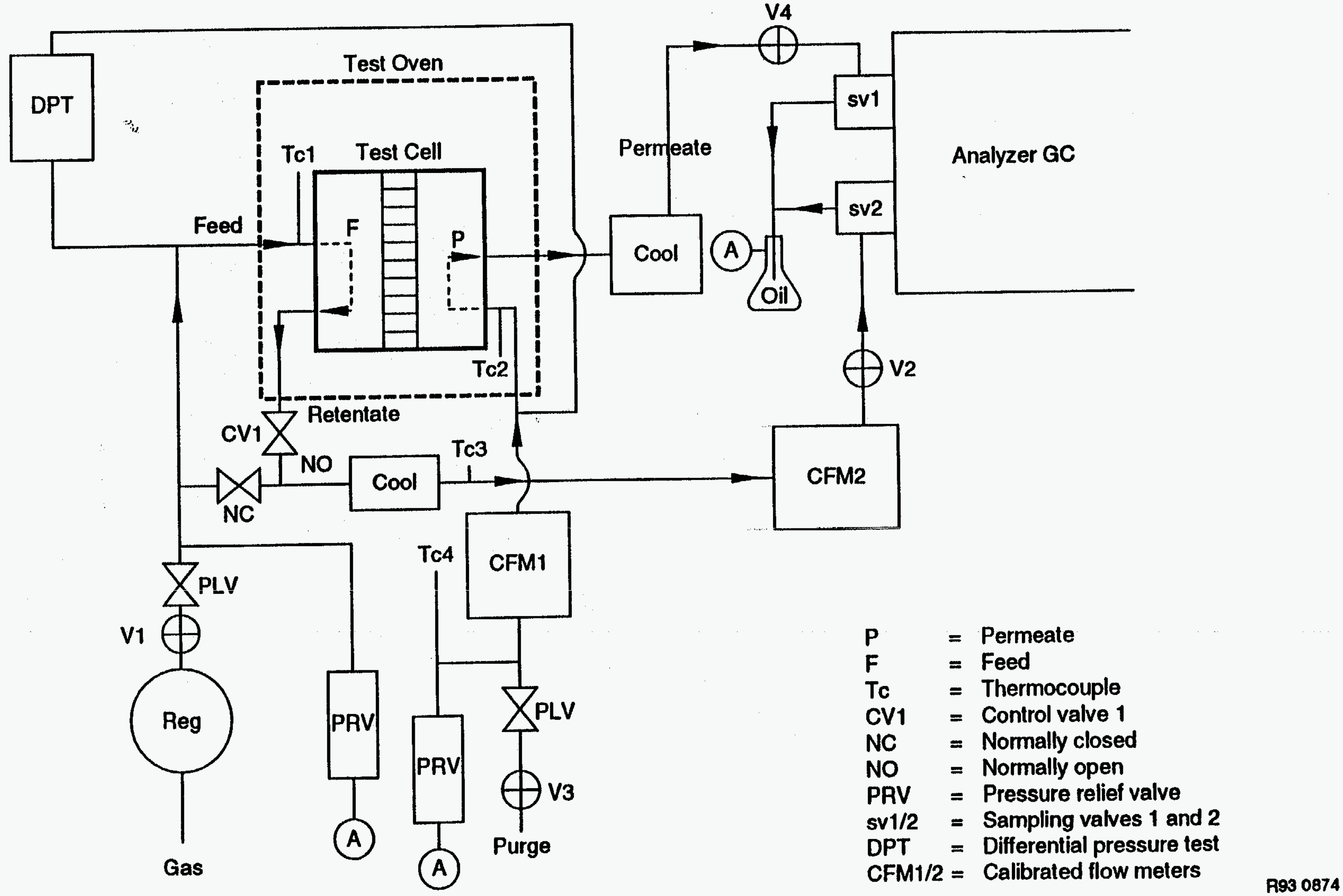

Figure 14. Mixed-component chromatographic detection method experimental configuration.

4. EXPERIMENTAL RESULTS AND DISCUSSION

4.1 VOC Transport Experiments

The measured VOC concentrations from each laboratory-scale waste drum trial are listed in Appendix A. The measured VOC concentrations in the polyethylene bottles are listed in Appendix B. Data characterizing the initial calibration curves, continuing calibration standards, and sample duplicates are summarized in Appendix C.

The percent relative standard deviations for the initial calibration standards were typically less than 2.5% with only five exceptions. The coefficient of determination, r^2, is a measure of linearity and for most calibration curves was greater than 0.995. The greatest difficulty was encountered with p-xylene. The values of r^2 for p-xylene ranged from 0.979 to 0.994. The difficulty encountered with p-xylene is possibly due to its high boiling point and the possibility of cold trapping. The percent relative standard deviations and r^2 values are listed in Table C.1 in Appendix C.

The validity of the initial calibration curves were checked using continuing calibration standards. The relative percent error for the CCS analytes were within ± 20%, with most being within ± 10%. Mean percent errors were all within 10% with only one exception. Tables listing the relative percent error for the CCS are found in Tables C.2-C.5 in Appendix C.

Precision was assessed through the analysis of sample duplicates and expressed as the relative percent difference. The relative percent differences were generally less than 25%. In test period IV, the relative percent difference for p-xylene on days 8 and 12 were greater than 100%. This is attributed to very low sample concentrations which were significantly below the linear dynamic range established by the initial calibration curves. Outside the linear dynamic range the precision and accuracy of the data is suspect, varying as much as ± 30-100% from the reported value. The relative percent differences for the duplicate samples are listed in Tables C.6-C.9 in Appendix C.

The drum and large bag headspace VOC concentrations were calculated from the calibration curve extrapolated using a loop ratio of 2.5 (low level manifold uses a 5.0-cm^3 sample loop and the high level manifold uses a 2.0-cm^3 sample loop). Upon review of the drum headspace and large bag headspace samples a possible systematic error was found in the system loop ratios. The error was apparently due to the efficiency of the sample being swept from the loop, the efficiency of the split ratio, and integration of broadened peaks. The data indicated that there was a variance in the loop ratio which varied with the analyte of interest. Low level standards A-III and B-III were randomly analyzed on each loop 5 times and their area counts were then compared. If the true loop ratio was exactly 2.5, the area counts for the standards sampled on the 5.0 cm^3 loop would be 2.5 times larger than the standards sample on the 2.0 cm^3 loop. The loop ratio for standard gas mixture A-III analytes methylene chloride, Freon-113, TCA, carbon tetrachloride, and TCE were established at 2.55 ± 0.04, 2.61 ± 0.03, 2.70 ± 0.04, 2.89 ± 0.13, and 2.95 ± 0.05, respectively. The loop for standard gas mixture B-III analytes cyclohexane and TCA were established at 2.6 ± 0.04 and 2.6 ± 0.02, respectively. The methanol, toluene, and p-xylene in the standard gas mixture overloaded the column on the 5.0 cm^3 loop, therefore an average system correction factor of 2.7 was used.

During the test periods I, II, and III samples were missed due to sample sequence errors. Samples 108-2SB2, 108-4SB4, and 108-2SB2D were missed during test period I and sample 212-3SB3 was mixed during test period II. Samples 314-3SB3, 314-4SB4, 314-2SB3D, 316-1SB4, 316-2SB4, and 319-3DH were missed during test period III.

Drums were disassembled to determined if there were any failures in the layers of confinement. The drum lid seals, drum feedthrough septa, large bag feedthrough septa, large bags, and small bags were all intact throughout all four test periods with the following exceptions. In test period I, two 1.0 mm holes were detected in small bag 3SB3 near the bulkhead feedthrough. A 2.0 mm hole was found in small bag 4SB4. The tape came undone on 4SB3 at the base of the horsetail; however, the bag was still sealed. Sample analyte concentrations from drum #2 headspace were significantly lower than the concentration from the matching replicate sample in drum #4 headspace. No determination could be made at the time for the discrepancy.

In test period II, two 3.0 mm slits were found in small bag 1SB4. The tape on the large bag horsetail drum #3 came undone and the horsetail unraveled, but the small piece of tape folded over the end of the horsetail did stay in place. Sample concentrations from drum #2 headspace again were significantly lower than the sample concentration from the matching replicate drum #4 headspace. It was determined that the sample transfer line was partially blocked and was replaced.

In test period III, the horsetail on 3SB1 and the large poly bags from drums #3 and #4 were open at the top but were still sealed at the base. Small poly bag 4SB3 was flat and appeared not have been filled with the standard gas mixture. In test period IV, the horsetail on 2SB1 was open at the top but still sealed at the base. The thermocouple probe for drum #4 was not placed in the drum; thus, there was an 0.125-in. hole in the side of the drum.

4.2 VOC-Polymer Permeability Measurements

4.2.1 Single-Component Pressure Change Method

The gas mixture solubility in the polyethylene bag was determined using the single-component pressure change method. The gas mixture solubility is defined as:

$$S_m = \frac{P_m}{D_m} \tag{22}$$

S_m = gas solubility in polymer, cm^3 (STP) (cm^{-3} polymer) (cm Hg)$^{-1}$

P_m = gas permeability in polymer, cm^3 (STP) cm cm^{-2} s^{-1} (cm Hg)$^{-1}$

D_m = gas diffusivity in polymer, $cm^{-2}\ s^{-1}$

The values of P_m and D_m were experimentally determined. Gas permeability in a polymer was calculated using experimental data.

$$P_m = \frac{P_2' V_2 L T_s}{T P_1 A P_s} \tag{23}$$

where

P_2' = experimental rate of change in pressure on permeate side of test cell (cm Hg) s^{-1}

V_2 = permeate volume, cm^3

T = experimental temperature, K

P_1 = feed gas pressure, cm Hg

A = membrane surface area, cm^2

L = membrane thickness, cm

T_S = standard temperature, K

P_S = standard pressure, cm Hg.

and gas diffusivity in the polymer was calculated as

$$D_m = \frac{L^2}{6T_l} \tag{24}$$

where

T_l = time lag, s

Permeabilities, diffusivities, and solubilities for the VOC-air mixtures on the polyethylene bag are listed in Table 5. The permeabilities of the single component mixtures in air were indistinguishable from compressed air alone as a result of the low sensitivity of the pressure swing method. The detection limit of this method was approximately 1% by volume. Permeabilities determined by the pure gas methods were composite permeabilities for the gas mixture. The

Table 5. Permeability, diffusivity and solubility of VOC-air mixtures in yellow polyethylene bag.

Test gas	Permeability (Ba)	Diffusivity ($cm^2\ s^{-1} \times 10^7$)	Solubility [cm^3 (cm^{-3} polymer) (cm Hg)$^{-1} \times 10^4$]
300 ppmv trichloroethylene in air	1.62 ± 0.15	9.39 ± 1.37	1.7 ± 0.3
1,006 ppmv methylene chloride in air	1.74 ± 0.04	5.94 ± 0.58	3.0 ± 0.3
994 ppmv trichloroethane in air	1.64 ± 0.04	6.81 ± 0.92	2.2 ± 0.3
1,010 ppmv Freon-113 in air	1.64 ± 0.06	7.86 ± 0.84	2.1 ± 0.3

permeability is a function of all gases in the mixture and should not be expected to represent any single component of the mixture.

4.2.2 Mixed-Component Chromatographic Detection Method

The permeability of specific VOC in a VOC-air mixture were determined via the mixed-component chromatographic detection method. The VOC permeability was calculated from Equation 23.

$$\rho = \frac{\Delta V_g T_s P_2 L}{\Delta t_{exp} T P_s A \Delta P_g} \qquad (25)$$

where

ΔV_g = partial volume of the permeating species in the flow, cm^3

ΔP_g = partial pressure differential of the permeating species across the membrane, cm Hg

Δt_{exp} = time for partial volume flow under experimental condition, s

P_2 = pressure on permeate side of the membrane, cm Hg

The partial volume of a particular gas was determined by multiplying the total volume of the bulk permeate by percent volume gas concentration in the bulk flow.

The calculated permeabilities assumed an ideal case of noninteracting-noncompeting gases. Actual interactions of various gases (i.e., the competition or co-solubility) in a mixture are difficult to assess. Calculated VOC permeabilities for different VOC-air mixtures are listed in Table 6.

Table 6. Measured VOC permeability from mixed-component chromatographic detection method.

VOC	Multiple VOC-air mixtures A-I_a (Ba)[a]	Multiple VOC-air mixtures A-III_a (Ba)	Single VOC-air mixture (Ba)
Methylene chloride	244 ± 37	313 ± 21	232 ± 15[b]
Freon-113	27.4 ± 2.6	54 ± 8.0	34.3 ± 1.3[c]
1,1,1-trichloroethane	138 ± 15	209 ± 14	83.1 ± 3.4[d]
Carbon tetrachloride	224 ± 16	161 ± 49	—[e]
Trichloroethylene	779 ± 40	311 ± 22	660 ± 15[f]

a. Ba = 10^{-10} cm^3 (STP) cm cm^{-2} s^{-1} $(cm\ Hg)^{-1}$.

b. 1,006 ppmv methylene chloride in air.

c. 1,010 ppmv Freon-113 in air.

d. 994 ppmv 1,1,1-trichloroethane in air.

e. Not measured.

f. 300 ppmv trichloroethylene in air.

The permeabilities varied depending upon whether the test gas contained a single VOC or a mixture of VOCs. Examination of the measured permeabilities for the gases at high and low VOC concentration showed some differences in the values. The difference may be the result that one or more of the VOCs may act as a plasticizer. This phenomenon needs to be investigated further.

During the experiment, the time required for the permeate to reach a steady state increased with the increased boiling point of the gaseous component of interest. A system limitation was identified to be the plumbing external to the permeation cell. Transfer lines and valving for the current system provided excessive dead-space and were operated at ambient temperature (23 to 28°C). Thus, it was difficult to obtain an equilibrium measurement for gases with boiling points above the 75 to 80°C range. Gases such as toluene (b.p. 111°C) and p-xylene (b.p. 135°C) in gas standard B-I_{1a} were generally not equilibrated within a 24-hour period. Permeabilities for VOC constituents in gas standard B-I_{1a} were not determined because it was not possible to obtain a steady-state measurement in the current system. These data will have to be measured when the system is redesigned to eliminate or reduce the deadspace.

Deviations presented in the tables are a measure of reproducibility and not of accuracy. Reasons for the observed variance lie in the difficulty of comparing chromatographic peaks, which differed by as much as an order of magnitude. Additional studies involving concentration and temperature profiles of single and multi-component mixtures should yield a better understanding of the conditions affecting the gas permeabilities. Slow equilibration can be overcome by redesigning the system to incorporate most of the plumbing and valving in a temperature-controlled oven. External lines that cannot be placed in the oven must be wrapped in heat tape and held above ambient temperature to inhibit surface binding of low-volatility components.

5. MODEL RESULTS AND DISCUSSION

The model equations presented in Section 2 were solved to estimate the VOC concentration as a function of time for those experiments where the VOC permeability was measured. Thus, model calculations of the waste drum and polyethylene bottle VOC transport experiments that used gas standard B-I are not presented in this report.

5.1 Model Parameter Determination

Many model parameters were measured or estimated from available process information. Other parameters that were not measured directly were estimated using the VOC transport model and lab-scale waste drum data from Trial 2.3. This trial was used because the drum temperature was constant and no leaks were identified in the small bags. Model parameters determined in this fashion were used in all other model calculations.

Model input included specifying the total surface area, diffusional area, void volume, bag thickness, and diffusional pathway length for small and large bags. Although every effort was made to prepare four small bags that were identical, occasionally one small bag was different from the other bags. In several experiments one small bag had a puncture in it, and in another experiment a small bag was unintentionally not filled with a gas mixture. Thus, the program was written to require model input for two small bags. One set of parameters specified bag parameters for three small bags assumed to be identical. The other set of parameters pertained to the fourth small bag. If all four small bags were identical, then the model parameters for the two small bags were identical.

5.1.1 Surface Areas

5.1.1.1 Permeable Area. The dimensions of the heat-sealed bags were 11 in. (27.9 cm) by 18 in. (45.7 cm). The total bag surface area was 400.0 in.^{2} (2,550 cm^2). In the case of the small bags sealed with horsetails, the horsetail base was between generally 11 and 12 in. (27.9 and 30.5 cm) from the bottom of the bag. In addition, approximately 1 in. (2.5 cm) of bag material was bunched together very closely below the horsetail. The total surface area of a small bag was estimated to be 400.0 in.^{2} (2,550 cm^2). The large-bag dimensions before closure by horsetail were 33 in. (83.8 cm) wide and 36 in. (91.4 cm) long. Allowing for approximately 6 in. (15.2 cm) in length, the maximum surface area of the large bag was estimated to be 1,980 in.^{2} (12,800 cm^2).

The actual bag surface area available for permeation is less than the total bag surface area. Small bags in intimate contact with each other, contact between small bags and the large bag, the large bag resting on the drum liner floor, and the overlapping and folding of the bags near the horsetail all decrease the total available surface area. The actual surface area of each bag in each drum could not be measured. For the lab-scale waste drums, the total permeable bag surface area was estimated to be 50% of the total bag surface area. The percentage of total bag surface area available to VOC permeation was estimated to the nearest 25%.

5.1.1.2 Diffusional Area. The cross-sectional diffusional area of a horsetail was estimated to be 0.002 in.^{2} (0.01 cm^2). Holes and slits observed in small bags upon removal from the drum were measured between 0.04 and 0.12 in. (0.1 and 0.3 cm) in length. The diffusional area of a hole in a small bag was estimated in the model to be 0.005 in.^{2} (0.03 cm^2). The cross-sectional area of the hole punched in the lid of the drum liner is 0.11 in.^{2} (0.71 cm^2).

5.1.2 Transport Lengths

All bags have a thickness of 0.004 in. (0.01 cm). The drum liner has a thickness of 0.090 in. (0.23 cm). Horsetail lengths of 6 in. (15.2 cm) were assumed. Model input for the diffusional length between drum liner and drum headspace void volumes was 0.47 in. (1.18 cm). Diffusion lengths across small bag punctures was estimated to be 0.17 in. (0.43 cm).

5.1.3 Void and Polymer Volumes

The small bags have an approximate internal volume of 240 in.^{3} (4,000 cm^3). Small bags with small holes were observed to be partially filled at the end of the test period. The bag volume could not be estimated due to extensive handling upon removal from the drum. Small bags with a visible puncture or tear were assumed to have a bag volume of approximately 120 in.^{3} (2,000 cm^3). A metal cage was placed inside the large bag before drum closure to assure that the shape of the bag was similar in each drum. The cage has a diameter of 18.6 in. (47.3 cm) and a height of 8.1 in. (20.6 cm). The final shape of the large bag was assumed to be a cylinder with a height 1 in. (2.5 cm) and a diameter 2 in. (5.1 cm) greater than that of the support cage. The internal volume of the large bag is estimated to be 3,050 in.^{3} (50,000 cm^3). Large bag void volume was the difference between the total estimated internal volume of the large bag and the total volume of the small bags.

The total volume of the lab-scale drum liner and drum were determined by weighing the mass of water that each container could hold. The total volume of the drum liner was determined to be approximately 3,800 in.^{3} (62,000 cm^3). Thus, the void volume inside the drum liner containing the large and small bags was estimated to be 730 in.^{3} (12,000 cm^3). The total void volume of the drum headspace outside the drum liner was determined to be approximately 980 in.^{3} (16,000 cm^3). The polyethylene bottles have a nominal void volume of 240 in.^{3} (4,000 cm^3).

The total polymer volume was calculated as the product of the total surface area of the polymer and the polymer thickness. The volume of any horsetail or bag edges was neglected.

5.1.4 VOC Transport Properties

5.1.4.1 VOC Permeability. The smaller value of the permeability coefficients for each VOC in gas mixture A listed in Table 6 was used in model calculations.

5.1.4.2 VOC Solubility in Polymers. The gas solubility for each VOC in gas mixture A are summarized in Table 7. Gas solubility in the polymer during the experiment was estimated using Henry's law

$$s = \frac{c_{voc}}{H_s} \tag{26}$$

where

s	=	gas solubility, cm^3 (STP) (cm^{-3} polymer) (cm Hg)$^{-1}$
c	=	VOC concentration in gas phase, mol cm^{-3}
H_s	=	Henry's constant = c_o/s_o
s_o	=	gas solubility at VOC concentration c_o, cm^3 (STP) (cm^{-3} polymer) (cm Hg)$^{-1}$.

Permeability experiments to determine the gas solubility in the drum liner could not be performed because the drum liner wall thickness was too great. Gas solubility in the polyethylene drum liner was estimated using the values in Table 5. In the case of carbon tetrachloride, an approximation of the VOC solubility in polyethylene was estimated using lab-scale results from Trial 2.3 and the VOC transport model. The solubility of 1,000 ppmv carbon tetrachloride in air at 77°F (25°C) in the polyethylene drum liner was estimated to be 3.3×10^{-4} cm^3 (STP) (cm^{-3} polymer) (cm Hg)$^{-1}$.

5.1.4.3 Transfer Coefficient η. The transfer coefficient in Equation (3) defines the rate of VOC uptake in a polymer film. The values for each VOC were determined using the experimental data from Trial 2.3 and are summarized in Table 7.

5.1.4.4 VOC-Air Diffusivity. The diffusivity of most VOCs in air at a given temperature and pressure were identified in the literature.[10] In the case where diffusivity data could not be identified, the VOC diffusivity in air was estimated using Equation (16). Equation (16) was also used to correct for any difference in temperature and pressure observed in the experiments.

5.1.4.5 H_2 Diffusion Characteristic across Carbon Composite Filter. The H_2 diffusion characteristic across a NFT-020 carbon composite filter was reported to be 44×10^{-7} mol s^{-1} (mol fraction)$^{-1}$ at 77°F (25°C).[7]

5.1.5 Initial VOC Concentrations

Initial VOC concentration in the small bags was assumed to be equal to the concentration of the feed gas mixture and zero in all other void volumes unless a small bag was punctured. In that case, the small bag was assumed to contain only 120 in.^{3} (2,000 cm^3) of the 240 in.^{3} (4,000 cm^3) of the gas mixture introduced in the bag. The initial large bag VOC concentration was calculated as the number of VOC moles introduced into the large bag divided by the large bag void volume.

Table 7. VOC transfer coefficients used in Equation (3).

VOC	η, sec^{-1}
Methylene chloride	1×10^{-6}
Freon-113	8×10^{-7}
Trichloroethane	4×10^{-6}
Carbon tetrachloride	8×10^{-6}
Trichloroethylene	4×10^{-6}

5.1.6 Temperature and Pressure

Two waste drums were placed in an environmental chamber to simulate the heating and cooling of waste drums that occur as the result of changes in environmental conditions. The daily temperature in the drum and drum liner headspace of these drums varied as a function of time. In order to simplify model calculations, equations defining the measured temperature as a function of time was determined for each void volume by performing a nonlinear regression analysis of the recorded temperature data. The equations estimating actual temperatures at a given time were accurate within 0.9°F (0.5°C). The first day of each test period began at $t = 0$ sec after all small bags were filled. All waste drums were at room temperature when the small bags were filled. The heating cycle began and ended at t_1 and t_2 seconds, respectively. The heating cycle lasted approximately four hours, or 14,400 seconds. In the case of $t_1 < t < t_2$, the time-dependent nature of the measured temperature in the drum headspace was described by the equation

$$T_{dh}(^oC) = 25.3899 + 20.345\left(1 - e^{-1.22 \times 10^{-4}\left[t - t_1 + 797.7\right]}\right) , \tag{27}$$

and the measured drum liner headspace temperature was described by the equation

$$T_{dl}(^oC) = 24.4287 + 22.2311\left(1 - e^{-1.014 \times 10^{-4}\left[t - t_1 + 723.29\right]}\right) . \tag{28}$$

During the cooldown period ($t > t_2$), the temperature in the drum headspace was described by the equation

$$T_{dh}(^oC) = 27.4542 + 41.456\, e^{-8.451 \times 10^{-5}\left[t - t_2 + 11583.4\right]} , \tag{29}$$

and the drum liner headspace temperature was described by the equation

$$T_{dl}(^oC) = 26.5389 + 31.320\, e^{-8.174\times10^{-5}\left[t-t_2\,+\,8370.18\right]} \quad . \tag{30}$$

After each 24-hour period, t was reset to zero. The temperature in the waste drum continued to cool until the heat cycle was reinitiated. In the case of $t < t_1$ (for all days except the first), the temperature in the drum headspace was described by the equation

$$T_{dh}(^oC) = 27.4542 + 41.456\, e^{-8.451\times10^{-5}\left[t-t_2\,+\,97983.4\right]} \quad , \tag{31}$$

and the drum liner headspace temperature was described by the equation

$$T_{dl}(^oC) = 26.5389 + 31.320\, e^{-8.174\times10^{-5}\left[t-t_2\,+\,94{,}770.2\right]} \quad . \tag{32}$$

The temperatures inside the large and small bags were not measured and were assumed to be the same as the drum liner headspace temperature.

The temperature in the drum headspace of a lab-scale waste drum maintained at ambient room temperature varied between 75.2 and 77.9°F (24 and 25.5°C) during all trials. A constant temperature of 76.5°F (24.7°C) was used in model calculations for the waste drums maintained at room temperature. The ambient pressure varied between 638.0 and 651.5 torr during the experiments. A constant pressure of 644.8 torr was used in all model calculations.

5.2 Model Results

The VOC transport model was used to estimate the VOC concentration within lab-scale waste drums as a function of time. Model calculations were performed using a computer program listed in Appendix D. The program used IMSL subroutines to solve a series of first-order differential equations. The program was run on a CRAY X-MP 216 supercomputer. Model predictions of the first measured small bag concentration were made at the approximate hour the samples were collected. All other model results are calculated at 24-hour intervals. Model input and output listing the predicted VOC concentration in the small bags, large bag, and drum headspace void volumes for all trial using gas mixture A are tabulated in Appendix E.

5.2.1 Model Accuracy

Some examples of model predictions of VOC concentrations in small bag void volumes in lab-scale waste drums maintained under different thermal environments are shown in Figures 15 and 16. Examples of model predictions of VOC concentrations in the large bag void volumes maintained under different thermal environments are shown in Figures 17 and 18. In each figure, a continuous function was defined that estimated the time dependence of predicted VOC concentrations during the experiment. Model values are also shown.

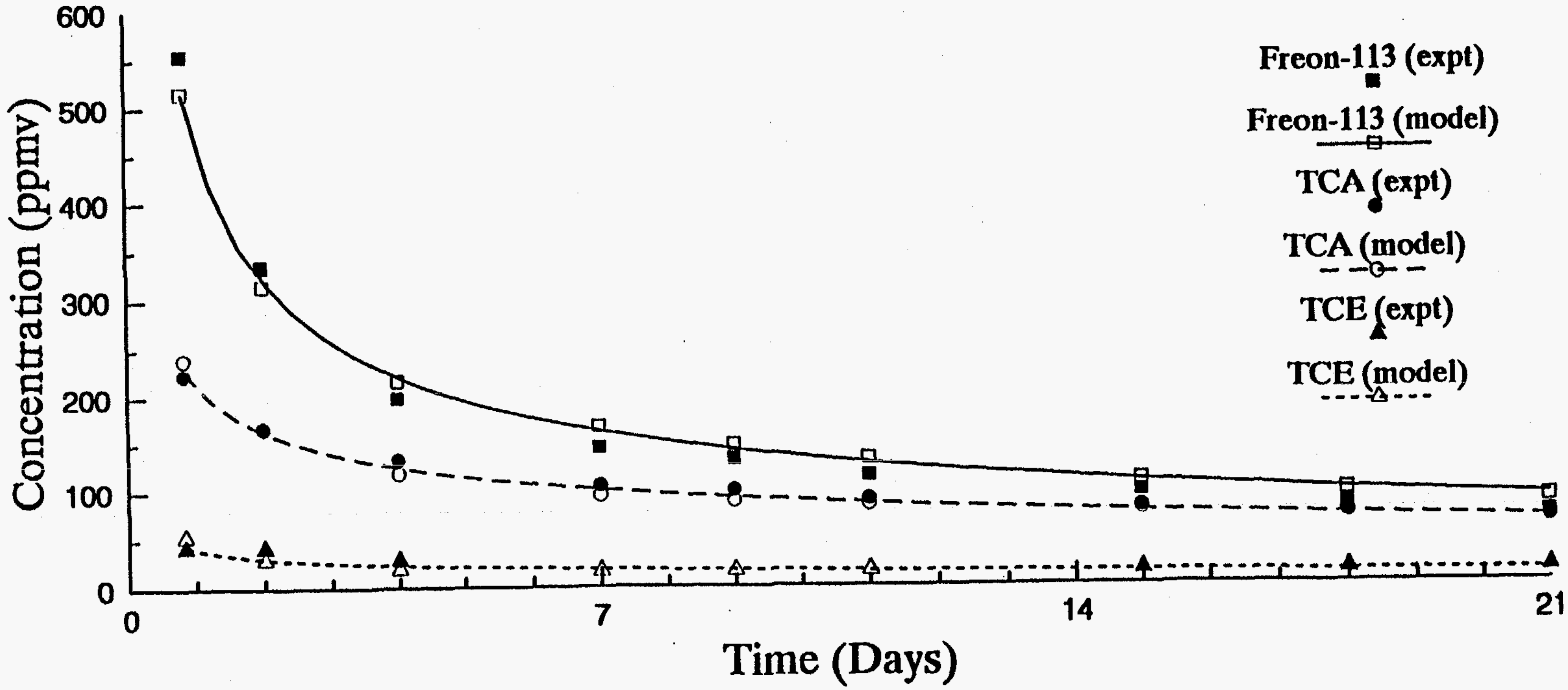

Figure 15. Model predictions and experimental data of average Freon-113, TCA, and TCE concentration in small bag void volumes of waste drum in variable-temperature environment (Trial 1.1).

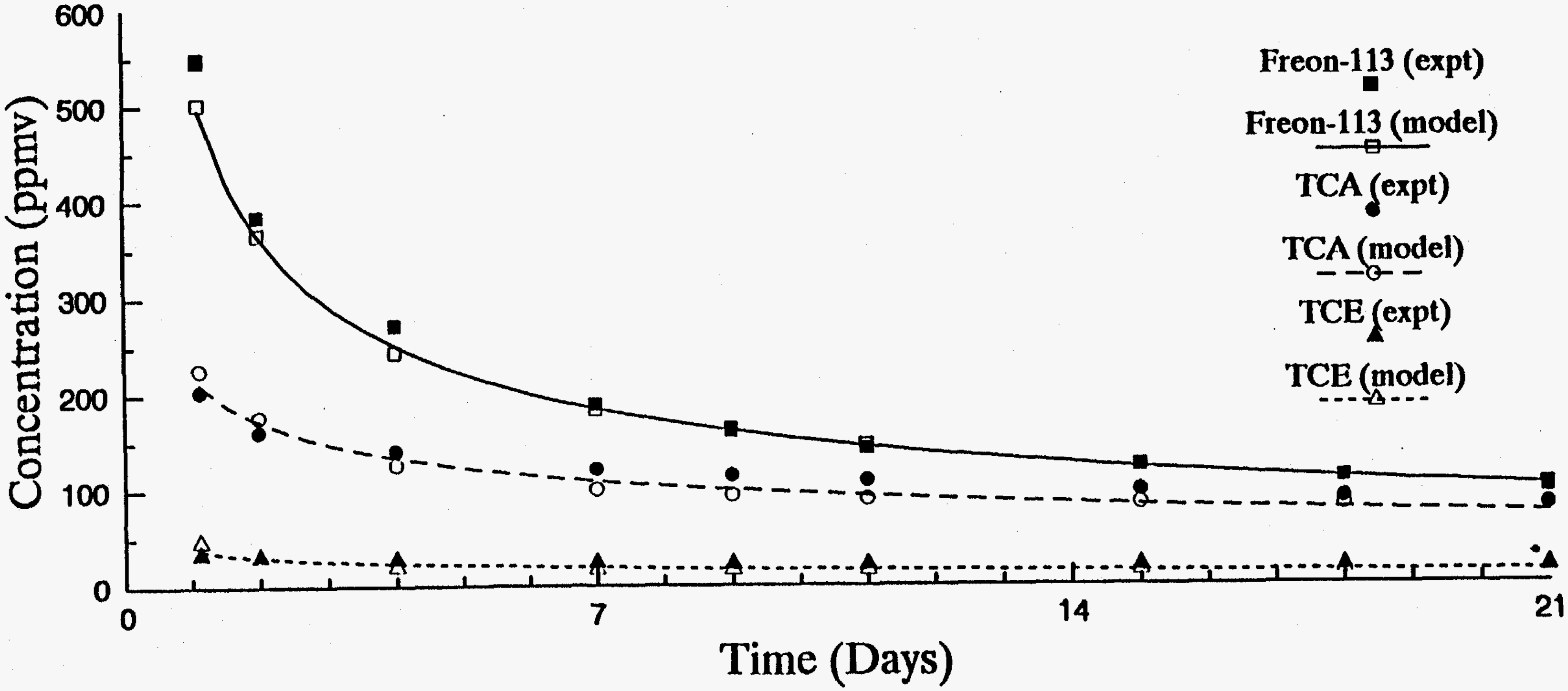

Figure 16. Model predictions and experimental data of average Freon-113, TCA, and TCE concentration in small bag void volumes of waste drum in constant-temperature environment (Trial 2.3).

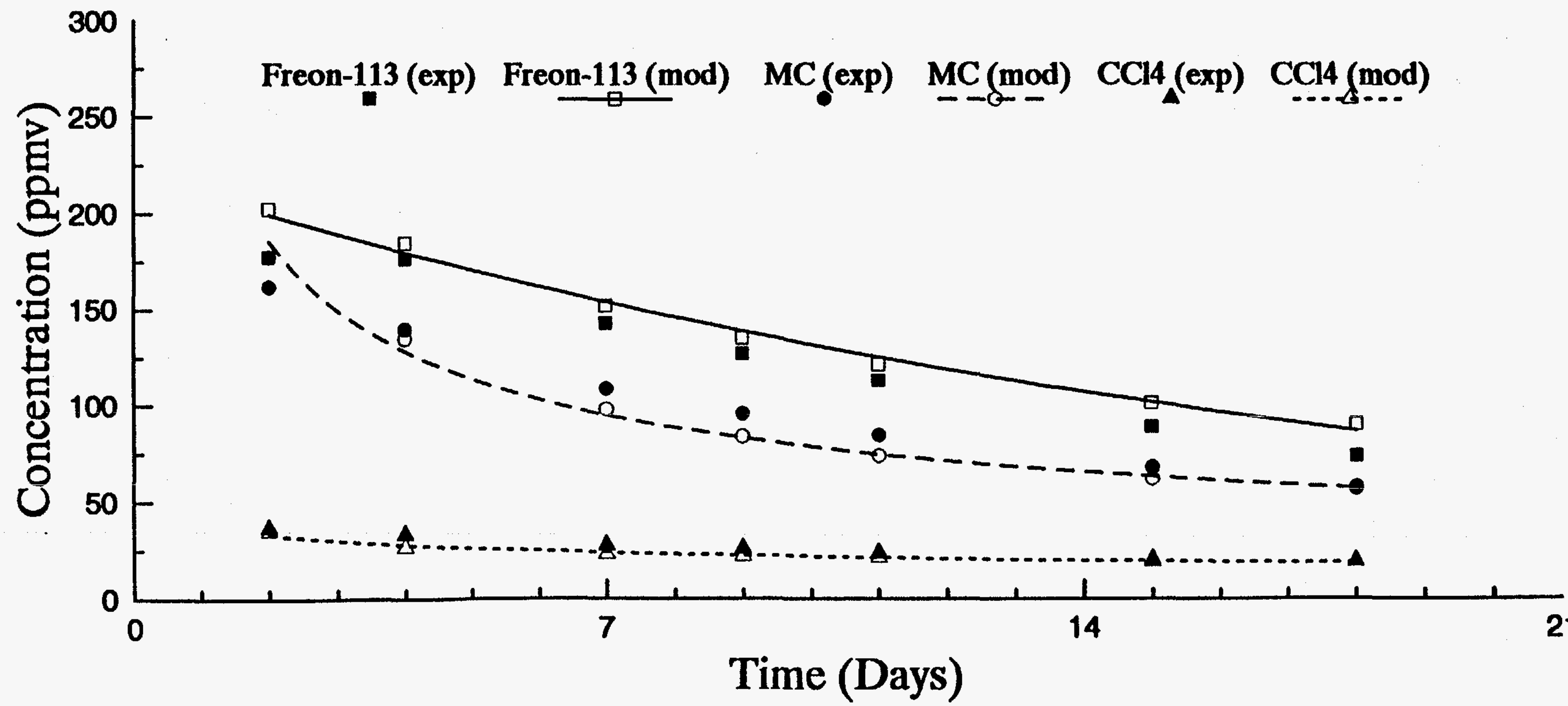

Figure 17. Model predictions and experimental data of Freon-113, methylene chloride (MC), and carbon tetrachloride (CCl_4) concentration in large bag void volume of waste drum in variable-temperature environment (Trial 2.1).

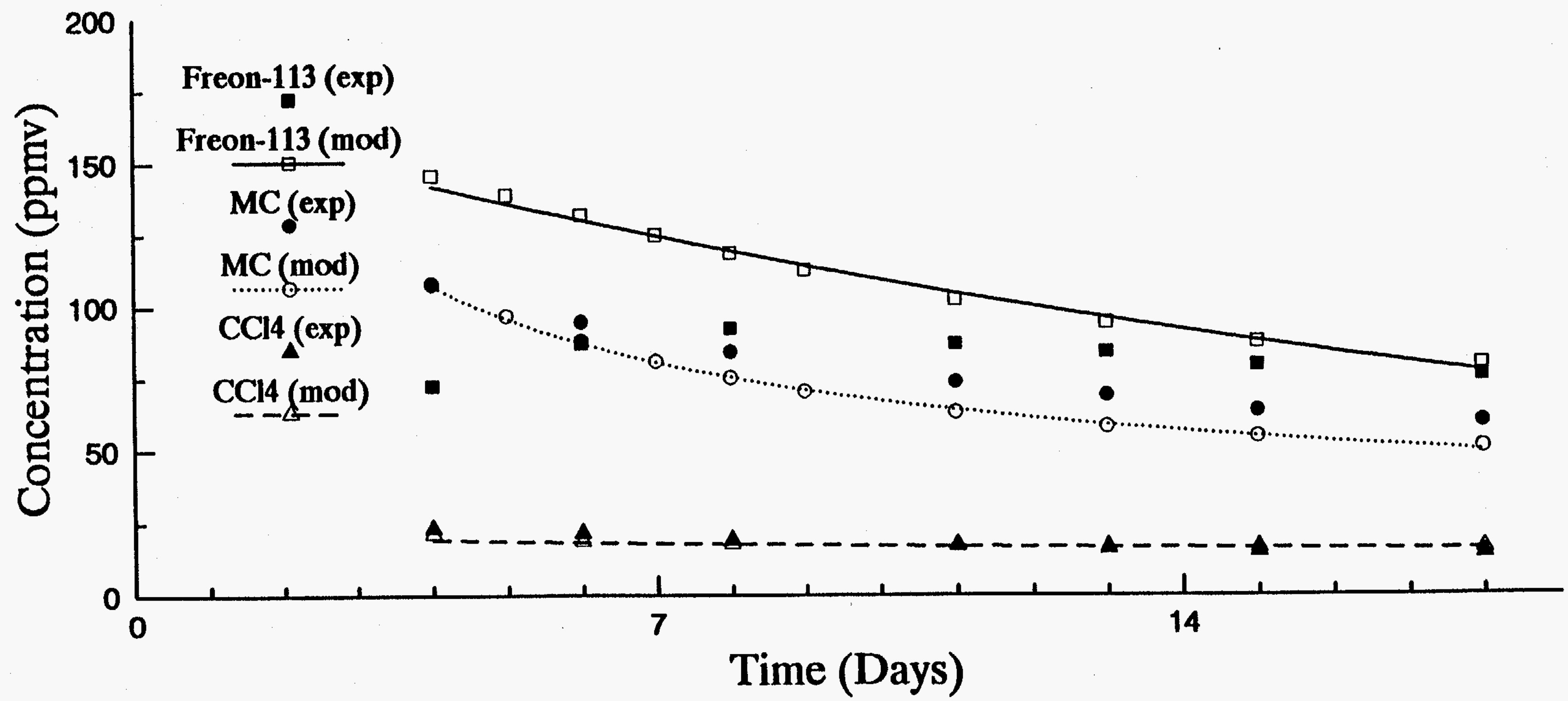

Figure 18. Model predictions and experimental data of Freon-113, methylene chloride (MC) and carbon tetrachloride (CCl_4), concentration in the large bag void volume of waste drum in constant-temperature environment (Trial 3.4).

The accuracy of model predictions of VOC concentration in each void volume in each trial was characterized by the mean absolute relative deviation defined as

$$|\bar{d}| = \sum_{i=1}^{N} \frac{\left| \left(c_{mod} - c_{exp} \right)_i \right|}{N\, c_o} \tag{28}$$

where

$|\bar{d}|$ = mean absolute relation deviation

c_{mod} = model prediction of VOC concentration at time t

c_{exp} = measured VOC concentration at time t

c_o = initial VOC concentration introduced into small bags

N = number of comparisons made during trial for a given void volume.

The mean absolute relative deviation for small bag, large bag, and drum headspace void volumes in each trial involving gas mixture A are summarized in Figures 19 through 21.

In most trials, the small bag mean absolute relative deviation for each VOC was less than 2%. The calculated deviation was much greater for Freon-113 in Trial 4 than for any other VOC in any trial. Trial 4 experiments were performed using a different gas mixture than was used in other trials. The gas was reanalyzed to check the Freon-113 concentration, but the analysis did not indicate any significant deviation from the value reported. No other possible explanation for the significantly higher measured Freon-113 concentration in Trial 4 could be determined. The large bag mean absolute relative deviation followed the same trends as observed for the small bags.

The mean absolute relative deviation for the drum headspace void volume in waste drums maintained at room temperature was less than 2% for a majority of the trials. Most mean absolute relative deviations for the drum headspace void volume in waste drums maintained under a variable-temperature environment were between 2% and 4%. The increase in the deviation between the model and experimental results in the heated drums was attributed to the failure of the model to account for increased VOC solubility in the polyethylene drum liner at higher temperatures.

5.2.2 Effect of Drum Temperature

The average concentrations of Freon-113 and TCA in the drum headspace of waste drums maintained in constant-temperature and variable-temperature environments are plotted as a function of time in Figure 22. The VOC concentration in the drum headspace of waste drums maintained at room temperature was consistently greater during the course of the 3-week

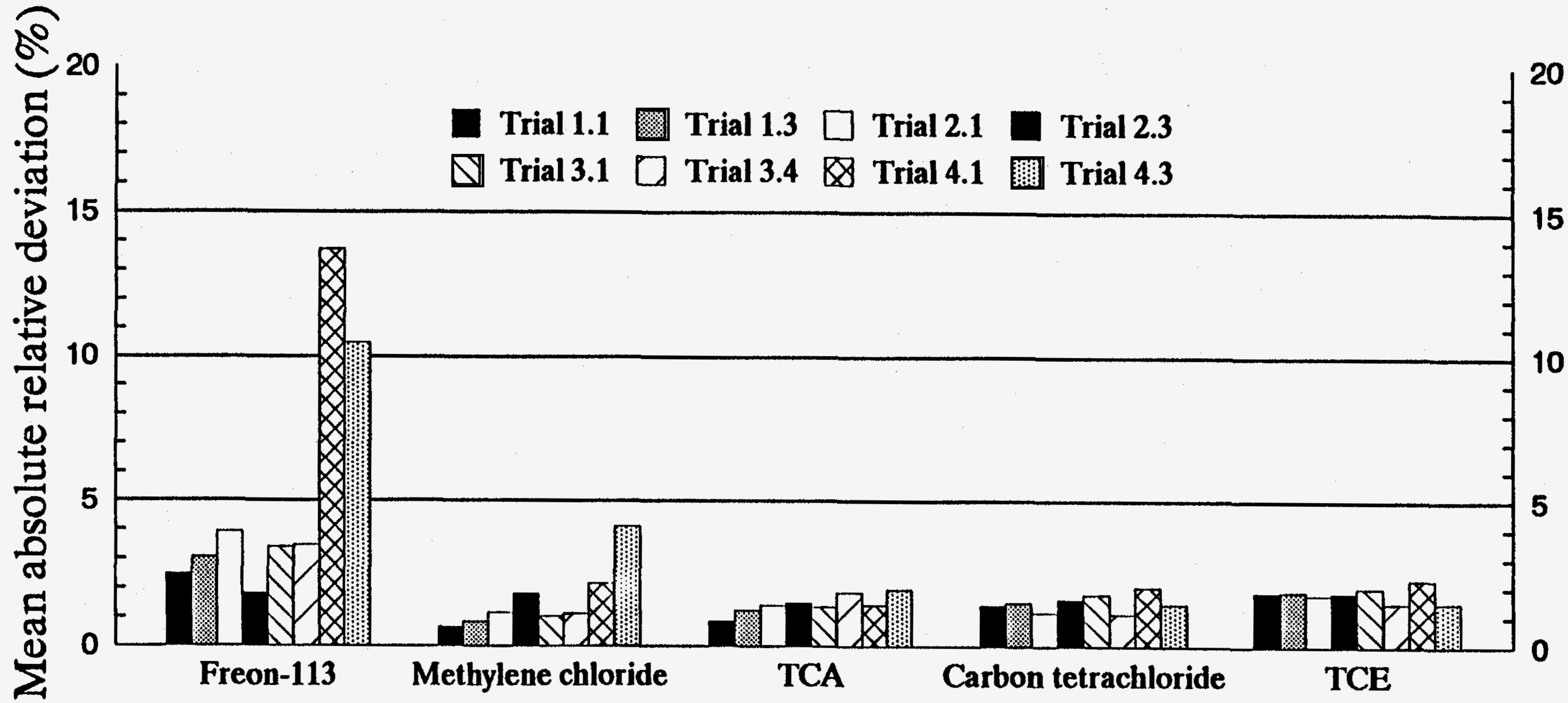

Figure 19. Mean absolute relative deviation of VOC concentration in small bags.

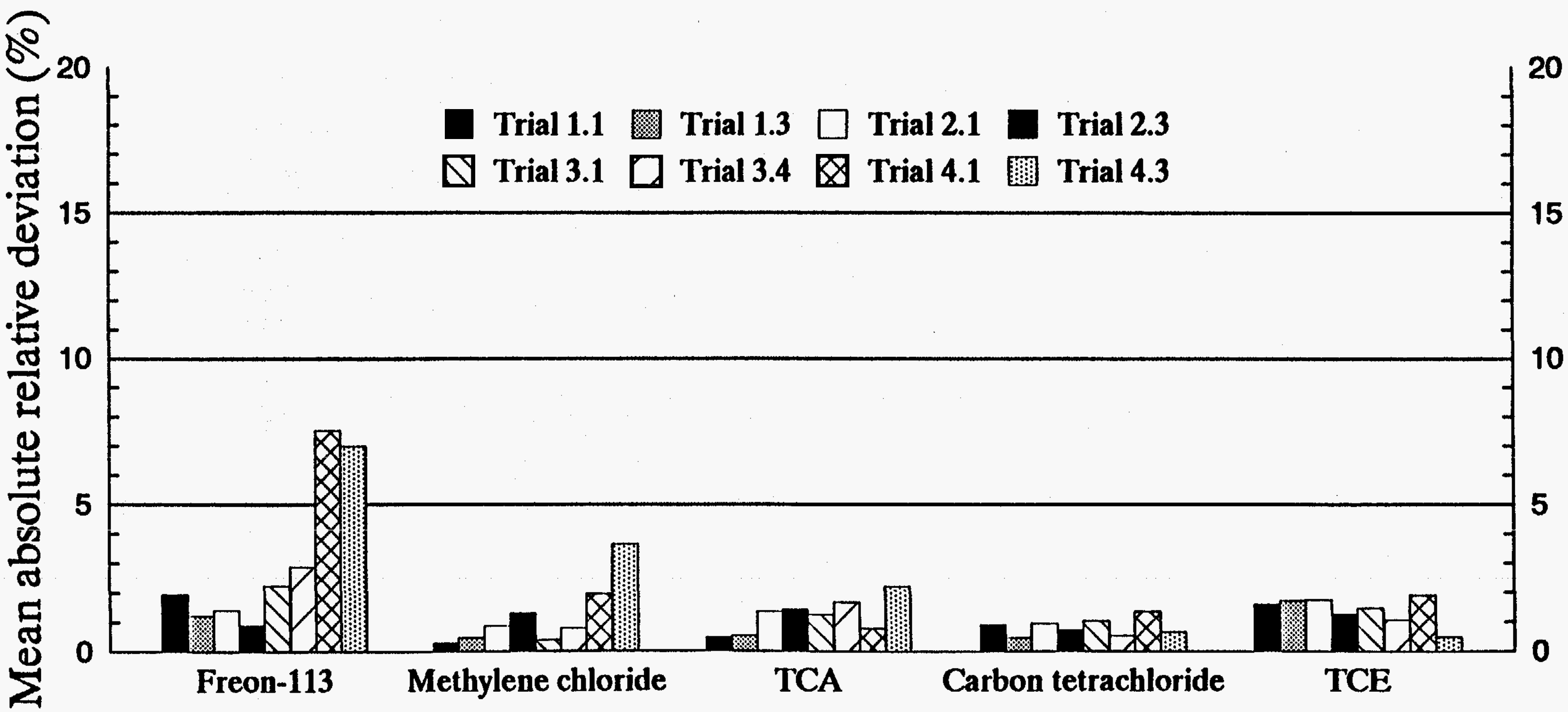

Figure 20. Mean absolute relative deviation of VOC concentration in large bags.

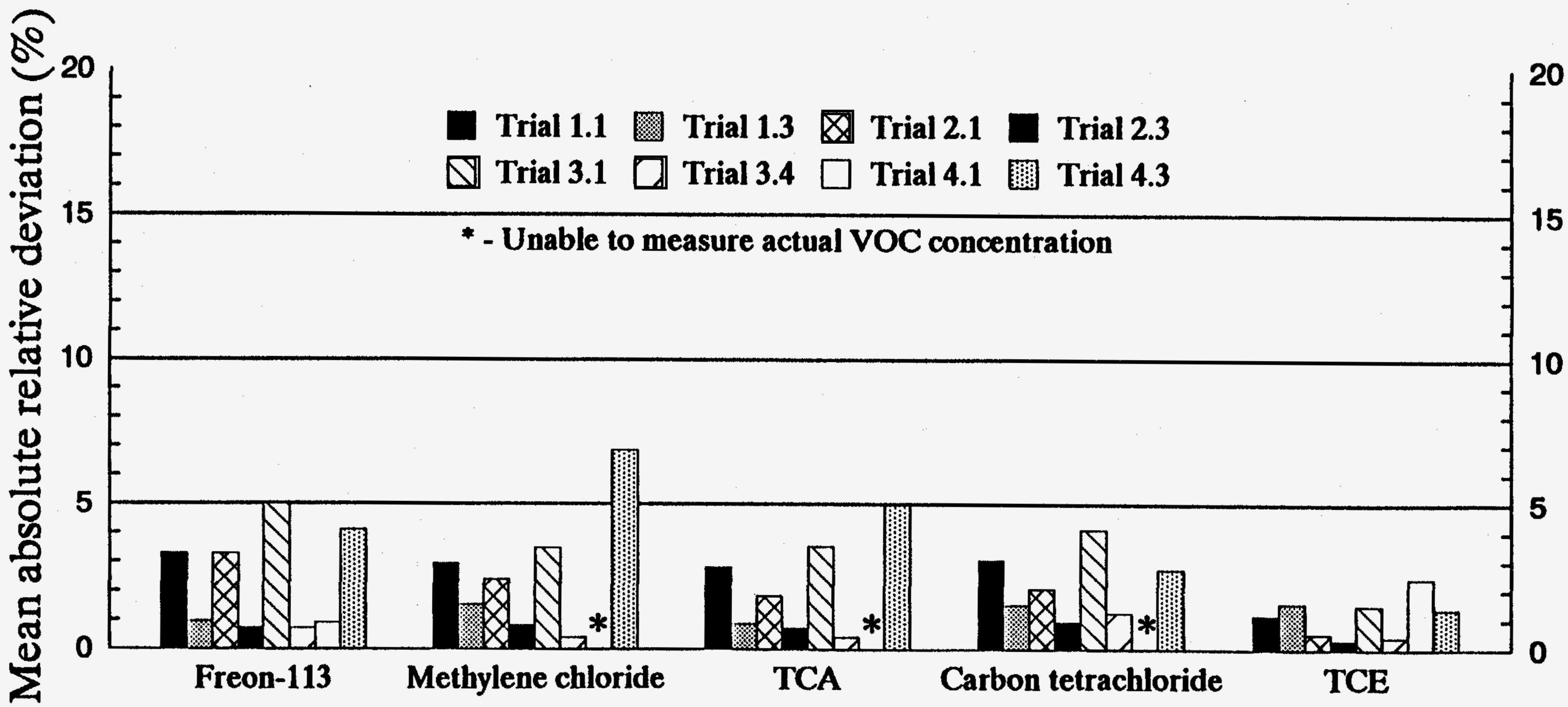

Figure 21. Mean absolute relative deviation of VOC concentration in drum headspace.

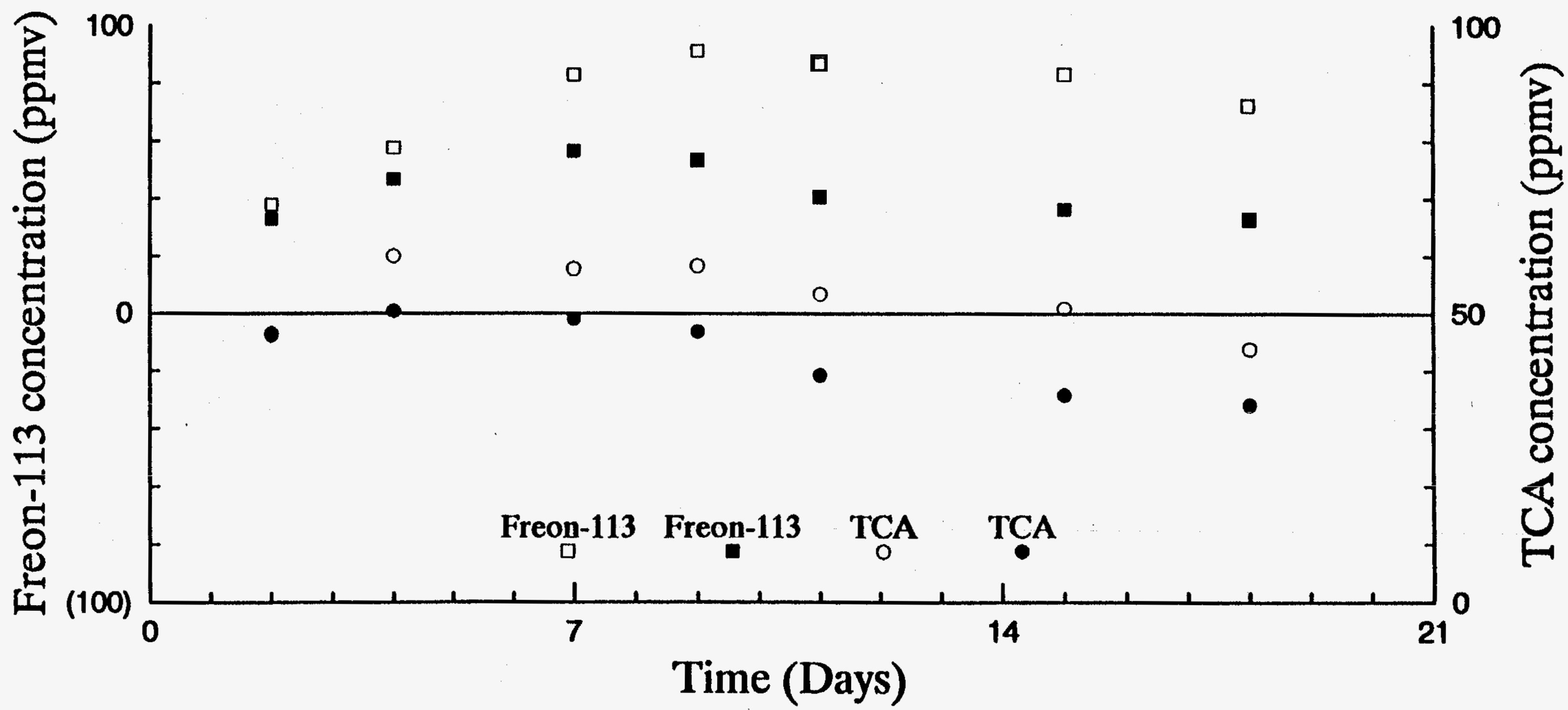

Figure 22. Average Freon-113 and 1,1,1-trichloroethane (TCA) concentration in drum headspace for constant-temperature (○,□) and variable-temperature (●,■) experiments.

experiment than that in the waste drums exposed to a variable heat source. The difference was attributed to an increase of VOC solubility in the polyethylene liner at higher temperatures and an increased rate of aspiration due to fluctuating drum temperature. Although the current model does not account for the temperature dependence of VOC solubility in the polymer drum liner, the model does predict lower drum headspace VOC concentrations in a waste drum exposed to thermal cycling than in a drum maintained at room temperature.

5.2.3 Effect of Small Bag Closure

The effect of the small bag closure type on VOC transport in the lab-scale drum cannot be determined from a direct comparison of measured VOC concentration in small bags. In several trials, a small bag was damaged. In addition, the time between the filling of the small bags and the first gas samples was not the same in each trial.

The model was used to estimate the relative importance of the VOC transport through a small bag horsetail compared to VOC permeation across the bag wall. Recall Equation (4)

$$V_{1,j} \frac{dy_{1,j}}{dt} = (\alpha\phi + \beta)_{1,j} [y_2 - y_1] - \gamma_{1,j}\phi \frac{ds_{1,j}}{dt} \tag{4}$$

where

$\alpha_{1,j} = (\rho A_P P/\Delta x_P)_{1,j}$

$\beta_{1,j} = (DA_D/\Delta x_D)_{1,j}$

$\phi_{1,j}$ = temperature and pressure correction, $76\ T_1/(273.15\ P)$

The value of $\alpha_{1,j}$ reflects the importance of VOC transport via permeation. The value of $\beta_{1,j}$ reflect the importance of VOC transport via diffusion. The ratio of $\alpha\phi/\beta$ provides a measure of which term is most important. A ratio value much greater than unity would indicate that VOC transport primarily occurs via permeation across the bag. A ratio value much less than unity would indicate that VOC transport via diffusion predominates. The ratio was calculated for the low-permeability Freon-113 using model parameters from Trial 2.3 and was greater than 500. This indicates that for lab-scale waste drums with no gas generation, VOC permeation out of the small polyethylene bags is much greater than diffusion through the horsetail. In the case of a punctured small bag with a hole similar in size as observed in the trials, the $\alpha\phi/\beta$ ratio was approximately six.

5.3 Effect of Parameter Values on Model Results

5.3.1 Permeable Surface Area

The effect of available permeable small bag surface area on VOC transport from small bags is shown in Figure 23. Model results demonstrate that the total bag surface area is not as important as knowledge of available permeable surface area. Use of the total bag surface area may result in an overestimation of the rate of VOC transport from a bag.

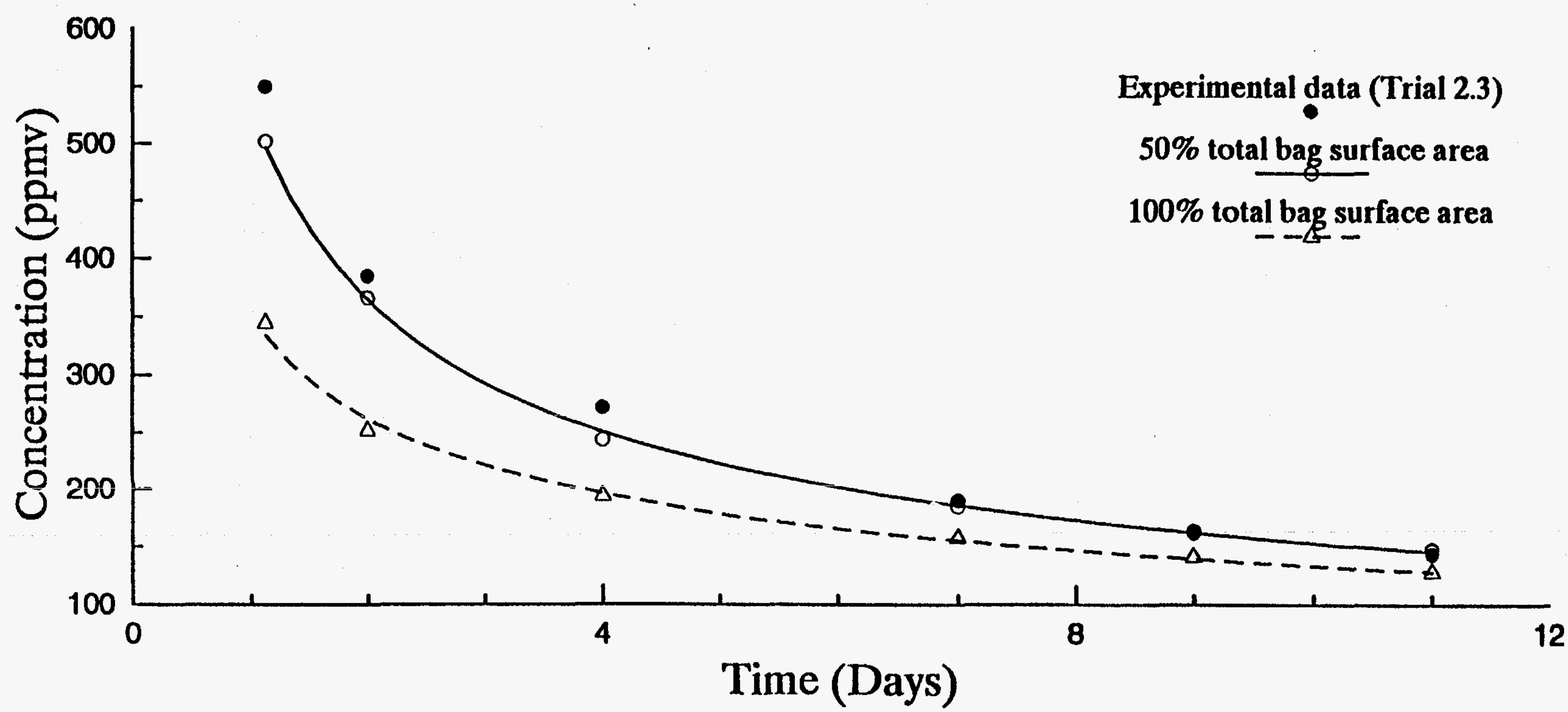

Figure 23. Predicted Freon-113 concentration in small bags as a function of available permeable small and large bag surface area.

5.3.2 Transport Length

The assumption that each void volume is a well-mixed region in which the VOC concentration is the same throughout the volume at any time is made for computational simplicity. The assumption is less appropriate when the area across which VOCs enter or exit a volume is relatively small as compared to the total void volume. This is the case for the drum liner and drum headspace void volumes. The specification of a diffusion length between two well-mixed volumes greater than actual thickness of the boundary separating the volumes is a simple means to better model VOC transport between the two volumes. The effect on the model diffusional length on the predicted VOC concentration difference between the drum liner and drum headspace void volumes is shown in Figure 24.

5.3.3 VOC Solubility in Polyethylene

The effect of neglecting VOC solubility in polyethylene on model predictions of the VOC concentration in the large bag and drum headspace void volumes is shown in Figure 25. Failure to account for any VOC solubility in polyethylene is equivalent to letting $\eta = 0$ in Equation (3). Model assumptions of VOC solubility in the polyethylene drum liner and the empirical determination of the transfer coefficient η used in Equation (3) results in a model that only approximates the general effect of VOC solubility in the drum liner on VOC concentration in the drum headspace. The nature of the experiments aggravated the significance of VOC solubility in the drum liner on experimental results. The VOC capacity of a drum liner represented a significant fraction of the total VOCs introduced initially into the waste drum.

5.3.4 Other Model Parameters

The effect of varying other model parameters was also investigated and shown to have little effect on model results. Model results did not vary significantly when the large bag void volume was decreased by 1,240 $in.^2$ (8,000 cm^2) and the drum liner void volume increased by the same amount.

Tests were performed on drum filters identical in design to those used on the lab-scale waste drums to determine if the lower VOC drum headspace concentration was the result of a higher VOC diffusion characteristic than would be predicted by Equation (17). The test cell was similar in size to a previous test apparatus.[7] Test results indicated that Equation (17) is an appropriate means of estimating the VOC diffusion characteristic across the drum filter.

5.4 Experimental and Model Refinements

A major feature of these VOC transport experiments was the transient nature of the VOC gas phase concentration as a result of having no VOC source in the waste drums. The presence of VOC-containing waste, such as a waste sludge, would replenish VOC molecules that had

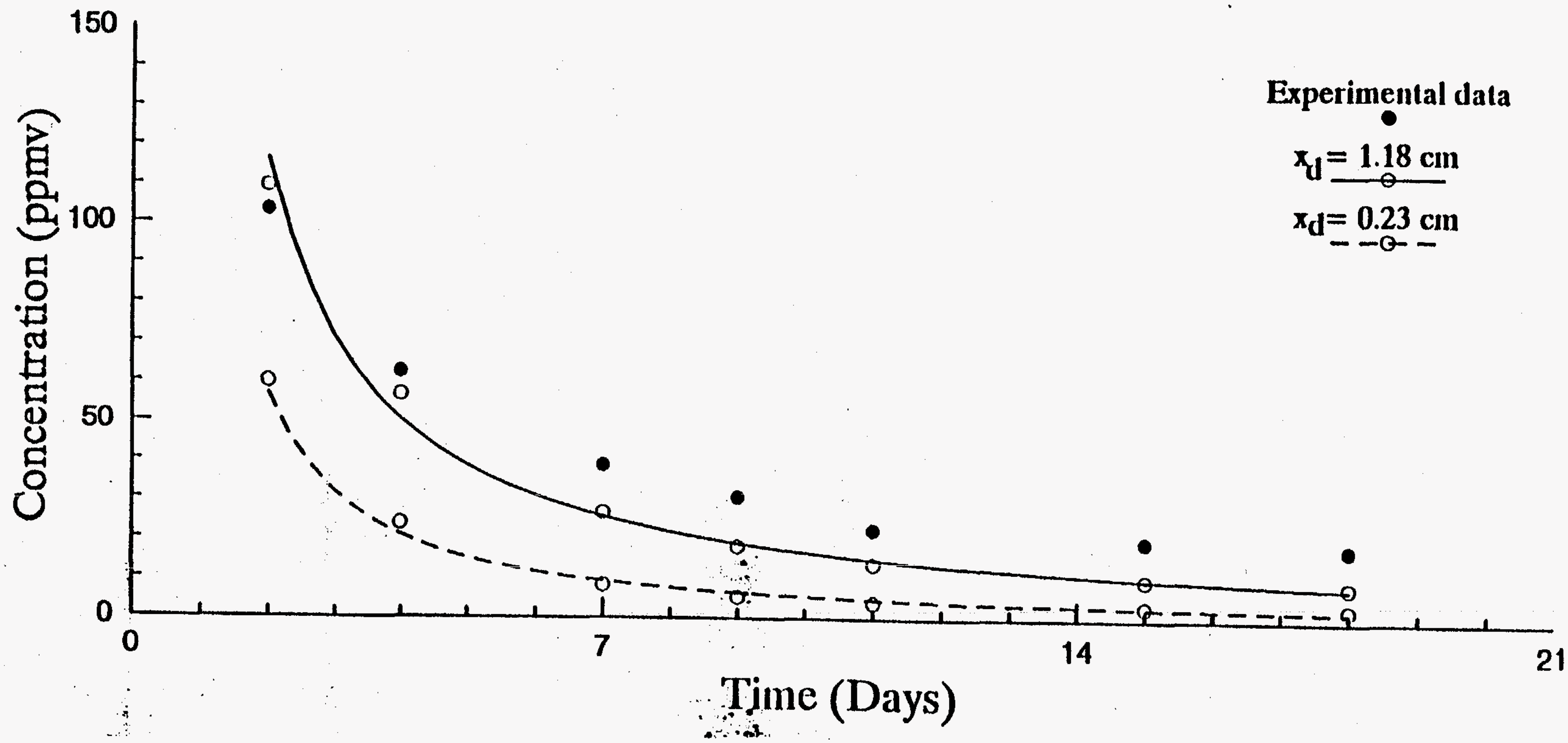

Figure 24. Predicted average TCA concentration difference between large bag and drum headspace void volumes in waste drums maintained at a constant temperature (Trial 2.3) as a function of diffusion lengths (x_d) across drum liner lid.

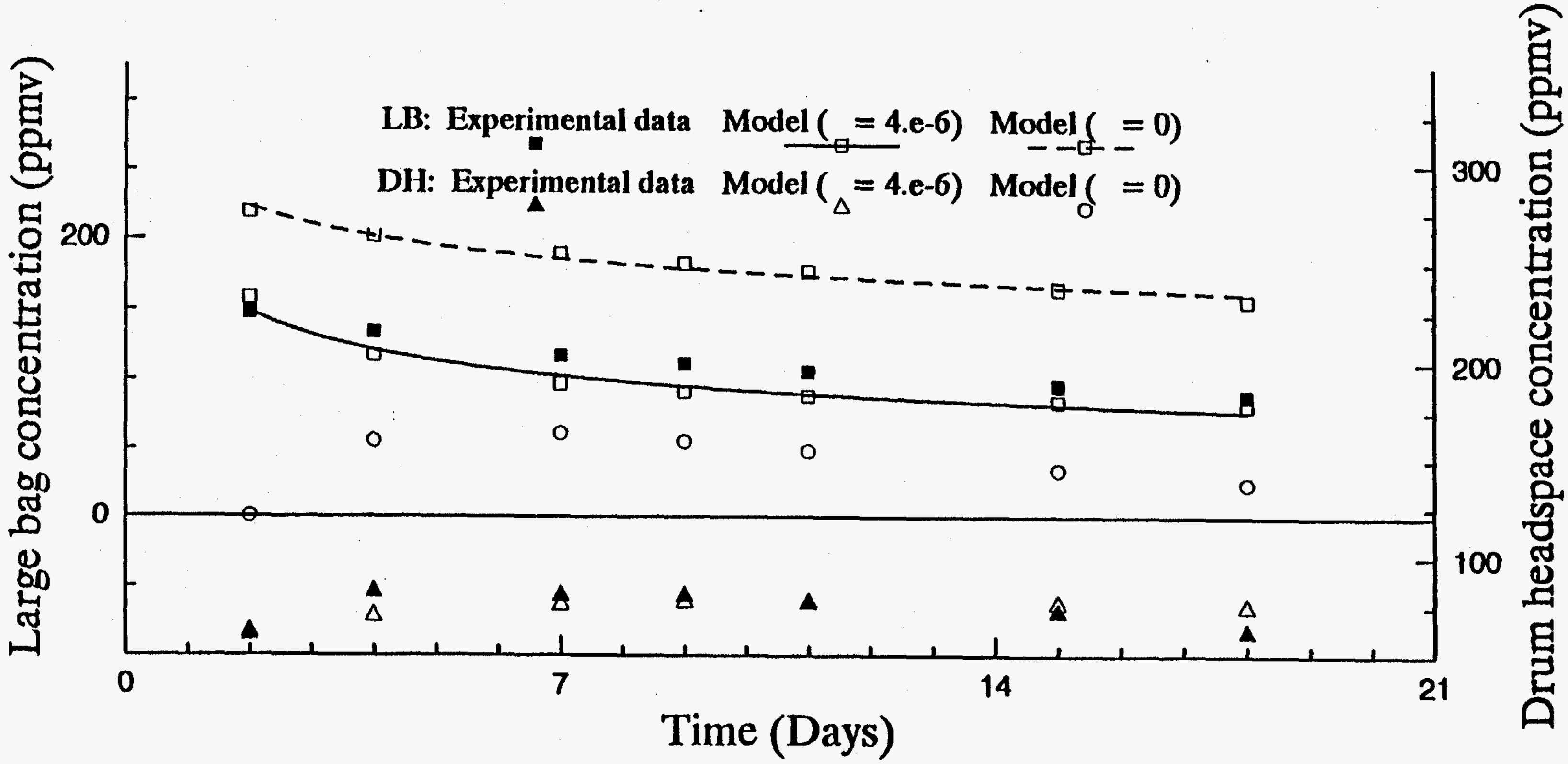

Figure 25. Comparison of experimental data (Trial 2.3) and model predictions of TCA concentration in large bags (LB) and drum headspace (DH) void volumes with and without (η = 0) VOC accumulation in polyethylene drum liner.

permeated and diffused out of the void volume. A drum containing such waste and kept in a constant-temperature environment should reach a quasi-steady state. A system at quasi-steady state appears to be at steady state over a short time period but is slowly changing with time. The transient behavior reflects the fact that as the VOC concentration in the waste slowly decreases, the VOC equilibria between the waste and surrounding gas phase also changes. The presence of a VOC source in the lab-scale waste drums would more closely simulate real waste. The effect of VOC solubility in the drum liner on the drum headspace VOC concentration should be diminished under quasi-steady state conditions.

Future work includes obtaining VOC permeability and solubility data for the components in gas mixture B and examining the capability of the VOC transport model of predicting the VOC concentration throughout the lab-scale waste drum. In addition, the rate of VOC transport out of the polymer bottles will be analyzed. Measurements of VOC permeabilities as a function of temperature and over a wider range of VOC concentrations will be made. Future simulated waste drum experiments will place VOC-contaminated simulated waste in waste drums and measure VOC concentration over a relatively long period of time. The applicability of the current model to predict the VOC concentration throughout a simulated waste drum containing VOC-contaminated waste will be investigated. Finally, a model that predicts VOC concentration throughout an actual waste drum based on process knowledge and the measured VOC concentration in the drum headspace will be developed and tested.

6. CONCLUSIONS

A VOC transport model has been developed that accurately predicts the VOC concentration in the void volumes within a simulated waste drum. The success of the model over a variety of operating conditions indicated that the model accounted for the important transport mechanisms within the waste drum and the accuracy of model parameters. Model and experimental results have demonstrated that the primary mechanisms of VOC transport from void volumes inside a waste drum were permeation and diffusion to an adjacent void volume with lower VOC concentration and solubilization into a polymer. The model estimated the effect of temperature on VOC permeability and diffusivity but did not account for increased VOC solubility at higher temperatures. Model results demonstrated the importance of knowing the available permeable surface area. Vapor permeabilities of five VOCs across polyethylene waste bags were experimentally measured. These model and experimental data will be useful in developing and testing a VOC transport model to predict VOC concentrations within actual waste drums.

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Appendix A

Measured VOC Concentrations in Lab-Scale Simulated Waste Drums

DRUM: 1.1 GAS: A TEMP: Variable SMALL BAG CLOSURE: horsetail

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC: 1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113). Initial concentration: 903 ppmv	1[a]	599.6	509.2	560.0	549.5	–	–
	2	357.6	–	309.8	–	198.8	13.1
	4	–	199.4	–	197.1	169.6	39.4
	7	–	145.3	–	144.2	128.4	40.9
	9	133.6	130.8	–	–	114.2	37.7
	11	–	113.5	–	113.5	100.8	32.2
	15	–	–	96.2	96.1	86.2	28.9
	18	83.5	–	81.7	–	72.4	25.0
	21	71.1	69.5	69.2	68.9	–	–
VOC: Methylene chloride. Initial concentration: 1012 ppmv	1[a]	207.6	204.2	203.7	202.1	–	–
	2	175.5	–	174.9	–	175.6	71.6
	4	–	138.4	–	137.6	132.1	63.1
	7	–	97.1	–	96.7	92.2	45.1
	9	88.2	87.7	–	–	83.2	40.8
	11	–	76.7	–	76.4	73.1	36.9
	15	–	–	65.8	66.0	62.8	35.3
	18	57.4	–	57.0	–	54.2	32.4
	21	51.6	51.3	51.1	50.9	–	–
VOC: 1,1,1-Trichloroethane. Initial concentration: 977 ppmv	1[a]	243.1	216.3	220.4	213.4	–	–
	2	168.1	–	166.0	–	151.9	43.7
	4	–	133.1	–	132.5	122.6	45.5
	7	–	105.1	–	104.6	95.4	42.1
	9	99.3	98.3	–	–	89.1	40.4
	11	–	88.8	–	88.6	80.4	37.7
	15	–	–	79.8	79.5	73.3	37.6
	18	71.9	–	71.5	–	65.2	35.6
	21	65.6	65.1	64.7	64.5	–	–
VOC: Carbon tetrachloride. Initial concentration: 305 ppmv	1[a]	53.5	50.3	50.1	48.8	–	–
	2	41.2	–	41.2	–	36.5	9.0
	4	–	32.3	–	32.1	28.5	9.3
	7	–	24.4	–	24.0	21.1	7.7
	9	23.0	23.0	–	–	19.6	7.3
	11	–	21.7	–	21.6	18.4	7.1
	15	–	–	18.8	18.8	16.5	7.1
	18	17.2	–	17.9	–	13.6	6.7
	21	14.4	14.5	15.9	14.2	–	–
VOC: Trichloroethylene. Initial concentration: 310 ppmv	1[a]	42.3	42.2	41.9	41.7	–	–
	2	41.0	–	40.9	–	37.5	15.0
	4	–	28.1	–	27.8	25.6	12.2
	7[b]	–	13.9	–	13.8	11.6	2.0
	9[b]	12.8	12.7	–	–	10.5	1.8
	11[b]	–	11.4	–	11.4	9.1	1.5
	15	–	–	14.0	14.1	12.6	6.9
	18	13.0	–	13.0	–	12.7	8.7
	21	12.9	12.7	12.7	12.7	–	–

Notes:
a. Sampled approximately 19 hours after filling small bags at t = 0.
b. Suspect data.

DRUM: 1.2 GAS: B TEMP: Variable SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM[a]
VOC:	1[b]	309.3	336.6	316.6	341.7	–	–
Methanol	2	217.8	221.6	–	–	181.1	20.5
	4	–	165.7	–	166.1	142.1	32.7
Initial concentration:	7	98.1[c]	–[d]	–	–	98.0	13.1
1002 ppmv	9	101.6	–	–	102.2	89.2	13.0
	11	–	81.8	81.6	–	74.1	15.0
	15	–	–	66.1	66.9	62.6	4.9
	18	48.9	–	49.2	–	47.0	3.4
	21	37.2	38.3	37.1	37.4	–	–
VOC:	1[b]	132.0	141.5	137.9	149.7	–	–
Cyclohexane	2	99.3	100.3	–	–	92.3	2.5
	4	–	82.1	–	82.4	76.6	4.6
	7	73.7[c]	–[d]	–	–	74.0	7.3
Initial concentration:	9	66.0	–	–	67.0	62.5	5.8
777 ppmv	11	–	58.6	58.3	–	54.5	8.8
	15	–	–	59.3	59.5	57.0	4.1
	18	47.2	–	47.0	–	45.1	4.3
	21	40.4	40.4	40.3	40.7	–	–
VOC:	1[b]	228.4	249.7	237.5	263.0	–	–
1,1,1-Trichloroethane	2	161.9	164.9	–	–	148.5	9.4
	4	–	135.0	–	135.3	124.7	13.6
Initial concentration:	7	112.0[c]	–[d]	–	–	111.0	10.5
1020 ppmv	9	103.2	–	–	103.9	95.9	8.4
	11	–	90.9	90.3	–	83.9	13.1
	15	–	–	87.0	87.3	82.5	3.4
	18	68.7	–	68.5	–	64.9	4.0
	21	58.1	58.3	58.0	58.7	–	–
VOC:	1[b]	36.8	36.6	36.9	37.0	–	–
Toluene	2	25.0	25.0	–	–	32.4	3.8
	4	–	19.5	–	19.6	25.5	4.0
Initial concentration:	7	23.7[c]	–[d]	–	–	29.8	10.8
	9	22.7	–	–	22.7	26.1	9.9
421 ppmv	11	–	21.6	21.7	–	24.0	10.8
	15	–	–	22.0	22.0	26.3	11.0
	18	19.1	–	19.1	–	22.4	10.5
	21	16.6	16.6	16.6	16.6	–	–
VOC:	1[b]	6.4	7.2	6.6	6.5	–	–
P-xylene	2	4.5	4.6	–	–	5.3	2.0
	4	–	4.4	–	4.5	5.1	2.2
	7	6.5[c]	–[d]	–	–	9.0	5.9
Initial concentration:	9	7.6	–	–	7.6	8.5	5.7
120 ppmv	11	–	8.4	8.1	–	12.3	7.3
	15	–	–	7.4	7.0	7.2	5.7
	18	8.3	–	7.9	–	8.1	6.6
	21	6.4	6.5	6.5	6.5	–	–

Notes:
- a. Suspect data.
- b. Sampled approximately 24 hrs after filling small bags at t = 0.
- c. 5-cc sample loop.
- d. No data detected.

DRUM: 1.3 GAS: A TEMP: Constant SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3[a]	SB4	L. BAG	DRUM
VOC:	1[b]	643.6	681.7	321.0	640.2	–	–
1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113)	2	–	519.3	–	468.9	179.2	11.8
	4	–	–	186.4	282.2	174.1	43.0
Initial concentration:	7	197.1	–	175.6	–	144.4	63.6
903 ppmv	9	171.3	–	–	163.1	138.7	64.1
	11	–	156.6	135.8	–	123.9	63.2
	15	131.9	–	123.8	–	115.2	68.5
	18	119.8	121.9	–	–	104.9	62.7
	21	109.5	111.7	104.0	108.2	–	–
VOC:	1[b]	207.9	200.0	207.7	204.4	–	–
	2	–	186.2	–	185.6	176.7	84.9
Methylene chloride	4	–	–	139.2	140.4	134.3	83.2
	7	102.5	–	107.0	–	97.8	70.3
	9	97.2	–	–	97.6	92.7	62.0
Initial concentration:	11	–	88.0	87.6	–	83.2	57.9
	15	79.2	–	78.7	–	75.8	57.0
1012 ppmv	18	71.3	71.6	–	–	68.2	51.6
	21	66.9	67.1	66.7	66.8	–	–
VOC:	1[b]	275.4	269.3	189.3	259.1	–	–
	2	–	189.7	–	186.3	161.5	53.6
1,1,1-Trichloroethane	4	–	–	142.1	143.8	131.2	67.5
	7	116.1	–	119.8	–	105.8	70.3
Initial concentration:	9	111.4	–	–	113.0	102.4	63.9
	11	–	103.7	102.7	–	91.2	60.6
977 ppmv	15	98.5	–	95.2	–	88.3	63.0
	18	88.6	89.1	–	–	81.8	58.6
	21	84.0	84.4	83.8	84.2	–	–
VOC:	1[b]	56.5	59.9	48.1	58.8	–	–
Carbon tetrachloride	2	–	45.4	–	45.3	39.2	12.1
	4	–	–	34.7	34.5	30.9	14.5
Initial concentration:	7	27.2	–	30.9	–	24.0	15.2
	9	27.1	–	–	27.6	23.3	13.3
305 ppmv	11	–	25.3	24.9	–	21.5	12.6
	15	22.7	–	22.8	–	20.1	13.2
	18	21.0	21.7	–	–	18.4	12.1
	21	19.1	19.5	19.4	19.3	–	–
VOC:	1[b]	43.7	43.9	43.4	43.7	–	–
Trichloroethylene	2	–	43.2	–	43.1	39.2	16.4
	4	–	–	29.5	29.6	27.0	17.2
	7[c]	15.1	–	17.4	–	12.9	4.9
Initial concentration:	9[c]	14.1	–	–	14.2	11.8	3.9
	11[c]	–	12.8	12.9	–	10.4	3.5
310 ppmv	15	15.3	–	15.4	–	13.7	9.0
	18	14.1	14.2	–	–	12.7	8.7
	21	14.1	14.1	14.0	14.0	–	–

Notes:
a. Small hole in bag.
b. Sampled approximately 20 hrs after filling small bags at t = 0.
c. Suspect data.

DRUM: 1.4 GAS: B TEMP: Constant SMALL BAG CLOSURE: horsetail

VOC	DAY	SB1	SB2	SB3	SB4[a]	L. BAG	DRUM
VOC:	1[b]	254.2	220.5	250.5	205.7	–	–
Methanol	2	–	169.8	176.0	–	149.1	115.6
	4	140.8	–	–	138.0	124.8	110.1
Initial concentration:	7	102.2	–	–	–[c]	102.7	89.7
1002 ppmv	9	110.7	107.6	–	–	97.4	87.8
	11	93.4	–	–	92.8	85.0	79.2
	15	–	–	87.3	86.5	82.0	75.8
	18	–	72.7	73.4	–	68.6	63.4
	21	61.7	62.2	62.5	62.0	–	–
VOC:	1[b]	111.8	97.9	106.8	89.9	–	–
Cyclohexane	2	–	76.1	77.8	–	71.4	56.4
	4	65.9	–	–	65.7	62.5	54.8
	7	69.4	–	–	–[c]	68.2	60.8
Initial concentration:	9	63.7	62.4	–	–	63.7	59.4
777 ppmv	11	56.4	–	–	56.3	53.5	49.6
	15	–	–	61.9	61.7	60.1	55.9
	18	–	52.4	52.4	–	50.9	47.7
	21	47.7	47.8	47.8	47.7	–	–
VOC:	1[b]	201.5	116.9	190.7	147.4	–	–
1,1,1-Trichloroethane	2	–	128.4	133.3	–	119.2	91.5
	4	111.5	–	–	110.5	104.9	92.2
Initial concentration:	7	106.9	–	–	–[c]	104.9	92.9
	9	100.8	98.7	–	–	93.5	84.1
1020 ppmv	11	89.7	–	–	89.2	84.6	78.3
	15	–	–	93.9	93.5	90.6	83.9
	18	–	79.7	79.7	–	76.7	71.8
	21	72.6	72.6	72.7	72.5	–	–
VOC:	1[b]	27.1	27.0	27.0	26.9	–	–
Toluene	2	–	18.1	18.1	–	24.4	16.5
	4	14.5	–	–	14.5	19.4	15.6
Initial concentration:	7	21.2	–	–	–[b]	21.0	23.1
	9	19.9	19.6	–	–	22.9	21.1
421 ppmv	11	43.8[c]	–	–	–[c]	21.4	19.9
	15	–	–	19.9	19.9	23.7	22.4
	18	–	17.6	17.6	–	20.9	20.0
	21	15.7	15.7	15.7	15.6	–	–
VOC:	1[b]	5.4	5.4	6.1	6.2	–	–
P-xylene	2	–	3.9	3.8	–	4.6	2.8
	4	3.9	–	–	3.8	4.5	3.4
	7	6.5	–	–	–[b]	7.3	6.9
Initial concentration:	9	7.2	7.2	–	–	7.7	7.2
120 ppmv	11	7.6	–	–	7.5	11.1	10.5
	15	–	–	6.7	6.6	6.8	6.8
	18	–	7.5	7.4	–	7.6	7.7
	21	6.2	6.2	6.2	6.1	–	–

Notes:

a. Small hole in bag.
b. Sampled approximately 26 hrs after filling small bags at t = 0.
c. No data detected.
d. Suspect data.

DRUM: 2.1 GAS: A TEMP: Variable SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3	SB4[a]	L. BAG	DRUM
VOC: 1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113) Initial concentration: 903 ppmv	1[b]	596.6	582.7	596.8	371.6	–	–
	2	408.3	–	417.7	–	177.1	7.5
	4	–	230.8	–	182.0	176.1	43.5
	7	–	160.5	–	148.9	142.8	46.0
	9	140.4	139.3	–	–	126.8	42.6
	11	–	123.7	–	116.8	112.9	35.5
	15	–	–	98.2	91.0	88.7	26.1
	18	81.0	–	81.3	–	73.9	24.3
	21	65.7	65.7	66.2	61.4	–	–
VOC: Methylene chloride Initial concentration: 1012 ppmv	1[b]	188.5	187.3	189.1	185.9	–	–
	2	165.7	–	165.8	–	161.8	63.5
	4	–	140.8	–	140.1	139.4	71.2
	7	–	110.4	–	109.6	108.7	56.8
	9	95.6	95.3	–	–	95.4	51.4
	11	–	85.5	–	85.3	84.4	44.8
	15	–	–	68.8	68.7	67.8	37.3
	18	58.5	–	58.5	–	57.8	35.8
	21	49.8	49.7	49.5	49.5	–	–
VOC: 1,1,1-Trichloroethane Initial concentration: 977 ppmv	1[b]	234.3	227.0	246.4	200.5	–	–
	2	168.8	–	170.4	–	153.6	48.4
	4	–	147.8	–	146.0	139.4	63.5
	7	–	121.9	–	120.4	115.3	55.7
	9	108.6	108.3	–	–	104.9	52.9
	11	–	99.7	–	98.8	95.9	47.0
	15	–	–	84.2	83.4	80.6	40.6
	18	77.4	–	77.8	–	75.8	41.0
	21	64.3	63.9	63.9	63.3	–	–
VOC: Carbon tetrachloride Initial concentration: 305 ppmv	1[b]	53.7	53.5	56.9	52.2	–	–
	2	40.4	–	40.4	–	36.6	10.8
	4	–	36.3	–	35.7	33.0	13.8
	7	–	29.8	–	29.8	27.5	12.2
	9	27.1	27.2	–	–	25.5	11.6
	11	–	25.5	–	25.5	23.4	10.1
	15	–	–	20.5	20.0	18.9	8.5
	18	19.3	–	20.1	–	18.9	8.8
	21	15.6	15.1	15.4	15.5	–	–
VOC: Trichloroethylene Initial concentration: 310 ppmv	1[b]	39.7	41.2	42.1	43.3	–	–
	2	32.2	–	32.2	–	29.6	10.9
	4	–	29.6	–	29.6	27.5	12.5
	7	–	24.4	–	24.2	22.5	11.9
	9	22.1	21.9	–	–	21.2	11.9
	11	–	20.7	–	20.6	19.8	11.2
	15	–	–	18.5	18.6	17.6	10.7
	18	18.8	–	18.8	–	18.0	11.4
	21	15.7	15.5	15.6	15.5	–	–

Notes:
a. Small hole in bag.
b. Sampled approximately 24 hrs after filling small bags at t = 0.

DRUM: 2.2 GAS: B TEMP: Variable SMALL BAG CLOSURE: horsetail

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM[a]
VOC:	1[b]	271.9	267.8	269.2	292.6	–	–
Methanol	2	204.1	202.9	–	–	171.1	24.1
	4	–	150.8	–	152.1	137.2	33.6
Initial concentration:	7	101.0	100.9	–	–	92.6	9.2
1002 ppmv	9	85.0	–	–	85.1	79.8	17.8
	11	–	73.8	71.3	–	69.9	8.1
	15	–	–	53.6	54.0	52.5	9.9
	18	42.8	–	42.7	–	42.7	19.4
	21	33.4	33.2	33.3	33.4	–	–
VOC:	1[b]	129.6	132.1	136.3	143.7	–	–
Cyclohexane	2	94.4	92.9	–	–	85.5	1.8
	4	–	80.7	–	81.4	79.0	8.9
	7	68.6	68.6	–	–	67.3	-4.2
	9	56.7	–	–	57.0	56.9	3.3
Initial concentration:	11	–	50.0	49.4	–	48.3	-3.6
777 ppmv	15	–	–	41.0	42.3	40.1	-1.1
	18	39.0	–	40.4	–	39.7	10.3
	21	27.8	27.7	27.7	27.7	–	–
VOC:	1[b]	222.9	222.5	228.4	247.7	–	–
1,1,1-Trichloroethane	2	155.7	154.5	–	–	139.8	8.7
	4	–	131.4	–	132.8	128.2	20.8
	7	112.3	111.9	–	–	109.3	1.6
Initial concentration:	9	94.2	–	–	94.6	93.5	12.2
1020 ppmv	11	–	82.2	80.8	–	80.9	1.2
	15	–	–	67.4	68.9	66.1	5.0
	18	61.4	–	62.8	–	61.9	19.5
	21	47.2	47.1	47.0	47.2	–	–
VOC:	1[b]	40.3	41.9	42.6	41.7	–	–
Toluene	2	27.9	26.4	–	–	33.0	5.0
	4	–	23.6	–	23.7	31.1	6.7
Initial concentration:	7	18.6	18.6	–	–	24.8	4.5
	9	15.3	–	–	15.3	20.9	5.3
421 ppmv	11	–	15.8	16.3	–	20.5	4.2
	15	–	–	13.8	14.6	17.8	4.9
	18	15.4	–	15.7	–	21.0	10.3
	21	10.0	9.9	10.0	9.9	–	–
VOC:	1[b]	9.3	9.8	9.9	9.7	–	–
P-xylene	2	6.2	5.9	–	–	6.5	3.2
	4	–	6.0	–	5.9	6.8	3.8
	7	5.2	5.1	–	–	6.0	3.6
Initial concentration:	9	4.6	–	–	4.4	5.0	3.1
	11	5.0	–	–	5.1	5.5	4.3
120 ppmv	15	–	–	4.9	4.9	4.7	3.3
	18	5.8	–	5.7	–	6.2	4.2
	21	3.9	3.9	4.0	4.0	–	–

Notes:
a. Suspect data (faulty sample line).
b. Sampled 25 hrs after filling small bags at t = 0.

DRUM: 2.3 GAS: A TEMP: Constant SMALL BAG CLOSURE: horsetail

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC: 1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113)	1[a]	582.0	506.8	570.0	537.3	–	–
	2	–	365.3	–	403.0	171.7	10.3
Initial concentration:	4	–	–	287.6	256.0	176.7	51.1
	7	189.7	–	190.0	–	152.4	73.2
903 ppmv	9	164.8	–	–	158.1	143.2	79.0
	11	–	143.5	–[b]	–	133.7	78.3
	15	125.7	–	90.9[c]	–	117.0	73.0
	18	112.8	111.2	–	–	104.6	57.0
	21	100.0	98.7	101.2	99.9	–	–
VOC:	1[a]	176.7	174.8	176.7	175.5	–	–
Methylene chloride	2	–	159.1	–	160.0	157.5	85.5
	4	–	–	138.9	139.0	138.0	96.9
	7	115.8	–	116.1	–	114.9	86.1
	9	106.8	–	–	107.2	106.9	82.2
Initial concentration:	11	–	110.6	–[b]	–	99.6	76.9
	15	87.7	–	67.4[c]	–	87.3	68.8
1012 ppmv	18	78.0	77.9	–	–	72.1	57.3
	21	69.4	69.8	70.0	69.8	–	–
VOC:	1[a]	213.5	191.6	208.9	200.3	–	–
1,1,1-Trichloroethane	2	–	160.0	–	162.2	147.8	59.7
	4	–	–	141.3	141.3	133.8	81.9
	7	121.6	–	121.9	–	116.6	80.0
Initial concentration:	9	114.6	–	–	114.7	111.1	79.9
	11	–	109.3	–[b]	–	105.8	76.7
977 ppmv	15	98.8	–	75.8[c]	–	95.9	71.6
	18	90.3	90.2	–	–	88.7	61.7
	21	82.2	82.3	82.4	82.3	–	–
VOC:	1[a]	47.2	45.1	46.9	45.8	–	–
Carbon tetrachloride	2	–	38.1	–	38.4	34.8	13.9
	4	–	–	34.2	33.7	31.3	18.0
Initial concentration:	7	28.9	–	29.9	–	26.3	17.9
	9	28.3	–	–	28.3	26.6	18.1
305 ppmv	11	–	27.0	–[b]	–	25.0	17.6
	15	23.4	–	17.6[c]	–	22.1	15.7
	18	22.0	21.8	–	–	20.8	13.7
	21	19.3	19.6	19.5	19.6	–	–
VOC:	1[a]	33.7	33.7	34.0	33.7	–	–
Trichloroethylene	2	–	30.9	–	30.8	28.7	13.1
	4	–	–	27.2	27.3	25.6	14.0
	7	23.2	–	23.2	–	21.8	14.0
Initial concentration:	9	21.7	–	–	21.8	20.9	14.4
	11	–	20.8	–[b]	–	19.9	14.1
310 ppmv	15	19.2	–	15.6[c]	–	18.1	13.4
	18	17.4	17.4	–	–	16.7	12.6
	21	16.1	16.1	16.1	16.1	–	–

Notes:
a. Sampled approximately 27 hrs after filling small bags at t = 0.
b. No data detected.
c. Suspect data.

DRUM: 2.4 GAS: B TEMP: Constant SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC: Methanol	1[a]	281.9	289.0	287.6	274.4	–	–
	2	–	207.9	209.3	–	173.2	92.5
Initial concentration:	4	139.8	–	–	140.9	125.2	92.8
1002 ppmv	7	111.1	–	–	111.5	104.3	86.5
	9	103.7	104.1	–	–	98.0	85.6
	11	96.7	–	–	96.6	92.9	83.7
	15	–	–	82.1	59.5[b]	80.5	72.3
	18	–	74.2	74.9	–	72.8	64.9
	21	65.7	66.0	66.3	67.0	–	–
VOC: Cyclohexane	1[a]	130.7	129.1	131.3	122.7	–	–
	2	–	105.2	106.2	–	97.6	46.6
Initial concentration:	4	78.0	–	–	77.9	75.9	51.7
777 ppmv	7	76.9	–	–	76.9	76.1	60.9
	9	68.1	68.0	–	–	68.8	57.2
	11	61.5	–	–	60.9	60.5	51.2
	15	–	–	55.0	37.0[b]	55.2	47.0
	18	–	48.8	48.9	–	49.8	42.1
	21	44.6	44.6	44.8	44.7	–	–
VOC: 1,1,1-Trichloroethane	1[a]	234.7	235.6	236.9	220.7	–	–
	2	–	175.8	177.0	–	155.6	71.9
Initial concentration:	4	126.8	–	–	126.4	122.1	84.4
1020 ppmv	7	124.5	–	–	124.6	122.6	100.3
	9	112.1	112.1	–	–	112.4	95.4
	11	101.5	–	–	100.7	101.4	87.2
	15	–	–	91.6	64.2[b]	91.5	79.1
	18	–	82.9	83.0	–	83.7	71.8
	21	76.1	76.0	76.2	76.2	–	–
VOC: Toluene	1[a]	31.6	31.2	31.4	31.1	–	–
	2	–	28.5	28.6	–	37.4	15.4
Initial concentration:	4	21.9	–	–	21.8	29.3	14.1
421 ppmv	7	18.6	–	–	18.5	25.3	16.2
	9	15.6	15.6	–	–	21.6	14.7
	11	15.2	–	–	15.2	21.2	15.4
	15	–	–	13.3	9.9[b]	18.5	14.2
	18	–	11.8	11.8	–	16.5	13.1
	21	10.4	10.4	10.4	10.4	–	–
VOC: P-xylene	1[a]	7.0	6.9	6.9	6.9	–	–
	2	–	6.2	6.2	–	7.2	3.9
Initial concentration:	4	5.8	–	–	5.7	6.8	5.6
120 ppmv	7	5.1	–	–	5.1	6.0	4.2
	9	4.5	4.5	–	–	5.1	3.7
	11	5.0	–	–	5.1	5.5	4.3
	15	–	–	4.6	4.1	5.1	4.1
	18	–	4.6	4.6	–	4.8	4.2
	21	4.0	4.0	4.0	4.0	–	–

Notes:
a. Sampled approximately 27 hrs after filling small bag at t = 0.
b. Suspect data.

DRUM: 3.1 GAS: A TEMP: Variable SMALL BAG CLOSURE: horsetail

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC:	1[a]	481.2	540.3	562.1	567.0	–	–
1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113)	2	178.2	–	181.6	–	172.0	26.5
	6	–	155.9	–	154.9	144.3	28.4
Initial concentration:	8	–	134.5	–	133.8	125.4	27.4
903 ppmv	11	110.4	112.0	–	–	104.0	18.2
	13	–	96.7	–	96.6	91.4	18.7
	15	–	–	85.9	–[b]	79.5	13.0
	18	69.6	–	70.7	–	65.7	8.3
	21	56.7	57.4	58.8	57.5	–	–
VOC:	1[a]	188.8	188.1	188.5	188.3	–	–
	4	145.1	–	144.8	–	145.0	47.3
Methylene chloride	6	–	112.2	–	112.3	111.2	41.2
	8	–	94.8	–	94.7	93.6	37.4
	11	77.8	78.2	–	–	77.0	31.7
Initial concentration:	13	–	70.4	–	70.6	70.3	31.6
1012 ppmv	15	–	–	61.4	–[b]	60.7	26.4
	18	53.4	–	53.0	–	52.7	23.1
	21	46.8	46.4	46.5	46.5	–	–
VOC:	1[a]	206.4	212.4	221.5	225.0	–	–
	4	154.3	–	153.2	–	149.6	41.9
1,1,1-Trichloroethane	6	–	117.8	–	117.3	113.2	38.1
	8	–	104.3	–	104.2	100.7	37.0
Initial concentration:	11[c]	90.5	91.7	–	–	87.9	32.6
	13	–	90.1	–	91.2	89.1	35.6
977 ppmv	15	–	–	78.3	–[b]	76.1	29.0
	18	66.7	–	67.1	–	65.0	25.4
	21	59.1	59.2	58.8	70.7	–	–
VOC:	1[a]	48.9	46.2	47.2	47.9	–	–
	4	36.7	–	35.5	–	34.3	7.1
Carbon tetrachloride	6	–	26.5	–	26.3	25.5	6.5
	8	–	23.0	–	23.4	21.9	6.3
Initial concentration:	11[c]	20.7	20.8	–	–	19.6	5.2
305 ppmv	13	–	20.1	–	20.9	19.6	5.4
	15	–	–	17.2	–[b]	16.6	4.2
	18	16.1	–	13.9	–	13.4	3.3
	21	12.5	13.2	12.5	12.5	–	–
VOC:	1[a]	37.2	36.0	37.0	37.1	–	–
	4	33.7	–	33.6	–	32.1	10.4
Trichloroethylene	6	–	21.7	–	21.7	20.8	8.3
	8	–	19.5	–	19.6	18.7	8.2
Initial concentration:	11[c]	17.6	18.1	–	–	16.8	8.1
	13	–	20.2	–	20.3	19.7	9.9
310 ppmv	15	–	–	17.0	–[b]	16.3	8.0
	18	14.6	–	14.8	–	14.1	7.4
	21	13.9	13.8	13.8	13.7	–	–

Notes:
a. Sampled approximately 21 hrs after filling small bags at t = 0.
b. No data detected.
c. Suspect data.

DRUM: 3.2 GAS: B TEMP: Variable SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC:	1[a]	315.6	286.0	274.5	303.3	–	–
Methanol	4	154.5	148.6	–	–	144.3	80.7
	6	–	127.9	–	127.9	119.6	69.3
Initial concentration:	8	107.0	106.6	–	–	100.7	64.8
987 ppmv	11	89.3	–	–	87.5	85.4	61.9
	13	–	73.4	55.6[b]	–	72.7	60.5
	15	–	–	63.9	–[c]	65.9	52.5
	18	59.0	–	58.9	–	58.1	35.6
	21	51.1	51.0	50.9	51.0	–	–
VOC:	1[a]	151.4	125.1	125.0	137.6	–	–
Cyclohexane	4	96.4	94.2	–	–	96.4	43.6
	6	–	76.0	–	75.9	75.3	36.7
	8	68.4	68.1	–	–	67.9	35.7
	11	62.5	–	–	62.8	63.0	32.3
Initial concentration:	13	–	55.4	38.1[b]	–	58.7	33.2
787 ppmv	15	–	–	48.3	–[c]	51.1	27.5
	18	40.7	–	40.9	–	40.8	15.1
	21	36.6	36.4	36.5	36.6	–	–
VOC:	1[a]	269.0	221.0	218.0	244.0	–	–
1,1,1-Trichloroethane	4	143.0	139.3	–	–	141.9	63.7
	6	–	116.1	–	116.0	114.1	54.5
	8	104.0	103.4	–	–	102.2	52.9
Initial concentration:	11	90.8	–	–	90.8	91.0	47.0
	13	–	78.5	53.4[b]	–	82.3	46.6
1054 ppmv	15	–	–	68.3	–[c]	71.7	38.5
	18	59.6	–	59.7	–	59.1	24.4
	21	52.7	52.3	52.4	52.5	–	–
VOC:	1[a]	34.4	33.8	33.8	34.2	–	–
Toluene	4	26.5	26.1	–	–	37.4	15.5
	6	–	18.2	–	18.3	26.0	11.1
Initial concentration:	8	16.1	16.1	–	–	23.1	10.8
	11	18.3	–	–	18.6	26.0	12.5
425 ppmv	13	–	17.1	12.1[b]	–	25.2	15.4
	15	–	–	15.3	–[c]	22.6	13.2
	18	11.4	–	11.7	–	16.4	4.2
	21	11.1	11.0	11.0	11.1	–	–
VOC:	1[a]	12.3	12.2	12.2	12.3	–	–
P-xylene	4	10.4	10.5	–	–	11.6	8.7
	6	–	10.8	–	9.6	10.6	8.9
	8	8.7	8.6	–	–	9.3	7.8
Initial concentration:	11	10.9	–	–	11.0	11.9	9.7
	13	–	16.1[b]	10.2[b]	–	9.2	9.0
99.2 ppmv	15	–	–	10.0	–[c]	10.5	9.1
	18	9.6	–	9.5	–	9.9	8.5
	21	9.9	9.9	9.9	9.9	–	–

Notes:
a. Sampled approximately 21 hrs after small bags filled at t = 0.
b. Suspect data.
c. No data detected.

DRUM: 3.3 GAS: B TEMP: Constant SMALL BAG CLOSURE: horsetail

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC:	1[a]	220.0	261.7	281.2	285.3	–	–
Methanol	4	–	143.8	–	125.0	131.2	45.2
	6	–	–	121.8	121.6	112.7	44.5
Initial concentration:	8	102.4	–	104.2	–	96.3	50.3
987 ppmv	11	88.6	–	–	88.7	82.9	36.5[b]
	13	–	80.4	–[c]	–	74.2	37.1[b]
	15	72.1	–	73.9	–	68.7	37.5
	18	68.4	67.6	–	–	62.8	–[c]
	21	61.9	62.2	63.4	61.3	–	–
VOC:	1[a]	99.6	118.2	120.2	122.1	–	–
	4	–	79.1	–	66.5	78.9	16.0
Cyclohexane	6	–	–	72.7	71.5	73.1	16.9
	8	66.9	–	67.0	–	67.8	23.7
	11	56.0	–	–	56.0	56.7	9.7[b]
Initial concentration:	13	–	52.0	–[c]	–	53.3	12.2[b]
787 ppmv	15	47.9	–	49.3	–	48.6	13.3
	18	46.0	46.0	–	–	46.9	–[c]
	21	43.5	43.8	43.6	43.6	–	–
VOC:	1[a]	158.5	204.8	213.5	216.9	–	–
	4	–	126.7	–	106.6	126.1	25.0
1,1,1-Trichloroethane	6	–	–	115.9	114.0	115.3	26.6
	8	106.6	–	107.0	–	107.2	38.3
Initial concentration:	11	90.1	–	–	90.2	90.4	14.8[b]
	13	–	83.7	–[c]	–	84.6	19.0[b]
1054 ppmv	15	77.3	–	79.7	–	77.6	21.0
	18	74.4	74.7	–	–	75.2	–[c]
	21	70.8	70.6	70.7	70.4	–	–
VOC:	1[a]	26.9	27.0	26.8	26.7	–	–
Toluene	4	–	17.8	–	15.2	25.0	3.4
	6	–	–	16.2	16.0	22.9	3.9
	8	14.3	–	14.3	–	20.4	4.9
Initial concentration:	11	11.9	–	–	11.9	16.8	3.4[b]
425 ppmv	13	–	10.5	–[c]	–	15.0	3.4[b]
	15	9.7	–	10.0	–	14.2	3.8
	18	9.3	9.3	–	–	13.5	–[c]
	21	8.9	9.0	8.9	9.0	–	–
VOC:	1[a]	11.3	11.4	11.3	11.3	–	–
	4	–	9.2	–	8.9	9.9	7.5
P-xylene	6	–	–	9.5	9.4	10.0	7.9
	8	8.4	–	8.4	–	8.9	7.3
Initial concentration:	11	9.9	–	–	9.8	10.3	8.7[b]
	13	–	12.3	–[c]	–	8.0	8.4[b]
99.2 ppmv	15	8.9	–	8.8	–	9.2	7.9
	18	9.4	9.3	–	–	9.7	–[c]
	21	9.6	9.7	9.7	9.6	–	–

Notes:
a. Sampled approximately 21 hrs after filling small bags at t = 0.
b. Suspect data.
c. No data detected.

DRUM: 3.4 GAS: A TEMP: Constant SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3[a]	SB4	L. BAG	DRUM
VOC: 1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113)	1[b]	610.0	637.3	57.1	619.9	–	–
	4	–	281.1	129.5	–	72.3	16.9
Initial concentration:	6	189.8	–	152.5	–	87.3	36.6
903 ppmv	8	150.4	–	–	152.5	92.1	52.8
	11	121.7	124.3	–	–	87.0	54.1
	13	107.9	–	–	–[c]	89.0	56.6
	15	–	–	84.0	100.1	79.4	53.4
	18	–	93.7	74.7	–	76.0	55.1
	21	85.1	85.6	57.3	85.3	–	–
VOC: Methylene chloride	1[b]	150.1	153.1	144.5	149.8	–	–
	4	–	111.7	100.9	–	108.0	66.6
	6	63.8	–	78.3	–	94.6	64.6
	8	85.5	–	–	85.3	84.1	62.9
Initial concentration:	11	75.5	75.4	–	–	73.7	55.5
1012 ppmv	13	70.2	–	–	–[c]	68.9	53.7
	15	–	–	61.0	64.7	63.5	49.5
	18	–	61.1	54.2	–	59.7	48.2
	21	56.2	56.4	44.2	56.2	–	–
VOC: 1,1,1-Trichloroethane	1[b]	205.1	231.1	141.1	209.4	–	–
	4	–	120.2	117.4	–	108.9	57.2
	6	106.1	–	85.8	–	98.6	60.7
	8	97.1	–	–	97.2	91.7	63.7
Initial concentration:	11	88.7	88.9	–	–	83.9	59.9
977 ppmv	13	84.1	–	–	–[c]	80.5	60.1
	15	–	–	73.7	78.9	75.0	55.8
	18	–	75.6	67.3	–	72.3	55.9
	21	70.7	70.6	55.4	70.7	–	–
VOC: Carbon tetrachloride	1[b]	39.9	44.7	33.5	40.9	–	–
	4	–	25.9	25.5	–	23.1	9.9
	6	23.1	–	18.7	–	21.4	11.2
Initial concentration:	8	20.8	–	–	21.0	18.9	11.4
305 ppmv	11	18.7	18.9	–	–	17.1	10.4
	13	17.3	–	–	–[c]	15.1	10.1
	15	–	–	15.2	16.3	14.1	9.6
	18	–	14.7	13.2	–	13.9	9.3
	21	13.8	13.6	10.3	13.9	–	–
VOC: Trichloroethylene	1[b]	29.3	29.4	28.9	29.3	–	–
	4	–	22.3	22.2	–	21.1	9.0
	6	18.5	–	15.4	–	17.5	8.7
	8	16.7	–	–	16.7	16.1	9.0
Initial concentration:	11	14.9	14.9	–	–	14.3	9.3
310 ppmv	13	14.4	–	–	–[c]	13.8	9.4
	15	–	–	12.5	13.0	12.4	8.7
	18	–	12.7	11.6	–	12.1	8.9
	21	11.8	11.8	10.0	11.8	–	–

Notes:
- a. Bag not initially filled with gas mixture.
- b. Sampled approximately 23 hrs after filling small bags at t = 0.
- c. No data detected.

DRUM: 4.1 GAS: A TEMP: Variable SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC: 1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113). Initial concentration: 1010 ppmv	1[a]	863.4	863.5	827.3	744.7	–	–
	2	596.0	–	552.4	–	275.4	77.3
	4	–	383.6	–	314.7	281.3	76.0
	7	–	291.3	–	272.4	253.3	81.9
	9	263.2	264.3	–	–	240.0	78.4
	11	–	244.1	–	236.2	220.7	74.4
	15	–	–	209.2	205.2	191.7	76.0
	18	192.7	–	189.3	–	178.5	71.5
	21	176.9	176.9	175.8	173.7	–	–
VOC: Methylene chloride. Initial concentration: 1010 ppmv	1[a]	181.1	179.4	173.6	172.7	–	–
	2	150.3	–	149.0	–	139.2	12.5[b]
	4	–	121.4	–	121.8	112.4	19.5[b]
	7	–	91.9	–	91.9	84.9	3.7[b]
	9	78.1	77.5	–	–	73.5	–[c]
	11	–	66.1	–	65.7	60.7	–[c]
	15	–	–	49.1	48.7	44.7	–[c]
	18	40.0	–	38.8	–	37.1	–[c]
	21	29.8	29.6	29.5	29.8	–	–
VOC: 1,1,1-Trichloroethane. Initial concentration: 1020 ppmv	1[a]	292.2	288.6	254.2	230.8	–	–
	2	169.5	–	164.1	–	142.0	–[c]
	4	–	138.4	–	139.9	121.5	–[c]
	7	–	114.3	–	111.9	100.4	–[c]
	9	101.9	101.2	–	–	93.1	–[c]
	11	–	9.8	–	90.8	82.3	–[c]
	15	–	–	75.2	74.7	67.5	–[c]
	18	71.2	–	70.3	–	66.2	–[c]
	21	58.7	58.9	59.5	61.4	–	–
VOC: Carbon tetrachloride. Initial concentration: 301 ppmv	1[a]	64.3	64.7	58.7	58.7	–	–
	2	45.8	–	45.8	–	38.4	–[c]
	4	–	38.7	–	39.8	32.9	–[c]
	7	–	33.7	–	33.5	28.5	–[c]
	9	30.3	29.4	–	–	27.5	–[c]
	11	–	28.1	–	28.4	24.9	–[c]
	15	–	–	23.4	24.0	21.1	–[c]
	18	21.5	–	21.8	–	20.2	–[c]
	21	20.4	20.6	20.5	21.2	–	–
VOC: Trichloroethylene. Initial concentration: 297 ppmv	1[a]	39.1	40.2	41.6	44.2	–	–
	2	34.8	–	34.7	–	30.9	6.0
	4	–	29.4	–	31.1	25.8	5.1
	7	–	24.6	–	24.7	22.1	5.5
	9	22.1	22.0	–	–	20.5	5.1
	11	–	20.7	–	20.7	18.8	4.7
	15	–	–	18.5	18.5	17.0	5.3
	18	20.2	–	20.2	–	18.9	5.2
	21	17.0	17.3	17.7	18.2	–	–

Notes:
a. Sampled approximately 23 hrs after filling small bags at t = 0.
b. Suspect data.
c. No data detected.

DRUM: 4.2 GAS: B TEMP: Variable SMALL BAG CLOSURE: horsetail

	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC:	1[a]	159.8	166.0	170.7	165.6	–	–
Methanol	2	135.8	137.7	–	–	117.0	67.6
	4	–	110.2	–	109.8	98.3	74.0
Initial concentration:	6	87.3	89.5	–	–	82.7	–
764 ppmv	9	76.8	–	–	75.8	71.9	58.6
	11	–	68.5	68.8	–	66.5	53.4
	15	–	–	57.0	57.2	54.5	45.0
	18	51.4	–	51.3	–	49.9	–
	21	46.2	46.2	46.2	45.8	–	–
VOC:	1[a]	149.8	154.7	161.5	155.5	–	–
	2	87.8	88.2	–	–	79.0	22.0
Cyclohexane	4	–	83.4	–	84.0	77.4	36.5
	7	63.5	63.9	–	–	59.3	–
	9	64.2	–	–	64.4	61.2	32.7
Initial concentration:	11	–	52.4	52.6	–	49.4	28.0
746 ppmv	15	–	–	41.9	41.7	39.3	22.4
	18	45.1	–	45.2	–	43.6	–
	21	37.9	38.1	37.6	37.9	–	–
VOC:	1[a]	308.9	305.2	269.1	244.7	–	–
	2	147.8	148.5	–	–	132.4	39.5
1,1,1-Trichloroethane	4	–	134.2	–	134.8	124.6	64.3
	7	106.0	106.4	–	–	98.8	#
Initial concentration:	9	102.8	–	–	102.9	98.4	57.4
	11	–	87.8	88.2	–	82.4	49.3
980 ppmv	15	–	–	70.9	70.6	66.4	39.6
	18	70.9	–	71.1	–	68.4	#
	21	60.4	60.7	60.3	60.5	–	–
VOC:	1[a]	28.6	29.5	30.0	30.7	–	–
	2	9.1[b]	9.2[b]	–	–	15.0[b]	–[c]
Toluene	4	–	12.2	–	12.8	19.2	–[c]
	7	3.2	3.2	–	–	9.0	–[c]
Initial concentration:	9	6.2	–	–	6.5	12.6	–[c]
398 ppmv	11	–	0.7	0.7	–	6.2	–[c]
	15	–	–	<0[b]	<0[b]	3.7	–[c]
	18	3.7	–	7.0	–	9.5	–[c]
	21	–[c]	–[c]	–[c]	–[c]	–	–
VOC:	1[a]	–[c]	–[c]	–[c]	–[c]	–	–
	2	–[c]	–[c]	–	–	–[c]	–[c]
P-xylene	4	–	–[c]	–	–[c]	–[c]	–[c]
	7	–[c]	–[c]	–	–	–[c]	–[c]
Initial concentration:	9	–[c]	–	–	–[c]	–[c]	–[c]
	11	–	–[c]	–[c]	–	–[c]	–[c]
99 ppmv	15	–	–	–[c]	–[c]	–[c]	–[c]
	18	–[c]	–	–[c]	–	–[c]	–[c]
	21	–[c]	–[c]	–[c]	–[c]	–	–

Notes:
a. Sampled approximately 23 hrs after filling small bags at t = 0.
b. Suspect data.
c. No data detected.

DRUM: 4.3 GAS: A TEMP: Constant SMALL BAG CLOSURE: horsetail

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113)	1[a]	705.6	705.4	747.7	738.5	–	–
	2	–	547.1	–	581.3	264.6	91.0
Initial concentration:	4	–	–	392.1	370.8	274.8	108.1
	7	303.2	–	315.5	–	254.6	111.8
1010 ppmv	9	272.9	–	–	271.3	241.1	130.5
	11	–	252.8	258.9	–	230.5	118.5
	15	228.8	–	230.8	–	209.5	107.6
	18	212.9	211.9	–	–	197.8	96.8
	21	202.2	201.7	203.6	201.8	–	–
VOC:	1[a]	144.2	143.6	146.9	143.9	–	–
Methylene chloride	2	–	121.5	–	122.0	114.2	25.9
	4	–	–	101.0	100.9	95.1	21.4
	7	82.0	–	82.4	–	76.3	10.0[b]
	9	71.6	–	–	71.6	66.4	17.5
Initial concentration:	11	–	63.7	63.9	–	59.1	8.2[b]
1010 ppmv	15	51.4	–	51.6	–	48.0	3.1[b]
	18	43.5	43.2	–	–	40.0	–[c]
	21	36.0	36.2	36.0	36.0	–	–
VOC:	1[a]	207.2	195.5	227.7	211.8	–	–
1,1,1-Trichloroethane	2	–	144.1	–	148.5	121.0	26.0
	4	–	–	117.1	116.1	103.3	30.3
	7	102.7	–	103.1	–	92.8	22.8[b]
Initial concentration:	9	92.4	–	–	92.5	83.7	30.9
1020 ppmv	11	–	87.2	87.1	–	78.9	22.7
	15	76.5	–	77.0	–	69.4	17.7
	18	70.6	70.5	–	–	64.6	11.2
	21	63.0	63.1	62.9	63.4	–	–
VOC:	1[a]	48.0	46.7	51.9	49.8	–	–
Carbon tetrachloride	2	–	39.2	–	39.0	32.5	11.0
	4	–	–	31.9	32.0	27.4	10.7
Initial concentration:	7	30.4	–	29.4	–	26.3	9.2
	9	26.2	–	–	26.0	22.8	11.1
301 ppmv	11	–	25.9	24.3	–	22.0	8.9
	15	22.2	–	21.1	–	19.5	7.7
	18	19.4	19.7	–	–	17.7	5.7
	21	18.6	18.6	18.7	18.6	–	–
VOC:	1[a]	31.1	31.1	31.1	31.0	–	–
Trichloroethylene	2	–	27.2	–	27.2	24.4	10.4
	4	–	–	21.9	21.9	19.8	10.1
	7	19.0	–	19.1	–	17.4	8.7
Initial concentration:	9	16.9	–	–	16.8	15.4	9.3
297 ppmv	11	–	15.9	15.9	–	14.6	8.1
	15	14.3	–	14.4	–	13.3	7.3
	18	13.6	13.6	–	–	12.6	6.8
	21	12.5	12.6	12.5	12.6	–	–

Notes:
a. Sampled approximately 25 hrs after filling small bags at t = 0.
b. Suspect data.
c. No data detected.

DRUM: 4.4 GAS: B TEMP: Constant SMALL BAG CLOSURE: heat seal

VOC	DAY	SB1	SB2	SB3	SB4	L. BAG	DRUM
VOC:	1[a]	161.5	169.5	162.7	170.5	–	–
Methanol	2	–	142.6	141.0	–	103.6	56.3
	4	113.1	–	–	113.7	89.8	58.8
Initial concentration:	7	89.2	–	–	93.9	78.1	59.2
764 ppmv	9	75.5	76.2	–	–	65.7	51.0
	11	67.5	–	–	68.8	61.9	49.3
	15	–	–	54.9	55.4	49.7	40.8
	18	–	49.2	49.3	–	44.8	36.6
	21	43.7	43.7	43.6	44.0	–	–
VOC:	1[a]	138.9	126.6	136.2	124.7	–	–
Cyclohexane	2	–	102.6	99.4	–	81.5	16.7
	4	85.5	–	–	85.7	73.5	25.8
	7	72.6	–	–	75.0	64.8	29.3
	9	65.6	65.7	–	–	58.6	27.5
Initial concentration:	11	59.4	–	–	59.5	53.6	27.9
746 ppmv	15	–	–	45.6	45.7	41.3	18.4
	18	–	41.1	41.1	–	36.9	14.2
	21	33.5	34.0	33.8	34.1	–	–
VOC:	1[a]	234.6	242.9	254.3	243.9	–	–
1,1,1-Trichloroethane	2	–	175.4	167.8	–	130.2	31.6
	4	142.1	–	–	142.7	119.5	47.3
	7	120.2	–	–	124.6	105.6	52.9
Initial concentration:	9	108.3	108.4	–	–	98.2	49.5
	11	98.9	–	–	99.1	88.3	45.5
980 ppmv	15	–	–	77.5	77.6	68.9	34.5
	18	–	69.5	69.3	–	61.2	27.7
	21	58.2	58.5	58.3	58.6	–	–
VOC:	1[a]	21.4	21.5	21.1	21.1	–	–
Toluene	2	–	11.8	12.0	–	17.9	–[c]
	4	8.7	–	–	8.8	15.5	–[c]
Initial concentration:	7	5.1	–	–	5.8	10.4	–[c]
	9	3.3	3.4	–	–	9.5	–[c]
398 ppmv	11	1.9	–	–	1.9	7.6	–[c]
	15	–	–	–[c]	–[c]	4.4	–[c]
	18	–	–[c]	–[c]	–	2.9	–[c]
	21	1.5	1.7	1.6	1.9	–	–
VOC:	1	–[c]	–[c]	–[c]	–[c]	–	–
P-xylene	2	–	–[c]	–[c]	–	–[c]	–[c]
	4	–[c]	–	–	–[c]	–[c]	–[c]
	7	–[c]	–	–	–[c]	–[c]	–[c]
Initial concentration:	9	–[c]	–[c]	–	–	–[c]	–[c]
	11	–[c]	–	–	–[c]	–[c]	–[c]
99 ppmv	15	–	–	–[c]	–[c]	–[c]	–[c]
	18	–	–[c]	–[c]	–	–[c]	–[c]
	21	–[c]	–[c]	–[c]	–[c]	–	–

Notes:
a. Sampled approximately 26 hrs after filling bags at t = 0.
b. Suspect data.
c. No data detected.

Appendix B

VOC Concentrations in Polyethylene Bottles

Table B-1 . VOC concentration (ppmv) in polyethylene bottles during transport experiment.

Sample day	Bottle number	Methanol	Cyclo-hexane	TCA	Toluene	p-xylene
Time 0	1	1,036.3	837.5	1,102.2	411.1	101.1
	2	1,096.0	875.7	1,151.2	437.5	112.4
	3	1,098.7	865.0	1,145.8	396.9	86.7
	4	1,095.4	862.2	1,142.4	392.7	84.9
Day 21	1	654.1	404.2	603.6	55.0	11.2
	2	823.3	449.9	674.3	57.2	11.3
	3	637.3	189.5	331.5	32.8	8.8
	4	641.1	201.2	351.9	32.2	8.7
Day 50	1	214.1	194.1	292.8	20.7	5.6
	2	396.3	250.0	384.4	22.5	5.7
	3	207.9	79.6	150.6	9.5	4.4
	4	213.3	87.5	166.2	7.4	4.3
Day 81	1	94.7	149.5	218.0	12.1	8.3
	2	235.5	210.7	323.8	13.7	8.4
	3	91.6	60.9	111.0	3.5	7.6
	4	92.8	65.3	121.0	1.5	7.4
Day 124	1	-40.2	134.0	175.1	-4.4	-4.2
	2	109.3	208.7	292.9	-2.8	-4.1
	3	-41.8	52.5	92.2	-12.3	-5.3
	4	-41.8	52.9	95.6	-13.9	-5.5

TCA—1,1,1-Trichloroethane

1—Large mouth with seal
2—Large mouth without seal
3—Small mouth with seal
4—Small mouth without seal

Appendix C

Statistics Characterizing Initial Calibration Curves, Continuing Calibration Curves, and Sample Duplicates

Table C-1. Percent relative standard deviations and coefficient of determination (R squared) values for initial calibration curves.

Test Numbe	Calibration Level	MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCl4	TCE
1	I	0.20	0.29	0.28	0.23	0.21	0.68	0.81	0.87	1.39	1.22
1	II	0.16	0.16	0.16	0.12	0.47	0.13	0.49	0.47	1.21	1.30
1	III	3.73	1.95	2.02	2.91	3.46	0.20	0.73	0.07	0.84	1.00
1	**R squared**	**0.999**	**0.999**	**0.999**	**0.997**	**0.984**	**0.998**	**1.000**	**0.998**	**0.999**	**1.000**
1	I	1.69	1.88	1.59	1.46	1.30	0.26	0.39	0.34	0.35	0.69
1	II	0.58	1.35	1.24	0.91	0.88	0.11	0.22	0.23	1.49	0.60
1	III	0.30	0.61	2.79	0.56	0.32	0.52	0.43	0.40	0.52	0.31
1	**R squared**	**0.999**	**0.998**	**0.998**	**0.990**	**0.985**	**0.998**	**1.000**	**1.000**	**0.998**	**1.000**
2	I	1.02	1.05	1.01	0.67	1.91	0.19	0.18	0.13	0.32	0.15
2	II	0.95	0.57	0.51	1.37	1.89	0.09	0.13	0.08	0.97	0.19
2	III	1.49	0.19	0.17	0.41	1.13	0.07	0.28	0.18	0.59	0.40
2	**R squared**	**0.999**	**0.999**	**1.000**	**0.998**	**0.994**	**0.998**	**1.000**	**1.000**	**0.999**	**1.000**
3	I	1.36	1.46	1.46	1.48	2.08	0.37	0.49	0.50	0.97	0.79
3	II	0.30	0.77	0.54	2.07	1.78	0.27	0.48	0.40	1.68	0.70
3	III	0.59	0.71	0.70	0.64	0.74	0.27	0.41	0.40	0.84	0.65
3	**R squared**	**0.999**	**0.999**	**0.999**	**0.998**	**0.971**	**0.998**	**1.000**	**1.000**	**0.998**	**1.000**
4	I	1.37	0.25	0.18	0.62	0.61	0.24	0.35	0.48	1.47	0.87
4	II	3.63	1.36	1.24	2.37	2.22	0.13	0.51	0.55	2.32	1.04
4	III	1.52	0.38	0.31	0.47	0.86	0.40	0.36	0.70	1.17	0.61
4	**R squared**	**0.997**	**0.999**	**1.000**	**0.997**	**0.979**	**0.987**	**0.997**	**0.999**	**0.999**	**0.999**

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - p-Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), MeCl2 - Methylene Chloride, CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene

Table C-2. Percent relative error for continuing calibration standard analytes for test period I.

CCS Day		MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
Day 2	Conc.	555.1	444.8	590.2	239.4	66.0	571.5	498.8	556.9	171.8	173.4
	%Rec	**111.2**	**118.0**	**116.2**	**113.5**	**113.2**	**120.3**	**110.6**	**112.3**	**115.3**	**113.3**
	Rel. % Error	**11.2**	**18.0**	**16.2**	**13.5**	**13.2**	**20.3**	**10.6**	**12.3**	**15.3**	**13.3**
Day 3	Conc.	568.6	444.1	592.4	244.5	69.7	563.1	472.3	540.0	159.5	151.0
	%Rec	**113.9**	**117.8**	**116.6**	**115.9**	**119.6**	**118.5**	**104.7**	**108.9**	**107.0**	**98.7**
	Rel. % Error	**13.9**	**17.8**	**16.6**	**15.9**	**19.6**	**18.5**	**4.7**	**8.9**	**7.0**	**-1.3**
Day 5	Conc.	576.2	446.4	593.7	242.8	61.6	592.5	530.9	584.0	181.3	187.5
	%Rec	**115.5**	**118.4**	**116.9**	**115.1**	**105.7**	**124.7**	**117.7**	**117.7**	**121.7**	**122.5**
	Rel. % Error	**15.5**	**18.4**	**16.9**	**15.1**	**5.7**	**24.7**	**17.7**	**17.7**	**21.7**	**22.5**
Day 8	Conc.	567.9	376.6	510.1	196.6	52.5	513.4	471.9	512.3	162.2	167.1
	%Rec	**113.8**	**99.9**	**100.4**	**93.2**	**90.1**	**108.1**	**104.6**	**103.3**	**108.9**	**109.2**
	Rel. % Error	**13.8**	**-0.1**	**0.4**	**-6.8**	**-9.9**	**8.1**	**4.6**	**3.3**	**8.9**	**9.2**
Day 10	Conc.	502.5	396.7	522.4	199.9	51.9	493.6	449.3	489.7	155.7	156.2
	%Rec	**100.7**	**105.2**	**102.8**	**94.7**	**89.0**	**103.9**	**99.6**	**98.7**	**104.5**	**102.1**
	Rel. % Error	**0.7**	**5.2**	**2.8**	**-5.3**	**-11.0**	**3.9**	**-0.4**	**-1.3**	**4.5**	**2.1**
Day 12	Conc.	511.7	401.3	525.6	192.6	48.1	497.5	438.8	486.0	149.6	150.0
	%Rec	**102.5**	**106.4**	**103.5**	**91.3**	**82.5**	**104.7**	**97.3**	**98.0**	**100.4**	**98.0**
	Rel. % Error	**2.5**	**6.4**	**3.5**	**-8.7**	**-17.5**	**4.7**	**-2.7**	**-2.0**	**0.4**	**-2.0**
Day 16	Conc.	505.2	370.4	499.4	184.1	54.6	507.5	462.3	502.3	155.5	161.3
	%Rec	**101.2**	**98.2**	**98.3**	**87.3**	**93.7**	**106.8**	**102.5**	**101.3**	**104.4**	**105.4**
	Rel. % Error	**1.2**	**-1.8**	**-1.7**	**-12.7**	**-6.3**	**6.8**	**2.5**	**1.3**	**4.4**	**5.4**
Day 19	Conc.	541.2	410.2	548.2	199.5	48.0	503.9	457.2	495.0	153.2	157.5
	%Rec	**108.5**	**108.8**	**107.9**	**94.5**	**82.3**	**106.1**	**101.4**	**99.8**	**102.8**	**102.9**
	Rel. % Error	**8.5**	**8.8**	**7.9**	**-5.5**	**-17.7**	**6.1**	**1.4**	**-0.2**	**2.8**	**2.9**
Day 22	Conc.	562.7	418.8	558.3	214.5	56.8	504.4	442.4	483.7	154.8	147.6
	%Rec	**112.8**	**111.1**	**109.9**	**101.7**	**97.4**	**106.2**	**98.1**	**97.5**	**103.9**	**96.5**
	Rel. % Error	**12.8**	**11.1**	**9.9**	**1.7**	**-2.6**	**6.2**	**-1.9**	**-2.5**	**3.9**	**-3.5**
Mean % Error		**8.9**	**9.3**	**8.1**	**0.8**	**-3.0**	**11.1**	**4.1**	**4.2**	**7.7**	**5.4**
Standard Deviation		**5.9**	**7.7**	**7.3**	**11.2**	**13.2**	**7.9**	**6.5**	**7.2**	**6.8**	**8.4**

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
% Rec - Percent Recovery, Rel. % Error - Relative Percent Error

Table C-3. Percent relative error for continuing calibration standard analytes for test period II.

CCS Day		MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
Day 2	Conc.	500.8	396.6	536.6	209.6	49.2	497.4	439.5	480.0	158.6	149.9
	%Rec	**100.4**	**105.2**	**105.6**	**99.3**	**84.4**	**104.7**	**97.5**	**96.8**	**106.4**	**98.0**
	Rel. % Error	**0.4**	**5.2**	**5.6**	**-0.7**	**-15.6**	**4.7**	**-2.5**	**-3.2**	**6.4**	**-2.0**
Day 3	Conc.	519.5	383.9	520.2	219.9	55.4	507.6	436.0	480.9	158.7	146.5
	%Rec	**104.1**	**101.8**	**102.4**	**104.2**	**95.0**	**106.9**	**96.7**	**97.0**	**106.5**	**95.8**
	Rel. % Error	**4.1**	**1.8**	**2.4**	**4.2**	**-5.0**	**6.9**	**-3.3**	**-3.0**	**6.5**	**-4.2**
Day 5	Conc.	515.0	382.6	520.1	211.7	52.7	513.4	451.2	497.2	162.3	158.0
	%Rec	**103.2**	**101.5**	**102.4**	**100.3**	**90.4**	**108.1**	**100.0**	**100.2**	**108.9**	**103.3**
	Rel. % Error	**3.2**	**1.5**	**2.4**	**0.3**	**-9.6**	**8.1**	**0.0**	**0.2**	**8.9**	**3.3**
Day 8	Conc.	510.1	373.5	507.5	212.0	58.0	506.4	452.5	492.6	156.4	155.8
	%Rec	**102.2**	**99.1**	**99.9**	**100.5**	**99.5**	**106.6**	**100.3**	**99.3**	**105.0**	**101.8**
	Rel. % Error	**2.2**	**-0.9**	**-0.1**	**0.5**	**-0.5**	**6.6**	**0.3**	**-0.7**	**5.0**	**1.8**
Day 10	Conc.	469.7	361.0	482.9	199.6	48.3	456.9	423.3	448.5	138.7	143.4
	%Rec	**94.1**	**95.8**	**95.1**	**94.6**	**82.8**	**96.2**	**93.9**	**90.4**	**93.1**	**93.7**
	Rel. % Error	**-5.9**	**-4.2**	**-4.9**	**-5.4**	**-17.2**	**-3.8**	**-6.1**	**-9.6**	**-6.9**	**-6.3**
Day 12	Conc.	465.8	347.6	470.0	199.0	51.9	468.6	421.3	434.0	116.3	136.3
	%Rec	**93.3**	**92.2**	**92.5**	**94.3**	**89.0**	**98.7**	**93.4**	**87.5**	**78.1**	**89.1**
	Rel. % Error	**-6.7**	**-7.8**	**-7.5**	**-5.7**	**-11.0**	**-1.3**	**-6.6**	**-12.5**	**-21.9**	**-10.9**
Day 16	Conc.	477.0	363.0	489.3	200.9	52.5	479.3	437.1	451.7	124.4	144.1
	%Rec	**95.6**	**96.3**	**96.3**	**95.2**	**90.1**	**100.9**	**96.9**	**91.1**	**83.5**	**94.2**
	Rel. % Error	**-4.4**	**-3.7**	**-3.7**	**-4.8**	**-9.9**	**0.9**	**-3.1**	**-8.9**	**-16.5**	**-5.8**
Day 19	Conc.	472.2	363.0	491.7	198.3	49.8	486.6	436.2	460.4	129.7	144.1
	%Rec	**94.6**	**96.3**	**96.8**	**94.0**	**85.4**	**102.4**	**96.7**	**92.8**	**87.0**	**94.2**
	Rel. % Error	**-5.4**	**-3.7**	**-3.2**	**-6.0**	**-14.6**	**2.4**	**-3.3**	**-7.2**	**-13.0**	**-5.8**
Day 22	Conc.	467.2	356.9	484.7	188.9	47.3	489.8	436.1	465.5	135.3	144.1
	%Rec	**93.6**	**94.7**	**95.4**	**89.5**	**81.1**	**103.1**	**96.7**	**93.9**	**90.8**	**94.2**
	Rel. % Error	**-6.4**	**-5.3**	**-4.6**	**-10.5**	**-18.9**	**3.1**	**-3.3**	**-6.1**	**-9.2**	**-5.8**
Mean % Error		**-2.1**	**-1.9**	**-1.5**	**-3.1**	**-11.4**	**3.1**	**-3.1**	**-5.7**	**-4.5**	**-4.0**
Standard Deviation		**4.5**	**4.1**	**4.3**	**4.5**	**5.9**	**4.0**	**2.3**	**4.3**	**11.5**	**4.4**

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
% Rec - Percent Recovery, Rel. % Error - Relative Percent Error

Table C-4. Percent relative error for continuing calibration standard analytes for test period III.

CCS Day		MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
Day 2	Conc.	525.2	394.3	522.4	212.4	57.0	511.9	463.8	503.7	157.1	161.0
	%Rec	**105.3**	**104.6**	**102.8**	**100.7**	**97.8**	**107.8**	**102.8**	**101.6**	**105.4**	**105.2**
	Rel. % Error	**5.3**	**4.6**	**2.8**	**0.7**	**-2.2**	**7.8**	**2.8**	**1.6**	**5.4**	**5.2**
Day 3	Conc.	531.3	378.8	507.8	200.2	58.7	505.7	457.7	498.2	160.7	158.5
	%Rec	**106.5**	**100.5**	**100.0**	**94.9**	**100.7**	**106.5**	**101.5**	**100.4**	**107.9**	**103.6**
	Rel. % Error	**6.5**	**0.5**	**0.0**	**-5.1**	**0.7**	**6.5**	**1.5**	**0.4**	**7.9**	**3.6**
Day 5	Conc.	519.6	369.9	497.4	193.0	54.7	494.5	444.1	482.1	151.3	152.8
	%Rec	**104.1**	**98.1**	**97.9**	**91.5**	**93.8**	**104.1**	**98.5**	**97.2**	**101.5**	**99.9**
	Rel. % Error	**4.1**	**-1.9**	**-2.1**	**-8.5**	**-6.2**	**4.1**	**-1.5**	**-2.8**	**1.5**	**-0.1**
Day 8	Conc.	527.4	326.2	439.5	187.2	56.8	461.9	425.0	455.0	142.6	145.4
	%Rec	**105.7**	**86.5**	**86.5**	**88.7**	**97.4**	**97.2**	**94.2**	**91.7**	**95.7**	**95.0**
	Rel. % Error	**5.7**	**-13.5**	**-13.5**	**-11.3**	**-2.6**	**-2.8**	**-5.8**	**-8.3**	**-4.3**	**-5.0**
Day 10	Conc.	514.7	342.6	456.4	202.4	61.8	459.2	422.8	453.7	142.1	144.6
	%Rec	**103.1**	**90.9**	**89.8**	**95.9**	**106.0**	**96.7**	**93.7**	**91.5**	**95.4**	**94.5**
	Rel. % Error	**3.1**	**-9.1**	**-10.2**	**-4.1**	**6.0**	**-3.3**	**-6.3**	**-8.5**	**-4.6**	**-5.5**
Day 12	Conc.	510.5	364.5	484.7	194.2	53.9	463.9	424.6	459.1	146.0	145.3
	%Rec	**102.3**	**96.7**	**95.4**	**92.0**	**92.5**	**97.7**	**94.1**	**92.6**	**98.0**	**95.0**
	Rel. % Error	**2.3**	**-3.3**	**-4.6**	**-8.0**	**-7.5**	**-2.3**	**-5.9**	**-7.4**	**-2.0**	**-5.0**
Day 16	Conc.	514.8	362.5	483.1	196.3	57.0	464.5	422.0	455.9	148.4	142.9
	%Rec	**103.2**	**96.2**	**95.1**	**93.0**	**97.8**	**97.8**	**93.6**	**91.9**	**99.6**	**93.4**
	Rel. % Error	**3.2**	**-3.8**	**-4.9**	**-7.0**	**-2.2**	**-2.2**	**-6.4**	**-8.1**	**-0.4**	**-6.6**
Day 19	Conc.	494.1	353.9	468.4	194.1	53.9	441.9	409.6	439.6	139.7	140.9
	%Rec	**99.0**	**93.9**	**92.2**	**92.0**	**92.5**	**93.0**	**90.8**	**88.6**	**93.8**	**92.1**
	Rel. % Error	**-1.0**	**-6.1**	**-7.8**	**-8.0**	**-7.5**	**-7.0**	**-9.2**	**-11.4**	**-6.2**	**-7.9**
Day 22	Conc.	515.3	367.7	484.4	212.9	62.3	450.3	419.3	452.4	155.9	144.6
	%Rec	**103.3**	**97.5**	**95.4**	**100.9**	**106.9**	**94.8**	**93.0**	**91.2**	**104.6**	**94.5**
	Rel. % Error	**3.3**	**-2.5**	**-4.6**	**0.9**	**6.9**	**-5.2**	**-7.0**	**-8.8**	**4.6**	**-5.5**
Mean % Error		**3.6**	**-3.9**	**-5.0**	**-5.6**	**-1.6**	**-0.5**	**-4.2**	**-5.9**	**0.2**	**-3.0**
Standard Deviation		**2.2**	**5.3**	**5.0**	**4.2**	**5.3**	**5.3**	**4.1**	**4.5**	**5.0**	**4.7**

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
% Rec - Percent Recovery, Rel. % Error - Relative Percent Error

Table C-5. Percent relative error for continuing calibration standard analytes for test period IV.

CCS Day		MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
Day 2	Conc.	447.6	405.1	504.5	214.3	52.8	362.1	446.2	531.3	264.2	166.5
	%Rec	**89.7**	**107.5**	**99.3**	**101.6**	**90.6**	**76.2**	**98.9**	**107.1**	**177.3**	**108.8**
	Rel. % Error	**-10.3**	**7.5**	**-0.7**	**1.6**	**-9.4**	**-23.8**	**-1.1**	**7.1**	**77.3**	**8.8**
Day 3	Conc.	417.6	350.6	463.8	197.9	56.7	387.9	447.9	457.3	136.3	140.2
	%Rec	**83.7**	**93.0**	**91.3**	**93.8**	**97.3**	**81.7**	**99.3**	**92.2**	**91.5**	**91.6**
	Rel. % Error	**-16.3**	**-7.0**	**-8.7**	**-6.2**	**-2.7**	**-18.3**	**-0.7**	**-7.8**	**-8.5**	**-8.4**
Day 5	Conc.	444.1	375.9	503.0	205.5	59.1	418.6	485.8	509.6	155.1	155.4
	%Rec	**89.0**	**99.7**	**99.0**	**97.4**	**101.4**	**88.1**	**107.7**	**102.7**	**104.1**	**101.6**
	Rel. % Error	**-11.0**	**-0.3**	**-1.0**	**-2.6**	**1.4**	**-11.9**	**7.7**	**2.7**	**4.1**	**1.6**
Day 8	Conc.	451.4	379.1	504.9	214.9	63.2	416.5	484.6	508.6	152.1	155.2
	%Rec	**90.5**	**100.6**	**99.4**	**101.8**	**108.4**	**87.7**	**107.5**	**102.5**	**102.1**	**101.4**
	Rel. % Error	**-9.5**	**0.6**	**-0.6**	**1.8**	**8.4**	**-12.3**	**7.5**	**2.5**	**2.1**	**1.4**
Day 10	Conc.	473.2	380.4	509.4	213.3	65.0	420.8	495.1	525.7	160.1	162.9
	%Rec	**94.8**	**100.9**	**100.3**	**101.1**	**111.5**	**88.6**	**109.8**	**106.0**	**107.4**	**106.5**
	Rel. % Error	**-5.2**	**0.9**	**0.3**	**1.1**	**11.5**	**-11.4**	**9.8**	**6.0**	**7.4**	**6.5**
Day 12	Conc.	473.8	381.4	507.3	217.7	66.8	420.1	495.2	527.9	164.3	162.4
	%Rec	**94.9**	**101.2**	**99.9**	**103.2**	**114.6**	**88.4**	**109.8**	**106.4**	**110.3**	**106.1**
	Rel. % Error	**-5.1**	**1.2**	**-0.1**	**3.2**	**14.6**	**-11.6**	**9.8**	**6.4**	**10.3**	**6.1**
Day 16	Conc.	488.0	404.7	546.0	231.9	68.7	447.0	522.4	543.0	155.7	164.8
	%Rec	**97.8**	**107.3**	**107.5**	**109.9**	**117.8**	**94.1**	**115.8**	**109.5**	**104.5**	**107.7**
	Rel. % Error	**-2.2**	**7.3**	**7.5**	**9.9**	**17.8**	**-5.9**	**15.8**	**9.5**	**4.5**	**7.7**
Day 19	Conc.	473.1	388.4	527.2	226.0	67.9	445.2	516.9	536.7	162.4	164.0
	%Rec	**94.8**	**103.0**	**103.8**	**107.1**	**116.5**	**93.7**	**114.6**	**108.2**	**109.0**	**107.2**
	Rel. % Error	**-5.2**	**3.0**	**3.8**	**7.1**	**16.5**	**-6.3**	**14.6**	**8.2**	**9.0**	**7.2**
Day 22	Conc.	476.3	395.7	530.9	229.9	67.3	434.3	511.0	531.7	153.1	165.1
	%Rec	**95.5**	**105.0**	**104.5**	**109.0**	**115.4**	**91.4**	**113.3**	**107.2**	**102.8**	**107.9**
	Rel. % Error	**-4.5**	**5.0**	**4.5**	**9.0**	**15.4**	**-8.6**	**13.3**	**7.2**	**2.8**	**7.9**
Mean % Error		**-7.7**	**2.0**	**0.5**	**2.8**	**8.2**	**-12.2**	**8.5**	**4.7**	**12.1**	**4.3**
Standard Deviation		**4.4**	**4.5**	**4.5**	**5.3**	**9.6**	**5.7**	**6.1**	**5.2**	**25.1**	**5.5**

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
% Rec - Percent Recovery, Rel. % Error - Relative Percent Error

Table C-6. Relative percent difference (RPD) for duplicate sample analyses during test period I.

(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
102-3SB4						774.6	228.9	303.2	68.0	49.0
102-3SB4D						758.7	225.2	291.7	65.1	48.4
RPD						2.07	1.63	3.87	4.36	1.23
103-3SB2						615.4	195.0	206.6	48.6	42.6
103-3SB2D						601.7	192.2	202.9	47.9	42.1
RPD						2.25	1.45	1.81	1.45	1.18
105-1SB2						248.7	162.9	156.7	39.3	34.4
105-1SB2D						247.0	162.7	163.3	41.3	37.5
RPD						0.69	0.12	-4.13	-4.96	-8.62
108-2SB2	No Data	No Data	No Data	No Data	No Data					
108-2SB2D	No Data	No Data	No Data	No Data	No Data					
RPD										
110-4SB2	108.3	* 65.7	101.5	* 18.6	* 6.4					
110-4SB2D	108.4	* 65.5	101.1	* 18.5	* 6.4					
RPD	-0.09	0.30	0.39	0.54	0.00					
112-2SB3	* 83.7	* 62.1	93.5	* 19.8	* 6.7					
112-2SB3D	* 83.3	* 70.4	101.3	* 24.3	* 7.6					
RPD	0.48	-12.53	-8.01	-20.41	-12.59					
116-1SB4						102.3	* 67.3	* 79.9	* 19.5	* 14.7
116-1SB4D						104.5	* 68.7	* 88.2	* 22.7	* 17.6
RPD						-2.13	-2.06	-9.88	-15.17	-17.96
119-4SB3	* 79.6	* 57.0	* 86.0	* 16.7	* 6.1					
119-4SB3D	* 79.5	* 57.1	* 86.1	* 16.6	* 6.1					
RPD	0.13	-0.18	-0.12	0.60	0.00					
122-3SB3						110.6	* 65.4	* 82.0	* 20.2	* 13.5
122-3SB3D						111.0	* 65.3	* 91.9	* 19.4	* 13.6
RPD						-0.36	0.15	0.12	4.04	-0.74

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene

RPD - Relative Percent Difference, * - Outside Linear Dynamic Range

Table C-7. Relative percent difference (RPD) for duplicate sample analyses during test period II.

(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
202-3SB4						579.2	180.4	203.3	48.3	35.5
202-3SB4D						568.0	179.0	198.8	48.2	35.2
RPD						1.95	0.78	2.24	0.21	0.85
203-3SB2						389.0	161.5	160.6	41.1	* 32.0
203-3SB2D						380.3	160.1	159.0	40.3	* 31.7
RPD						2.26	0.87	1.00	1.97	0.94
205-1SB2						240.3	138.7	143.7	36.9	* 29.6
205-1SB2D						213.4	127.7	135.5	36.5	* 29.8
RPD						11.86	8.26	5.87	1.09	-0.67
208-2SB2	106.7	* 59.3	96.8	* 16.5	* 4.9					
208-2SB2D	106.0	75.5	112.8	* 16.4	* 7.4					
RPD	0.66	-24.04	-15.27	0.61	-40.65					
210-4SB2	107.4	* 61.8	100.7	* 14.9	* 4.8					
210-4SB2D	107.6	* 61.8	100.7	* 14.9	* 4.8					
RPD	-0.19	0.00	0.00	0.00	0.00					
212-2SB3	* 73.0	* 47.8	* 77.1	* 15.0	* 5.0					
212-2SB3D	* 74.1	* 56.9	* 86.4	* 19.4	* 5.8					
RPD	-1.50	-17.38	-11.38	-25.58	-14.81					
216-1SB4						* 89.0	* 64.3	* 76.6	* 19.9	* 17.4
216-1SB4D						* 78.8	* 58.2	* 74.3	* 19.7	* 18.5
RPD						12.16	9.96	3.05	1.01	-6.13
219-4SB3	* 74.2	* 46.0	* 76.6	* 10.9	* 4.3					
219-4SB3D	* 74.2	* 46.0	* 76.6	* 10.9	* 4.3					
RPD	0.00	0.00	0.00	0.00	0.00					
222-3SB3						95.9	* 65.1	* 75.2	* 20.3	* 15.4
222-3SB3D						95.3	* 64.6	* 75.1	* 20.6	* 15.4
RPD						0.63	0.77	0.13	-1.47	0.00

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
RPD - Relative Percent Difference, * - Outside Linear Dynamic Range

Table C-8. Relative percent difference (RPD) for duplicate sample analyses during test period III.

(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
302-3SB4	286.5	128.5	229.0	* 26.6	* 9.6					
302-3SB4D	271.1	123.6	219.5	* 26.2	* 9.5					
RPD	5.52	3.89	4.24	1.52	1.05					
305-3SB2	149.7	80.5	129.8	* 18.6	* 8.7					
305-3SB2D	144.3	78.5	126.5	* 18.3	* 8.6					
RPD	3.67	2.52	2.58	1.63	1.16					
307-1SB2						168.5	112.2	118.0	* 28.9	* 22.4
307-1SB2D						* 86.6	* 65.3	* 72.8	* 17.8	* 16.3
RPD						64.21	52.85	47.38	47.54	31.52
309-2SB2	108.9	* 67.5	103.3	* 16.2	* 8.5					
309-2SB2D	104.4	74.7	109.7	* 21.5	* 9.6					
RPD	4.22	-10.13	-6.01	-28.12	-12.15					
312-4SB2						119.6	* 70.8	* 80.4	* 17.6	* 14.0
312-4SB2D						119.1	* 71.2	* 80.4	* 17.7	* 14.0
RPD						0.42	-0.56	0.00	-0.57	0.00
314-2SB3	* 51.9	* 35.2	* 49.4	* 11.4	9.1					
314-2SB3D	No Data	No Data	No Data	No Data	No Data					
RPD										
316-1SB4						No Data	No Data	No Data	No Data	No Data
316-1SB4D						* 83.7	* 59.4	71.1	* 14.7	* 16.1
RPD										
319-4SB3						* 76.5	* 52.4	* 62.5	* 11.5	* 10.9
319-4SB3D						* 48.8	* 38.5	* 45.6	* 7.8	* 8.7
RPD						44.21	30.58	31.27	38.34	22.45
322-3SB3	* 59.3	* 41.3	* 67.3	* 8.0	* 7.9					
322-3SB3D	* 57.4	* 41.2	* 67.2	* 8.0	* 7.6					
RPD	3.26	0.24	0.15	0.00	3.87					

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene

RPD - Relative Percent Difference, * - Outside Linear Dynamic Range

Table C-9. Relative percent difference (RPD) for duplicate sample analyses during test period IV.

(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	Freon	MeCl2	TCA	CCL4	TCE
402-3SB4						562.8	142.3	226.9	88.3	* 33.7
402-3SB4D						554.8	140.0	219.5	84.5	* 33.3
RPD						**1.43**	**1.63**	**3.32**	**4.40**	**1.19**
403-3SB2						447.0	120.7	132.8	35.8	* 24.9
403-3SB2D						439.2	119.3	130.6	34.8	* 24.7
RPD						**1.76**	**1.17**	**1.67**	**2.83**	**0.81**
405-1SB2						337.9	130.8	142.1	40.2	* 29.9
405-1SB2D						326.7	130.9	150.1	43.9	35.2
RPD						**3.37**	**-0.08**	**-5.48**	**-8.80**	**-16.28**
408-2SB2	* 81.0	* 64.2	105.8	* 3.3	ND					
408-2SB2D	* 79.9	74.8	116.9	* 10.6	ND					
RPD	**1.37**	**-15.25**	**-9.97**	**-105.04**						
410-4SB2	* 72.2	* 66.3	108.7	* 3.4	ND					
410-4SB2D	* 72.4	* 66.0	108.2	* 3.3	ND					
RPD	**-0.28**	**0.45**	**0.46**	**2.99**						
412-2SB3	* 65.3	* 53.3	88.1	* 0.7	ND					
412-2SB3D	* 65.0	* 60.8	95.5	* 6.1	ND					
RPD	**0.46**	**-13.15**	**-8.06**	**-158.82**						
416-1SB4						193.1	* 56.4	* 81.7	* 25.0	* 20.0
416-1SB4D						195.0	* 57.7	* 89.8	* 27.7	* 23.1
RPD						**-0.98**	**-2.28**	**-9.45**	**-10.25**	**-14.39**
419-4SB3	* 46.7	* 42.3	* 71.9	ND	ND					
419-4SB3D	* 46.8	* 42.2	* 71.9	ND	ND					
RPD	**-0.21**	**0.24**	**0.00**							
422-3SB3						186.1	* 40.8	* 67.7	* 19.1	* 13.5
422-3SB3D						185.7	* 40.8	* 67.9	* 19.1	* 13.6
RPD						**0.22**	**0.00**	**-0.29**	**0.00**	**-0.74**

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
RPD - Relative Percent Difference, * - Outside Linear Dynamic Range, ND - Not Detected

Appendix D

Computer Program of VOC Transport Model for Lab-Scale Simulated Waste Drums

```
c
c program calculates the VOC concentration as a function of time
c in a simulated waste drum.  The drum contains small poly bags initially
c filled with VOC-containing air.  These bags were placed in a large poly
c bag inside a 90-mil rigid polyethylene liner, inside a vented metal drum.
c------------------------------------------------------------------------
c  allows user to specify different model parameters for one small bag
c  the parameters for other three small bags are the same.  this allows user
c  to describe situations where one bag may be smaller, have a leak, etc.
c------------------------------------------------------------------------
c  model accounts for VOC accumulation in poly bags and liner
c----------------------------------------------------------------------
c  model allows user to specify if drum temperature is constant or variable
c------------------------------------------------------------------------
c  The program utilizes an IMSL routine to solve a series of first-order
c  ordinary differential equations.
c
      character*32 test,ifname,ofname,vocid(9)
      real aa(1,1),yy(5,5),yz(9),sb1(5,21),sb2(5,21),lb(5,21),dh(5,21)
      real param(50),p,d,ap(5),ad(5),v(5),xp(5),xd(5),mw
      integer ivoc(5)
      common/qq/p,d,ap,ad,v,xp,xd,pi,patm,pHg,dfh,c0,mw,temp0,
     #vpb,vpc,y0,s0c0,nft,thr1
      common/ss/s6,s7,s8,s9
      external fcn,ivpag,sset
c---------------------
c input
c---------------------
      write(*,9)
   9  format(1x,'Enter name of input data file  ')
      read(*,*)ifname
      open(unit=3,file=ifname,status='unknown')
c---------------------------------------------------------------------
c User provided input
c   nvoc - number of VOCs in drum
c   y(i,n) - i-th VOC concentration in n-th layer of confinement, (mol/cm3)
c          n=1, small bag headspace (for 3 identical bags)
c          n=2, small bag headspace (for 4th small bag)
c** allows user to specify unique conditions of one of four small bags
c          n=3, large bag headspace
c          n=4, drum liner headspace
c          n=5, drum headspace
c   ap(n) - permeation surface area around n-th layer of confinement (cm2)
c   ad(n) - cross-sectional area for diffusion out of n-th layer
c               of confinement (cm2)
c   xp(n) - thickness of permeable surface (cm)
c   xd(n) - length of diffusional path between layers of confinement (cm)
c   v(n) - void volume in n-th layer of confinement (cm3)
c *********************************************************************
c   ivoc - VOC identification number
c        1 - CCl4    2 - cyclohexane    3 - methanol    4 - CH2Cl2
c        5 - toluene    6 - TCA    7 - TCE    8 - Freon-113    9 - p-xylene
c *********************************************************************
      vocid(1)='carbon tetrachloride'
      vocid(2)='cyclohexane'
      vocid(3)='methanol'
      vocid(4)='methylene chloride'
      vocid(5)='toluene'
      vocid(6)='1,1,1-trichloroethane'
      vocid(7)='trichloroethylene'
      vocid(8)='Freon-113'
      vocid(9)='p-xylene'
```

```
c   yvoc(i) - concentration of VOC i in drum headspace, ppmv
c   nft -  if = 1, temperature = constant
c          if = 2, temperature = f(t)
c   thr1 - approximate number of hours after t=0 when heating cycle begins
c   thr2 - approximate number of hours after t=0 when small bags first sampled
c   temp - drum temperature, C
c   pHg - atmospheric pressure, cm Hg
c   dfh - carbon composite filter H2-diffusion constant, mol/s/mol fraction
c-----------------------------------------------------------------------
c initial conditions
      read(3,*)test,ofname
      open(unit=2,file=ofname,status='unknown')
      read(3,*)nvoc
c   neq - number of layers of confinement inside waste drum
      neq=5
      do 8 i=1,nvoc
         read(3,*)ivoc(i),(yy(i,j),j=1,neq)
  8   continue
      read(3,*)(ap(j),ad(j),v(j),xp(j),xd(j),j=1,neq)
      read(3,*)nft,thr1,thr2,temp,pHg,dfh
c-----------------------------------------------------------------------
c r0 - gas constant (cm3 atm/mol K)
c patm - atmospheric pressure (atm)
      r0=82.06
      pi=3.141592654
c convert pHg (cm Hg) to patm (atm)
      patm=pHg/76.0
c temp0 - initial drum temperature, K
      temp0=temp+273.2
c c0 - initial gas concentration in each layer of confinement (mol/cm3)
      c0=patm/(r0*temp0)
cccccc*****************************************************************
cccccc    calculate concentration throughout waste drum for each VOC
cccccc*****************************************************************
      nv=nvoc
      do 43 i=1,nv
c---------------
c convert VOC gas concentration from ppmv to mol/cm3
         do 37 j=1,neq
            yz(j)=yy(i,j)*c0*1.e-6
  37     continue
c VOC conc. in polymer walls (6(3); 9(1) -small bag, 7 -large bag, 8 - liner)
c (cm3 VOC/cm3 polymer)
         yz(6)=0.
         yz(7)=0.
         yz(8)=0.
         yz(9)=0.
         nq=9
c y0 - initial VOC concentration in gas feed, mol/cm3
         y0=yz(1)
c-----------------------------------------------------------------------
c set param to default values
         mxparm=50
         CALL SSET(mxparm,0.0,param,1)
         param(4)=150000
         param(10)=2
c param(12): 1=Adams' method;  2=Gear's backward difference method
         param(12)=2
c-----------------------------------------------------------------------
c initialization of other variables
c t - time (sec)
         t=0.
```

```
c tol - error tolerance
        tol=1.e-6
        ido=1
c---------------
c  mw - VOC molecular weight
c  p - VOC permeability coefficient across polyethylene (cm3 cm/cm2 s cmHg)
c  d - diffusivity (cm2/s) of VOC in air
c  s0c0 - VOC solubility in polymer/VOC gas conc. [cm3/cm3 poly/atm/(mol/cm3)]
        call vprop(ivoc(i),c0,mw,p,d,vpb,vpc,s0c0)
c***********************************************************************
c calculation of VOC concentrations inside waste drum over 21 days
c***********************************************************************
c  nh - counter
        nh=0
        do 20 is=1,21
c subroutine to calculate time interval, dtend (sec)
  24       call dti(yz(1),dtend)
           tend=t+dtend
c calculation of VOC concentration in each volume inside waste drum
           CALL IVPAG(ido,nq,fcn,fcnj,aa,t,tend,tol,param,yz)
c--------------------------------------------------------------------------
c output (every simulated 24 hrs)
           if((((t/3600.).gt.thr2).and.(nh.eq.0)).or.(((t/86400.)
     $.gt.is).and.(nh.eq.1)))then
             if(nh.eq.0)ist=1
             if(nh.eq.1)ist=is
c convert VOC concentration (mol/cm3) to ppmv
             sb1(i,ist)=(yz(1)/c0)*1.e6
             sb2(i,ist)=(yz(2)/c0)*1.e6
             lb(i,ist)=(yz(3)/c0)*1.e6
             dh(i,ist)=(yz(5)/c0)*1.e6
             nh=1
           else
             goto 24
           end if
  20    continue
c-------------------------------------------
c final call to release workspace
c-------------------------------------------
        ido=3
        CALL IVPAG(ido,nq,fcn,fcnj,aa,t,tend,tol,param,yz)
   43 continue
c-------------------------------------------
c  output
c-------------------------------------------
      write(2,88)
  88  format(1x,//)
      write(2,89)test
  89  format(15x,a10)
      write(2,92)
  92  format(43x,'Initial VOC concentration (ppmv)')
      write(2,93)
  93  format(41x,'3 small',3x,'1 small',3x,'Large',4x,'Drum',6x,'Drum')
      write(2,94)
  94  format(43x,'bags',6x,'bag',6x,'bag',5x,'liner',3x,'headspace')
      nv=nvoc
      do 105 i=1,nv
      write(2,97)vocid(ivoc(i)),yy(i,1),yy(i,2),yy(i,3),yy(i,4),yy(i,5)
  97  format(15x,a24,3x,f6.1,3x,f6.1,2x,f6.1,3x,f6.1,4x,f6.1)
 105  continue
      write(2,*)' '
      write(2,99)
```

```
 99  format(15x,'Model parameters:')
     write(2,101)
101  format(32x,'Ap(cm2)',2x,'Ad(cm2)',2x,'V(cm3)',3x,'xp(cm)',
    #3x,'xd(cm)')
     write(2,107)ap(1),ad(1),v(1),xp(1),xd(1)
107  format(15x,'3 small bags',5x,2(f6.0,4x,f4.2,4x),f5.2)
     write(2,109)ap(2),ad(2),v(2),xp(2),xd(2)
109  format(15x,'1 small bag',6x,2(f6.0,4x,f4.2,4x),f5.2)
     write(2,111)ap(3),ad(3),v(3),xp(3),xd(3)
111  format(15x,'Large bag',8x,2(f6.0,4x,f4.2,4x),f5.2)
     write(2,113)ap(4),ad(4),v(4),xp(4),xd(4)
113  format(15x,'Drum liner',7x,2(f6.0,4x,f4.2,4x),f5.2)
     write(2,117)ap(5),ad(5),v(5),xp(5),xd(5)
117  format(15x,'Drum headspace',3x,2(f6.0,4x,f4.2,4x),f5.2)
     write(2,*)' '
     write(2,131)temp
131  format(15x,'Initial drum temperature (C):',2x,f4.1)
     if(nft.eq.1)then
       write(2,133)
133    format(15x,'Drum temperature during the trial:  constant')
     else
       write(2,135)
135    format(15x,'Drum temperature during the trial:  variable')
       write(2,137)thr1
137    format(15x,'Heating cycle began approximately ',f4.1,
    #' hrs after t=0')
     end if
     write(2,139)thr2
139  format(15x,'First samples collected from small bags',1x,
    #'approximately ',f4.1,' hrs after t=0')
     write(2,141)pHg
141  format(15x,'Ambient pressure (cm Hg):',2x,f4.1)
     write(2,143)dfh
143  format(15x,'Hydrogen diffusion characteristic across filter',1x,
    #'(mol/mol fraction/s):',2x,e12.5)
     write(2,*)' '
     write(2,145)
145  format(15x,'Predicted small bag concentrations (ppmv):')
     write(2,147)vocid(ivoc(1)),vocid(ivoc(2)),vocid(ivoc(3)),
    #vocid(ivoc(4)),vocid(ivoc(5))
147  format(20x,a20,5x,a14,a21,3x,a22,1x,a22)
     write(2,153)
153  format(15x,'Day ',1x,2('3 small',2x,'1 small',5x),'3 small",2x,
    #'1 small',7x,2('3 small',2x,'1 small',6x))
     write(2,154)
154  format(22x,2('bags',5x,'bag',9x),'bags',5x,'bag',11x,
    #2('bags',5x,'bag',10x))
     do 160 in=1,21
        write(2,155)in,(sb1(j,in),sb2(j,in),j=1,nvoc)
155     format(15x,i2,4x,3(f5.1,4x,f5.1,7x),2x,2(f5.1,4x,f5.1,7x))
160  continue
     write(2,163)test
163  format(1x,11(/),15x,a10,' (continued)')
     write(2,*)' '
     write(2,245)
245  format(15x,'Other predicted VOC concentrations (ppmv):')
     write(2,247)vocid(ivoc(1)),vocid(ivoc(2)),vocid(ivoc(3)),
    #vocid(ivoc(4)),vocid(ivoc(5))
247  format(20x,a20,5x,a14,a21,3x,a22,1x,a22)
     write(2,253)
```

```
 253  format(15x,'Day ',1x,2(1x,'Large',4x,'Drum',7x),1x,'Large',4x
     #'Drum',9x,2(1x,'Large',4x,'Drum',7x))
      write(2,254)
 254  format(22x,2('bag',3x,'headspace',6x),'bag',3x,'headspace',8x,
     #2('bag',3x,'headspace',6x))
      do 260 in=1,21
         write(2,255)in,(lb(j,in),dh(j,in),j=1,nvoc)
 255     format(15x,i2,4x,3(f5.1,4x,f5.1,7x),2x,2(f5.1,4x,f5.1,7x))
 260  continue
      stop
      end

      SUBROUTINE FCN(neq,t,y,yp)
      real y(neq),yp(neq),p,d,ap(5),ad(5),v(5),xp(5),xd(5),q
      real mw
      common/qq/p,d,ap,ad,v,xp,xd,pi,patm,pHg,dfh,c0,mw,temp0,
     #vpb,vpc,y0,s0c0,nft,thr1
      common/ss/s6,s7,s8,s9
c
c assume temperature inside poly bags and drum liner are same
c for polyethylene:  log Pf = K - 0.22 (PIvoc)
c       K = c1 - c2/T, T(K)    c2=3700.
c for liquids
c       P=Pf/Pvap(sat'd)
c therefore  (P1/P2) =  [Pf/Pvap(sat'd)]1/[Pf/Pvap(sat'd)]2
c
c assume same ratio relationship describes temperature effect for VOC gases
c permeability,diffusivity data for 25 C = 298.15 K
      t0=temp0
      call linert(nft,thr1,t0,t,tk,dt4)
      p1=10**(-3700/t0+vpb/(vpc+t0))
      p2=10**(-3700/tk+vpb/(vpc+tk))
      ptk=(p2/p1)*p
c assume diffusivity is proportional to T**1.823/P, T(K)
      dtk=d*(1./patm)*(tk/t0)**1.823
c dh2 - estimated H2-air diffusivity at 25 C, 1 atm  (cm2/s)
      dh2=0.611*(298.15/273.15)**1.823
c stp - P/RT (gmol/cm3) at standard pressure (1 atm) and temperature (273.2K)
      stp=1./(82.05*273.15)
c ptc - convert cm3 (STP) to cm3 (actual T,P)
      ptc=stp*(82.05*tk/patm)
c----------------------------------------------------------------------
c yp - first derivative of y with respect to t
c----------------------------------------------------------------------
c small bag (3 identical bags)
      s6=s0c0*patm*(y(1)+y(3))
      a=0.5*ptk*ap(1)*pHg*ptc/xp(1)
      b=dtk*ad(1)/xd(1)
c  g1 - fraction of moles in v(1) relative to v(3)
      g1=y(1)*v(1)/(y(1)*v(1)+y(3)*v(3))
      z1=ap(1)*xp(1)*stp
c rate of change of VOC concentration in innermost layer of confinement
      yp(1)=(a+b)*(y(3)-y(1))/v(1)-g1*yp(6)*z1/v(1)
c note: rate of VOC leaving three identical small bags and entering v(3)
      q=3.*(a+b)*(y(3)-y(1))
c----------------------------------------------------------------------
c small bag (one different bag)
      s9=0.
      a=0.5*ptk*ap(2)*pHg*ptc/xp(2)
      b=dtk*ad(2)/xd(2)
      if(y(2).gt.1.e-10)then
```

```
c  g2 - fraction of moles in v(2) relative to v(3)
        g2=y(2)*v(2)/(y(2)*v(2)+y(3)*v(3))
        z2=ap(2)*xp(2)*stp
        s9=s0c0*patm*(y(2)+y(3))
      else
        g2=0.
      end if
c rate of change of VOC concentration in one different small bag
      yp(2)=(a+b)*(y(3)-y(2))/v(2)-g2*yp(9)*z2/v(2)
c note: rate of VOC leaving one different small bag and entering v(3)
      q=q+(a+b)*(y(3)-y(2))
c-----------------------------------------------------------------------
c rate of change of VOC concentration in large poly bag
      s7=0.
      a=0.5*ptk*ap(3)*pHg*ptc/xp(3)
      b=dtk*ad(3)/xd(3)
        if(y(3).gt.1.e-10)then
c  g3 - fraction of moles in v(3) relative to v(4)
          g3=y(3)*v(3)/(y(3)*v(3)+y(4)*v(4))
          z3=ap(3)*xp(3)*stp
          s7=s0c0*patm*(y(3)+y(4))
        else
          g3=0.
        end if
      yp(3)=(-q+(a+b)*(y(4)-y(3))-3*(1-g1)*yp(6)*
     #z1-g3*yp(7)*z3-(1-g2)*yp(9)*z2)/v(3)
      q=(a+b)*(y(4)-y(3))
c
c rate of change of VOC concentration in liner headspace
      s8=0.
        if(y(4).gt.1.e-10)then
c  g4 - fraction of moles in v(4) relative to v(5)
          g4=y(4)*v(4)/(y(4)*v(4)+y(5)*v(5))
          g5=1-g4
          z4=ap(4)*xp(4)*stp
          s8=s0c0*patm*(y(4)+y(5))
        else
          g4=0.
          g5=0.
        end if
      a=ptk*ap(4)*pHg*ptc/xp(4)
      b=dtk*ad(4)/xd(4)
      if(dt4.gt.0.)then
        x4=y(4)*dt4/tk
      else
        x4=y(5)*dt4/tk
      end if
      yp(4)=(-q+(a+b)*(y(5)-y(4))-(1-g3)*yp(7)*
     #z3-g4*yp(8)*z4)/v(4)-x4
      q=(a+b)*(y(5)-y(4))
c
c rate of change of VOC concentration in drum headspace
      call headspt(nft,thr1,t0,t,t5,dt5)
      df=dfh*dtk/dh2
      if(dt5.gt.0.)then
        x5=y(5)*t5*(dt4/tk**2+dt5/t5**2)
      else
        x5=0.
      end if
      yp(5)=(-q-df*y(5)/c0-g5*yp(8)*z4)/v(5)+x4-x5
c
c rate of change of VOC content per small bag wall(6) - (three identical bags),
```

```
c     large bag(7), liner(8), small bag wall (9) - (one different bag)
c VOC-specific values for ak; specify which VOC using vpb
c carbon tetrachloride (vpb=1242.43)
      if(vpb.eq.1242.43)ak=8.e-6
c methylene chloride (vpb=1325.9)
      if(vpb.eq.1325.9)ak=1.e-6
c TCA (vpb=2136.6)
      if(vpb.eq.2136.6)ak=4.e-6
c TCE (vpb=1018.6)
      if(vpb.eq.1018.6)ak=4.e-6
c Freon-113 (vpb=1099.9)
      if(vpb.eq.1099.9)ak=8.e-7
c assume solubility is proportional to VOC concentration
      yp(6)=ak*(s6-y(6))
      yp(7)=ak*(s7-y(7))
      yp(8)=ak*(s8-y(8))
      yp(9)=ak*(s9-y(9))
      return
      end

      SUBROUTINE FCNJ(neq,t,y,dypdy)
      real y(neq),dypdy(*)
      return
      end

      subroutine vprop(i,c0,amw,pm,df,b,c,s0c0)
      real mw(9),p(9),d(9),vpb(9),vpc(9),sc(9)
c mw(i) - molecular weight of compound i
c p(i) - VOC i permeability across polyethylene at 25C, cm3 cm/cm2 s cm Hg
c df(i) - diffusion of VOC i in air at 25 C (Reference = ?)
c vpb(i) - Antoine equation coefficient, B, for i-th component
c vpc(i) - Antoine equation coefficient, C (K), for i-th component
c sc(i) - VOC solubility in polymer/[VOC]gas, (cm3 VOC/cm3 poly)(cm3/mol VOC)
c---------------------------------------------------------------------------
c 1 = carbon tetrachloride
      mw(1)=153.82
      p(1)=161.e-10
      d(1)=0.0828
      vpb(1)=1242.43
      vpc(1)=-43.15
c assumed value for normalized solubility
      sc(1)=0.025/(1000.*c0*1.e-6)
c 2 = cyclohexane
      mw(2)=84.1
      p(2)=1860.e-10
      d(2)=0.0750
      vpb(2)=1203.526
      vpc(2)=-50.287
      sc(2)=0.
c 3 = methanol
      mw(3)=32.0
      p(3)=19.e-10
      d(3)=0.152
      vpb(3)=1473.11
      vpc(3)=-43.15
      sc(3)=0.
c 4 = methylene chloride
      mw(4)=84.9
      p(4)=244.e-10
      d(4)=0.104
      vpb(4)=1325.9
      vpc(4)=-20.55
```

```
      sc(4)=0.023/(1006.*c0*1.e-6)
c 5 = toluene
      mw(5)=92.1
      p(5)=1100.e-10
      d(5)=0.0849
      vpb(5)=1343.943
      vpc(5)=-53.773
      sc(5)=0.
c 6 = TCA
      mw(6)=133.4
      p(6)=138.e-10
      d(6)=0.0794
      vpb(6)=2136.6
      vpc(6)=29.65
      sc(6)=0.017/(994.*c0*1.e-6)
c 7 = TCE
      mw(7)=131.4
      p(7)=311.e-10
      d(7)=0.0875
      vpb(7)=1018.6
      vpc(7)=-80.45
      sc(7)=0.013/(300.*c0*1.e-6)
c 8 = Freon-113
      mw(8)=187.4
      p(8)=27.e-10
c estimated diffusivity (Wilke-Lee eqn)
      d(8)=0.062
      vpb(8)=1099.9
      vpc(8)=-45.65
      sc(8)=0.016/(1010.*c0*1.e-6)
c 9 = p-xylene
      mw(9)=106.2
      p(9)=1000.e-10
      d(9)=0.0670
      vpb(9)=1453.43
      vpc(9)=-57.840
      sc(9)=0.
c
      amw=mw(i)
      pm=p(i)
      df=d(i)
      b=vpb(i)
      c=vpc(i)
      s0c0=sc(i)
      return
      end

      subroutine dti(y,dt)
      real ap(5),ad(5),v(5),xp(5),xd(5),mw
      common/qq/p,d,ap,ad,v,xp,xd,pi,patm,pHg,dfh,c0,mw,temp0,
     #vpb,vpc,y0,s0c0,nft,thrl
      pdy=y*(p*ap(1)*pHg/xp(1)+d*ad(1)/xd(1))/v(1)
      dt=60.*(1.e-15/pdy)**(0.25)
      return
      end

      subroutine linert(nft,thrl,t0,t,tk,dtl)
      x=t/86400.
      n=int(t)/86400
      dt=x-n
      tr=dt*86400.
      if(nft.eq.1)then
```

```
  tk=t0
  dtl=0.
else if(nft.eq.2)then
  thr=t/60.
  if(thr.lt.thrl)then
    tk=t0
    dtl=0.
  else
    if(dt.lt.14280./86400.)then
      tk=273.15+24.4287+22.231*(1.-exp(-1.014e-4*(tr+723.29)))
      dtl=22.231*1.014e-4*exp(-1.014e-4*(tr+723.29))
    else
      tk=273.15+26.539+31.32*exp(-8.174e-5*(tr+8370.18))
      dtl=-31.32*8.174e-5*exp(-8.174e-5*(tr+8370.18))
    end if
  end if
end if
return
end

subroutine headspt(nft,thrl,t0,t,tk,dth)
x=t/86400.
n=int(t)/86400
dt=x-n
tr=dt*86400.
if(nft.eq.1)then
  tk=t0
  dtl=0.
else if(nft.eq.2)then
  thr=t/60.
  if(thr.lt.thrl)then
    tk=t0
    dtl=0.
  else
    if(dt.lt.14280./86400.)then
      tk=273.15+25.3899+20.345*(1.-exp(-1.22e-4*(tr+797.7)))
      dth=20.345*1.22e-4*exp(-1.22e-4*(tr+797.7))
    else
      tk=273.15+27.454+41.456*exp(-8.451e-5*(tr+11583.84))
      dth=-8.451e-5*41.456*exp(-8.451e-5*(tr+11583.84))
    end if
  end if
end if
return
end
```

Appendix E

Computer Program Output for Lab-Scale Simulated Waste Drum VOC Transport Experiments

Trial 1.1

	Initial VOC concentration (ppmv)				
	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1012.0	1012.0	0.0	0.0	0.0
Freon-113	903.0	903.0	0.0	0.0	0.0
1,1,1-trichloroethane	977.0	977.0	0.0	0.0	0.0
carbon tetrachloride	305.0	305.0	0.0	0.0	0.0
trichloroethylene	310.0	310.0	0.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.01	4000.	0.01	15.00
1 small bag	2550.	0.01	4000.	0.01	15.00
Large bag	12800.	0.01	34000.	0.01	15.00
Drum liner	10000.	0.71	12000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7

Drum temperature during the trial: variable

Heating cycle began approximately 20.0 hrs after t=0

First samples collected from small bags approximately 19.0 hrs after t=0

Ambient pressure (cm Hg): 64.5

Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	229.0	229.0	515.9	515.9	239.7	239.7	63.7	63.7	53.5	53.5
2	182.0	182.0	314.1	314.1	166.2	166.2	38.0	38.0	29.0	29.0
3	157.1	157.1	249.7	249.7	136.8	136.8	30.8	30.8	21.8	21.8
4	138.0	138.0	216.7	216.7	118.8	118.8	27.3	27.3	18.6	18.6
5	122.7	122.7	195.7	195.7	107.4	107.4	25.4	25.4	17.1	17.1
6	110.3	110.3	180.2	180.2	99.9	99.9	24.1	24.1	16.3	16.3
7	100.2	100.2	167.6	167.6	94.6	94.6	23.3	23.3	15.7	15.7
8	91.9	91.9	156.8	156.8	90.7	90.7	22.6	22.6	15.4	15.4
9	85.2	85.2	147.4	147.4	87.8	87.8	22.1	22.1	15.1	15.1
10	79.6	79.6	139.1	139.1	85.4	85.4	21.7	21.7	14.9	14.9
11	75.0	75.0	131.7	131.7	83.4	83.4	21.3	21.3	14.7	14.7
12	71.1	71.1	125.0	125.0	81.7	81.7	20.9	20.9	14.5	14.5
13	67.9	67.9	119.0	119.0	80.1	80.1	20.6	20.6	14.4	14.4
14	65.1	65.1	113.5	113.5	78.7	78.7	20.3	20.3	14.2	14.2
15	62.8	62.8	108.6	108.6	77.4	77.4	20.1	20.1	14.1	14.1
16	60.7	60.7	104.1	104.1	76.1	76.1	19.8	19.8	13.9	13.9
17	58.9	58.9	100.1	100.1	74.9	74.9	19.5	19.5	13.8	13.8
18	57.4	57.4	96.4	96.4	73.7	73.7	19.3	19.3	13.7	13.7
19	56.0	56.0	93.0	93.0	72.5	72.5	19.0	19.0	13.5	13.5
20	54.7	54.7	89.9	89.9	71.4	71.4	18.8	18.8	13.4	13.4
21	53.6	53.6	87.0	87.0	70.3	70.3	18.6	18.6	13.3	13.3

Trial 1.1 (continued)

Other predicted VOC concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace
1	220.6	91.0	153.5	6.1	208.9	39.6	54.4	7.6	49.3	12.5
2	177.8	117.6	197.8	32.1	156.4	61.2	35.6	11.8	27.7	11.9
3	154.1	110.1	195.6	51.3	130.9	65.4	29.7	14.6	21.2	12.3
4	135.6	100.1	185.4	63.2	115.2	67.8	26.8	16.5	18.4	12.9
5	120.7	91.3	174.0	69.2	105.1	69.7	25.0	17.6	17.0	13.3
6	108.7	84.0	163.2	71.6	98.3	70.9	23.9	18.3	16.2	13.5
7	98.9	78.0	153.4	71.9	93.5	71.6	23.1	18.7	15.7	13.6
8	90.9	73.1	144.5	71.2	90.0	71.8	22.5	18.8	15.4	13.6
9	84.4	69.0	136.6	70.0	87.2	71.7	22.0	18.9	15.1	13.6
10	78.9	65.6	129.5	68.5	85.0	71.3	21.6	18.8	14.9	13.5
11	74.4	62.8	123.0	67.0	83.1	70.7	21.2	18.6	14.7	13.5
12	70.7	60.4	117.2	65.5	81.4	70.1	20.9	18.5	14.5	13.4
13	67.5	58.4	111.9	64.1	79.9	69.3	20.6	18.3	14.4	13.3
14	64.8	56.6	107.2	62.7	78.5	68.4	20.3	18.1	14.2	13.2
15	62.5	55.0	102.8	61.5	77.1	67.5	20.0	17.9	14.1	13.1
16	60.5	53.6	98.9	60.4	75.9	66.6	19.8	17.7	13.9	13.0
17	58.8	52.4	95.3	59.3	74.7	65.7	19.5	17.5	13.8	12.9
18	57.2	51.3	92.0	58.3	73.5	64.8	19.3	17.3	13.7	12.8
19	55.8	50.2	89.0	57.2	72.4	63.8	19.0	17.1	13.5	12.7
20	54.6	49.3	86.2	56.3	71.3	62.9	18.8	16.9	13.4	12.6
21	53.5	48.4	83.7	55.4	70.2	62.0	18.5	16.6	13.3	12.4

Trial 1.3

	Initial VOC concentration (ppmv)				
	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1012.0	1012.0	58.0	0.0	0.0
Freon-113	903.0	903.0	52.0	0.0	0.0
1,1,1-trichloroethane	977.0	977.0	53.0	0.0	0.0
carbon tetrachloride	305.0	305.0	17.0	0.0	0.0
trichloroethylene	310.0	310.0	18.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.00	4000.	0.01	0.23
1 small bag	2550.	0.03	2000.	0.01	0.43
Large bag	12800.	0.01	35000.	0.01	15.00
Drum liner	10000.	0.71	13000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7

Drum temperature during the trial: constant

First samples collected from small bags approximately 20.0 hrs after t=0

Ambient pressure (cm Hg): 64.5

Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	237.9	228.8	587.8	358.1	263.3	216.1	70.2	58.9	55.5	52.6
2	189.4	186.6	381.7	220.4	175.0	167.5	40.9	38.9	30.8	29.9
3	164.8	162.8	297.3	204.0	143.9	139.7	32.8	31.9	23.1	22.7
4	146.2	144.7	249.9	196.5	125.1	122.4	28.9	28.4	19.6	19.4
5	131.4	130.2	220.4	188.1	113.1	111.4	26.7	26.4	17.9	17.8
6	119.4	118.4	200.2	178.8	105.2	104.1	25.3	25.1	17.0	16.9
7	109.7	108.8	185.0	169.6	99.8	99.0	24.3	24.2	16.4	16.4
8	101.7	101.0	172.9	160.9	96.0	95.4	23.7	23.6	16.1	16.0
9	95.1	94.5	162.8	153.0	93.2	92.8	23.1	23.1	15.8	15.8
10	89.7	89.2	154.1	145.7	91.0	90.7	22.7	22.7	15.6	15.6
11	85.2	84.8	146.5	139.2	89.3	89.1	22.4	22.4	15.5	15.4
12	81.4	81.1	139.7	133.3	87.9	87.7	22.2	22.1	15.3	15.3
13	78.3	78.0	133.7	127.9	86.8	86.6	21.9	21.9	15.2	15.2
14	75.6	75.4	128.3	123.1	85.7	85.6	21.7	21.7	15.1	15.1
15	73.4	73.2	123.4	118.7	84.8	84.7	21.6	21.5	15.0	15.0
16	71.5	71.3	119.0	114.8	84.0	83.8	21.4	21.4	14.9	14.9
17	69.8	69.7	115.0	111.1	83.2	83.1	21.2	21.2	14.8	14.8
18	68.4	68.2	111.3	107.9	82.4	82.3	21.1	21.1	14.7	14.7
19	67.1	67.0	108.0	104.9	81.7	81.6	20.9	20.9	14.7	14.7
20	66.0	65.9	105.0	102.1	81.0	80.9	20.8	20.8	14.6	14.6
21	65.0	64.9	102.3	99.6	80.4	80.3	20.7	20.6	14.5	14.5

Trial 1.3 (continued)

Other predicted VOC concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace
1	225.1	79.8	162.0	5.9	210.4	34.2	55.9	6.8	50.5	11.7
2	184.3	114.0	197.8	26.2	162.3	56.7	37.6	10.7	29.2	11.6
3	161.1	111.4	198.4	43.0	136.4	62.4	31.3	13.5	22.4	12.0
4	143.3	103.9	191.3	55.4	120.4	66.1	28.1	15.6	19.3	12.7
5	129.1	96.3	182.0	63.6	110.0	69.1	26.2	17.1	17.7	13.2
6	117.5	89.8	172.5	68.5	103.1	71.4	25.0	18.1	16.9	13.6
7	108.1	84.4	163.5	71.2	98.4	73.2	24.1	18.8	16.4	13.8
8	100.4	80.0	155.3	72.6	94.9	74.3	23.5	19.2	16.0	13.9
9	94.0	76.3	147.8	73.0	92.4	75.1	23.0	19.4	15.8	14.0
10	88.8	73.3	141.1	72.9	90.4	75.5	22.6	19.5	15.6	14.0
11	84.4	70.7	135.0	72.5	88.8	75.6	22.3	19.6	15.4	14.0
12	80.8	68.6	129.5	72.0	87.5	75.6	22.1	19.6	15.3	14.0
13	77.8	66.8	124.5	71.3	86.4	75.4	21.9	19.5	15.2	14.0
14	75.2	65.2	120.0	70.7	85.4	75.1	21.7	19.5	15.1	14.0
15	73.0	63.9	115.9	70.1	84.5	74.8	21.5	19.4	15.0	13.9
16	71.1	62.7	112.2	69.4	83.7	74.4	21.3	19.3	14.9	13.9
17	69.5	61.7	108.8	68.9	82.9	74.0	21.2	19.2	14.8	13.8
18	68.1	60.8	105.7	68.3	82.2	73.5	21.0	19.1	14.7	13.8
19	66.9	60.0	102.9	67.8	81.5	73.0	20.9	19.0	14.6	13.7
20	65.8	59.2	100.3	67.3	80.8	72.5	20.8	18.9	14.6	13.7
21	64.8	58.5	98.0	66.8	80.2	72.0	20.6	18.7	14.5	13.6

Trial 2.1

	Initial VOC concentration (ppmv)				
	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1012.0	1012.0	58.0	0.0	0.0
Freon-113	903.0	903.0	52.0	0.0	0.0
1,1,1-trichloroethane	977.0	977.0	53.0	0.0	0.0
carbon tetrachloride	305.0	305.0	17.0	0.0	0.0
trichloroethylene	310.0	310.0	18.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.00	4000.	0.01	0.23
1 small bag	2550.	0.03	2000.	0.01	0.43
Large bag	12800.	0.01	35000.	0.01	15.00
Drum liner	10000.	0.71	13000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7
Drum temperature during the trial: variable
Heating cycle began approximately 21.0 hrs after t=0
First samples collected from small bags approximately 24.0 hrs after t=0
Ambient pressure (cm Hg): 64.5
Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	218.7	214.7	485.8	276.3	220.7	203.4	56.5	51.8	46.9	45.0
2	181.4	179.2	326.9	211.6	164.2	158.7	37.5	36.1	28.7	28.0
3	156.4	154.8	256.4	200.7	134.7	131.5	30.3	29.7	21.5	21.3
4	137.2	136.0	219.4	190.5	117.0	115.0	27.0	26.7	18.5	18.3
5	121.9	120.9	196.4	179.0	105.7	104.5	25.1	24.9	17.0	16.9
6	109.5	108.7	179.8	167.7	98.3	97.5	23.9	23.8	16.2	16.1
7	99.4	98.8	166.7	157.2	93.2	92.7	23.0	23.0	15.7	15.7
8	91.2	90.7	155.6	147.8	89.5	89.1	22.4	22.4	15.3	15.3
9	84.5	84.1	146.1	139.3	86.6	86.3	21.9	21.9	15.1	15.1
10	79.0	78.6	137.7	131.7	84.3	84.1	21.5	21.5	14.9	14.9
11	74.4	74.1	130.2	124.8	82.4	82.2	21.1	21.1	14.7	14.7
12	70.6	70.3	123.4	118.7	80.7	80.5	20.8	20.8	14.5	14.5
13	67.3	67.2	117.4	113.1	79.1	79.0	20.5	20.5	14.3	14.3
14	64.6	64.5	112.0	108.1	77.7	77.6	20.2	20.2	14.2	14.2
15	62.3	62.2	107.1	103.6	76.4	76.3	19.9	19.9	14.1	14.0
16	60.3	60.2	102.6	99.4	75.1	75.0	19.7	19.6	13.9	13.9
17	58.5	58.4	98.5	95.7	73.9	73.8	19.4	19.4	13.8	13.8
18	56.9	56.9	94.9	92.2	72.7	72.6	19.2	19.1	13.6	13.6
19	55.5	55.5	91.5	89.1	71.6	71.5	18.9	18.9	13.5	13.5
20	54.3	54.2	88.4	86.2	70.5	70.4	18.7	18.7	13.4	13.4
21	53.2	53.1	85.6	83.6	69.4	69.3	18.4	18.4	13.3	13.3

Trial 2.1 (continued)

Other predicted VOC concentrations (ppmv):

Day	methylene chloride Large bag	methylene chloride Drum headspace	Freon-113 Large bag	Freon-113 Drum headspace	1,1,1-trichloroethane Large bag	1,1,1-trichloroethane Drum headspace	carbon tetrachloride Large bag	carbon tetrachloride Drum headspace	trichloroethylene Large bag	trichloroethylene Drum headspace
1	211.5	103.4	185.0	12.5	196.8	47.6	49.1	8.8	43.5	12.9
2	177.2	118.6	202.0	36.2	154.3	62.5	35.0	12.2	27.4	12.2
3	153.4	110.7	195.8	54.7	128.9	66.1	29.3	14.8	21.0	12.5
4	134.8	100.5	184.6	65.5	113.4	68.2	26.4	16.6	18.2	13.0
5	120.0	91.5	172.8	70.8	103.5	69.7	24.8	17.7	16.9	13.3
6	108.0	84.0	161.9	72.7	96.9	70.7	23.7	18.4	16.1	13.5
7	98.2	77.9	151.9	72.8	92.2	71.3	22.9	18.7	15.6	13.6
8	90.2	73.0	143.0	71.8	88.8	71.3	22.3	18.8	15.3	13.6
9	83.7	68.8	135.1	70.4	86.1	71.1	21.8	18.8	15.1	13.6
10	78.3	65.4	127.9	68.8	83.9	70.7	21.4	18.7	14.9	13.5
11	73.9	62.5	121.4	67.2	82.0	70.0	21.1	18.5	14.7	13.5
12	70.1	60.1	115.6	65.6	80.4	69.3	20.7	18.4	14.5	13.4
13	67.0	58.0	110.4	64.1	78.9	68.5	20.4	18.2	14.3	13.3
14	64.3	56.2	105.6	62.7	77.5	67.6	20.2	18.0	14.2	13.2
15	62.0	54.6	101.3	61.3	76.2	66.7	19.9	17.8	14.0	13.1
16	60.1	53.3	97.4	60.1	74.9	65.7	19.6	17.6	13.9	13.0
17	58.3	52.0	93.8	59.0	73.7	64.8	19.4	17.3	13.8	12.9
18	56.8	50.9	90.5	57.9	72.6	63.9	19.1	17.1	13.6	12.7
19	55.4	49.9	87.5	56.9	71.4	63.0	18.9	16.9	13.5	12.6
20	54.2	48.9	84.8	55.9	70.3	62.0	18.6	16.7	13.4	12.5
21	53.1	48.0	82.3	55.0	69.2	61.1	18.4	16.5	13.3	12.4

Trial 2.3

	Initial VOC concentration (ppmv)				
	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1012.0	1012.0	0.0	0.0	0.0
Freon-113	903.0	903.0	0.0	0.0	0.0
1,1,1-trichloroethane	977.0	977.0	0.0	0.0	0.0
carbon tetrachloride	305.0	305.0	0.0	0.0	0.0
trichloroethylene	310.0	310.0	0.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.01	4000.	0.01	15.00
1 small bag	2550.	0.01	4000.	0.01	15.00
Large bag	12800.	0.01	34000.	0.01	15.00
Drum liner	10000.	0.71	12000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7

Drum temperature during the trial: constant

First samples collected from small bags approximately 27.0 hrs after t=0

Ambient pressure (cm Hg): 64.5

Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	221.4	221.4	501.4	501.4	226.3	226.3	58.4	58.4	46.8	46.8
2	190.0	190.0	365.8	365.8	177.0	177.0	41.5	41.5	31.2	31.2
3	165.4	165.4	286.6	286.6	146.0	146.0	33.3	33.3	23.3	23.3
4	146.8	146.8	243.7	243.7	127.0	127.0	29.3	29.3	19.8	19.8
5	132.0	132.0	217.3	217.3	114.8	114.8	27.0	27.0	18.0	18.0
6	120.0	120.0	198.9	198.9	106.7	106.7	25.6	25.6	17.1	17.1
7	110.2	110.2	184.8	184.8	101.1	101.1	24.6	24.6	16.5	16.5
8	102.1	102.1	173.3	173.3	97.2	97.2	23.8	23.8	16.1	16.1
9	95.5	95.5	163.5	163.5	94.2	94.2	23.3	23.3	15.8	15.8
10	90.0	90.0	155.0	155.0	92.0	92.0	22.9	22.9	15.6	15.6
11	85.5	85.5	147.5	147.5	90.2	90.2	22.5	22.5	15.4	15.4
12	81.7	81.7	140.8	140.8	88.7	88.7	22.3	22.3	15.3	15.3
13	78.5	78.5	134.8	134.8	87.5	87.5	22.0	22.0	15.2	15.2
14	75.9	75.9	129.3	129.3	86.4	86.4	21.8	21.8	15.1	15.1
15	73.6	73.6	124.4	124.4	85.5	85.5	21.6	21.6	15.0	15.0
16	71.6	71.6	120.0	120.0	84.6	84.6	21.5	21.5	14.9	14.9
17	70.0	70.0	116.0	116.0	83.8	83.8	21.3	21.3	14.8	14.8
18	68.5	68.5	112.3	112.3	83.1	83.1	21.2	21.2	14.7	14.7
19	67.2	67.2	109.0	109.0	82.3	82.3	21.0	21.0	14.6	14.6
20	66.1	66.1	105.9	105.9	81.6	81.6	20.9	20.9	14.6	14.6
21	65.1	65.1	103.1	103.1	81.0	81.0	20.7	20.7	14.5	14.5

Trial 2.3 (continued)

Other predicted VOC concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace
1	213.2	94.6	157.1	7.4	199.5	41.7	50.2	7.6	43.2	11.4
2	184.9	112.6	189.5	22.0	164.5	55.2	38.2	10.3	29.6	11.2
3	161.7	110.4	196.2	39.0	138.5	61.3	31.8	13.1	22.6	11.7
4	143.9	103.1	191.3	52.1	122.2	65.4	28.5	15.4	19.4	12.5
5	129.7	95.8	182.8	60.9	111.7	68.6	26.5	16.9	17.8	13.1
6	118.1	89.4	173.5	66.4	104.5	71.2	25.2	18.0	16.9	13.5
7	108.6	84.1	164.6	69.5	99.6	73.1	24.3	18.7	16.4	13.7
8	100.8	79.8	156.4	71.0	96.0	74.4	23.7	19.1	16.0	13.9
9	94.4	76.2	148.9	71.7	93.4	75.3	23.2	19.4	15.8	13.9
10	89.1	73.2	142.2	71.7	91.3	75.8	22.8	19.6	15.6	14.0
11	84.8	70.7	136.1	71.5	89.7	76.0	22.5	19.6	15.4	14.0
12	81.1	68.6	130.6	71.0	88.3	76.0	22.2	19.6	15.3	14.0
13	78.0	66.8	125.6	70.5	87.1	75.9	22.0	19.6	15.2	14.0
14	75.4	65.3	121.0	70.0	86.1	75.7	21.8	19.6	15.1	14.0
15	73.2	63.9	116.9	69.4	85.2	75.3	21.6	19.5	15.0	13.9
16	71.3	62.8	113.2	68.9	84.3	74.9	21.4	19.4	14.9	13.9
17	69.7	61.8	109.7	68.3	83.6	74.5	21.3	19.3	14.8	13.8
18	68.3	60.8	106.6	67.8	82.8	74.1	21.1	19.2	14.7	13.8
19	67.0	60.0	103.8	67.4	82.1	73.6	21.0	19.1	14.6	13.7
20	65.9	59.3	101.2	66.9	81.4	73.1	20.8	19.0	14.5	13.7
21	64.9	58.6	98.8	66.5	80.7	72.6	20.7	18.8	14.5	13.6

Trial 3.1

	Initial VOC concentration (ppmv)				
	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1012.0	1012.0	0.0	0.0	0.0
Freon-113	903.0	903.0	0.0	0.0	0.0
1,1,1-trichloroethane	977.0	977.0	0.0	0.0	0.0
carbon tetrachloride	305.0	305.0	0.0	0.0	0.0
trichloroethylene	310.0	310.0	0.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.01	4000.	0.01	15.00
1 small bag	2550.	0.01	4000.	0.01	15.00
Large bag	12800.	0.01	34000.	0.01	15.00
Drum liner	10000.	0.71	12000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7
Drum temperature during the trial: variable
Heating cycle began approximately 22.0 hrs after t=0
First samples collected from small bags approximately 21.0 hrs after t=0
Ambient pressure (cm Hg): 64.5
Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	224.7	224.7	495.9	495.9	231.4	231.4	60.6	60.6	50.8	50.8
2	182.0	182.0	314.2	314.2	166.3	166.3	38.0	38.0	29.0	29.0
3	157.1	157.1	249.8	249.8	136.8	136.8	30.8	30.8	21.8	21.8
4	138.0	138.0	216.7	216.7	118.8	118.8	27.3	27.3	18.6	18.6
5	122.7	122.7	195.7	195.7	107.4	107.4	25.4	25.4	17.1	17.1
6	110.3	110.3	180.2	180.2	99.9	99.9	24.1	24.1	16.3	16.3
7	100.2	100.2	167.6	167.6	94.6	94.6	23.3	23.3	15.7	15.7
8	91.9	91.9	156.8	156.8	90.7	90.7	22.6	22.6	15.4	15.4
9	85.2	85.2	147.4	147.4	87.8	87.8	22.1	22.1	15.1	15.1
10	79.6	79.6	139.1	139.1	85.4	85.4	21.7	21.7	14.9	14.9
11	75.0	75.0	131.7	131.7	83.4	83.4	21.3	21.3	14.7	14.7
12	71.1	71.1	125.0	125.0	81.7	81.7	20.9	20.9	14.5	14.5
13	67.9	67.9	119.0	119.0	80.1	80.1	20.6	20.6	14.4	14.4
14	65.1	65.1	113.5	113.5	78.7	78.7	20.3	20.3	14.2	14.2
15	62.8	62.8	108.6	108.6	77.4	77.4	20.1	20.1	14.1	14.1
16	60.7	60.7	104.1	104.1	76.1	76.1	19.8	19.8	13.9	13.9
17	59.0	59.0	100.1	100.1	74.8	74.8	19.5	19.5	13.8	13.8
18	57.4	57.4	96.4	96.4	73.7	73.7	19.3	19.3	13.7	13.7
19	56.0	56.0	93.0	93.0	72.5	72.5	19.0	19.0	13.5	13.5
20	54.7	54.7	89.9	89.9	71.4	71.4	18.8	18.8	13.4	13.4
21	53.6	53.6	87.0	87.0	70.3	70.3	18.6	18.6	13.3	13.3

Trial 3.1 (continued)

Other predicted VOC concentrations (ppmv):

Day	methylene chloride Large bag	methylene chloride Drum headspace	Freon-113 Large bag	Freon-113 Drum headspace	1,1,1-trichloroethane Large bag	1,1,1-trichloroethane Drum headspace	carbon tetrachloride Large bag	carbon tetrachloride Drum headspace	trichloroethylene Large bag	trichloroethylene Drum headspace
1	216.9	95.7	159.5	7.3	204.9	42.3	52.4	7.9	47.0	12.5
2	177.8	117.6	197.8	32.1	156.4	61.2	35.6	11.8	27.7	11.9
3	154.1	110.1	195.6	51.3	130.9	65.3	29.7	14.6	21.2	12.3
4	135.6	100.1	185.4	63.2	115.2	67.8	26.8	16.5	18.4	12.9
5	120.7	91.3	174.0	69.2	105.1	69.7	25.0	17.6	17.0	13.3
6	108.7	84.0	163.2	71.6	98.3	70.9	23.9	18.3	16.2	13.5
7	98.9	78.0	153.4	71.9	93.5	71.5	23.1	18.7	15.7	13.6
8	90.9	73.1	144.5	71.2	90.0	71.8	22.5	18.8	15.4	13.6
9	84.4	69.0	136.6	69.9	87.2	71.7	22.0	18.9	15.1	13.6
10	79.0	65.6	129.4	68.5	85.0	71.3	21.6	18.8	14.9	13.5
11	74.4	62.8	123.0	67.0	83.0	70.7	21.2	18.7	14.7	13.5
12	70.7	60.4	117.2	65.5	81.4	70.0	20.9	18.5	14.5	13.4
13	67.5	58.3	111.9	64.1	79.9	69.2	20.6	18.3	14.4	13.3
14	64.8	56.6	107.2	62.8	78.5	68.4	20.3	18.1	14.2	13.2
15	62.5	55.0	102.8	61.5	77.1	67.5	20.0	17.9	14.1	13.1
16	60.5	53.7	98.9	60.4	75.9	66.6	19.8	17.7	13.9	13.0
17	58.8	52.4	95.3	59.3	74.7	65.7	19.5	17.5	13.8	12.9
18	57.2	51.3	92.0	58.3	73.5	64.8	19.3	17.3	13.7	12.8
19	55.9	50.2	89.0	57.3	72.4	63.8	19.0	17.1	13.5	12.7
20	54.6	49.3	86.2	56.3	71.3	62.9	18.8	16.9	13.4	12.6
21	53.5	48.4	83.7	55.4	70.2	62.0	18.5	16.6	13.3	12.4

Trial 3.4

Initial VOC concentration (ppmv)

	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1012.0	0.0	0.0	0.0	0.0
Freon-113	903.0	0.0	0.0	0.0	0.0
1,1,1-trichloroethane	977.0	0.0	0.0	0.0	0.0
carbon tetrachloride	305.0	0.0	0.0	0.0	0.0
trichloroethylene	310.0	0.0	0.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.00	4000.	0.01	0.23
1 small bag	2550.	0.00	100.	0.01	0.23
Large bag	12800.	0.01	36000.	0.01	15.00
Drum liner	10000.	0.71	14000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7

Drum temperature during the trial: constant

First samples collected from small bags approximately 24.0 hrs after t=0

Ambient pressure (cm Hg): 64.5

Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	172.4	164.6	517.6	106.4	189.8	155.6	49.3	40.3	38.0	34.9
2	142.6	138.7	338.7	140.9	134.1	124.1	31.3	28.6	23.2	21.9
3	123.8	121.1	249.9	148.1	109.5	103.7	24.8	23.6	17.2	16.7
4	109.7	107.6	202.3	145.3	94.8	91.2	21.8	21.1	14.6	13.3
5	98.6	96.8	174.3	139.1	85.5	83.1	20.1	19.7	13.4	7.6
6	89.5	88.1	156.1	132.0	79.4	77.8	19.0	18.8	12.7	11.4
7	82.2	81.0	143.1	125.1	75.3	74.2	18.3	18.1	12.3	15.3
8	76.2	75.2	133.0	118.7	72.4	71.6	17.8	17.6	12.1	11.8
9	71.2	70.4	124.7	112.8	70.2	69.7	17.4	17.3	11.9	13.2
10	67.1	66.5	117.7	107.5	68.6	68.2	17.1	17.0	11.7	10.2
11	63.8	63.2	111.7	102.7	67.4	67.0	16.9	16.8	11.6	15.1
12	61.0	60.5	106.3	98.3	66.3	66.0	16.7	16.6	11.5	9.1
13	58.6	58.2	101.6	94.4	65.4	65.2	16.5	16.4	11.4	7.4
14	56.6	56.3	97.3	90.9	64.7	64.4	16.3	16.3	11.3	12.8
15	55.0	54.7	93.5	87.7	64.0	63.8	16.2	16.2	11.3	17.7
16	53.5	53.3	90.0	84.8	63.3	63.2	16.1	16.1	11.2	4.0
17	52.3	52.1	86.9	82.2	62.8	62.6	16.0	15.9	11.1	6.9
18	51.2	51.0	84.1	79.8	62.2	62.0	15.9	15.8	11.1	17.7
19	50.3	50.1	81.5	77.6	61.7	61.5	15.7	15.7	11.0	14.3
20	49.4	49.3	79.2	75.6	61.2	61.0	15.6	15.6	10.9	9.3
21	48.7	48.6	77.1	73.8	60.7	60.5	15.5	15.5	10.9	10.6

Trial 3.4 (continued)

Other predicted VOC concentrations (ppmv):

Day	methylene chloride Large bag	methylene chloride Drum headspace	Freon-113 Large bag	Freon-113 Drum headspace	1,1,1-trichloroethane Large bag	1,1,1-trichloroethane Drum headspace	carbon tetrachloride Large bag	carbon tetrachloride Drum headspace	trichloroethylene Large bag	trichloroethylene Drum headspace
1	164.5	66.2	108.8	3.7	155.4	28.7	40.2	5.6	34.8	9.2
2	138.6	85.9	141.6	15.2	123.9	43.1	28.6	8.1	21.9	8.9
3	121.0	84.3	148.1	28.1	103.6	47.6	23.6	10.2	16.7	9.1
4	107.5	78.6	145.1	38.5	91.1	50.3	21.1	11.8	14.4	9.5
5	96.8	72.8	138.8	45.8	83.1	52.5	19.7	12.9	13.3	9.9
6	88.1	67.8	131.8	50.4	77.8	54.1	18.7	13.7	12.6	10.2
7	81.0	63.7	124.8	53.1	74.2	55.4	18.1	14.1	12.3	10.3
8	75.2	60.2	118.4	54.5	71.6	56.2	17.6	14.4	12.0	10.4
9	70.4	57.4	112.6	55.1	69.6	56.7	17.3	14.6	11.9	10.5
10	66.5	55.1	107.3	55.1	68.2	57.0	17.0	14.7	11.7	10.5
11	63.2	53.1	102.5	54.9	67.0	57.1	16.8	14.7	11.6	10.5
12	60.5	51.5	98.2	54.5	66.0	57.0	16.6	14.7	11.5	10.5
13	58.2	50.1	94.3	54.0	65.2	56.9	16.4	14.7	11.4	10.5
14	56.3	48.9	90.8	53.5	64.4	56.7	16.3	14.6	11.3	10.5
15	54.7	47.9	87.6	53.0	63.8	56.4	16.2	14.6	11.2	10.5
16	53.3	47.0	84.7	52.5	63.1	56.1	16.1	14.5	11.2	10.4
17	52.1	46.2	82.1	52.0	62.6	55.8	15.9	14.4	11.1	10.4
18	51.0	45.5	79.7	51.5	62.0	55.4	15.8	14.3	11.0	10.3
19	50.1	44.9	77.5	51.1	61.5	55.0	15.7	14.3	11.0	10.3
20	49.3	44.3	75.6	50.7	61.0	54.7	15.6	14.2	10.9	10.2
21	48.6	43.8	73.7	50.3	60.5	54.3	15.5	14.1	10.9	10.2

Trial 4.1

Initial VOC concentration (ppmv)

	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1010.0	1010.0	0.0	0.0	0.0
Freon-113	1010.0	1010.0	0.0	0.0	0.0
1,1,1-trichloroethane	1020.0	1020.0	0.0	0.0	0.0
carbon tetrachloride	301.0	301.0	0.0	0.0	0.0
trichloroethylene	297.0	297.0	0.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.00	4000.	0.01	0.23
1 small bag	2550.	0.00	4000.	0.01	0.23
Large bag	12800.	0.01	34000.	0.01	15.00
Drum liner	10000.	0.71	12000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7

Drum temperature during the trial: variable

Heating cycle began approximately 23.0 hrs after t=0

First samples collected from small bags approximately 23.0 hrs after t=0

Ambient pressure (cm Hg): 64.5

Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	220.4	220.4	534.1	534.1	234.0	234.0	57.2	57.2	46.3	46.3
2	181.6	181.6	351.8	351.8	173.6	173.6	37.5	37.5	27.8	27.8
3	156.8	156.8	279.5	279.5	142.8	142.8	30.4	30.4	20.9	20.9
4	137.7	137.7	242.4	242.4	124.1	124.1	27.0	27.0	17.8	17.8
5	122.4	122.4	219.0	219.0	112.2	112.2	25.0	25.0	16.4	16.4
6	110.0	110.0	201.6	201.6	104.2	104.2	23.8	23.8	15.6	15.6
7	100.0	100.0	187.5	187.5	98.7	98.7	23.0	23.0	15.1	15.1
8	91.7	91.7	175.5	175.5	94.7	94.7	22.3	22.3	14.7	14.7
9	85.0	85.0	165.0	165.0	91.6	91.6	21.8	21.8	14.5	14.5
10	79.4	79.4	155.6	155.6	89.1	89.1	21.4	21.4	14.3	14.3
11	74.8	74.8	147.3	147.3	87.1	87.1	21.0	21.0	14.1	14.1
12	71.0	71.0	139.8	139.8	85.3	85.3	20.7	20.7	13.9	13.9
13	67.7	67.7	133.1	133.1	83.6	83.6	20.4	20.4	13.8	13.8
14	65.0	65.0	127.0	127.0	82.2	82.2	20.1	20.1	13.6	13.6
15	62.6	62.6	121.5	121.5	80.8	80.8	19.8	19.8	13.5	13.5
16	60.6	60.6	116.5	116.5	79.4	79.4	19.5	19.5	13.3	13.3
17	58.8	58.8	112.0	112.0	78.1	78.1	19.3	19.3	13.2	13.2
18	57.3	57.3	107.8	107.8	76.9	76.9	19.0	19.0	13.1	13.1
19	55.9	55.9	104.0	104.0	75.7	75.7	18.8	18.8	13.0	13.0
20	54.6	54.6	100.6	100.6	74.5	74.5	18.6	18.6	12.8	12.8
21	53.4	53.4	97.4	97.4	73.4	73.4	18.3	18.3	12.7	12.7

Trial 4.1 (continued)

Other predicted VOC concentrations (ppmv):

Day	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace
1	213.1	99.6	184.3	9.7	209.6	46.7	49.9	8.1	42.9	11.9
2	177.5	117.3	221.1	35.9	163.3	63.9	35.1	11.6	26.6	11.4
3	153.8	109.8	218.7	57.4	136.7	68.2	29.3	14.4	20.4	11.8
4	135.3	99.9	207.4	70.6	120.3	70.8	26.4	16.3	17.6	12.3
5	120.5	91.1	194.7	77.4	109.8	72.7	24.7	17.4	16.2	12.7
6	108.5	83.8	182.6	80.0	102.6	74.0	23.6	18.1	15.5	12.9
7	98.7	77.8	171.6	80.4	97.6	74.7	22.8	18.4	15.0	13.0
8	90.7	72.9	161.7	79.6	93.9	75.0	22.2	18.6	14.7	13.0
9	84.2	68.9	152.8	78.2	91.0	74.8	21.7	18.6	14.5	13.0
10	78.8	65.5	144.8	76.6	88.7	74.4	21.3	18.5	14.3	13.0
11	74.3	62.6	137.6	74.9	86.7	73.8	20.9	18.4	14.1	12.9
12	70.5	60.3	131.1	73.3	84.9	73.1	20.6	18.3	13.9	12.8
13	67.4	58.2	125.2	71.7	83.4	72.3	20.3	18.1	13.8	12.7
14	64.7	56.4	119.9	70.2	81.9	71.4	20.0	17.9	13.6	12.7
15	62.4	54.9	115.1	68.8	80.5	70.5	19.8	17.7	13.5	12.5
16	60.4	53.5	110.6	67.5	79.2	69.5	19.5	17.5	13.3	12.4
17	58.7	52.3	106.6	66.3	77.9	68.6	19.3	17.2	13.2	12.3
18	57.1	51.1	102.9	65.1	76.7	67.6	19.0	17.0	13.1	12.2
19	55.7	50.1	99.6	64.0	75.5	66.6	18.8	16.8	13.0	12.1
20	54.5	49.2	96.5	63.0	74.4	65.7	18.5	16.6	12.8	12.0
21	53.4	48.3	93.6	62.0	73.2	64.7	18.3	16.4	12.7	11.9

Trial 4.3

	Initial VOC concentration (ppmv)				
	3 small bags	1 small bag	Large bag	Drum liner	Drum headspace
methylene chloride	1010.0	1010.0	0.0	0.0	0.0
Freon-113	1010.0	1010.0	0.0	0.0	0.0
1,1,1-trichloroethane	1020.0	1020.0	0.0	0.0	0.0
carbon tetrachloride	301.0	301.0	0.0	0.0	0.0
trichloroethylene	297.0	297.0	0.0	0.0	0.0

Model parameters:

	Ap(cm2)	Ad(cm2)	V(cm3)	xp(cm)	xd(cm)
3 small bags	2550.	0.01	4000.	0.01	15.00
1 small bag	2550.	0.01	4000.	0.01	15.00
Large bag	12800.	0.01	34000.	0.01	15.00
Drum liner	10000.	0.71	12000.	0.23	1.18
Drum headspace	0.	0.00	16000.	0.00	0.00

Initial drum temperature (C): 24.7

Drum temperature during the trial: constant

First samples collected from small bags approximately 24.0 hrs after t=0

Ambient pressure (cm Hg): 64.5

Hydrogen diffusion characteristic across filter (mol/mol fraction/s): 0.44000E-05

Predicted small bag concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag	3 small bags	1 small bag
1	227.1	227.1	592.2	592.2	248.6	248.6	61.7	61.7	48.2	48.2
2	189.6	189.6	409.1	409.1	184.8	184.8	41.0	41.0	29.9	29.9
3	165.1	165.1	320.6	320.6	152.4	152.4	32.8	32.8	22.4	22.4
4	146.5	146.5	272.6	272.6	132.6	132.6	28.9	28.9	19.0	19.0
5	131.8	131.8	243.0	243.0	119.9	119.9	26.7	26.7	17.3	17.3
6	119.8	119.8	222.4	222.4	111.4	111.4	25.2	25.2	16.3	16.3
7	110.0	110.0	206.7	206.7	105.6	105.6	24.2	24.2	15.8	15.8
8	101.9	101.9	193.8	193.8	101.4	101.4	23.5	23.5	15.4	15.4
9	95.3	95.3	182.9	182.9	98.4	98.4	23.0	23.0	15.2	15.2
10	89.9	89.9	173.4	173.4	96.0	96.0	22.6	22.6	15.0	15.0
11	85.3	85.3	165.0	165.0	94.2	94.2	22.2	22.2	14.8	14.8
12	81.5	81.5	157.4	157.4	92.7	92.7	22.0	22.0	14.7	14.7
13	78.4	78.4	150.7	150.7	91.4	91.4	21.7	21.7	14.5	14.5
14	75.7	75.7	144.7	144.7	90.3	90.3	21.5	21.5	14.4	14.4
15	73.4	73.4	139.2	139.2	89.3	89.3	21.4	21.4	14.3	14.3
16	71.5	71.5	134.2	134.2	88.3	88.3	21.2	21.2	14.3	14.3
17	69.8	69.8	129.7	129.7	87.5	87.5	21.0	21.0	14.2	14.2
18	68.4	68.4	125.6	125.6	86.7	86.7	20.9	20.9	14.1	14.1
19	67.1	67.1	121.9	121.9	86.0	86.0	20.7	20.7	14.0	14.0
20	66.0	66.0	118.5	118.5	85.2	85.2	20.6	20.6	13.9	13.9
21	64.9	64.9	115.3	115.3	84.5	84.5	20.5	20.5	13.9	13.9

Trial 4.3 (continued)

Other predicted VOC concentrations (ppmv):

	methylene chloride		Freon-113		1,1,1-trichloroethane		carbon tetrachloride		trichloroethylene	
Day	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace	Large bag	Drum headspace
1	217.9	88.1	166.1	6.4	214.1	39.7	52.1	7.0	44.3	10.9
2	184.5	112.4	212.0	24.6	171.7	57.7	37.7	10.2	28.3	10.7
3	161.4	110.2	219.5	43.6	144.6	64.0	31.3	13.0	21.7	11.2
4	143.6	102.9	214.0	58.3	127.6	68.2	28.1	15.2	18.6	12.0
5	129.4	95.6	204.4	68.1	116.6	71.6	26.1	16.7	17.1	12.5
6	117.8	89.2	194.1	74.2	109.2	74.3	24.9	17.8	16.2	12.9
7	108.4	84.0	184.1	77.7	104.0	76.3	24.0	18.4	15.7	13.1
8	100.6	79.6	174.9	79.5	100.3	77.7	23.3	18.9	15.4	13.3
9	94.3	76.0	166.6	80.2	97.5	78.6	22.9	19.2	15.1	13.4
10	89.0	73.0	159.0	80.2	95.3	79.1	22.5	19.3	14.9	13.4
11	84.6	70.5	152.2	79.9	93.6	79.4	22.2	19.4	14.8	13.4
12	80.9	68.4	146.0	79.5	92.2	79.4	21.9	19.4	14.6	13.4
13	77.9	66.7	140.4	78.9	91.0	79.2	21.7	19.4	14.5	13.4
14	75.3	65.1	135.4	78.3	89.9	79.0	21.5	19.3	14.4	13.4
15	73.1	63.8	130.8	77.6	88.9	78.6	21.3	19.2	14.3	13.3
16	71.2	62.7	126.6	77.0	88.1	78.2	21.1	19.1	14.2	13.3
17	69.5	61.6	122.8	76.4	87.2	77.8	21.0	19.0	14.2	13.2
18	68.1	60.7	119.3	75.9	86.5	77.3	20.8	18.9	14.1	13.2
19	66.9	59.9	116.1	75.3	85.7	76.8	20.7	18.8	14.0	13.1
20	65.8	59.1	113.2	74.8	85.0	76.3	20.6	18.7	13.9	13.1
21	64.8	58.5	110.5	74.4	84.3	75.8	20.4	18.6	13.9	13.0