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THE EFFECT OF WATER COMPOSITION ON THE AIR STRIPPING OF VOLATILE ORGANIC COMPOUNDS FROM GROUNDWATER

by
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A thesis
submitted under the supervision of
Dr. Ronald L. Droste, PEng

presented to the University of Ottawa
in partial fulfillment of the requirements
for the degree of Master of Applied Science
in Civil Engineering

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ABSTRACT

The occurrence of volatile synthetic organic compounds in our environment has increased significantly in recent years to a point were approximately one half of all water supplies are affected. The objective of this study was to examine the effect of water composition (i.e., conductivity) on the air stripping of volatile organic compounds (VOC) using a countercurrent packed column.

Henry's Law constants were determined for various VOC of environmental significance: $CH_2=CCl_2$; CH_3CHCl_2; $CHCl_3$; $ClCH_2CH_2Cl$; CH_3CCl_3; CCl_4; $CCl_2=CHCl$; C_6H_6; $CHBr_3$; and $C_6H_5CH_3$. The experimental technique consisted of the multiple equilibration of an aqueous solution with the measurement of the liquid-phase VOC concentration. Henry's Law constants were determined using a two-factor, three-level factorial design over a range of temperature ($10^oC < T < 30^oC$) and conductivity ($300\ \mu mho/cm < C < 2300\ \mu mho/cm$).

The mass transfer experiments were performed to establish the effect of liquid and gas flow rates, conductivity and packing type on the air stripping of VOC and to evaluate the various mass transfer correlations available (e.g., Sherwood and Holloway, 1940, Shulman et al., 1955, Onda et al., 1968). The experiments were conducted using a four-factor, three-level fractional factorial design consisting of 27 runs (Bacon, 1970): liquid flow rate 2, 3, 4 L/min, gas flow rate 25, 50, 75 L/min, conductivity 300, 1300, 2300 µmho/cm and packing porosity, 6.4 mm Raschig rings (porosity 62%), 12.8 mm Raschig rings (64%) and 12.8 mm Intalox saddles (72%). The experiments were conducted in random order and analyzed by the procedure developed by Lamarche, 1986 and Munz, 1985. The factorial analysis was performed by a SAS general linear regression analysis. The results of the experiments and regression analysis are shown in Appendix E.

The equilibria studies indicated that the Henry's Law constants increase by approximately 30 to 40% with every 10°C change in temperature and decrease approximately 5 to 15% with every 1000 µmho/cm change in conductivity. SAS analysis of the equilibria runs showed that temperature was highly significant and conductivity was only slightly significant in the determination of H_C.

The mass transfer studies indicated that the Onda et al. correlation gave the best prediction of K_La for VOC (SEE = ± 3.6%) of the correlations studied. The mass transfer studies indicated that KLa decreased by approximately 3 to 5% with every 1000 µmho/cm change in conductivity. SAS analysis of the mass tranfer experiments indicated that the liquid flow rate was a highly significant factors in the determination of K_La and to a lesser degree conductivity and packing porosity while K_La is not significantly affected by changes in the gas flow rate.

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A special thank you to my family and friends who have always been there when I needed them the most; I will never forget that.

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GLOSSARY

Fundamental Quantities:

L = length (m, cm, or mm)
M = mass (kg, g, mg or μg)
P = pressure (atm, Pa, or mmHg)
T = temperature (°K or °C)
C = conductivity (μmho/cm)
t = time (days, hours, minutes, or seconds)

Thermodynamic Phase Equilibria:

C_G = equilibrium gas concentration $[M/L^3]$
C_L = liquid-phase concentration $[M/L^3]$
C_{LS} = equilibrium liquid concentration $[M/L^3]$
C_S = solubility of component i $[M/L^3]$
f_C = cosolvent mole fraction [-]
f_{Li} = liquid fugacity of component i [P]
f_{Ri} = reference fugacity of pure component i [P]
f_{Vi} = vapour fugacity of component i [P]
H_C = dimensionless Henry's Law constant [-]
H_{Ci} = dimensionless Henry's Law constant for component i [-]
H_{Si} = solute Henry's Law constant in cosolvent $[P\ L^3/M]$
H_{Mi} = solute Henry's Law constant in mixture $[P\ L^3/M]$
H_{Wi} = solute Henry's Law constant in water $[P\ L^3/M]$
H_{Xi} = Henry's Law coefficient of component [P]
K_A = equilibrium constant [-]
K_{OW} = octanol/water partition coefficient [-]
k_S = "salt-out" coefficient $[L^3/M]$
P = total ambient pressure [P]
p_i = partial pressure of component i [P]
p_{Oi} = vapour pressure of the pure solution [P]
R = universal gas constant $[P\ L^3/M/T]$
T = temperature [T]
T_A = ambient temperature [T]

Te = equilibrium temperature [T]
v_S = molar volume of the solution [-]
x_3 = liquid-phase mole fraction for cosolvent [-]
x_i = liquid-phase mole fraction of component i [-]
x_{Si} = mole fraction solubility of component i [-]
x_1 = liquid-phase mole fraction for water [-]
y_i = gas-phase mole fraction of component i.[-]
ΔH^o = change in enthalpy at standard temperature and pressure [-]
γ_{Ci} = solubility activity coefficient in cosolvent [-]
γ_i = symmetric activity coefficient of component i [-]
γ_i^* = asymmetric activity coefficient of component i [-]
γ_{Mi} = solubility activity coefficient in mixture [-]
γ_{Wi} = solubility activity coefficient in water [-]
μ = ionic strength of aqueous solution [-]
ϕ_{Vi} = fugacity coefficient of component i
α_{13} = empirical Margules parameter [-]

Mass Transfer Models:

A = interfacial area $[L^2]$
C = concentration $[M/L^3]$
C_G = gas-phase concentration $[M/L^3]$
$C_{int,G}$ = initial gas-phase concentration $[M/L^3]$
$C_{int,L}$ = initial liquid-phase concentration $[M/L^3]$
C_L = liquid-phase concentration $[M/L^3]$
D = diffusion coefficient $[L^3/t]$
D_G = gas diffusion coefficient $[L^2/t]$
D_L = liquid diffusion coefficient $[L^2/t]$
H_C = dimensionless Henry's Law coefficient [-]
K = overall mass transfer coefficient $[L^2/t]$
k = individual mass transfer coefficient $[L^2/t]$
K_G = overall gas mass transfer coefficient $[L^2/t]$
k_G = individual gas mass transfer coefficient $[L^2/t]$
K_L = overall liquid mass transfer coefficient $[L^2/t]$
k_L = individual liquid mass transfer coefficient $[L^2/t]$

m = mass [M]
R_G = gas-phase mass transfer resistance [-]
R_L = liquid-phase mass transfer resistance [-]
R_T = overall mass transfer resistance [-]
s = fractional rate of surface renewal of area exposed to penetration [1/t]
t_e = eddy exposure time [t]
δ = film thickness [L]
δ_G = gas interfacial thickness [L]
δ_L = liquid interfacial thickness [L]

Countercurrent Packed Column Design:

A = adsorption factor, $H_C (Q_L/Q_G)$ [-]
a = specific interfacial area [L^2]
A^* = cross-sectional area [L^2]
a_t = total specific surface area of packing [L^2/L^3]
a_W = specific wetted packing area [L^2/L^3]
C_G = gas-phase concentration [M/L^3]
C_L = liquid-phase concentration [M/L^3]
C_{LS} = equilibrium liquid-phase concentration [M/L^3]
D_G = gas-phase diffusion coefficient [L^2/t]
D_L = liquid-phase diffusion coefficient [L^2/t]
d_P = diameter of packing [L^2]
d_S = diameter of sphere equal to a unit of packing [L]
FCF = Finney's correction factor [-]
g = gravitational constant [L/t^2]
G_M = gas mass flux [$M/L^2/t$]
HTU = height of a transfer unit [L]
K_La = overall mass transfer constant [1/t]
k_La = individual mass transfer constant [1/t]
L = superficial liquid velocity [$L^3/L^2/t$]
L_M = liquid mass flux [$M/L^2/t$]
M = volumetric mass transfer area [L^3]
M_T = total mass balance [M]

n = Sherwood and Holloway empirical constant [-]
NNTU = number of transfer units due to end effects [-]
NTU = number of transfer units [-]
p_L = liquid density $[M/L^3]$
P_{Oi} = vapour pressure of component i [P]
Q_G = gas flow rate $[L^3/t]$
Q_L = liquid flow rate $[L^3/t]$
s = Sherwood and Holloway empirical constant [-]
S = stripping factor, (QG/QL)/HC [-]
sol_i = molar solubility of component i $[1/L^3]$
β = total liquid holdup constant [-]
TNTU = net number of transfer units, (NTU - NNTU) [-]
V_G = gas volume $[L^3]$
V_L = liquid volume $[L^3]$
Z = total depth of packing [L]
γ_G = gas-phase activity coefficient [-]
γ_L = liquid-phase activity coefficient [-]
α = Sherwood and Holloway empirical constant [-]
σ = variance of the residuals [-]
σ_C = critical surface tension of packing material $[E/L^2]$
σ_L = liquid-phase surface tension $[E/L^2]$
μ_G = gas-phase viscosity [P t]
μ_L = liquid-phase viscosity [P t]
ϕ_T = total liquid holdup [-]
ε = porosity [-]
ε_D = dry packing porosity [-]

CHAPTER 1

INTRODUCTION

1.0 BACKGROUND

1.1 Groundwater Contamination

Almost five of six public water systems in the United States rely on groundwater as their primary water supply and many of the nation's larger cities augment their surface water supplies with groundwater. This means that in the U.S. at least 73 million people drink groundwater in one form or another (AWWA, 1985a). In Ontario, Canada there are 250 provincial and municipally run water supply systems supplied by groundwater supplying approximately one-third of the people of the province.

1.2 Synthetic Volatile Organic Chemicals

It has been said that the number of synthetic chemicals now totals 1.8 million and is growing at a rate of 250,000 new formulations annually of which 300 to 500 reach the stage of commercial production with a global production of 100 to 200 million tons (Stumm and Morgan, 1981). Approximately one-third of the total production of these compounds will find their way into the environment.

Volatile organic compounds (VOC) are a general category of synthetic organic chemicals that includes low-molecular weight, volatile aliphatic and aromatic hydrocarbons, many of which are halogenated (Westrick, 1984). The presence of VOC in groundwater has increased considerably in the past few years. This prompted the U.S. Environmental Protection Agency (EPA) to initiate three studies to quantify the occurrence of VOC in groundwater: Brass, 1981; EPA, 1982; and Westrick, 1984. The studies indicated that the five most commonly found compounds in groundwater and drinking water supplies were: trichloroethylene; 1,1,1-trichloroethane; tetrachloroethylene; cis- and/or trans-1,2-dichloroethylene; and 1,1-dichloroethane. Also commonly found in drinking water supplies were the five trihalomethanes: chloroform; bromodichloromethane; dibromochloromethane; dichloroiodomethane; and bromoform. However, the presence of these compounds is thought to be due to the effect of chlorination on drinking water.

The findings of studies on groundwater contamination have lead the environmental regulatory agencies in both Canada and the United States to introduce strict regulations on the levels of effluent concentrations of an extensive number of priority pollutants. Under the Municipal and Industrial Strategy for Abatement (MISA) program in Ontario, Canada in 1987, the Ontario Ministry of the Environment (MOE) released a draft report listing 40 priority pollutants to be included in the environmental monitoring program being proposed for the province.

In 1985, the U.S. EPA under the Safe Drinking Water Act proposed National Drinking Water Regulations and Maximum Contaminant Levels for the following eight VOC commonly found in drinking water: trichloroethylene; carbon tetrachloride; 1,1,1-trichlorethane; vinyl chloride; 1,2-dichloroethane; benzene; 1,1-dichloroethylene; and p-dichlorobenzene. Also the regulation proposes monitoring, reporting and public notification requirements for these eight VOC and 51 other VOC (EPA, 1985).

The most common processes used to remove VOC from an aqueous stream are adsorption in an activated carbon process, oxidation through a chemical reaction process, degradation in a biological process and transfer to the atmosphere (volatilization or stripping) in a gas/liquid contacting process. This study investigated the use of air stripping to remove VOC from an aqueous stream.

1.3 Objectives

The ultimate goals of this research were to quantify the thermodynamic properties of low molecular weight halogenated organic solutes in aqueous solution, and to expand the understanding of mass transfer phenomena in countercurrent packed column processes to remove volatile contaminants of environmental significance from liquid streams.

The specific objectives of this research were:

1. To determine the Henry's Law constants of low molecular weight halogenated organic solutes, chosen for their environmental significance, over a temperature range of $10^{o}C < T < 30^{o}C$.
2. To quantify the effect of water composition (i.e., ionic strength) on the Henry's Law constants of low molecular weight halogenated organic solutes in aqueous solutions.
3. To assess the effect of water composition (i.e., ionic strength) on the mass transfer coefficients for the selected volatile organic compounds in a countercurrent packed column.
4. To verify the performance of the mass transfer correlations developed by Sherwood and Holloway, 1940, Shulman et al., 1955a to 1963 and Onda et al., 1968 under variable water composition (i.e., ionic strength) conditions.

CHAPTER 2

LITERATURE REVIEW

2.0 INTRODUCTION

2.1 THEORETICAL THERMODYNAMIC BACKGROUND

2.1.1 Vapour-Liquid Equilibria of Dilute Solutions

The equilibrium between two phases for a solute at a given temperature and pressure exits when the fugacities (or activities or chemical potential) in the phases are equal (Munz, 1985). Therefore, in the case of a vapour-liquid equilibrium process

$$f_{Vi} = f_{Li} \qquad (2.1)$$

where f_{Vi} = vapour-phase fugacity of component i
f_{Li} = liquid-phase fugacity of component i.

The fugacity is a measure of the escaping tendency of a compound from a phase. The vapour-phase fugacity is defined as

$$f_{Vi} = y_i \phi_{Vi} P \qquad (2.2)$$

where y_i = mole fraction of component i
ϕ_{Vi} = fugacity coefficient of component i
P = total ambient pressure.

At low pressure and ambient temperature (i.e., air stripping column), the molecular interaction is assumed to be negligible. This means the vapour-phase will behave ideally. Therefore, the fugacity coefficient becomes unity and the fugacity equation reduces to

$$f_{Vi} = y_i \; P = p_i \tag{2.3}$$

where p_i = partial pressure of component i.

The liquid-phase fugacity can be expressed as (Munz, 1985)

$$f_{Li} = x_i \; \gamma_i \; f_{Ri} \tag{2.4}$$

where x_i = mole fraction of component i
f_{Ri} = pure component reference fugacity
γ_i = liquid-phase symmetric activity coefficient of component i.

For a dilute solution, f_{Ri} is a function of temperature only and can be set equal to the vapour pressure of the pure solution, p_{Oi}. Substituting Eqs 2.4 and 2.3 into 2.1 yields

$$p_i = x_i \; \gamma_i \; p_{Oi} \tag{2.5}$$

Munz and Roberts, 1982 showed from thermodynamics of a dilute solution that the activity coefficient can be approximated by the reciprocal of the solubility (i.e., $\gamma_i = {x_{Si}}^{-1}$ where x_{Si} = mole fraction solubility of component i).

Considering solute that is only slightly soluble in water, the vapour-liquid equilibrium can be expressed in terms of the Henry's Law constant or air-water partition coefficient. Mackay and Wolkoff, 1973 showed that for very dilute solutions, the phase equilibrium can be represented by the linear relationship:

$$H_{Xi} = \frac{p_{Oi}}{x_{Si}} \tag{2.6}$$

Substituting Eq. 2.6 into Eq. 2.5 reduces Eq. 2.5 to

$$p_i = H_{Xi} \; x_i \tag{2.7}$$

which is one form of Henry's Law.

A statement of Henry's Law is "The mass of a slightly soluble gas that dissolves in a definite mass of a liquid at a given temperature is very nearly directly proportional to the partial pressure of that gas" (Weast et al., 1984). The equilibrium between the two phases can be represented by the following linear relationship (Munz, 1985)

$$\lim_{xi \to 0} \left(\frac{f_{Vi}}{x_i}\right) = H_{Xi} \qquad (2.8)$$

According to Munz and Roberts, 1982, a dilute solution corresponds to a mole fraction content less than 0.01. In the literature, the Henry's Law coefficient has been expressed in several other forms

$$H = \frac{p_{Oi}}{C_{Si}} \qquad (2.9)$$

$$H_C = \frac{C_G}{C_{LS}} \qquad (2.10)$$

where C_{Li} = solubility concentration of component i
C_G = equilibrium gas concentration
C_{LS} = equilibrium liquid concentration
H = Henry's Law constant [atm m^3 / mol]
H_C = dimensionless Henry's Law constant.

Eq. 2.9 is the most commonly used form for environmental applications. However , H_C is the easiest form to use in engineering calculations. These two expressions are related by

$$H_{Xi} = H_C \, R \, T \qquad (2.11)$$

where R = Universal gas constant
T = absolute temperature.

2.1.1.1 Temperature Effects

The strong relationships between temperature and solubility and temperature and vapour pressure are well documented in Smith and van Ness, 1975. Eq. 2.9 would indicate that an equally strong relationship should also exist between temperature and the Henry's Law constant (Mackay and Shiu, 1981).

Using thermodynamic principles Kavanaugh and Trussell, 1980 represented the relationship of temperature and H_C as a van't Hoff equation

$$\frac{d(\ln(K_A))}{dT_A} = \frac{\Delta H^o}{R\ T_A^2} \qquad (2.12)$$

where K_A = reaction equilibrium constant
T_A = ambient temperature
R = universal gas constant
ΔH^o = change in enthalpy at STP.

The equilibrium constant of a vapour-liquid system is the Henry's Law constant, H. By assuming that the change in enthalpy is independent of temperature and substituting H for K_A, Eq. 2.12 can be integrated directly to yield

$$\ln(H) = \frac{-\Delta H^o}{R\ T_A} + A \qquad (2.13)$$

where A = constant of integration.

The equation indicates that an increase in temperature will result in an increase in the Henry's Law coefficient. Munz, 1985 developed a similar equation using an equation relating temperature and vapour pressure (Clausius-Clapeyron Equation) and an equation derived from the Gibbs energy analysis relating temperature and the activity coefficient. Munz, 1985 found that

$$\log H_C = A - \frac{B}{T} \qquad (2.14)$$

where T = temperature

A and B = constants of integration.

This equation represents the temperature dependency of H_C satisfactorily for small temperature intervals of approximately 20-30°C and for the precision required in environmental applications. Singley et al., 1980 arrived at a relationship similar to Eq. 2.14. Experimentation proved that a 10°C increase in temperature can result in a 60% increase in the Henry's Law constant. Thus, temperature may well represent the main parameter influencing the rate of removal of VOC from a liquid-phase.

2.1.1.2 Solute Concentration Effects

In the case of hydrophobic compounds it is commonly assumed that Henry's Law will apply as long as the solubility does not exceed approximately 10^{-2} mole fraction. H_C should be directly affected by solute concentration since the activity coefficient will vary directly with concentration (Mackay and Shiu, 1981). Munz, 1985 and 1987 observed both theoretically and experimentally the effect of solute concentration on H_C and found no significant decrease. The author concluded that Henry's Law constants are constant with respect to solute concentration for the compounds studied up to a solute mole fraction of 10^{-3}. Singley et al., 1980 also analyzed the solute concentration effects over a concentration range between 0.1 and 100 µg/L and found that the concentration effects were insignificant. Yurteri et al., 1987 conducted a similar study on the effects of solute concentration on H_C and concluded that H_C was independent of solute concentration in pure-water within the ranges where the assumption of linear vapour-liquid equilibria (i.e., Henry's Law) holds.

2.1.1.3 Cosolvent Effects

The effect of a cosolvent or cosolute concentration was studied by Munz, 1985 and Munz and Roberts, 1987. In general, the addition of a cosolvent to a water system will increase the solubility of nonpolar solute since most cosolvents are generally less polar than water. Munz, 1985 hypothesized that the best cosolvent for a nonpolar solute is a cosolvent with a polarity that closely matches that of the solute. To assess the polarity of solvents and solute, the log octanol/water partition coefficient, log (K_{OW}) can be used. The smaller the K_{OW} value, the more polar and hydrophilic a solute will be. Table 2.1 lists the K_{OW} for many common solvents and VOC.

According to Munz, 1985, the effect of a cosolvent on the solubility (or activity coefficient) of a nonpolar solute (such as a VOC) can be represented mathematically by assuming that a mixed solvent is simply a linear combination of its component solvents. Therefore,

$$\log \left(\frac{H_{Mi}}{H_{Wi}}\right) = f_C \operatorname{Log} \left(\frac{H_{Si}}{H_{Wi}}\right) \qquad (2.15)$$

where f_C = the cosolvent mole fraction
H_{Si} = solute Henry's Law constant in cosolvent
H_{Mi} = solute Henry's Law constant in mixture
H_{Wi} = solute Henry's Law constant in water

For a relatively soluble cosolvent and nonpolar solute the ratio $H_{Si}/H_{Wi} < 1$ and therefore, it follows that the ratio $H_{Mi}/H_{Wi} < 1$. From Eq. 2.15, it follows that a solute's Henry's Law constant will be smaller in a mixed solvent than in pure water, and therefore, its solubility will be greater. This is referred to as a "solubilizing effect".

Compound	Log (K_{OW}) at 20°C
Trichloroethylene	2.29
Carbon Tetrachloride	2.72
Benzene	2.01
1,1,1-Trichloroethane	2.49
Chloroform	1.95
Water	-1.38
Methanol	-0.77

Table 2.1 - Log (K_{OW}) for Common Solvents and VOC (Munz, 1985 and Verschueren, 1977)

and 3) cosolvent. The Henry's Law constant (H_{Mi}) for the solution was expressed as

$$\ln(H_{Mi}) = x_1 \ln(H_{Wi}) + x_3 \ln(H_{Si}) - \alpha_{13}\, x_1\, x_3 \qquad (2.16)$$

where α_{13} = empirical Margules parameter
x_1 = liquid-phase mole fraction for water
x_3 = liquid-phase mole fraction for cosolvent

Munz, 1985 noted that this was only a simple model and could only be applied to nonpolar cosolvents. For a cosolvent that is less polar than water, the solubility of a nonpolar solute in the cosolvent will be larger than in water and therefore $H_{Si} < H_{Wi}$ according to Eq. 2.15. Thus, according to Eq. 2.16, $H_{Mi} < H_{Wi}$.

2.1.1.4 Water Composition Effects

The effect of water composition on Henry's Law constants has not been studied to a great extent and has not been clearly analyzed. The effect of water composition (i.e., ionic strength) has been studied by Yurteri et al., 1987, Gossett, 1987 and Nicholson et al., 1984. The Henry's Law constant is given by Yurteri et al., 1987 as

$$H_{Ci} = \gamma_{Li}\ p_i\ (\frac{v_S}{R\ T_e}) \qquad (2.17)$$

where H_{Ci} = dimensionless Henry's Law constant for component i

v_S = molar volume of the solution

T_e = equilibrium temperature

γ_{Li} = liquid-phase activity coefficient.

In the equation, vapour pressure is a function of temperature, while the activity coefficient and molar volume are functions mainly of solvent composition (i.e., ionic strength).

The activity coefficient of nonelectrolytes in aqueous solutions can be predicted using an empirical equation of the form (Snoeyink and Jenkins, 1980)

$$\log \gamma_i = k_S\ \mu \qquad (2.18)$$

where k_S = salting-out coefficient

μ = ionic strength of aqueous solution.

The values for k_S vary from 0.01 to 0.15 for most nonionic or molecular solutes. Value of k_S for common environmental solutes are shown on Table 2.2. The equation indicates a direct relationship between activity coefficient and ionic strength. Thus, as the ionic strength increases, the activity coefficient will increase. An increase in the activity coefficient (or ionic strength) of a solute in an aqueous solution inversely affects the solubility of the solute, therefore H_C will increase. This is known as the "salting-out effect".

Yurteri et al., 1987 studied the effect of ionic strength and found that the Henry's Law constant of VOC can increase as much as 35% in complex mixtures. As noted by Gossett, 1984 the salinity must reach a level greater than 0.2 M KCl to cause a 10% increase in the apparent H value.

Compound	k_S (L/mol)
Trichloroethylene	0.186
1,1,1-Trichloroethane	0.193
1,1-Dichloroethane	0.145

Table 2.2 - "Salting-out" Coefficients, k_S for Common VOC (Gossett, 1887)

2.1.2 Mass Transfer Models

Mass transfer models have been proposed to describe phase mass transport by many authors, Lewis and Whitman, 1924, Higbie et al., 1935, Danckwerts, 1951, Toor and Marchello, 1958 and Dobbins, 1956. In all models, the change in mass per unit time is proportional to the product of a mass transfer coefficient times a driving force such as a concentration, density, or pressure difference. The main difference between the various models is the way in which the mass transfer coefficient is expressed and the basic underlying assumptions.

2.1.2.1 The Two-Film Theory

The two-film theory was developed and introduced by Lewis and Whitman, 1924. The model describes the mass transport between two phase at the interface in a turbulent system (Fig. 2.1). The three main assumptions of the model are that transport across the boundary layers is solely controlled by molecular diffusion; the boundary layer is a thin or stagnant laminar layer on both sides of the interface; and both phases are in equilibrium at the interface. It is also assumed that steady-state diffusion applies at the boundary layer.

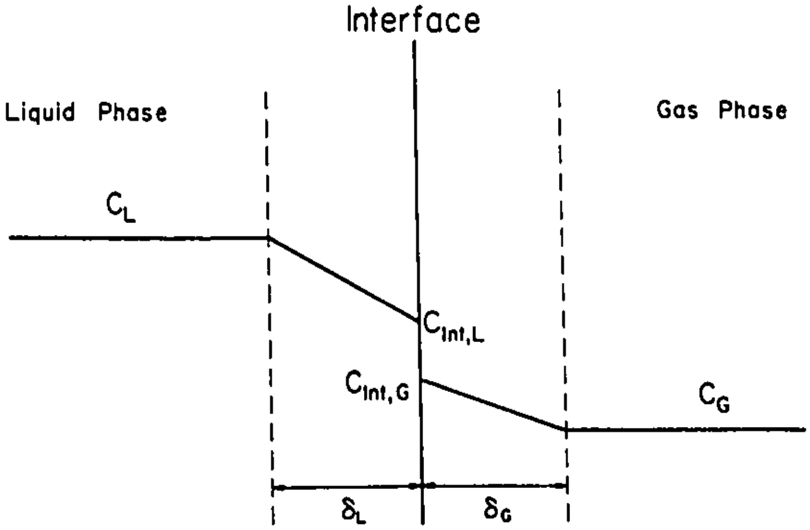


Figure 2.1 - Concentration Profiles According to the Two-film Model (Munz, 1985)

The mass transport to the interface can be written as

$$- \frac{dm}{dt} = D\ A\ \frac{dC}{dx} = A\ \frac{D_L}{\delta_L}\ (C_L - C_{int,L}) \qquad (2.19)$$

and the mass transport from the interface can be written as

$$- \frac{dm}{dt} = D\ A\ \frac{dC}{dx} = A\ \frac{D_G}{\delta_G}\ (C_{int,G} - C_G) \qquad (2.20)$$

where D = diffusion coefficient
δ = film thickness
m = mass
A = interfacial area
C = concentration.

D/δ is known as the individual mass transfer coefficient, k. Therefore, for the liquid film (L)

$$k_L = \frac{D_L}{\delta_L} \qquad (2.21)$$

and for the gas film (G)

$$k_G = \frac{D_G}{\delta_G} \qquad (2.22)$$

Algebraic manipulation of Eqns 2.21 and 2.22 and the use of Henry's Law yields for the gas film

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{H_C}{k_L} \qquad (2.23)$$

and for the liquid film

$$\frac{1}{K_L} = \frac{1}{k_L} + \frac{1}{H_C\ k_G} \qquad (2.24)$$

Assuming that Henry's Law holds true at the interface and that

$$dm/dt = K_L\ (C_L - C_S) \qquad (2.25)$$

where $C_S = C_G/H_C$

then the overall resistance can be expressed as the sum of the individual gas and liquid-phase resistances.

$$R_T = R_L + R_G \qquad (2.26)$$

where RT = overall mass transfer resistance
$R_L = (k_L)^{-1}$
$R_G = (H_C\ k_G)^{-1}$.

This leads to the expression

$$\frac{R_L}{R_G} = \frac{H_C k_G}{k_L} \qquad (2.27)$$

Mackay and Leinonen, 1975 and Mackay et al., 1979 stated that the resistances of the two phases are equal ($R_L = R_G$)

when the value of $H = 1.6 \times 10^{-4}$ [atm·m^3/mol] (or $H_C = 6.5 \times 10^{-3}$), implying that $k_G/k_L = 150$. However, Munz, 1985 uses the criterion that the liquid-phase resistance controls the overall mass transfer when more than 95% of the total resistance is represented by the liquid-phase resistance. Using $k_G/k_L = 150$ estimated by Mackay and Leinonen, 1975 and Mackay et al., 1979, an $H_C > 0.13$ satisfies the 95% criterion. Fig. 2.2 illustrates the relationship between k_G/k_L and H_C. The contribution of the liquid-phase resistance can be found by similarly rearranging Eq. 2.26 to yield for the gas-phase

$$\frac{R_G}{R_T} = \frac{1}{(1 + ((k_G/k_L)\ H_C))} \qquad (2.28)$$

Thus, as H_C increases, the gas-phase resistance becomes insignificant (Roberts and Levy, 1985).

$$\frac{R_L}{R_T} = \frac{1}{(1 + ((k_G/k_L)\ H_C)^{-1})} \qquad (2.29)$$

2.1.2.2 The Penetration Theory

Penetration theory was introduced by Higbie, 1935 and is based on the circulation of small turbulent eddies from the bulk phase reaching the interface, where they remain for a short and constant period of time (steady state not obtained) before returning to the bulk phase. During the time that the eddies reaches the interface, solute molecules penetrate into the eddy, by a process of unsteady-state or transient molecular diffusion. Using Fick's second law, the process can be described by:

$$\frac{dC}{dt} = D \frac{d^2C}{dx^2} \qquad (2.30)$$

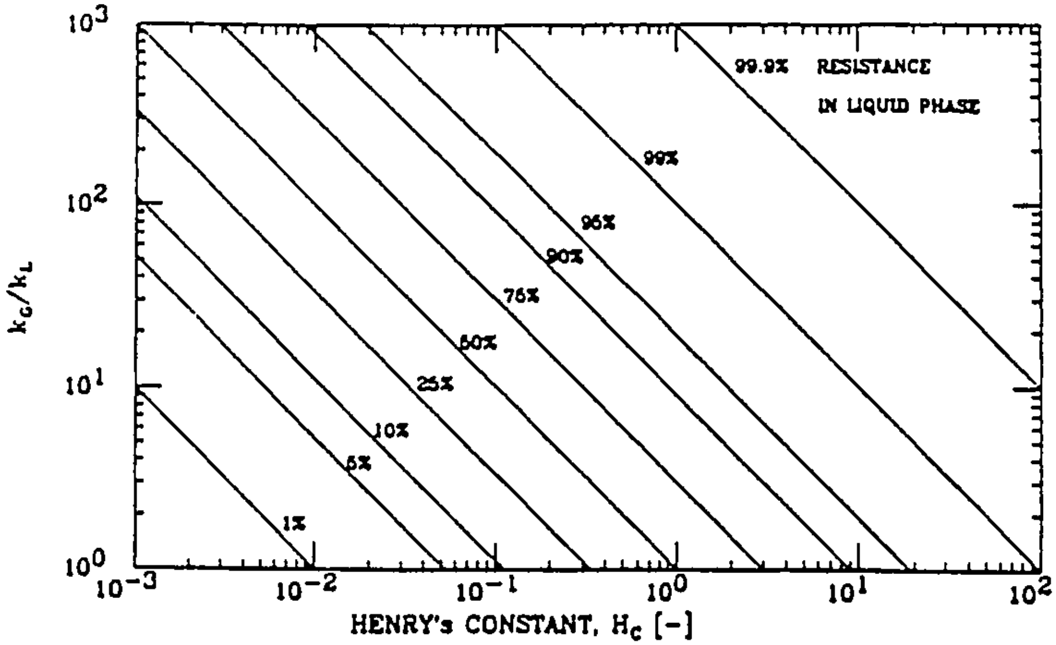


Figure 2.2 - Percent Resistance in Liquid-Phase as a Function of the Ratio of Mass Transfer Coefficient (k_G, k_L) and Henry's Law Constants (H_C) (Munz, 1985)

with initial conditions

$$t = 0,\ 0 \le x \le \infty,\ C = C_L \qquad (2.31)$$

and boundary conditions

$$t > 0,\ x = 0,\ C = C_{int,L} \qquad (2.32)$$

$$t > 0,\ x = \infty,\ C = C_L \qquad (2.33)$$

the expression obtained for the average mass transfer over the exposure time, t_e of any eddy is

$$\frac{dm}{dt} = 2\left(\frac{D_L}{\pi\, t_e}\right)^{1/2} A\,(C_{int,L} - C_L) \qquad (2.34)$$

The mass transfer coefficient is

$$k_L = 2 \left(\frac{D_L}{\pi \, t_e}\right)^{1/2} \qquad (2.35)$$

Penetration theory predicts a square-root dependence for the diffusion coefficient on k_L while two-film theory predicts a first-power dependence.

2.1.2.3 **The Surface-Renewal Theory**

The surface-renewal theory was introduced by Danckwerts, 1951 as an extension of penetration theory. In the surface-renewal theory the residence time t_e of an eddy at the interval is allowed to vary randomly from zero to infinity. The renewal residence time distribution is compared to that of the penetration on Fig. 2.3. From analysis of the surface age distribution function, Danckwerts developed an expression for the average mass transfer normal to the phase boundary

$$\frac{dm}{dt} = A \; (C_{int,L} - C_L) \; D^{1/2} \int_0^\infty \frac{s \; e^{-t}}{(\pi \; t)^{1/2}} \, dt \qquad (2.36)$$

$$= A \; (C_{int,L} - C_L) \; (D \; s)^{1/2} \qquad (2.37)$$

where s = fractional rate of surface renewal of the area exposed to penetration.

The mass transfer coefficient is

$$k_L = (D \; s)^{1/2} \qquad (2.38)$$

As in the penetration theory the mass transfer coefficient is proportion to the square-root of the molecular diffusiv-

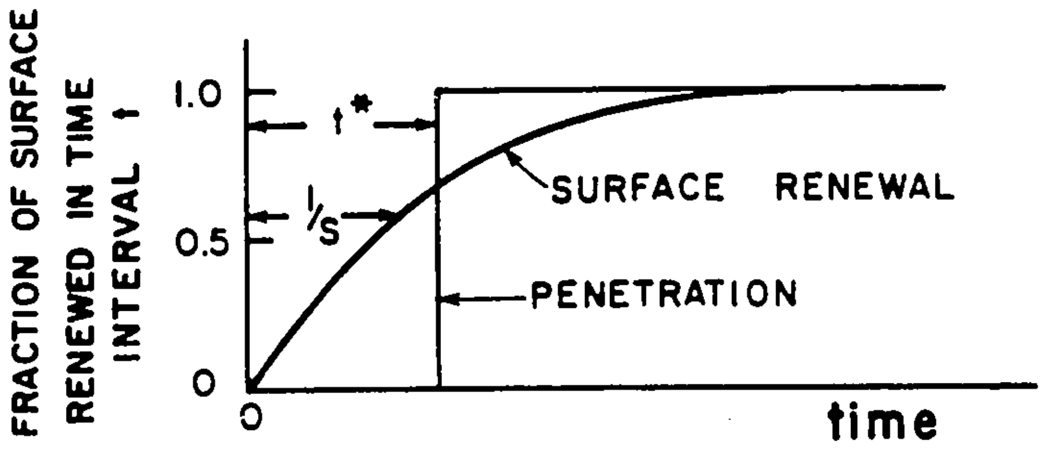


Figure 2.3 - Distribution of Turbulent Eddies in the Surface Layer According to the Penetration and Surface-renewal Theories (Munz, 1985)

ity. Penetration theory shows the fractional rate of removal, s to be equal to

$$s = \frac{4}{\pi} \frac{1}{t_e} \tag{2.39}$$

2.1.2.4 The Film-Penetration Theory

The film-penetration theory was presented by Dobbins, 1956 and Toor and Marchello, 1958 and was based on all the previous theories. The theory employs a resistant laminar surface layer as in the two-film theory and surface renewal by eddies as in the penetration theory. Thus, the theory obeys both $k \propto D^{1/2}$ for the eddies and $k \propto D$ for the laminar surface layer. The transfer equation follows Fick's second Law

$$\frac{dC}{dt} = D \frac{d^2C}{dx^2} \qquad (2.40)$$

with initial condition

$$t = 0,\ 0 \le x \le \infty,\ C = C_L \qquad (2.41)$$

and boundary conditions

$$t > 0, x > 0,\ C = C_{int,L} \qquad (2.42)$$

$$t > 0,\ x = \delta,\ C = C_L \qquad (2.43)$$

The primary difference to the penetration theory is the second boundary condition ($x = \delta$). Like the penetration theory, a variable surface age distribution was used and the resulting mass transfer equations are:

for the eddies,

$$\frac{dm}{dt} = A\ (C_{int,L} - C_L)\ (D\ s)^{1/2} (1 + 2 \sum_{n=1}^{\infty} \exp(-2\ n\ \delta\ (s/D)^{1/2})) \qquad (2.44)$$

for the laminar surface layer,

$$\frac{dm}{dt} = A\ (C_{int,L} - C_L)\ \frac{D}{s}\ (1 + 2 \sum_{n=1}^{\infty} (\frac{1}{(1 + n^2\ \pi^2\ (D/s\ \delta^2))})) \qquad (2.45)$$

When the rate of surface renewal is high, Eq. 2.44 reduces to the penetration theory. While when the rate is low, Eq. 2.45 reduces to the two-film theory.

Fig. 2.4 shows a comparison of the three theories and shows how they are asymtotic at their extremes.

2.1.2.5 Comparison of Theories

Several other methods have been proposed but the most common methods to determine the mass transfer between the vapour and liquid-phase were presented above. The advantages and disadvantages of the models are described below.

The difficulty in applying all the theories is in the measurement of parameters such as film thickness δ, the time of exposure t^*, or the fractional rate of surface renewal, s. The application of the penetration theory requires the measurement of both t^* and s, therefore it is almost impossible to apply this method and its accuracy is very hard to assess.

The advantage of the use of the two-film theory is the assumption that the total resistance to mass transfer is the sum of the gas and liquid-phase resistances. Munz and Roberts, 1982 noted experiments conducted by Goodgame and Sherwood, 1954 to test the concept of the two-film theory found that the additivity of resistance predicted their experimental data both when using the two-film or surface-renewal methods.

2.2 MASS TRANSFER THEORY APPLIED TO PACKED COLUMNS

Air stripping in countercurrent packed columns has been studied by numerous authors; Al-Dhowalia, 1982, Amy and Cooper, 1986, Amy et al., 1987, Ball et al., 1984, Byers and Morton, 1985, Gross and TerMaath, 1985, Hand et al., 1986, Kavanaugh and Trussell, 1980, Kavanaugh and Trussell, 1981, Lamarche, 1986, Munz, 1985, Nirmalakhandan et al., 1987, Pekin and Moore, 1985, Roberts et al., 1982, Roberts et al., 1985, Roberts and Levy, 1985, Stallings et al., 1985, and Umphres et al., 1983, as a method for removal of VOC from a liquid-phase (i.e., groundwater).

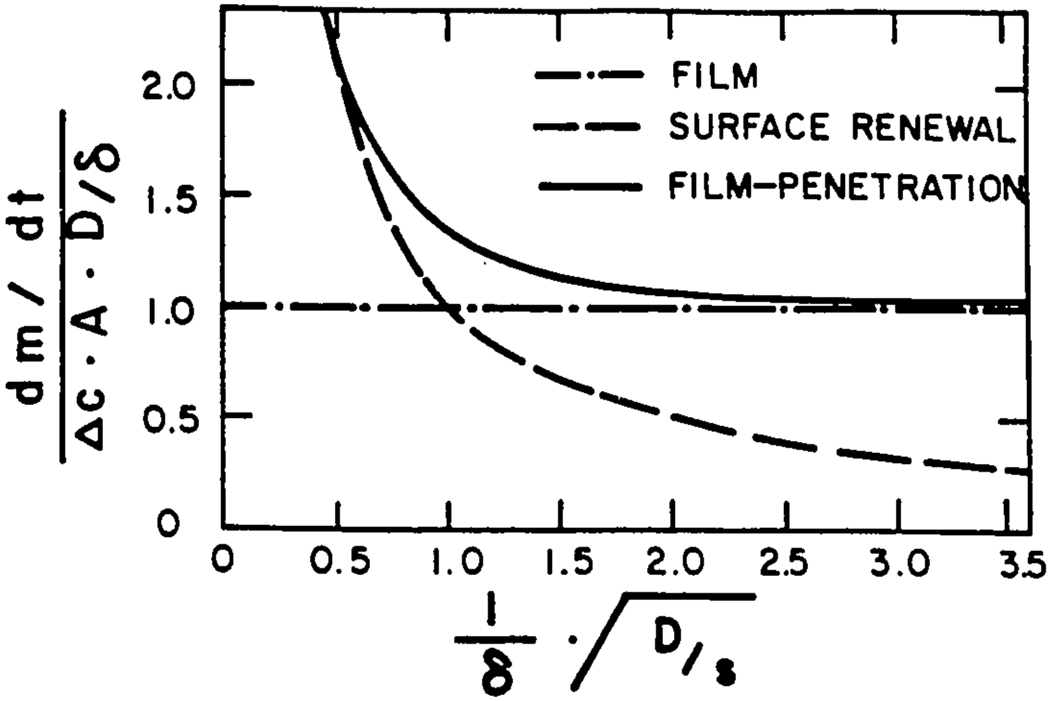


Figure 2.4 - Mean Transfer Rate as a Function of Exposure (Munz, 1985)

2.2.1 Countercurrent Packed Column Design

In the design of a countercurrent packed column the following assumptions were made: the process is isothermal; the overall liquid mass transfer coefficient, K_L, is considered constant with respect to time and position in the column and dependent only on temperature; equilibrium is described by Henry's Law; only one solute is transferred and is independent of the other solute in the system; the process is at steady state (i.e., constant gas and liquid flow rates and influent gas and liquid concentrations); dilute liquid and gas streams (i.e., the gas and liquid flowrates are not influenced by the amount of solute stripped or adsorbed); and the gas and liquid flows are plug flow in the column.

A countercurrent packed column is shown schematically on Fig. 2.5. The units used in the design equations will be in terms of volumetric concentrations (mol/m^3 or g/m^3) to correspond to the literature (Munz, 1985 and Treybal, 1980). Also, to simplify the presentation only the liquid-phase analysis will be used. The mass flux in the packed column is described by

$$-\frac{dm}{dt} = K_L\, M\, (C_L - C_{LS}) \qquad (2.46)$$

where M = volumetric mass transfer area
C_L = liquid-phase concentration
C_{LS} = liquid-phase equilibrium concentration.

Considering the volume dV in the schematic, the total packing surface area available for mass transfer is

$$dM = a\ X\ dZ \qquad (2.47)$$

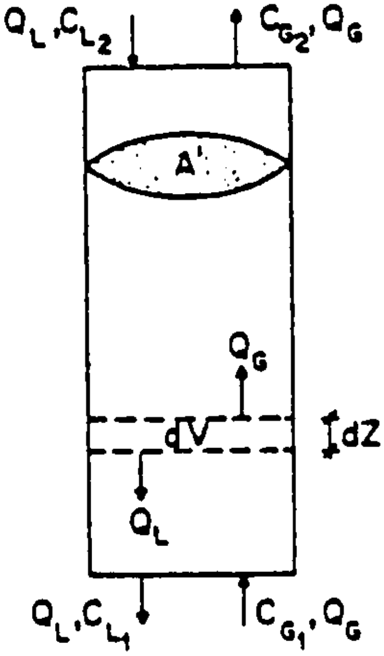


Figure 2.5 - Countercurrent Packed Column Mass Balance Schematic

where a = specific interfacial area per unit volume of packing

X = column cross-sectional area.

Substituting Eq. 2.47 into 2.46 yields

$$d(Q_L C_L) = K_L \, dM \, (C_L - C_{LS}) \tag{2.48}$$

$$= K_L \, a \, X \, dZ \, (C_L - C_{LS}) \tag{2.49}$$

Integrating Eq. 2.49 over the entire height of the column yields

$$Z = \int_0^Z dZ = \left(\frac{L}{K_L a}\right) \int_{C_{L2}}^{C_{L1}} \frac{dC_L}{(C_{LS} - C_L)} \tag{2.50}$$

$$Z = (HTU) \; (NTU) \tag{2.51}$$

where L = the superficial liquid velocity

HTU = height of a transfer unit

NTU = number of transfer units for the liquid-phase.

An HTU can be thought of as a measure of the mass transfer resistance or efficiency of the equipment, while a NTU is a measure of the difficulty of separation (Cussler, 1984). Thus,

$$HTU = \frac{L}{K_L a} \tag{2.52}$$

$$NTU = \int_{C_{L2}}^{C_{L1}} \frac{dC_L}{(C_{LS} - C_L)} \tag{2.53}$$

The expression for the mass balance of the volume dV gives

$$Q_L \, dC_L = Q_G \, dC_G \qquad (2.54)$$

Integrating Eq. 2.54 over the depth of the column, Z yields

$$C_G = C_{G1} + \frac{Q_L}{Q_G} (C_L - C_{L1}) \qquad (2.55)$$

where CG and CL occurs at any Z. Introducing the equilibrium condition into Eq. 2.55 gives

$$CLS = \frac{C_G}{H_C} = \frac{1}{H_C} (C_{G1} + \frac{Q_L}{Q_G} (C_L - C_{L1})) \qquad (2.56)$$

Substituting Eq. 2.56 into 2.53 and integrating gives

$$NTU = \frac{1}{(1 - A)} \ln (\frac{(C_{L2} - C_{G1}/H_C)(1 - A)}{(C_{L1} - C_{G1} H_C)} + A) \qquad (2.57)$$

where A = absorption factor = $H_C \, (Q_L/Q_G)$.

Assuming that the solute concentration in the influent gas is equal to zero ($C_{G1} = 0$) and S = stripping factor = A^{-1} = $(Q_G/Q_L) \, / \, H_C$, Eq. 2.57 reduces to

$$NTU = \frac{S}{(S - 1)} \ln (\frac{(C_{L1}/C_{L2})(S - 1) + 1}{S}) \qquad (2.58)$$

as used by Roberts et al. 1985 and Kavanaugh and Trussell 1980. Combining Eqs 2.52 and 2.58 with Eq. 2.51 yields

$$Z = \frac{L}{K_L a} \frac{S}{(S - 1)} \ln (\frac{(C_{L1}/C_{L2})(S - 1) + 1}{S}) \qquad (2.59)$$

The stripping factor is also known as an equilibrium capacity factor. The stripping factor will have a direct effect on the efficiency of any air stripping process (Munz 1985 and Treybal 1980). If S > 1, the gas-phase capacity of the column is sufficient to remove the total amount of the solute present in the influent. If $S < 1$, the performance of the column is limited by equilibrium and the fractional removal is asymptotic to the value of the stripping factor (i.e., $(1 - C_{L1}/C_{L2}) \rightarrow S$ as $Z \rightarrow \infty$).

2.2.2 Liquid-Phase Mass Transfer Coefficient Correlations

Mass transfer coefficients have been studied by numerous authors (Sherwood and Holloway, 1940, Shulman, 1955, and Onda et al., 1968) and correlations have been proposed. The correlations were developed from experimental data obtained through experimentation using limited operating condition ranges and component physical properties (i.e., packing types and column designs). The coefficients are directly dependent upon liquid properties, gas and liquid flow rates, and packing properties. A brief description of the most widely accepted correlations are presented below. The liquid-phase mass transfer coefficient correlations have also been reviewed by Au-Yeung and Ponter, 1983 and Roberts et al., 1985.

2.2.2.1 Sherwood and Holloway Correlation

Sherwood and Holloway's (1940) correlation was developed from experiments dealing with the desorption of carbon dioxide, oxygen or hydrogen from water in a packed column using a variety of packing types. This represented the first extensive investigation into the liquid-phase mass transfer coefficient. The Sherwood and Holloway (1940) correlation has been the most widely used correlation for air stripping of VOC. The correlation was based on the assumption that the gas-phase resistance is negligible compared to that of the liquid-phase. In the experiments conducted, it was estimated that the gas-phase resistance represented approximately 1% of the total resistance and therefore, could be neglected (Sherwood and Holloway, 1940). It was concluded that the measured overall coefficient was equivalent to the liquid coefficient over the range studied.

Sherwood and Holloway, 1940 developed the following correlation for the experimental data

$$\frac{K_L a}{D_L} = \alpha \left(\frac{L}{\mu_L}\right)^{1-n} \left(\frac{\mu_L}{p_L D_L}\right)^{1-S} \qquad (2.60)$$

where D_L = liquid-phase diffusion coefficient
μ_L = liquid-phase viscosity
p_L = liquid density.

Packing Type	d_S	α	n
3/8 in Raschig rings	0.0064	550	0.46
1/2 in Raschig rings	0.0128	280	0.35
1/2 in Berl saddles	0.0128	150	0.28

Table 2.3 - Sherwood and Holloway Correlation Constants (Sherwood and Holloway, 1940)

The constant s was found to be 0.5, and values for α and n for the different packing types are given on Table 2.3. The solute molecular diffusion coefficient in water is calculated by the Wilke-Chang method (Lyman et al., 1982). The correlation was developed using imperial units and to convert the correlation to SI units it is necessary to add conversion constants (10.764 and 0.3048) (Roberts et al., 1982 and 1985). Therefore, Eq. 2.58 becomes

$$\frac{K_L a}{D_L} = 10.764\ \alpha \left(\frac{0.3048\ L}{\mu_L}\right)^{1-n} \left(\frac{\mu_L}{p_L D_L}\right)^{1-S} \qquad (2.61)$$

The experimental conditions for which the equation applies are summarized below.

Liquid flow: $0.27 < L < 43$ kg m^{-2} s^{-1}
Gas flow: $0.04 < G < 1.8$ kg m^{-2} s^{-1}
Temperature: 5 to $40^{o}C$
Packing: 3/8, 1/2, 1, 1.5, and
2 in Raschig rings
1/2, 1, 1.5 in Berl saddles
3 in spiral tiles

2.2.2.2 Shulman Correlation

Shulman et al., 1955 introduced a mass transfer coefficient correlation based on the separate estimation of the gas and liquid-phase coefficients and interfacial area. The model was developed from data gathered through experimentation with the vaporization of solid naphthalene packing and k_Ga data provided by Fellinger, 1941 for the absorption of ammonia into water. The model recognizes the importance of both the gas and liquid-phase resistance in the overall resistance. The model was recommended by Treybal, 1980.

The resulting correlation for the liquid-phase resistance was empirically derived and expressed as

$$\frac{K_L d_S}{D_L} = 25.1 \left(\frac{d_S L_M}{\mu_L}\right)^{0.45} \left(\frac{\mu_L}{p_L D_L}\right)^{0.5} \qquad (2.62)$$

where d_S = diameter of a sphere having the same surface area as a unit of packing.

The correlation derived for the gas-phase coefficient is expressed as

$$\frac{K_G d_S}{\mu_L} = 1.195 \ (1 - \varepsilon)^{0.36} \left(\frac{d_S G_M}{\mu_G}\right)^{0.64} \left(\frac{\mu_L}{p_G D_G}\right)^{0.33} \qquad (2.63)$$

where D_G = solute molecular diffusion coefficient in air

ε = wet porosity of packing ($\varepsilon = \varepsilon_D - \phi_t$).

The solute molecular diffusion coefficient in air was calculated by the Fuller, Schettler, and Giddings method (Lyman et al., 1982). The experimental conditions for which the equation applies are summarized below.

Liquid flow: $0.27 < L < 43$ kg·m^{-2}·s^{-1}
Gas flow: $0.14 < G < 1.4$ kg·m^{-2}·s^{-1}
Temperature: 5 to 40^{o}C
Packing: 1/2, 1, 1.5 in Raschig rings
1/2, 1, 1.5, 2 in Berl saddles

2.2.2.3 Onda Correlation

The Onda model (Onda et al., 1968) like the Shulman model distinguishes the difference between k_L, k_G, and a. The model is based on the two-resistance model and the importance of both the gas and liquid-phase resistances. The correlation for the liquid-phase coefficient, K_L, was developed from experimental data gathered from a number of sources (Fujita, 1956, Hikita, 1956, Onda et al., 1959 and 1968, and Sherwood and Holloway, 1940)

$$K_L \left(\frac{p_L}{\mu_L g}\right)^{1/3} = 0.0057 \left(\frac{L_M}{a_W \mu_L}\right)^{2/3} \left(\frac{\mu_L}{p_L D_L}\right)^{-0.5} (a_t d_p)^{0.4} \qquad (2.64)$$

where a_W = specific wetted packing area, which was estimated as a function of the liquid flow rate, packing properties and liquid properties

$$\frac{a_W}{a_t} = 1 - \exp\left(-1.45 \left(\frac{\sigma_C}{\sigma_L}\right)^{0.75} \left(\frac{L_M}{a_t \mu_L}\right)^{0.1} \left(\frac{L_M{}^2 a_t}{p_L{}^2\ g}\right)^{-0.05} \left(\frac{L_M{}^2}{p_L \sigma_L a_t}\right)^{0.2}\right) \qquad (2.65)$$

For the gas-phase coefficient, K_G, adsorption and vaporization data were correlated to produce the following equation

$$\frac{K_G}{a_t D_G} = 5.23 \left(\frac{G_M}{a_t \mu_G}\right)^{0.7} \left(\frac{\mu_G}{p_G D_G}\right)^{1/3} (a_t d_p)^{-2} \qquad (2.66)$$

Onda, 1968 recommends that the constant, 5.23, should be changed to 2.0 for small packing (d_p < 15 mm). Onda developed the correlations for the following experimental conditions

Liquid flow: $0.8 < L < 43$ kg·m^{-2}·s^{-1}
Gas flow: $0.014 < G < 1.7$ kg·m^{-2}·s^{-1}
Temperature: 5 to 40^{o}C
Packing: 1/2, 1, 1.5, 2 in Raschig rings
6, 8, 10 mm Raschig rings
1/2, 1, 1.5 in Berl saddles
1/2, 1 in Spheres
13, 25 mm rods
1 inch Pall rings

2.2.2.4 Summary of Correlations

The three models have been studied and evaluated by different authors in an attempt to determine their application to air stripping of VOC (Au-Yeung and Ponter, 1983, Ball et al., 1984, Roberts et al., 1985, Lamarche, 1986, and Staudinger et al., 1990).

The main advantage of the Sherwood and Holloway model is that it is easy to apply and it is well tested for a wide range of operating conditions and packing properties. Ball et al., 1984 studied the Sherwood and Holloway model and determined that the model provided a reasonably good means of calculating the mass transfer coefficient for most VOC except low volatility compounds such as bromoform. Ball explained that the poor fit of the Sherwood and Holloway model for low volatility compounds was because the gas-phase resistance could not be considered insignificant and must not be ignored as in the Sherwood and Holloway model. Roberts et al., 1985 evaluated the three models for the air stripping of VOC and concluded that the Onda model provided the best agreement between the predicted and observed values for the mass transfer coefficients. The studies indicated that the gas-phase resistance should not be ignored, as in the Sherwood and Holloway model, unless the stripping factor, S, exceeds a minimum of approximately 10.

Shulman's model was considered to be cumbersome in its application because of its use of a series of graphs to estimate the effective interfacial area for adsorption and desorption (Roberts et al., 1985). Treybal, 1980 introduced a set of correlations, to take the place of the graphs, to aid in the calculation of the effective interfacial area.

The Onda model was found to be the most reliable model for predicting the mass transfer coefficients for VOC (Charpenter, 1976, Roberts et al., 1985 and Staudinger et al., 1990). Shulman, 1960, however, showed that the effective interfacial area is not directly proportional to the wetted area as proposed by Onda. It has also been noted that the Onda model is not general enough and should only be applied to Raschig rings and water systems (Au-Yeung and Ponter, 1983). Staudinger et al., 1990 found that the Onda correlation predicted the mass transfer rate constants within an average standard deviation of 17 percent corresponding to a ± 30 percent accuracy value for design purposes based on a 90 percent confidence limit.

As noted by Au-Yeung and Ponter, 1983 and Roberts et al., 1985, no published correlation can accurately predict the mass transfer coefficients of VOC for all operating conditions and packing properties. Each correlation was developed for a specific set of conditions and only within these conditions can they be used with any degree of accuracy.

2.3 EXPERIMENTAL DESIGN

The principle of experimentation is either to discover something new about a process or to compare the effect of several factors on some phenomena. In engineering and scientific research, an experimenter's objectives are generally to confirm or to explore a process. If an experiment is to be performed most efficiently, an experimental design based on statistical planning should be employed. In a statistically designed experiment, the experiment is planned such that the appropriate data are collected and analyzed using a statistical method, resulting in a valid and objective conclusion (Montgomery, 1984).

2.3.1 Factorial Experimental Design

In a study of the effect of two or more factors on a response, factorial designs are the most efficient (Montgomery, 1984). A factorial design allows all possible combinations of the levels of the factors to be investigated with each complete trial or replication of the experiment. The effect of a factor is defined as the change in response caused by a change in the level of a factor. Factorial designs not only allow for the determination of the main factor effects but also the effects caused by the interaction among factors.

The use of factorial design has three main advantages (Montgomery, 1984);

1) It is more efficient than the sequential design because it requires a smaller number of observations to evaluate the same response. In a two-factor, two-level experiment, the sequential design would require six observations (one replicate for each observation) to estimate the effect of the factors using average responses; however, using a factorial design only four observations would be required to measure the same effects. The reduction is due to the unneeded replication required in the sequential design.
2) By use of a factorial design it is possible to estimate the interactive effects among factors where in a sequential design the interactive effects are considered to be insignificant. This could cause misleading conclusions when the interactive effects are not insignificant.
3) Finally, factorial designs allow effects of a factor to be estimated at several levels of the other factor, yielding conclusions that are valid over a wider range of experimental conditions.

A generalized factorial design would result in the following "complete" linear equation (Bacon, 1976):

$$\begin{aligned} E(Y) = \beta_0 &+ \beta_1 x_1 + \dots + \beta_K x_K \\ &+ \beta_{12} x_1 x_2 + \dots + \beta_{K-1,K} x_{K-1} x_K \\ &+ \beta_{123} x_1 x_2 x_3 + \dots + \beta_{K-2,K-1,K} x_{K-2} x_{K-1} x_K \\ &+ \dots \\ &+ \beta_{12\dots K} x_1 x_2 \dots x_K + \varepsilon_K \end{aligned} \tag{2.67}$$

The equation includes the main effects plus all interaction effects. All experimentation in this study was carried out using a three-level factorial design. The three-level design allows the linearity of the model to be accessed. In a two-level design the linearity of the model is not known as an infinite number of curves can go through two points.

As the number of factors and levels increase the number of treatment combinations in a factorial experiment increases rapidly. To illustrate this in a three-factor, three-level experiment 27 experimental runs are required, however, by increasing the number of factors to four the number of runs increases to 81. Table 2.4 illustrates the buildup in runs for various types of factorial experiments. Along with the increase in the number of runs comes an increase in the number of higher order interactions. This becomes a problem when trying to explain higher order interactions when they are found to be significant.

f	3^f	Main Effect	Order of Interaction			
			1st	2nd	3rd	4th
2	9	2	1			
3	27	3	3	1		
4	81	4	6	3	1	
5	243	5	10	6	5	1

Table 2.4 - Build-up of Experimental Runs for Various Factorial Designs (Hicks, 1980)

To reduce the number of observations required, a design is made where only a fraction of the total number of runs can be run. This is known as a fractional replication or fractional design. The main assumption of the fractional design is that the higher order interactions are insignificant and can be ignored. The higher order interactions are assumed to become part of the error in the model. For example in a four-factor, three-level design both the 2nd and 3rd order interactions are considered to be insignificant. Under these conditions the 81 runs required to perform a four-factor, three-level analysis can be reduced by one-third and would require only 27 runs to evaluate the main and first order interactions. It cannot be stressed enough that the higher order interactions must not exist before a fractional design can be considered. Other criteria considered when using a fractional design are: the design was rotatable; the design lends itself to orthogonal blocking and the economics of the smaller number of runs required.

CHAPTER 3

EXPERIMENTAL DESIGN

3.0 INTRODUCTION

The objective of this section is to outline the experimental procedure and the experimental design used for conducting the Henry's Law constant and air stripping experiments. The chapter is divided into three major sections: 1) Vapour-Liquid Equilibria Experiments; 2) VOC Analytical Methods; and 3) Mass Transfer Experiments.

3.1 VAPOUR-LIQUID EQUILIBRIUM

The goal of the vapour-liquid equilibria experiments was to obtain reliable air-water partitioning coefficients (Henry's Law constants) for use in the mass transfer experiments to be conducted separately. The experiments were used to interpret the effects of temperature, ionic strength and molecular polarity on the thermodynamic behavior of the selected VOC.

3.1.1 Experimental Design

The literature sites numerous techniques to measure the Henry's Law constants of volatile compounds:

a) Direct determination by measuring the gas and liquid-phase concentration of an equilibrated solution;

b) Equilibration Partitioning in Closed System (EPICS);

c) Multiple Equilibration (ME) of a closed system; and
d) other techniques such as vapour pressure and solubility measurements, and batch air stripping in a bubble column.

A brief description of each technique will be presented below.

3.1.1.1 Direct Determination

The Direct Determination technique is based on a measurement of both the gas and liquid concentrations of an equilibrated solution. The Henry's Law constant, H_C may be determined using Henry's Law

$$H_C = C_G/C_L \tag{3.1}$$

where CG and CL are the equilibrium gas and liquid concentrations, respectively.

3.1.1.2 Equilibration Partitioning in Closed System (EPICS)

The EPICS technique was introduced by Lincoff and Gossett, 1984 and is based on the comparison of mass balances in two similar systems. The equation for the mass balance in a closed system is expressed as

$$M_T = C_L V_L + C_G V_G \tag{3.2}$$

where C_L and C_G = solute liquid and gas concentration
V_L and V_G = liquid and gas volumes.

By the use of two identical vessels containing the same amount of solute, M_T, at the same temperature and ionic strength but with different liquid volumes, an expression for H_C can be derived using Henry's Law, $H_C = C_G/C_L$

$$H_C = \frac{(C_{GA}/C_{GB})V_{LA} - V_{LB}}{V_{GB} - (C_{GA}/C_{GB})V_{GB}} \qquad (3.3)$$

or, rewritten in terms of liquid concentrations

$$H_C = \frac{(C_{LB}/C_{LA})V_{LB} - V_{LA}}{V_{GA} - (C_{LB}/C_{LA})V_{GB}} \qquad (3.4)$$

3.1.1.3 Multiple Equilibration (ME)

The ME technique was introduced by McAuliffe, 1971 and Munz, 1985 and is based on the analysis of the gas or liquid-phase concentration after successive phase equilibrations. The technique requires the use of a variable volume container such as a hypodermic syringe. A volume of liquid, V_L, having a solute concentration of C_{Lo} is introduced into the syringe. Then a known volume of gas, V_G, is added and allowed to equilibrate under closed conditions. A total mass balance yields

$$C_{Lo}V_{L1} = C_{L1}V_{L1} + C_{G1}V_{G1} \qquad (3.5)$$

after substitution of the Henry's Law constant, $H_C = C_G/C_L$, the equation becomes

$$C_{Lo} = C_{G1}\left(\frac{1}{H_C} + \frac{V_{G1}}{V_{L1}}\right) \qquad (3.6)$$

After each successive equilibration the gas is expelled and an equal amount of solute-free gas is reintroduced into the syringe so that the V_G/V_L ratio remains constant. After the nth successive equilibration, Eq. 3.5 becomes

$$C_{Ln-1} = C_{Gn}\left(\frac{1}{H_C} + \frac{V_{Gn}}{V_{Ln}}\right) \qquad (3.7)$$

Substituting Eq. 3.7 into Eq. 3.5 starting with the nth equilibration and working back to the first equilibration yields

$$C_{Gi} = \frac{C_{Lo}H_C}{[1 + (V_G/V_L)H_C]^n} \qquad (3.8)$$

or in logarithmic form

$$\log C_{Gi} = \log(C_{Lo}H_C) - n \{\log[1 + (V_G/V_L)H_C]\}) \qquad (3.9)$$

Using a semi-logarithmic plot of log C_{Gi} versus n, where n is the number of equilibrations and i = 1 to n, H_C may be determined from the slope and the initial liquid concentration from the intercept

$$\text{slope} = -\log [1 + (V_G/V_L)H_C] \qquad (3.10)$$

$$\text{intercept} = \log (C_{Lo}H_C) \qquad (3.11)$$

On the other hand, if liquid concentrations are to be measured, Eq. 3.9 becomes

$$\log C_{Li} = \log C_{Lo} - n \{\log[1 + (V_G/V_L)H_C]\} \qquad (3.12)$$

with i = 0 to n, regression analysis yields

$$\text{slope} = -\log [1 + (V_G/V_L)H_C] \qquad (3.13)$$

$$\text{intercept} = \log (C_{Lo}) \qquad (3.14)$$

3.1.1.4 Other Methods

As shown by Mackay and Wolkoff, 1973 for solutes with a low water miscibility (hydrophobic), H_C may be expressed as

$$H_C = \frac{P_{Oi}}{C_L} \qquad (3.15)$$

where if C_{Li} is expressed in term of solubility, H_C may be rewritten as

$$H_C = \frac{P_{0i}}{sol_i \; R \; T} \qquad (3.16)$$

where P_{0i} = vapour pressure of component i
sol_i = molar solubility of component i.

As noted by Mackay and Shiu, 1981 this method is subject to error when the solubility of the solute in water exceeds a mole fraction of 0.01; however, for most environmental situations concentrations are much lower.

The technique of batch air stripping in a bubble column was introduced by Mackay et al., 1979 and is based on passing a gas phase through a vessel containing a dissolved solute such that equilibration is reached between the rising gas bubbles and the solute in the water. The slope of the line on a semi-logarithmic plot of the falling liquid concentration versus time is used to determine H_C. The technique is popular because the need to measure exact concentrations is not needed, thereby eliminating the preparation of standard curves.

3.1.2 Selection of Experimental Method

The selection of the most appropriate method to determine H_C was based upon the difficulty required to perform the analysis, availability of equipment, sensitivity, and reproducibility. Firstly, as noted by Mackay and Shiu, 1981, the use of the vapour pressure and solubility data for calculating H_C is subject to error if the solute mole fraction exceeds a few percentage points. Also the vapour pressure and solubility data are not available for all VOC. Therefore this technique was not be used to determine H_C but was only used as a check of the experimentally determined values. The batch air stripping technique required a specialized setup and therefore was not investigated for use in this study. The direct determination technique required the determination of both the gas and liquid concentrations. The gas phase of halogenated compounds are usually analyzed by direct injection into a GC, a technique known as Head-Space Analysis, while the liquid phase is usually analyzed by a purge and trap technique. This two step analysis would require additional sample handling and transfers, thereby introducing possible errors. Therefore the method was considered unacceptable.

Of the two remaining methods, EPICS and ME, the EPICS techniques was the most desirable due to it considerably easier steps and shorter analysis time. However as discussed by Lincoff and Gossett, 1984, the EPICS technique has a maximum sensitivity when the ratio of liquid volumes, V_{LA}/V_{LB} is large. This would necessitate the use of very large equilibration vessels (>500 ml) if acceptable sensitivity was to be achieved. A vessel of this size was not readily available. Munz, 1985 also found inconsistent results with the EPICS technique. Therefore, the ME technique with liquid-phase analysis was chosen for determining the experimental H_C values to be used in the mass transfer experiments.

3.1.3 Experimental Design

The study was designed on a two-factor, three-level factorial design. The objective of the experiment was to determine the effect of temperature and conductivity of the Henry's Law constants of VOC in water. The two factors in the design were temperature and conductivity. The study was conducted at three levels for greater accuracy and so the interaction between the two factors could be assessed.

The study was initiated through the necessity to treat groundwater contaminated by leachate from a landfill site in

Gloucester, Ontario, Canada. According to Jackson, 1983, the Gloucester site leachate contained a wide range of VOC in concentrations ranging from 11 µg/L to 7155 µg/L for toluene and chloroform, respectively. The contaminants present at the Gloucester site are shown in Table 3.1. The solutes to be used were chosen based on the concentration levels at the Gloucester site. This criterion was also used by Lamarche, 1986 for a similar study of the same site. The VOC selected from the Gloucester site leachate, also chosen by Lamarche, were: 1,1-dichloroethane (CH_3CHCl_2); 1,2-dichloroethane ($ClCH_2CH_2Cl$); chloroform ($CHCl_3$); toluene ($C_6H_5CH_3$); and trichloroethylene ($CCl_2=CHCl$). All the above VOC are present in moderate to high levels in the Gloucester site and represent a wide range volatility and solubility.

Compound	Concentration (µg/L)
Trichloroethylene	227
1,2-Dichloroethane	352
Toluene	11
1,1-Dichloroethane	492
Chloroform	7155

Table 3.1 - Gloucester Landfill Site Contaminant Levels (Jackson and Graham, 1983)

A second criterion used to select the solutes to be investigated was their environmental significance. As previously mentioned, the U.S. EPA under the Safe Water Drinking Act proposed a National Drinking Water Regulation setting Recommended Maximum Contamination Levels (RMCL) and Maximum Contaminant Levels (MCL) for eight VOC in drinking water: trichloroethylene; carbon tetrachloride (CCl_4); 1,1,1-trichloroethane (CH_3CCl_3); vinyl chloride; 1,2-dichloroethane; benzene (C_6H_6); 1,1-dichloroethylene ($CH_2=CCl_2$); and p-dichlorobenzene. The RMCL and MCL set by the U.S. EPA are shown in Table 3.2. Due to the concern expressed by the U.S. EPA the above VOC were added to the

Compound	RMCL (mg/L)	MCL (mg/L)
Trichloroethylene	Zero	0.005
Carbon Tetrachloride	Zero	0.005
Vinyl Chloride	Zero	0.001
1,2-Dichloroethane	Zero	0.005
Benzene	Zero	0.005
1,1-Dichloroethylene	0.007	0.007
1,1,1-Trichloroethane	0.2	0.2
p-Dichlorobenzene	0.75	0.75

Table 3.2 - USEPA Priority Pollutants RMCL and MCL (EPA, 1985)

solutes being investigated in this study. Vinyl chloride and p-dichlorobenzene were not able to be analyzed under the current setup and therefore were not included in the study.

Bromoform ($CHBr_3$) was also investigated due to its very low Henry's Law constant and frequent occurrence in drinking water. It should also be noted that under the MISA program initiated by the MOE a list of priority pollutants was drafted. This list included all the VOC investigated.

The conductivity levels investigated were selected based on the levels commonly found in Ontario drinking water. These levels were determined by the conductivity values indicated in the MOE Operating Summary Water Supply System 1976 (MOE,1976). The conductivity values for groundwater water supplies in Ontario range from approximately 300 µmho/cm at Cache Bay to 2300 µmho/cm at Alfred, Ontario. The conductivity of the groundwater at the Gloucester site was found to be 1300 µmho/cm (Jackson et al., 1983).

Run#	X1 (μmho/cm)	X2 (^{o}C)
1	1300	10
2	2300	10
3	1300	20
4	2300	20
5	1300	30
6	2300	30
7	300	20
8	300	30
9	300	10

X1 = Conductivity
X2 = Temperature

Table 3.3 - Factorial Design of Phase Equilibria Experiments

The experiments were conducted at conductivities of 300, 1300, and 2300 μmho/cm covering the groundwaters previously mentioned.

The experiments were conducted at temperatures of 10, 20, and 30^{o}C which were commonly used in many past studies in order to make comparisions (Munz, 1985 and Lamarche, 1986).

3.1.4 Experimental Procedure

The experiments were conducted in a 50 mL gas-tight syringe (Hamilton Company) with a Teflon Luer-Lok fitting. The syringes were fitted with Mininert Teflon syringe valves to create a gas-tight seal on the end of the syringe during the experiment.

All experiments were conducted with distilled water, further purified by a Milli-Q, Reagent-Grade Water System (Waters Canada), adjusted to the required conductivity for the day's experiment by the addition of $CaCl_2$ (BDH Chemicals). The conductivity was measured using a Radiometer

Copenhagen Conductivity Meter (type CDM 2e) which was calibrated and checked prior to every experiment. All experiments were conducted in duplicate to ensure accuracy. The syringes were rinsed with the Milli-Q solution and then filled with 22 mL of the solution. The syringe was then spiked with 3 mL of the standard solute solution to bring the total liquid volume, V_L, to 25 mL. The syringe was then mixed by a tiny magnetic mixing bar inserted into the syringe for approximately 2 minutes. The initial concentration, C_{L0}, was measured by spiking 1 mL of the liquid into a 5 mL syringe previously filled with 4 mL of Milli-Q solution. The sample was immediately injected into the purge-and-trap vessel and analyzed by the GC (to be discussed in Section 3.2).

Immediately after injection of the sample, a volume of air was introduced into each of the syringes such that $V_L/V_G = 1$ and then the syringes were sealed with the mininert valves (see Fig. 3.1). The experiments were conducted in a Forma Lab environmental chamber where the temperature could be maintained to within 0.5^{o}C. The syringes were placed in the environmental chamber on a Fisher Shaker Water Bath (model 127) fitted with a platform to hold the syringes. The syringes were shaken for approximately 80 min. (analysis time required for the two samples for each equilibration) at about 2 cycles/s. After the equilibration period, the gas was expelled under a fume hood and the liquid concentration, C_{L1}, was determined. This procedure was carried out five times, for a total of six replicate liquid concentration measurements.

After completion of an experiment the equilibration syringes were rinsed several times with deionized water. Then the syringes were rinsed with methanol several times and allowed to air dry overnight inside the fume hood. Also all mininert valves and mini-stirring bar were rinsed with

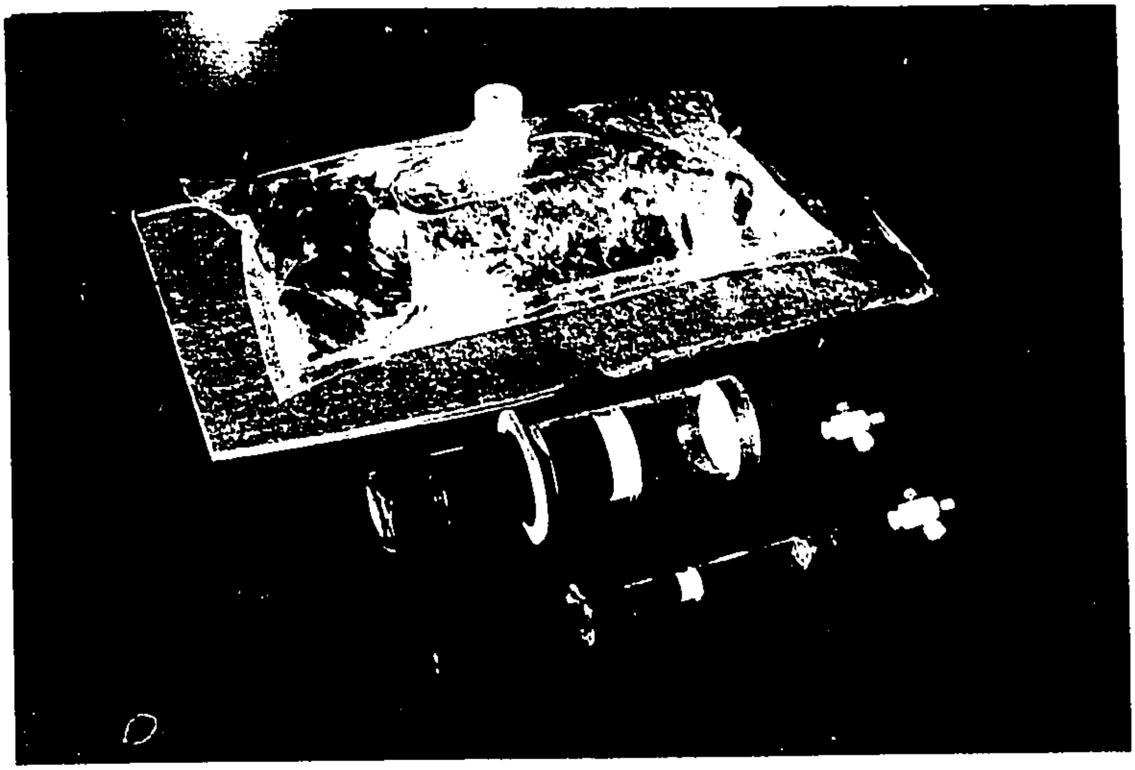


Figure 3.1 - Equilibrium Vessel for ME Experiments

methanol and deionized water several times and then allowed to air dry over night. All sampling syringes were rinsed with methanol and deionized water between samples.

3.2 VOC ANALYTICAL METHODS

3.2.1 Analytical Design

Several methods have been published for the analysis of VOC in water. The two most commonly used methods for analyzing VOC in water are the liquid-liquid extraction and the purge-and-trap methods. The two methods have been compared by Dressman et al., 1979 and Kirshen, 1981. The procedures for both the liquid-liquid extraction and the purge-and-trap methods were presented in detail by Dressman et al., 1979 and therefore, will not be presented here. The advantages of the liquid-liquid extraction (LLE) method are that it is simple, direct, inexpensive, and requires less time as compared to the purge-and-trap (PAT) method. However, it has numerous disadvantages such as

1) The electron capture detector used for the LLE method is not as selective as the flame ionization detector used in a standard PAT analysis therefore the PAT method is considered more reliable without confirmatory data,
2) The resolution of a VOC peak in LLE analysis is not as great as in PAT analysis, and
3) Nonvolatile interference has been noted in LLE analysis; this interference is not present in PAT analysis.

Dressman et al., 1979 recommended that the LLE method be used only for routine analysis of VOC and only in conjunction with a PAT analysis to identify the compounds present in the sample. It was concluded that the PAT analysis was the best method for the analysis of VOC.

3.2.2 Analytical Procedure

The VOC were analyzed using a Varian Vista 6000 gas chromatograph employing a flame ionization detector. The analytical column was a 2.44 m long by 3 mm SP-1000 column packed with 60/80 Carbopack-B (Supelco Inc.). The operating parameter were as follows: column temperature 45^{o}C for 3 min increasing at 8^{o}C/min to 210^{o}C holding for 5.63 min; injector temperature 210^{o}C; detector temperature 210^{o}C; attenuation 512; sensitivity 10^{-11}; carrier gas nitrogen at 30 mL/min; detector gases air at 300 mL/min and hydrogen at 30 mL/min.

The samples were concentrated using a Tekmar Liquid Sample Concentrator LSC-2 (Tekmar Company). The samples were purged for 11 min with nitrogen at 30 mL/min and adsorbed on a Tenax trap. After purging was completed the VOC were desorbed from the trap for 4 min by the carrier gas and analyzed by the GC. All samples were injected into the purge and trap vessel and the start switch was pressed for automatic analysis. The output peaks from the detector were identified, and quantified by a computerized data handling software package, Waters 820 (Waters Canada).

The detector signal was calibrated by injection of a set of external standards. A standard solution was prepared containing all the solutes to be analyzed. Three standards were made, one corresponding to each of the conductivities to be studied. The standards were prepared using Milli-Q water. The standards were prepared in ultra-clean Tedlar sampling bags (Cole Palmer) with Teflon faced septa closures. Approximately 1 L of water was added to each bag. The exact amount added was determined by weighing the bag. Approximately 7 mL of HPLC grade methanol was added to each bag to aid in dissolving the VOC. Known amounts of each of the solutes were injected into each bag to achieve concentrations in accordance with Table 3.1. The exact amount injected into the standards bag were determined and the actual concentrations in the bags were recalculated. The actual concentrations were used to calculate the calibration curves for the solute standards. Known amounts of the standard solution were spiked into a 5 mL sampling syringe for immediate injection into the purge vessel and analysis for the different solutes. Seven different concentrations were injected for each standard.

The calibration curves for each solute were evaluated by the Waters 820 integration software and stored for later use on the computer. The calibration curves are presented in Appendix A. The standards were periodically rerun throughout the course of the Henry's Law and air stripping experiments to ensure linearity of the detector. All solutes exhibited a linear response ($R^2 > 0.99$) for all concentrations studied (see Appendix A).

3.3 MASS TRANSFER EXPERIMENTS

3.3.1 Design of Packed Column

Figure 3.2 shows a schematic of the experimental apparatus for the countercurrent packed-column studies. The apparatus was similar to that used by Lamarche, 1986. The column consisted of plexiglas pipe, inside diameter of 101.6 mm, cut into section of 304.8 mm in length (see Fig. 3.2). The entire column consisted of six sections. The sections were joined by plexiglas sleeves, inside diameter of 114.3 mm, that were sealed with Viton o-rings. The top and bottom sections were designed such that end effects were minimized. The liquid distributor cap was approximately 38 mm above the top of the packing, while the bottom of the packing was approximately 152.4 mm from the bottom of the column. The column was fitted with packing support plates and liquid redistributors between every section of the column.

The experiments were conducted with three different packings; 6.4 and 12.8 mm ceramic Raschig rings, 12.8 mm ceramic Intalox saddles, shown on Fig. 3.3. All the packings were obtained from The Norton Company, Ohio. The ratio of column diameter to packing size was $d_C/d_P = 8$ for the 12.8 mm packing and 16 for the 6.4 mm packing. Treybal, 1982 recommended that the $d_C/d_P > 15$ to eliminate channelling in the column. Channelling occurs when the liquid flow is not a uniform time distribution (plug flow) and liquid flows down the walls of the column faster than in the packing.

The amount of channelling present in the column under various experimental conditions (liquid and gas flow rates)

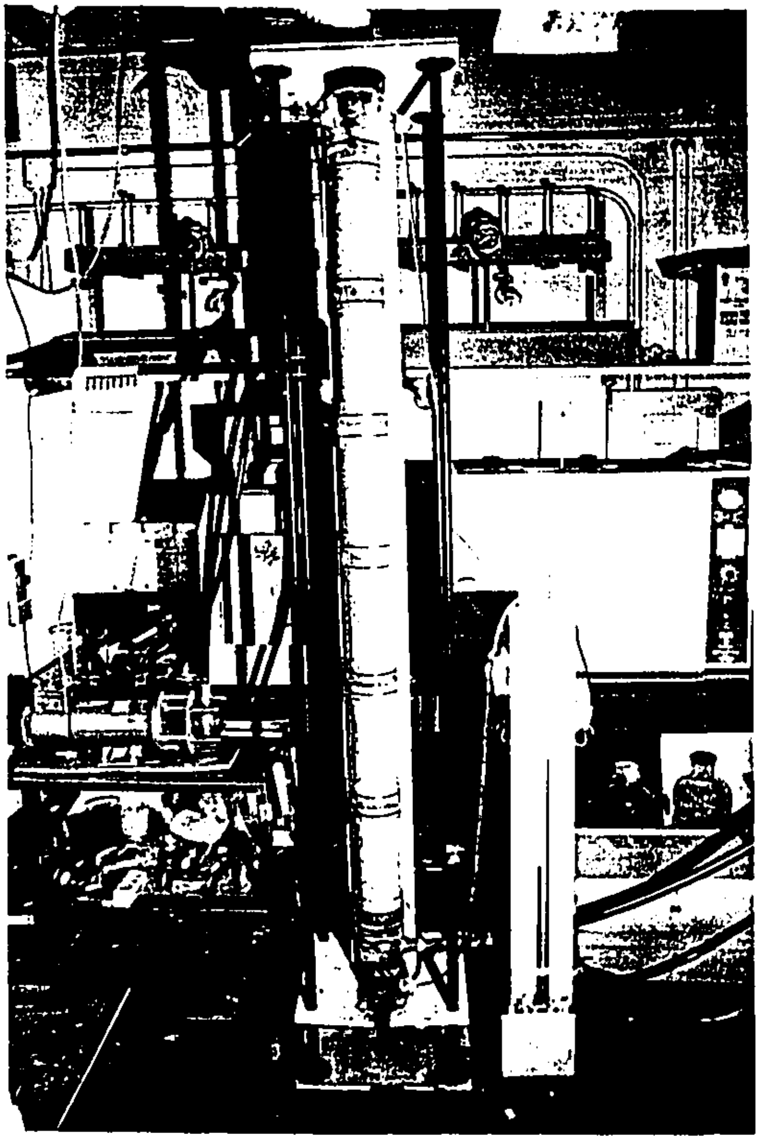


Figure 3.2 - Countercurrent Packed Column

and packing types was evaluated by column tracer studies. The tracer studies were performed and analyzed in accordance with Sater and Levenspiel, 1966 and Levenspiel and Smith, 1957. The tracer studies are presented in Appendix F and

Figure 3.3 - Experimental Packing used in Countercurrent Packed Column Runs

discussed in Section 4.2.2. To ensure maximum randomness in the packing, the column was packed in a water tank at a depth of at least 100 mm below the water surface as recommended by the manufacturer. The porosity of the packing was measured by Lamarche, 1985 in a previous study. The packing properties can be found in Table 3.4.

The influent liquid flow rate was controlled using a 19 mm brass gate valve. The flow rate was measured with a Signet magnetic flowmeter calibrated initially using a known volume container and a stopwatch. The liquid level at the bottom of the column was maintained just above the bottom of column by means of a siphon tube to act as an air seal. The air flow was provided by a Brunner air compressor (model H-63) (Durham Bush). The gas flow rate was controlled by a gate valve on the compressor tank and measured using a Gilmont shielded bypass rotameter with a glass float (Cole

Packing Type	d_P	a_t	ε_D	d_S
1/4 in R.R.	0.0064	764	0.62	0.0056
1/2 in R.R.	0.0128	407	0.64	0.0122
1/2 in I.S.	0.0128	623	0.65	0.0081

d_P = diameter of packing
a_t = total specific area of packing
ε_D = dry packing porosity
d_S = diameter of a sphere equal to a unit of packing

Table 3.4 - Experimantal Packing Properties (Ludwig, 1979)

Parmer). The rotameter was calibrated by the manufacturer prior to installation. The pressure at the entrance of the rotameter was measured with an open ended U-tube filled with water. The pressure drop across the column packing was measured with another U-tube filled with red guage oil (specific gravity 0.827).

Influent and effluent samples were taken from three-way valves (see Fig. 3.4) located on the inflow pipe at the top of the column and on the outflow pipe at the bottom, respectively. The valves were fitted with Luer-Lok fittings to provide a proper fit with the sampling syringe.

The effluent gas was released to the atmosphere through the fume hood. The effluent liquid was pumped from the collector reservoir to a set of four aeration tanks setup in series under the fume hood to remove any remaining VOC before releasing the effluent water to the drain.

3.3.2 Experimental Design

The experiment was designed as a four-factor, three-level fractional factorial design as shown on Table 3.5. The fractional design was employed to reduce the number of experiments from 81, required for a full factorial design

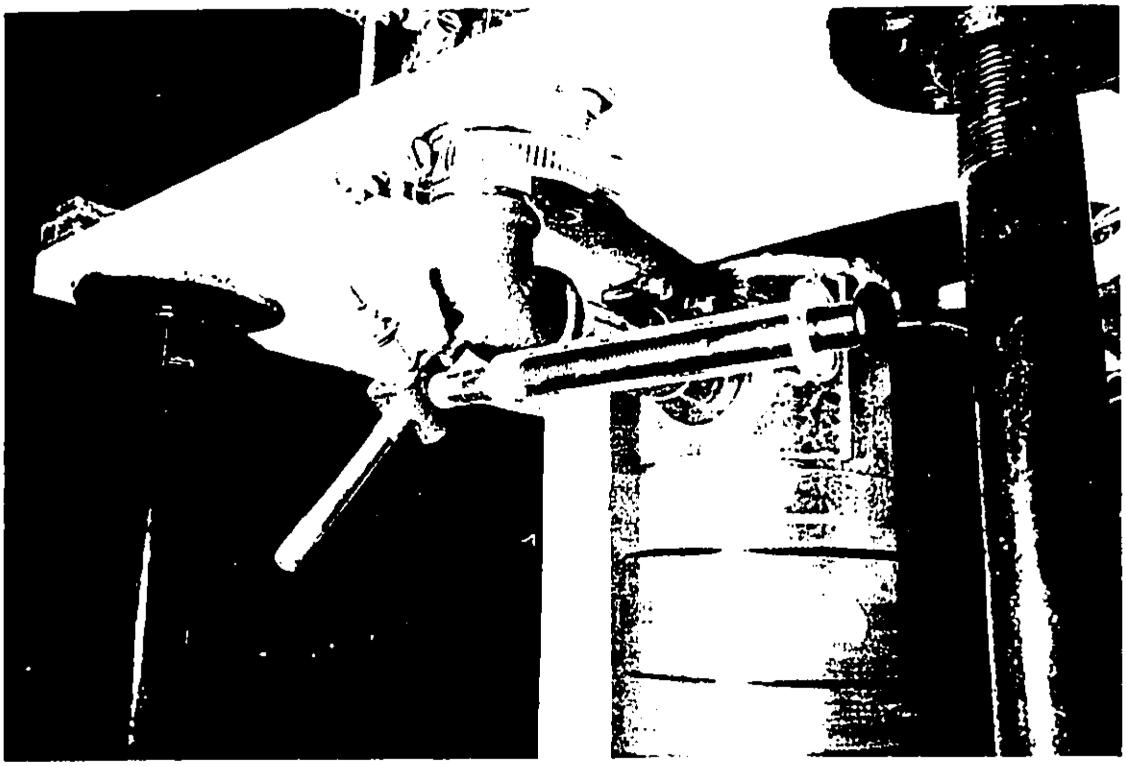


Figure 3.4 - Influent and Effluent 3-way Sampling Valve

(i.e., 3^4), to 27 runs. The main assumption made in the fractional factorial design is that the effect of the higher order interactions (i.e., ABC, ABD, ACD, BCD, and ABCD) can be ignored. This assumption is generally valid in most cases (Bacon, 1976). The four factors to be used are liquid flow rate, gas flow rate, conductivity, and packing type. Three levels of each factor were used to ensure the accuracy of parameters, and the linearity of the model.

The liquid and gas flow rates used in the air stripping experiments were chosen so that flooding of the column would not occur while maximizing the gas to liquid ratio. The second criterion used to select the flow rates was to select a flow rate within the range of gas and liquid flow rates used in the mass transfer correlations. To assess the possibility of flooding in the column, Fig. 3.5 from Treybal 1980 was used. Each experimental run was evaluated using the Fig. 3.5 so that the gas pressure drop was less than 400 N/m2/m

RUN #	X1 (L/min)	X2 (L/min)	X3 (μmho/cm)	X4 (-)
1	2	25	1300	2
2	4	25	1300	2
3	2	75	1300	2
4	4	75	1300	2
5	3	50	300	1
6	3	50	2300	1
7	3	50	300	3
8	3	50	2300	3
9	2	50	1300	1
10	4	50	1300	1
11	2	50	1300	3
12	4	50	1300	3
13	3	25	300	2
14	3	75	300	2
15	3	25	2300	2
16	3	75	2300	2
17	2	50	300	2
18	4	50	300	2
19	2	50	2300	2
20	4	50	2300	2
21	3	25	1300	1
22	3	75	1300	1
23	3	25	1300	3
24	3	75	1300	3
25	3	50	1300	2
26	3	50	1300	2
27	3	50	1300	2

X1 = Liquid flow rate
X2 = Gas flow rate
X3 = Conductivity
X4 = Packing Type, 1 - 6.4 mm Raschig rings
2 - 12.8 mm Raschig rings
3 - 12.8 mm Intalox saddles

Table 3.5 - Fractional Factorial Design for Mass Transfer Experiments

depth of packing recommended by Treybal, 1980. Typically, packing manufacturer's recommend a gas pressure drop from 200 to 400 N/m2/m depth of packing for the design of air strippers. Ball et al., 1981 concluded that for the optimum design of an air stripper a gas pressure drop of less than 50 N/m2/m depth of packing and a stripping factor greater than 5 should be used. The liquid and gas flow rates for the experiments were selected such that the predicted gas pressure drop (see Fig. 3.5) was less than the 400 N/m2/m depth of packing given by Treybal but greater than the 50 N/m2/m depth of packing specified by Ball. The levels selected for the experiments were

Liquid flow rates:	2,3,4 L/min (4.1,6.2,8.2 Kg/m^2/s)
Gas flow rates:	25,50,75 L/min (0.06,0.12,0.19 Kg/m^2/s)

The conductivity levels used in the mass transfer experiments were the same as those used in the Henry's Law experiments, namely 300, 1300, and 2300 µmho/cm.

The packing types used in the experimental run were 6.3 mm Raschig rings, 12.5 mm Raschig rings, and 12.5 mm Intralox saddles. These packings were also used by Lamarche 1985.

All other parameters such as temperature, and influent VOC concentration were held constant (± 10%) throughout the experimental runs.

3.3.3 Experimental Procedure

The preparation for each experiment commenced on the day prior to running the experiment while the current experiment was being analyzed. Firstly, the main reservoir was filled to a depth of 70 cm with tap water. The temperature of the water entering the tank was adjusted to be approximately at ambient temperature. The conductivity of the tapwater was adjusted to correspond to the experimental value by the addition of granulated $CaCl_2$ (Fisher Scientific and BDH Chemical) according to a conductivity correlation developed for the tank. The correlation is presented in

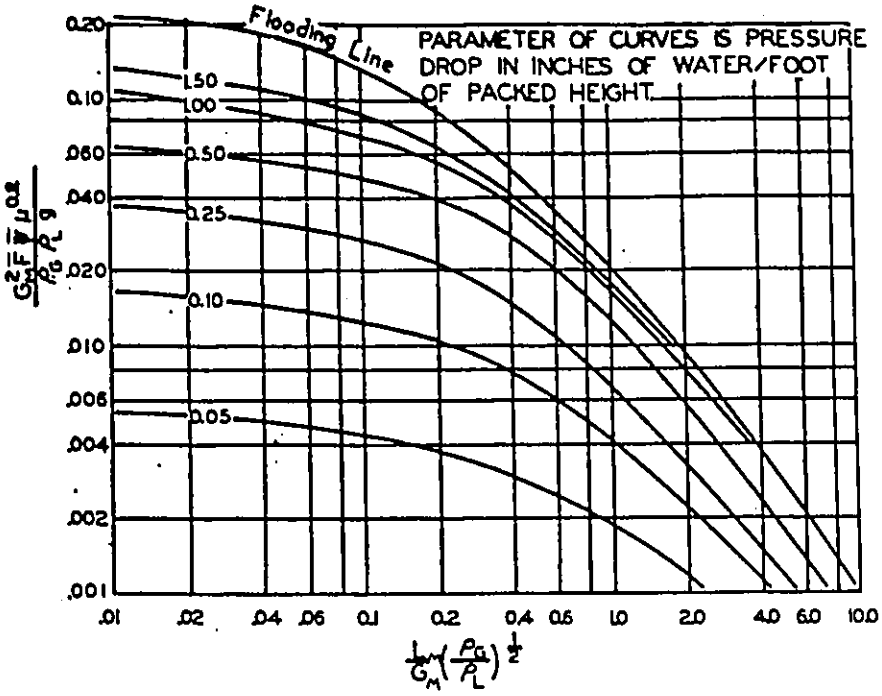


Figure 3.5 - Flooding and Pressure Drop in Packed Columns

Appendix B. The tank was covered and mixed overnight by a mechanical mixer to allow the temperature and conductivity to stabilize. The temperature and conductivity were checked and corrected the following day prior to starting the run. The VOC solution was prepared on the day prior to the experimental run. Approximately 500 mL of Milli-Q water adjusted to the experiments conductivity using powdered $CaCl_2$ was added to a 4.1 L Tedlar gas sampling bag fitted with a teflon faced septa closure. Also 500 mL of commercial grade methanol (BDH Chemicals) was added to the bag to help in dissolving the VOC. The volume of methanol was calculated to ensure that the final methanol molar fraction in the experimental water would be below the molar limit of $3X10^{-3}$ molar set by Munz, 1985 so that the cosolvent effects could be considered to be negligible. The bag was then mixed for two hours on a shaker table to ensure that the bag was completely mixed and the temperature returned to ambient.

After mixing, the air in the bag was removed using a Multiflex pump fitted with a hypodermic needle for insertion into the bag through the septa closure. The organics were spiked into the bag using a 1000 µL gas tight syringe and hand mixed for one minute between injections. The bag was then set on a shaker table to mix overnight. On the next day, the VOC solution was transferred into a 20.3 L Tedlar bag containing 3.5 L of Milli-Q water (conductivity adjusted). Then the air was removed and the bag was mixed on a shaker table for one hour before starting the experiment.

While the sample bag was mixing, water and air were allowed to flow through the column so that all contaminants from the previous experiment would be removed. Before each experiment, the magnetic flow meter (Signet) used for measuring the liquid flow was calibrated according to the manufacturer's instructions.

The VOC pump and inlet line were flushed with a mixture of 1 L of tap water and 100 mL of methanol to remove any residual VOC left there. Then the air bubbles were removed from all influent pipes by venting the pipes to the atmosphere. The presence of air bubbles could cause flow variations and variation in VOC concentration due to adsorption and desorption of VOC to and from the bubbles. The liquid and air flows were then adjusted to the required rates and allowed to settle. The flow rates were adjusted periodically when required. After mixing was completed, the VOC solution bag was connected to the VOC inlet pump, ensuring that no air was introduced into the system. The organic pump was started and the flow was adjusted to approximately 40 mL/min. The system was allowed to run for one hour before the first pair of samples (influent and effluent samples) were taken to ensure that steady state was reached. Five pairs of 5 mL samples were taken at five minute intervals. Before each sample was collected approximately 20 mL of liquid was allowed to flow through the sampling valve so that a fresh sample was taken each time. The air bubbles in the sampling syringes were then removed under the fume hood, and the syringes were capped with a Mininert valve and stored in a refrigerator until they could be analyzed. The samples were analyzed in the order in which they were taken and in accordance with the analytical method described earlier (Section 3.2.2).

During the collection of the samples, operating parameters for the experiment such as conductivity, influent and effluent liquid temperature, compressor air temperature, lab and compressor room temperature, liquid, VOC, and air flowrate, and manometer pressures were recorded. The instruments were read at the beginning and the end of experiment with the high and low values being recorded.

CHAPTER 4

RESULTS AND DISCUSSION

4.0 INTRODUCTION

The chapter is separated into two main sections: 1) Vapour-liquid equilibria; and 2) Mass transfer coefficients. The discussion will evaluate the effect of the results on the air stripping process, the possible experimental errors and the engineering significance of the findings.

4.1 VAPOUR-LIQUID EQUILIBRIA EXPERIMENTS

The Henry's Law constants were determined for various VOC of environmental significance: $CH_2{=}CCl_2$; CH_3CHCl_2; $CHCl_3$; $ClCH_2CH_2Cl$; CH_3CCl_3; CCl_4; $CCl_2{=}CHCl$; C_6H_6; $CHBr_3$; and $C_6H_5CH_3$. The Henry's Law constants were determined over a range of temperature ($10^oC < T < 30^oC$) and conductivity ($300\ \mu mho/cm < C < 2300\ \mu mho/cm$). The results of the experiments are presented in Appendix B.

4.1.1 Evaluation of ME Results

The Henry's Law constants were determined using the ME technique discussed previously. The experimental concentration data were analyzed by the following linear least-squares regression

$$\log C_{Li} = \log C_{Lo} - \log \left(1 + \frac{V_G}{V_L} H_C\right)^n \qquad (3.12)$$

where C_{Li} = final liquid concentration of compound i
C_{Lo} = initial liquid concentration of compound i
V_L = volume of liquid in equilibration vessel
V_G = volume of air in equilibration vessel
i = 0 to n
n = number of equilibration steps conducted.

Resulting output from the ME analysis is presented on Tables B.1 to B.10 in Appendix B. Typical plots of the linear regression and corresponding residuals for chloroform are shown on Figs 4.1 and 4.2, respectively.

Evaluation of the residuals is a powerful diagnostic tool for checking model adequacy and error structure of the data. The assumption is that the residuals should be randomly and normally distributed if the model and method of regression are appropriate. Analysis of the residual plots from the Henry's Law constants experiments indicates that no trends or patterns exist in the data. Therefore, the log-linear regression was considered an appropriate procedure for analyzing the data.

4.1.2 Assessment of Experimental Errors

Numerous possible experimental and analytical errors could affect the determination of the Henry's Law constants in the ME experiments. The errors are discussed below.

Losses occurring from the equilibration vessel will cause a decrease in the concentration of the VOC, thereby, artificially increasing the Henry's Law constants. The tightness of the equilibration vessel was evaluated by determining the change in concentration of the sealed vessel over time. Two syringes were spiked with 3000 µL of the standard solution and mixed with a mini-magnetic mixer for

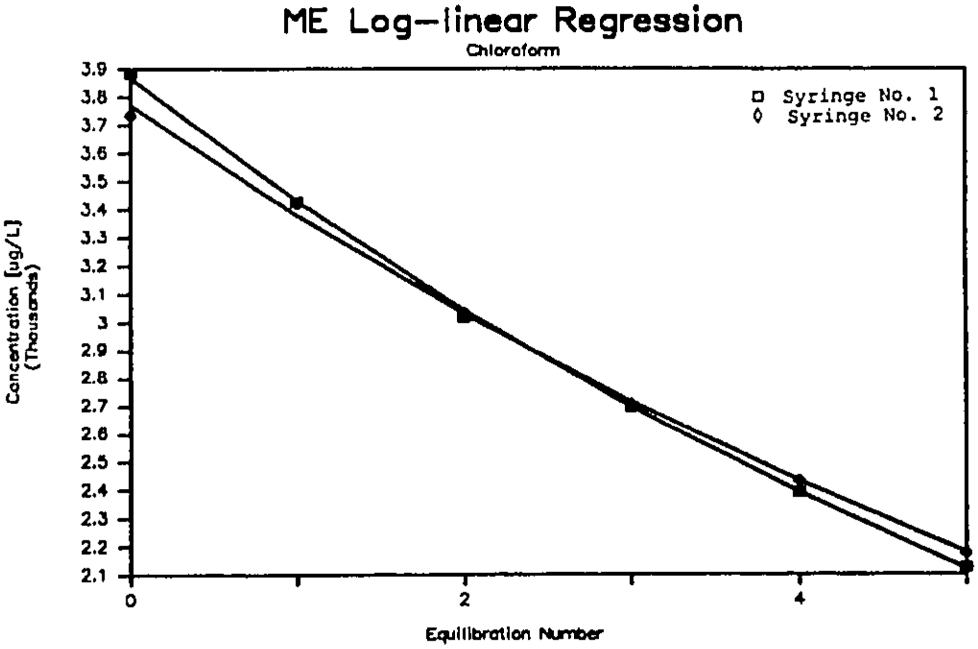


Figure 4.1 - Typical ME Linear Regression Plot for $CHCl_3$

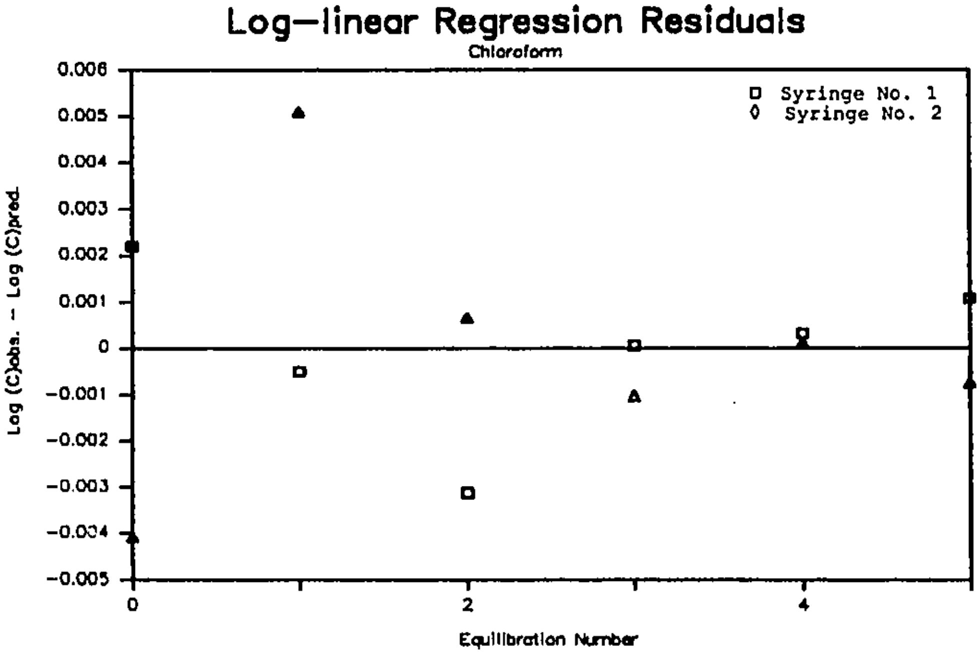


Figure 4.2 - Typical ME Residual Plot for $CHCl_3$

one hour. The initial concentration was then determined and the two syringes were placed in the environmental chamber to mix overnight. The concentration was determined after 24, 48 and 72 hours. The results are shown in Appendix C. The concentration was found to decrease 10% from the initial concentration over the 72 hour period. Based on these findings, the losses were assumed to be insignificant over the approximate 6 hour duration of the experiment.

Equilibrium between the gas and liquid-phase is an essential part of the determination of the Henry's Law constant by the ME technique. The equilibrium of the VOC was not specifically determined in this study, however, as noted by Dietz and Singley, 1979, approximately 1 minute of "vigorous handshaking" of headspace vials is sufficient for equilibrium to be reached. Munz, 1985 judged that based on the variability in the equilibration times used in the experiments and reproducibility of the results he obtained, equilibrium must have been achieved between the phases. Since the equilibration time used in this work exceeds that of Munz, 1985 and Dietz and Singley, 1979 it was assumed that true equilibrium between the phases was attained. The reproducibility noted by Munz, 1985 was also found in this work.

Liquid and gas volumes were adjusted for each equilibration in the ME technique and are subject to errors associated with the measurements. Munz, 1985 used a classical error propagation technique to evaluate the error associated with a change in the gas or liquid volume. The error in H_C due to V_L and V_G can be estimated by

$$\frac{\Delta H_C}{H_C} = ((\frac{\Delta V_G}{V_G})^2 + (\frac{\Delta V_L}{V_L})^2)^{1/2} \qquad (4.1)$$

The experiments were conducted using 50 mL syringes having 1 mL graduations. Throughout the experiment, V_L/V_G was set equal to 1. The largest error will occur with the smallest value of V_L and V_G. The smallest value of V_L and V_G is 20 mL occurring during the 5th equilibration. Munz, 1985 determined that the absolute error associated with each volume measurement was < 0.1 mL, therefore the error in H_C due to V_L and V_G is approximately ± 1%.

Adsorption and/or absorption of VOC by the glass or Teflon parts of the syringes could cause a decrease in the concentration in the syringe over time. The amount of adsorption and absorption was examined by Munz, 1985 and he found that no significant decrease in concentration was found during his experiments.

The Henry's Law constants were determined using the exponential form of Eq. 3.12. Solving for H_C yields

$$H_C = \left(\left(\frac{C_{Lo}}{C_{Li}}\right)^{1/n} - 1\right) \frac{V_L}{V_G} \qquad (4.2)$$

Munz, 1985 showed that it was possible to obtain a measure of the analytical error by taking the partial derivative with respect to C_{Lo} and C_{Li} and adding the square terms as in typical error propagation calculations (Crandell and Seabloom, 1970).

$$\frac{\Delta H_C}{H_C} = \frac{1}{n} \left(\frac{1}{H_C} \frac{V_L}{V_G} + 1\right) \left(\left(\frac{\Delta C_{Lo}}{C_{Lo}}\right)^2 + \left(\frac{\Delta C_{Ln}}{C_{Ln}}\right)^2\right)^{1/2} \qquad (4.3)$$

The actual analytical error in the replicate GC measurements was not specificly investigated, however, the experimental results from the two syringes showed good repeatability for the determination of H_C within ± 5%. The manufacturers have also noted that the error associated with the analysis of replicate samples can range from 20 to 30% (Roberts, 1982).

4.1.3 Effect of Temperature on the Henry's Law Constants

The experimental values of the Henry's Law constants, H_C, determined from the ME analysis were fitted to the following equation

$$\log_{10} H_C = -\frac{B}{T} + A \qquad (4.4)$$

where T is the absolute temperature to determine their temperature dependence. As noted by Hanson, 1985 bias can occur when log-linear regressions are employed. Bias is introduced by taking the logarithm of the data. The bias is evident when the residuals are back-transformed. In a least-squares regression the sum of the log-transformed residuals will be equal to zero but when back-transformed the sum of the residuals will not equal zero. This occurs because the logarithmic transform is non-linear causing the larger observations to be reduced proportionally more than the smaller values. Hanson, 1985 showed that if the residuals are normally distributed, the following formula can be used to approximate the bias introduced due to the non-linearity of a natural log transform

$$FCF = \exp\left(\frac{\sigma^2}{2}\right) \qquad (4.5)$$

where FCF = Finney's correction factor, and σ = variance of the residuals. For the data transformed using base 10 logarithms, Eq. 4.5 becomes

$$FCF = \exp\left(2.65\ \sigma^2\right) \qquad (4.6)$$

The value of σ can be approximated by the standard error of estimate of the regression. The back-transformed values for H_C determined from the log-linear regression analysis were multiplied by FCF to remove any bias caused by the transform.

Figures 4.3 to 4.12 convey the temperature dependence of the Henry's Law constants for the VOC investigated in the study: $CH_2{=}CCl_2$; CH_3CHCl_2; $CHCl_3$; $ClCH_2CH_2Cl$; CH_3CCl_3; CCl_4; $CCl_2{=}CHCl$; C_6H_6; $CHBr_3$; and $C_6H_5CH_3$. The solid line represents the best fit line for the three conductivities studied (i.e., 300, 1300, and 2300 μmho/cm), according to Eq. 4.4.

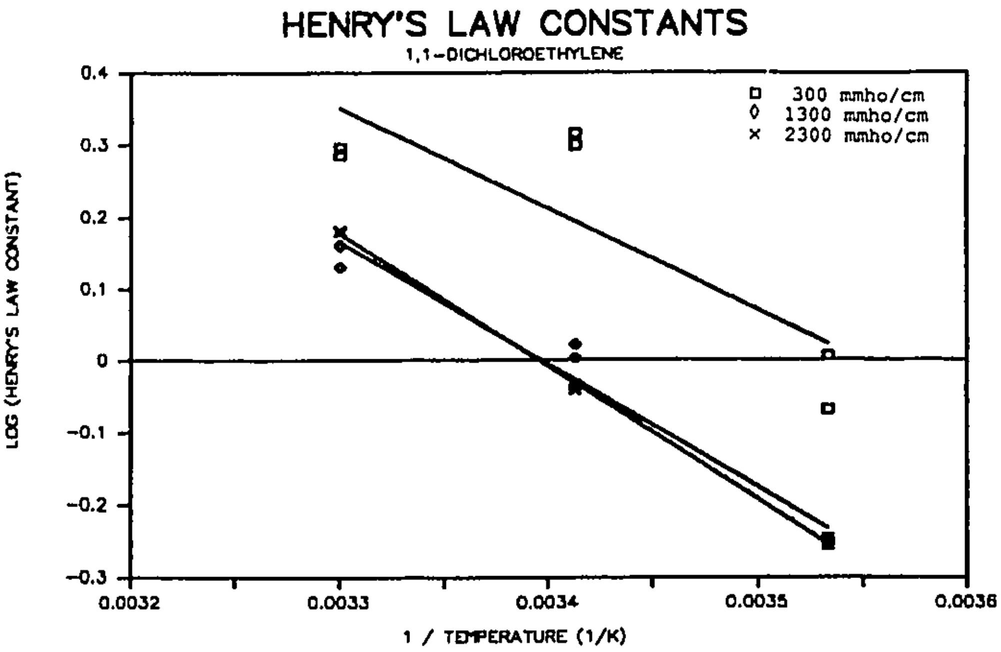


Figure 4.3 - Temperature Dependency of the Henry's Law Constants for $CH_2=CCl_2$

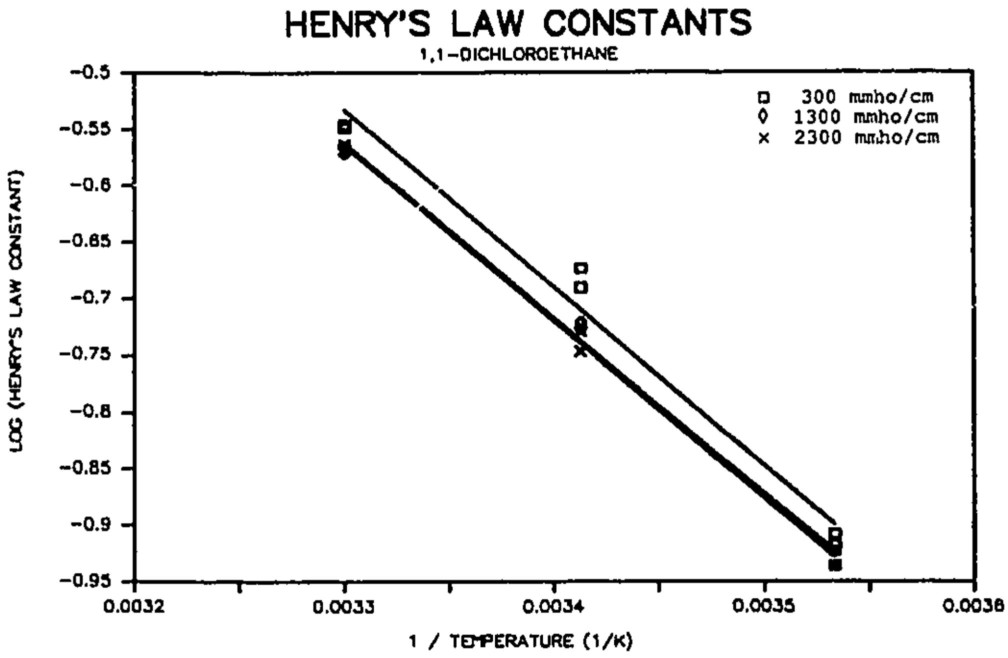


Figure 4.4 - Temperature Dependency of the Henry's Law Constants for CH_3CHCl_2

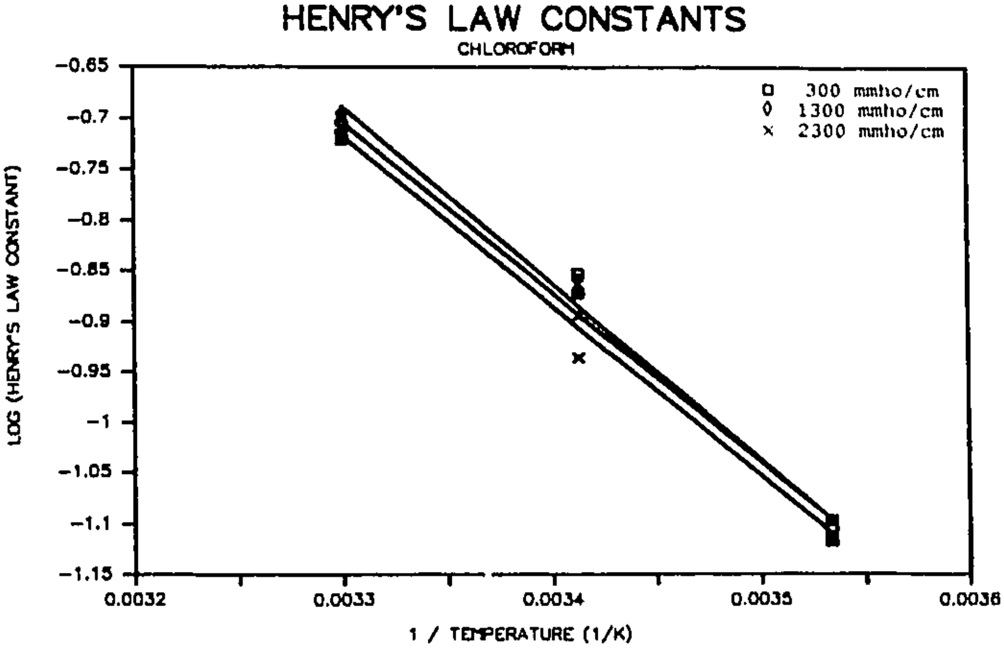


Figure 4.5 - Temperature Dependency of the Henry's Law Constants for $CHCl_3$

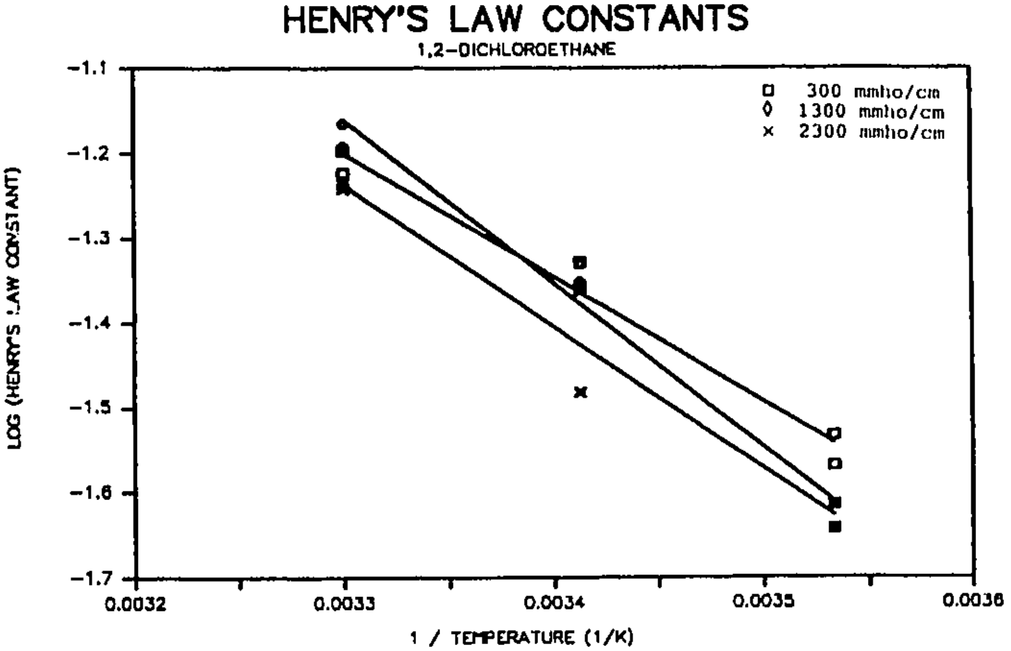


Figure 4.6 - Temperature Dependency of the Henry's Law Constants for $ClCH_2CH_2Cl$

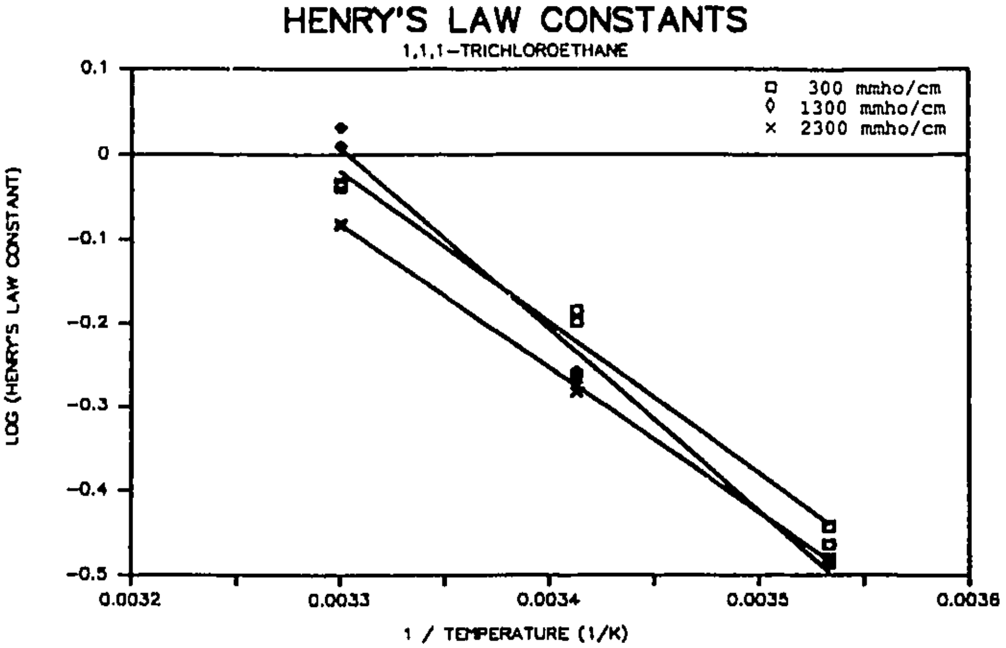


Figure 4.7 - Temperature Dependency of the Henry's Law Constants for CH_3CCl_3

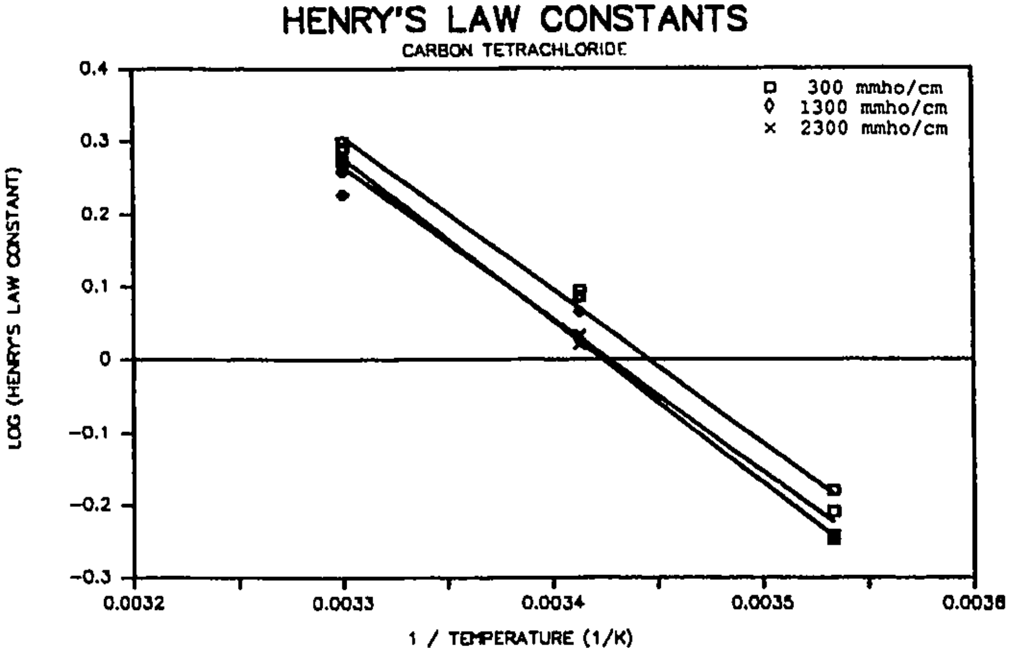


Figure 4.8 - Temperature Dependency of the Henry's Law Constants for CCl_4

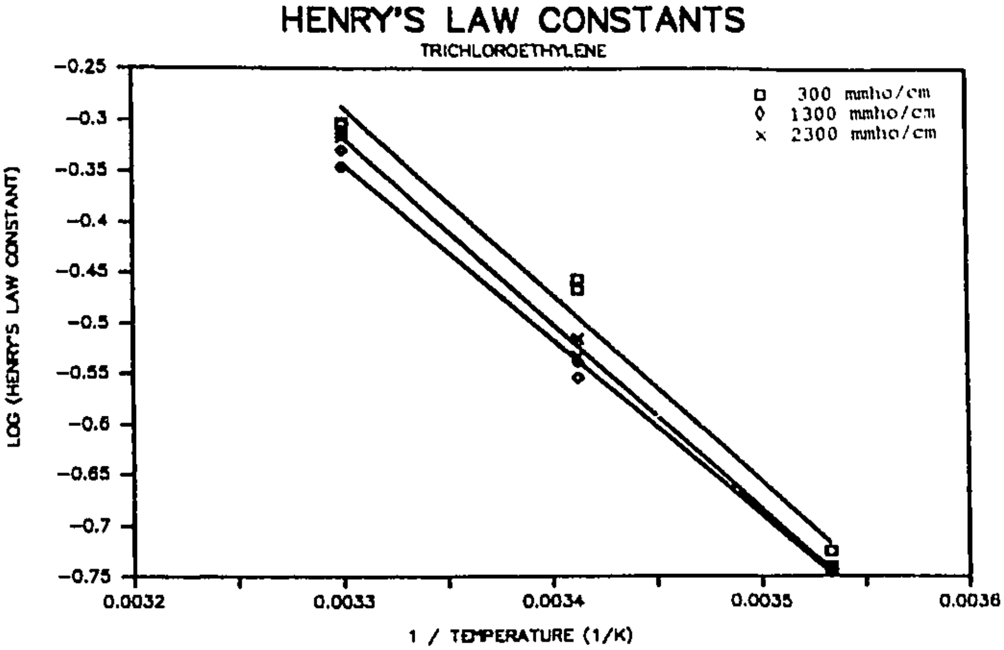


Figure 4.9 - Temperature Dependency of the Henry's Law Constants for $CCl_2=CHCl$

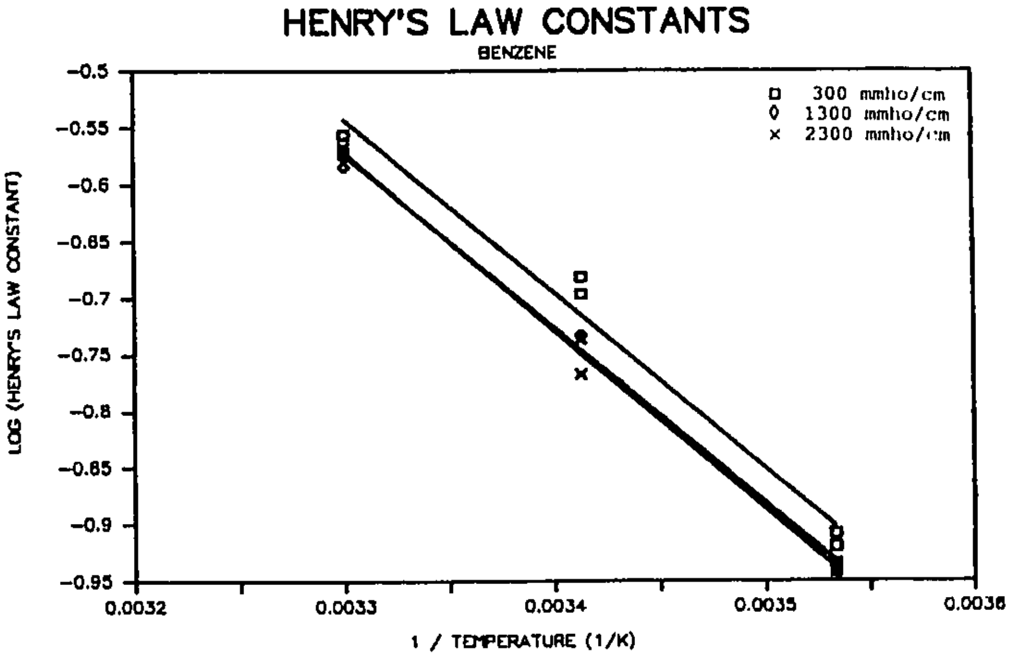


Figure 4.10 - Temperature Dependency of the Henry's Law Constants for C_6H_6

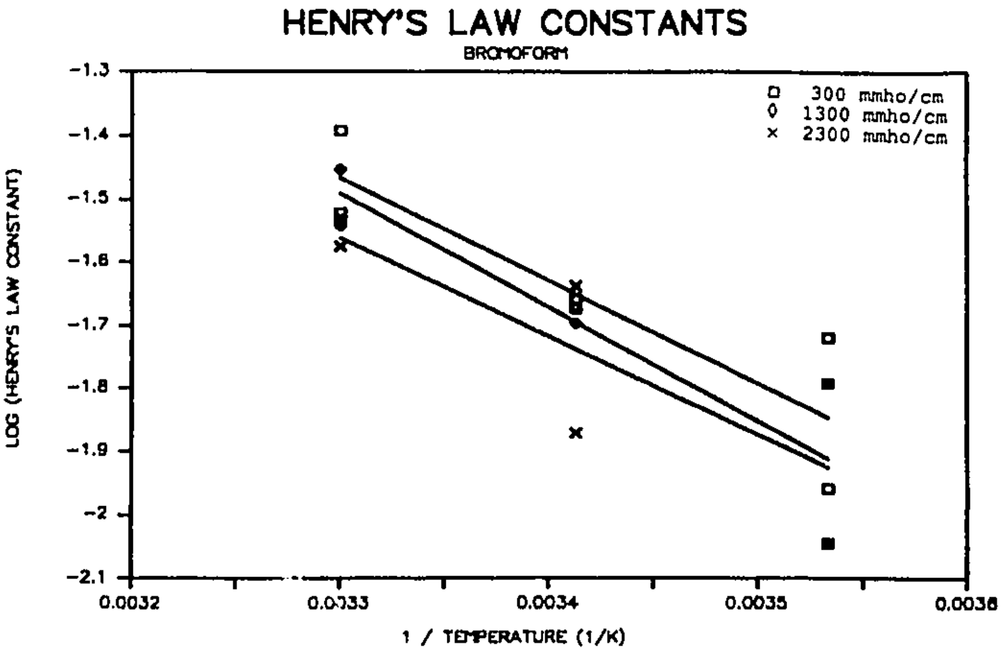


Figure 4.11 - Temperature Dependency of the Henry's Law Constants for $CHBr_3$

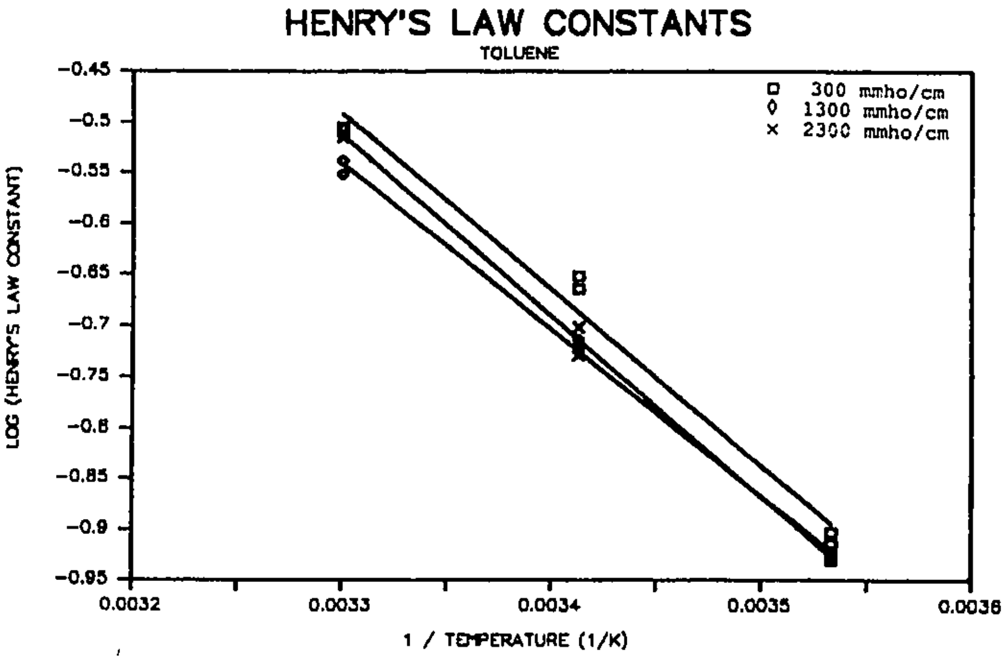


Figure 4.12 - Temperature Dependency of the Henry's Law Constants for $C_6H_5CH_3$

The equations for the regression lines and the coefficient of determinations (R^2) are shown on Table B.11 in Appendix B. The results of each individual experiment are also presented on Tables B.1 to B.10 in Appendix B.

Temperature dependency of Henry's Law constants has been studied in the past by Hunter-Smith 1983, Lamarche 1986, Leighton and Calo 1981, Lincoff and Gossett 1984, Munz 1985, and Nicholson et al. 1984. Various methods were used by the authors to determine the constants: ME method with gas-phase analysis (Hunter-Smith 1983), EPICS method with liquid-phase analysis (Lamarche 1986), purge-and-trap technique (Leighton and Calo 1981), EPICS method with gas-phase analysis (Lincoff and Gossett 1984 and Gossett 1987), ME method with gas and liquid-phase analysis (Munz 1985), and bubble-column technique (Nicholson et al. 1984).

To compare the various Henry's Law constant temperature relations the data in the above articles were converted to the dimensionless Henry's Law constant, H_C and fitted to Eq. 4.4 used in this study. The resulting equations were plotted and presented on Figures 4.13 to 4.17. The equation corresponding to a conductivity of 300 µmho/cm was used to represent the temperature dependancy in this study. This will approximate that conductivity used by previous authors since no conductivities or ionic strengths were noted in previous studies and the studies were generally conducted using deionized water. Also plotted on the figure where available was the temperature dependent equations developed from vapour pressure and solubility data, where available, according to Eq. 2.9. The vapour pressure data was taken from Boublik et al., 1984 and the solubility data was found in Horvath, 1982 (Chapter 8).

The data were converted to the units found in Eq. 2.9 and the best fit line was determined by a log-linear regression procedure. The solubility data for $CH_2{=}CCl_2$ were not available and the only previous study was performed by Gossett, 1987. No previous studies were found in the case of

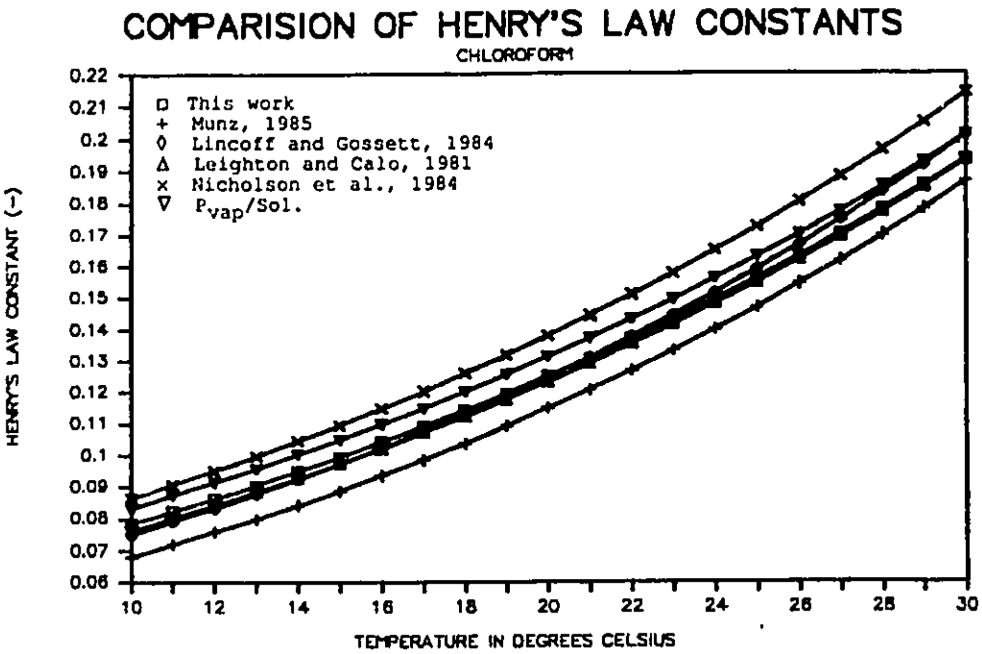


Figure 4.13 - Comparison of the Temperature Dependency of Henry's Law Constants for $CHCl_3$

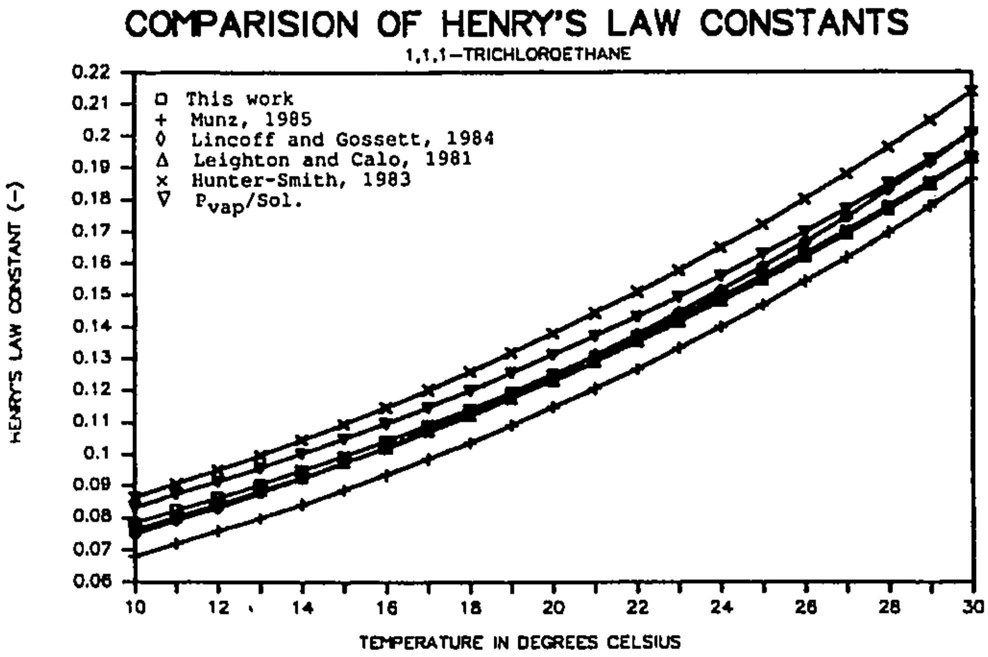


Figure 4.14 - Comparison of the Temperature Dependency of Henry's Law Constants for CH_3CCl_3

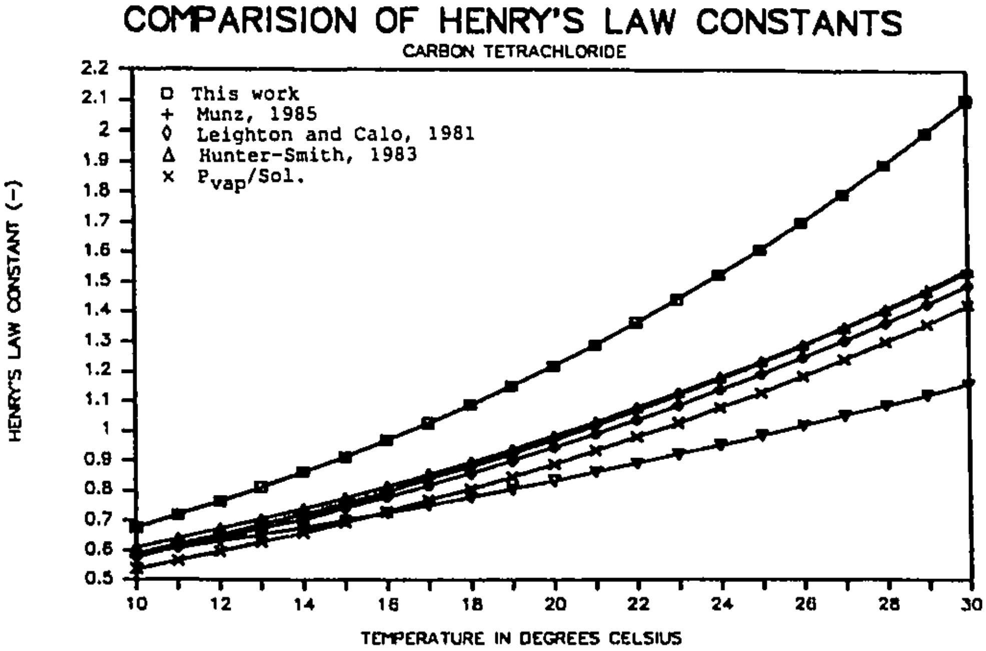


Figure 4.15 - Comparison of the Temperature Dependency of Henry's Law Constants for CCl_4

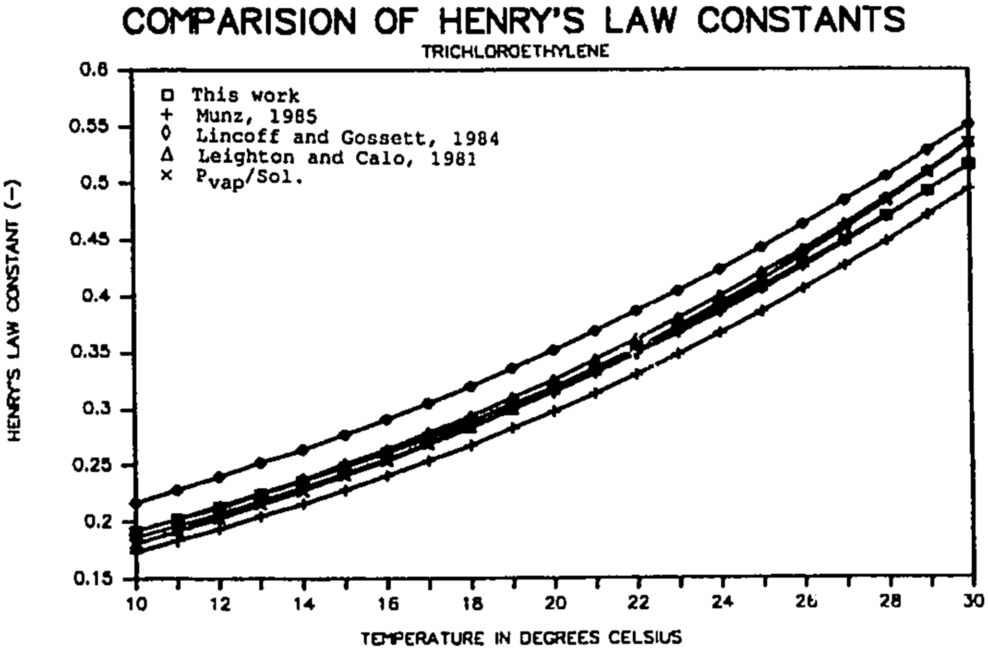


Figure 4.16 - Comparison of the Temperature Dependency of Henry's Law Constants for $CCl_2=CHCl$

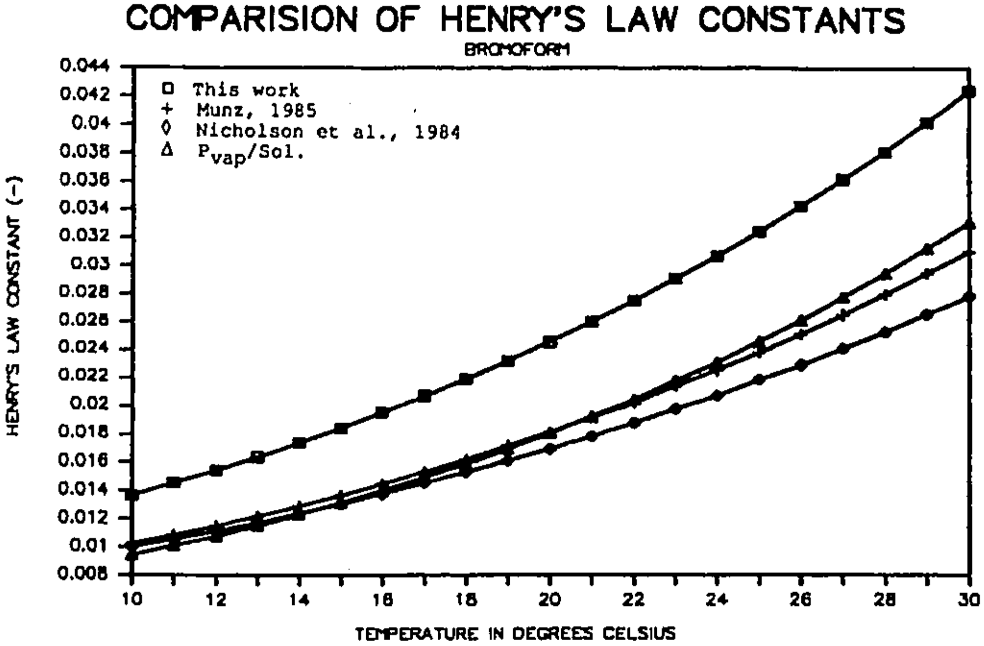


Figure 4.17 - Comparison of the Temperature Dependency of Henry's Law Constants for $CHBr_3$

$ClCH_2CH_2Cl$, CH_3CHCl_2, C_6H_6 and $C_6H_5CH_3$ and as such these compound were not included in the analysis.

The plots indicate good agreement between Henry's Law constants measured in this study and those measured in the previous studies except for the following compounds: CH_3CCl_3, CCl_4 and $CHBr_3$. For these compounds the temperature dependant equations were significantly higher than in the previous studies for the same temperature range (i.e., $10^oC < T < 30^oC$). The differences for CH_3CCl_3 and CCl_4 could be due to analytical errors caused by the interference of the two compounds. The two compounds elute from the GC column approximately at the same time: the column retention times for CH_3CCl_3 and CCl_4 were 14.8 min and 15.2 min, respectively. The closeness of the retention times caused the GC peaks to overlap slightly and could result in an integration error. The error would be a constant in the determination of all of the two VOC concentrations and would result in subsequent errors in the determination of H_C. In the case of $CHBr_3$, the difference from the previous studies could be a result of the poor regression lines. The coefficient of determination for the temperature dependant equations of CHBr3 are significantly lower than the other VOC (e.g., average $R^2 = 0.797$ for $CHBr_3$ and average $R^2 = 0.987$ for the other VOC). Due to the low volatility of $CHBr_3$, an error was be introduced because of the small concentration changes that occur during each equilibration in the ME experiments. This would result in a significantly greater variation in the H_C values calculated.

4.1.4 **Effect of Water Composition on the Henry's Law Constants**

The experimentally determined values for the Henry's Law constants were fitted to the following equation

$$\log_{10} H_C = B \log_{10} C + A \qquad (4.7)$$

where C is the conductivity in μmho/cm. Bias was removed by use of Finney's correction factor previously discussed.

Figures 4.18 to 4.27 show the conductivity dependence of the Henry's Law constant of the VOC investigated. The solid line represents the best fit line for each of the three temperatures studied (i.e., 10, 20, and 30°C), according to Eq. 4.7. The equations for the regression lines and the coefficient of determinations (R^2) are shown on Table B.12 in Appendix B. The results of each individual experiments are also presented on Table B.1 to B.10 in Appendix B.

The dependence of Henry's Law constants on water composition has been studied in the past by Gossett, 1987, Nicholson et al., 1984 and Yurteri et al., 1987. The three studies were rather limited in their scope as they only looked at a small number of VOC (e.g., Gossett, 1987: $CCl_2=CHCl$; $ClCH_2CH_2Cl$; CH_3CHCl_2; and $CHCl_3$, Nicholson et al., 1984: $CHCl_3$; $CHBr_3$; $CHCl_2Br$; and $CHClBr_2$ and Yurteri et al., 1987: CCl_2=CHCl; and $C_6H_5CH_3$) and for a specific range of conductivity (e.g., Nicholson et al., 1984: 0; 578; 1094 μmho/cm and Yurteri et al., 1987: 0; 625; 6250 μmho/cm). Also the studies were only conducted at 20°C. To compare the conductivity results of the various reports to those found in this report, the Henry's Law constants and conductivities were converted to those used in this study and fitted to Eq. 4.7. The equations are shown on Figures 4.28 to 4.31.

The plots indicate that there is very little agreement between the previous studies and this work. All previous studies indicate that the an increase in conductivity will result in an slight increase in H_C. Yurteri, 1987 noted, however, that due to irregularities in the observed data it was not possible to point out any specific trends in HC with any of the factors that were tested. Gossett, 1987 indicated that the salinity must reach substantial values to exert significant impact. For example, conductivity must reach 12500 μmho/cm to cause a greater than 10% increase in HC.

The result from this work indicate that an increase in conductivity will result in a slight decrease in H_C. However the slope of the regression line in only slightly less than zero and if studied over a greater conductivity range it may become positive. The discrepancy between the past studies, the theory and this work could be a result of:

1. All studies including this work used a limited number of experimental points (e.g., n = 3).

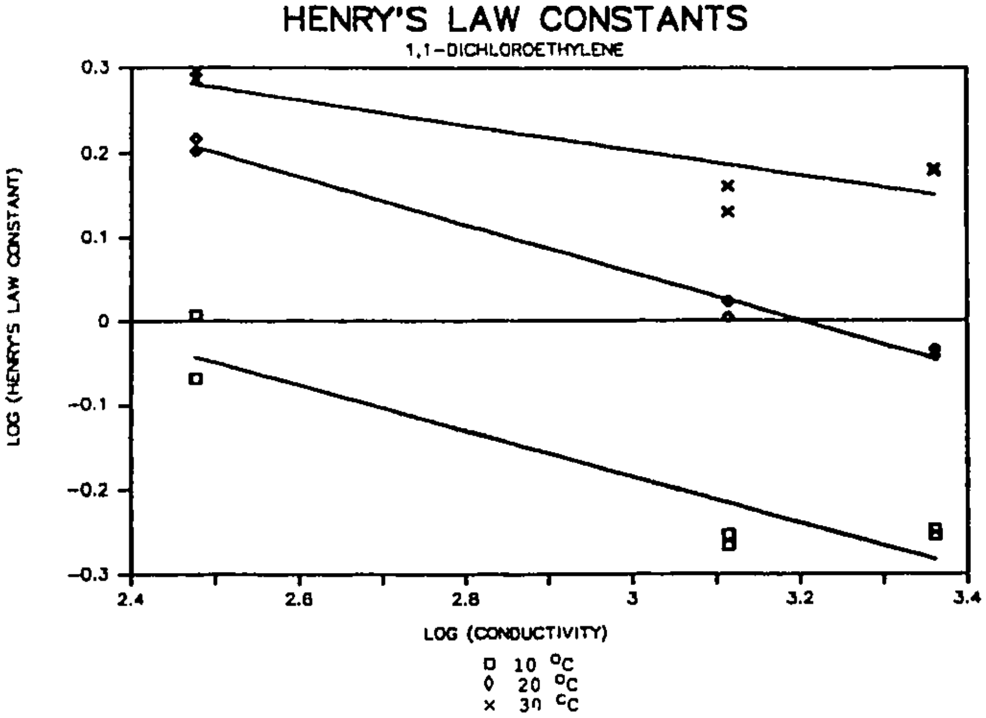


Figure 4.18 - Water Composition Dependency of the Henry's Law Constants for $CH_2=CCl_2$

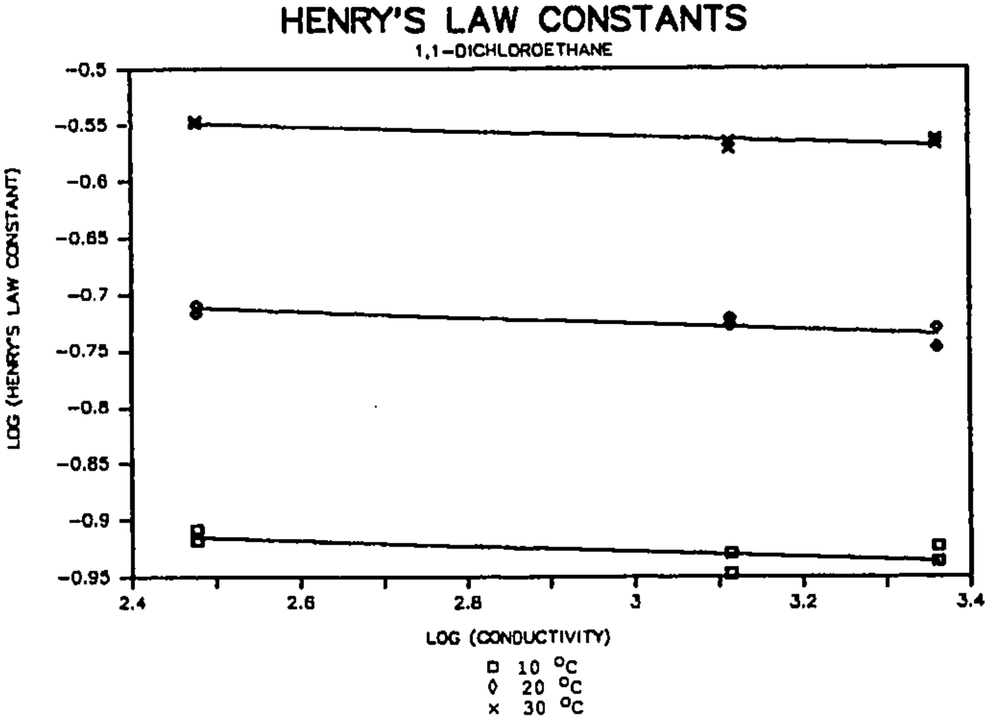


Figure 4.19 - Water Composition Dependency of the Henry's Law Constants for CH_3CHCl_2

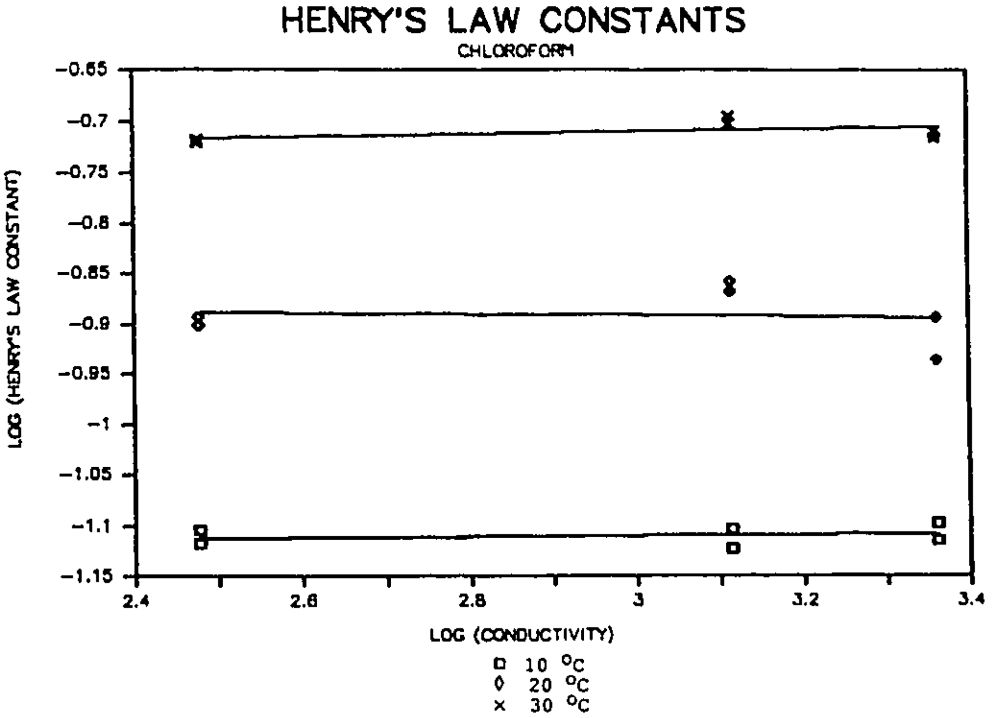


Figure 4.20 - Water Composition Dependency of the Henry's Law Constants for $CHCl_3$

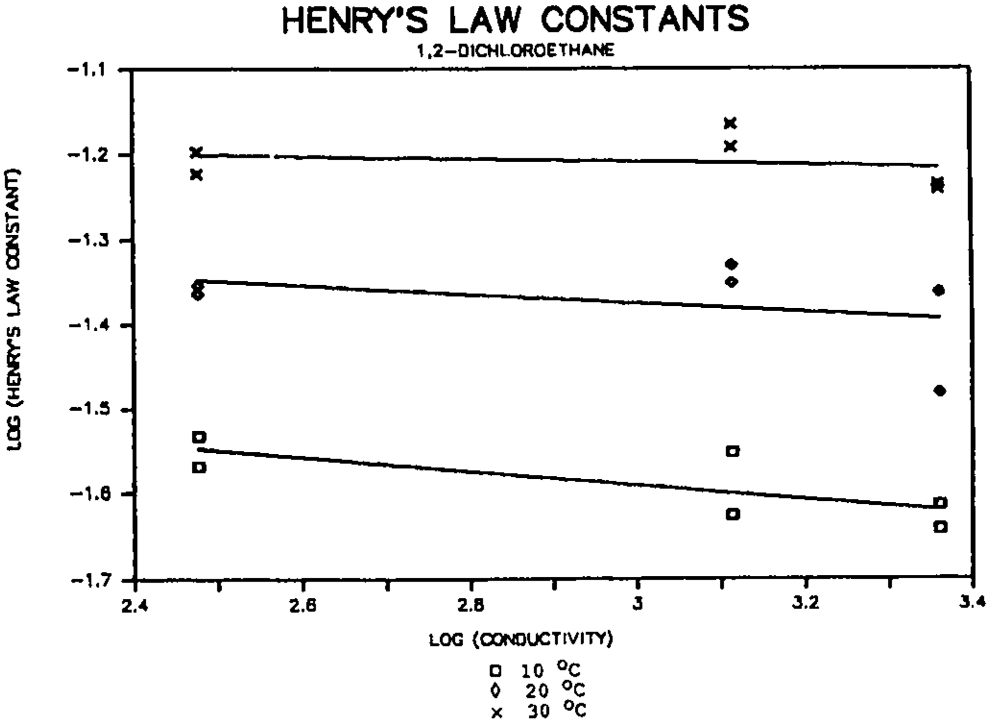


Figure 4.21 - Water Composition Dependency of the Henry's Law Constants for $ClCH_2CH_2Cl$

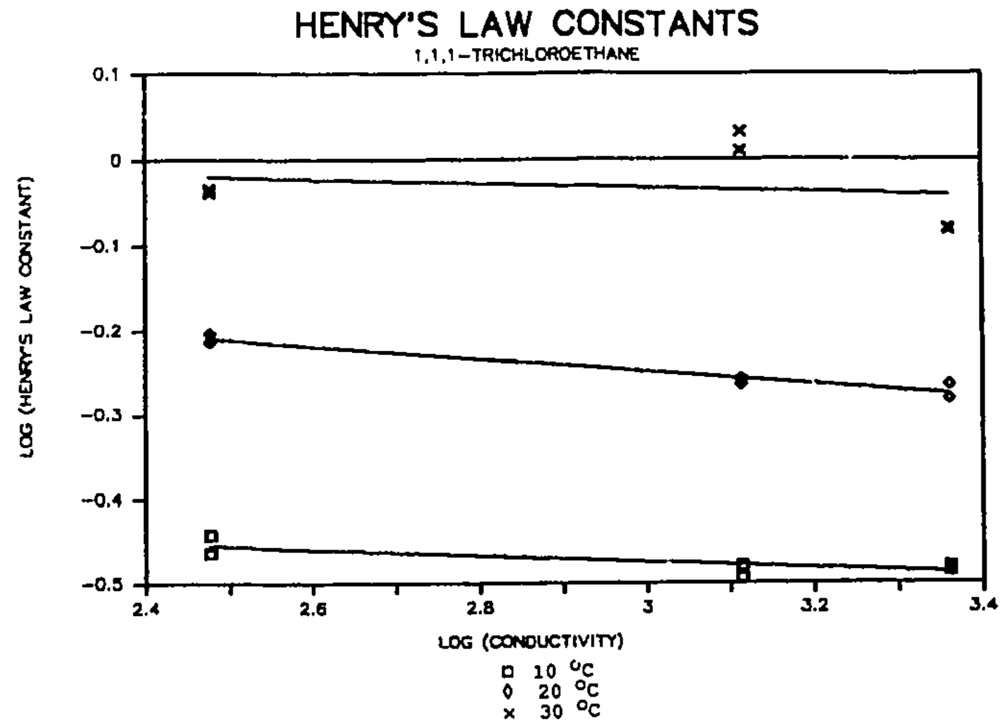


Figure 4.22 - Water Composition Dependency of the Henry's Law Constants for CH_3CCl_3

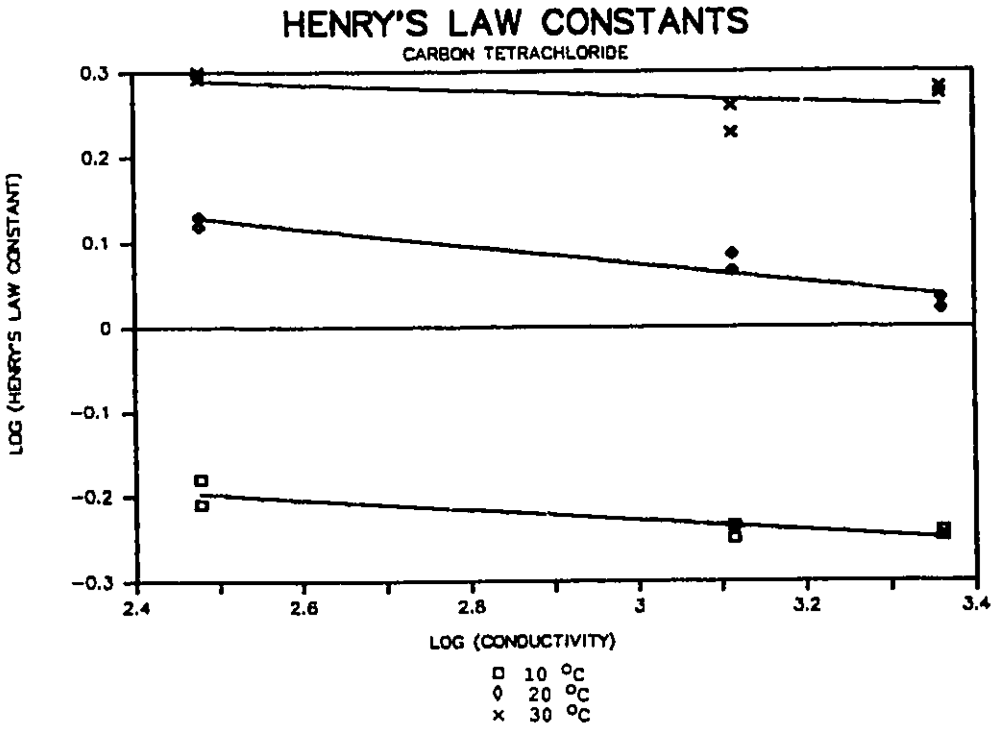


Figure 4.23 - Water Composition Dependency of the Henry's Law Constants for CCl_4

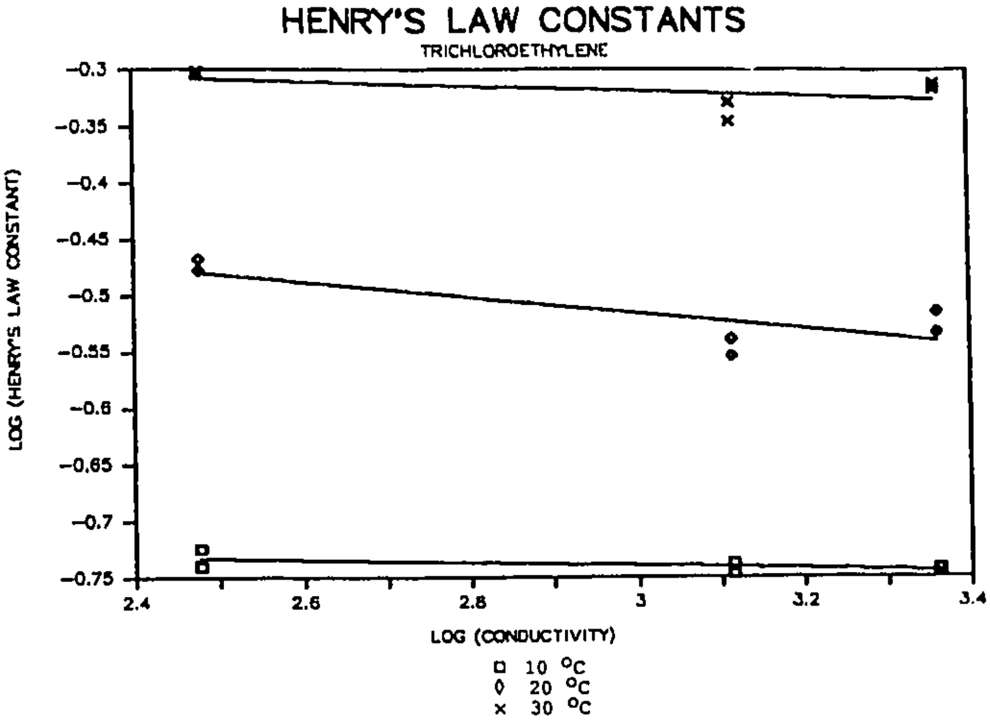


Figure 4.24 - Water Composition Dependency of the Henry's Law Constants for $CCl_2{=}CHCl$

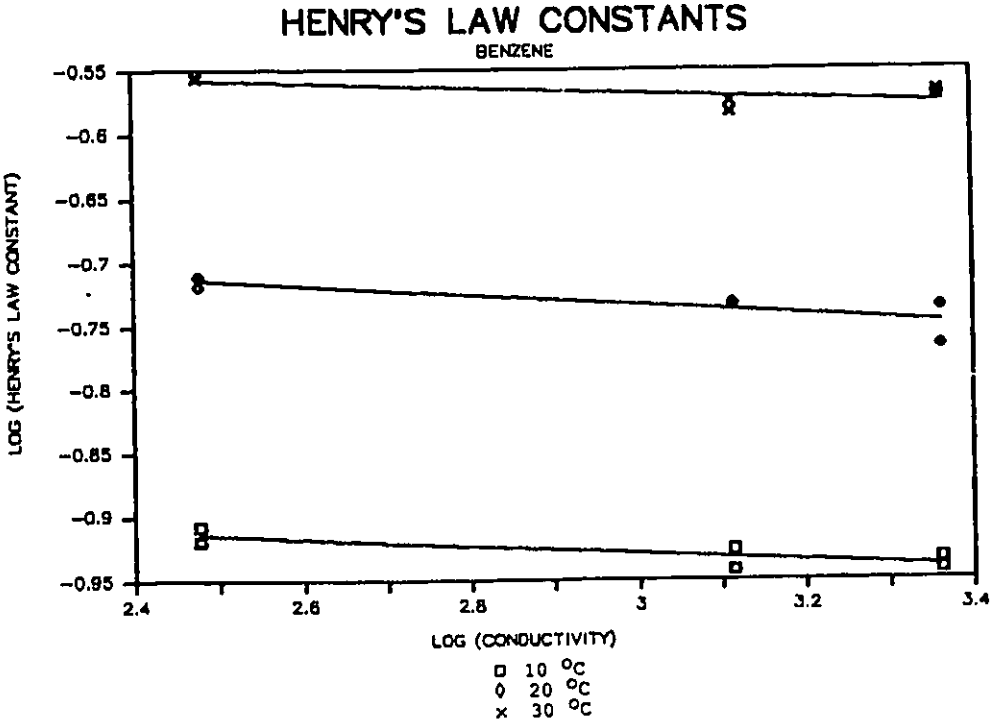


Figure 4.25 - Water Composition Dependency of the Henry's Law Constants for C_6H_6

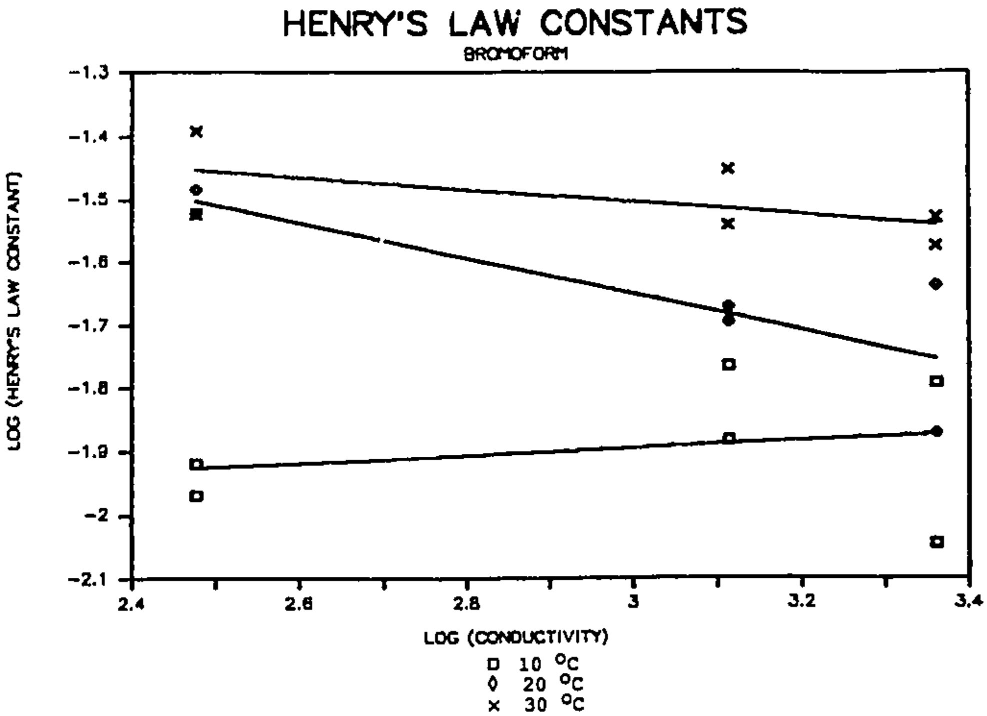


Figure 4.26 - Water Composition Dependency of the Henry's Law Constants for $CHBr_3$

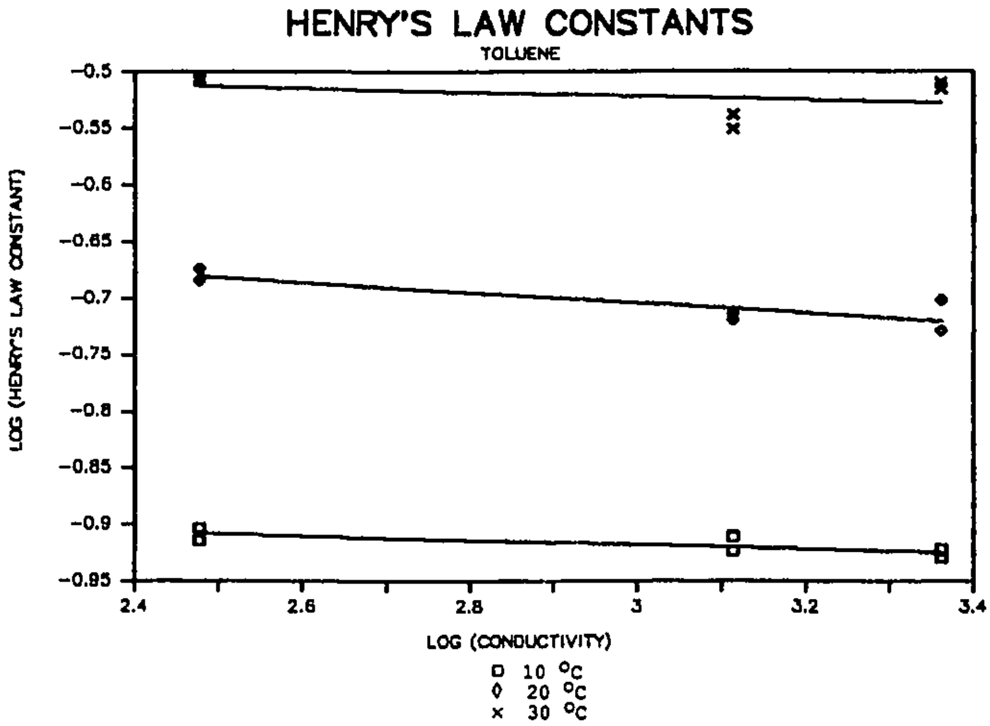


Figure 4.27 - Water Composition Dependency of the Henry's Law Constants for $C_6H_5CH_3$

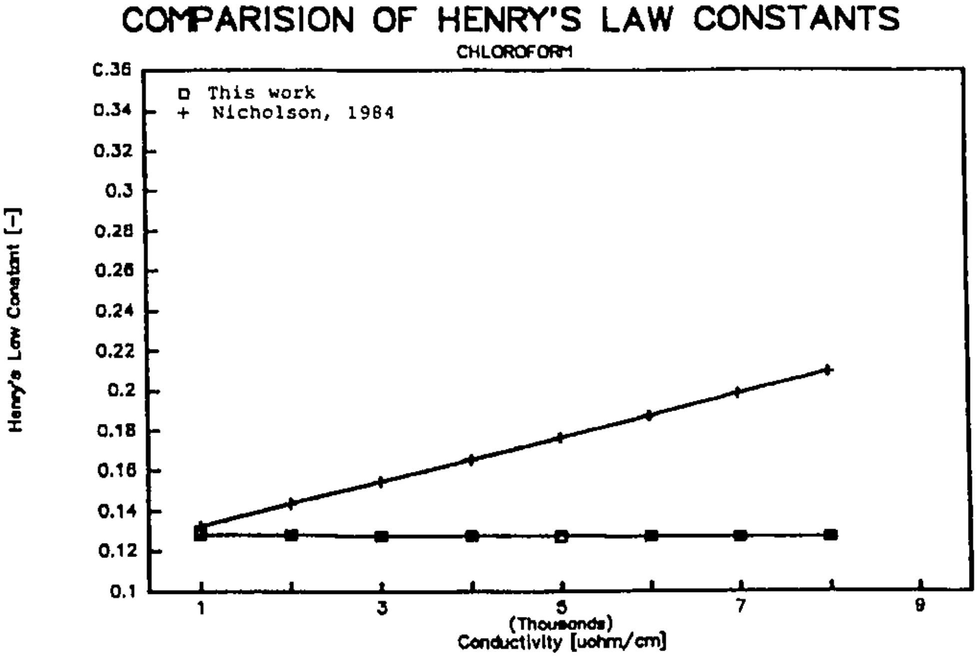


Figure 4.28 - Comparison of the Water Composition Dependency of Henry's Law Constants for $CHCl_3$

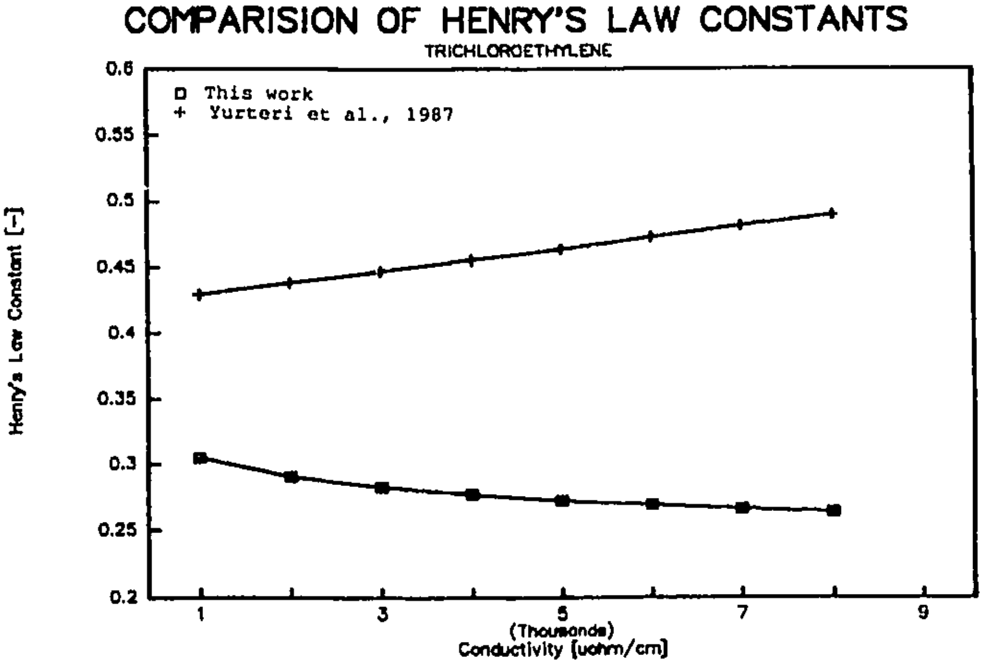


Figure 4.29 - Comparison of the Water Composition Dependency of Henry's Law Constants for $CCl2=CHCl$

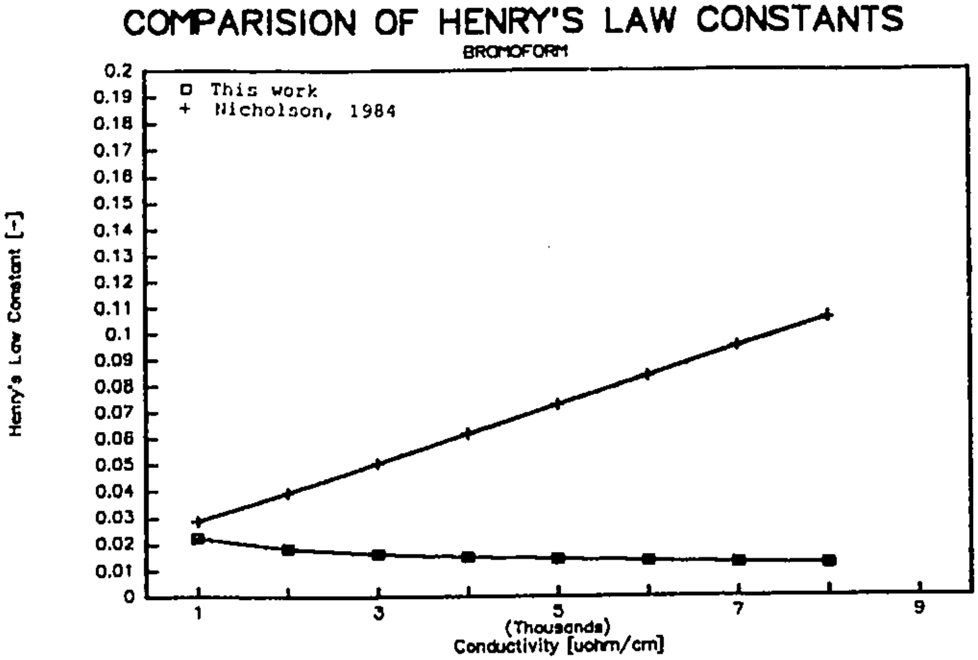


Figure 4.30 - Comparison of the Water Composition Dependency of Henry's Law Constants for $CHBr_3$

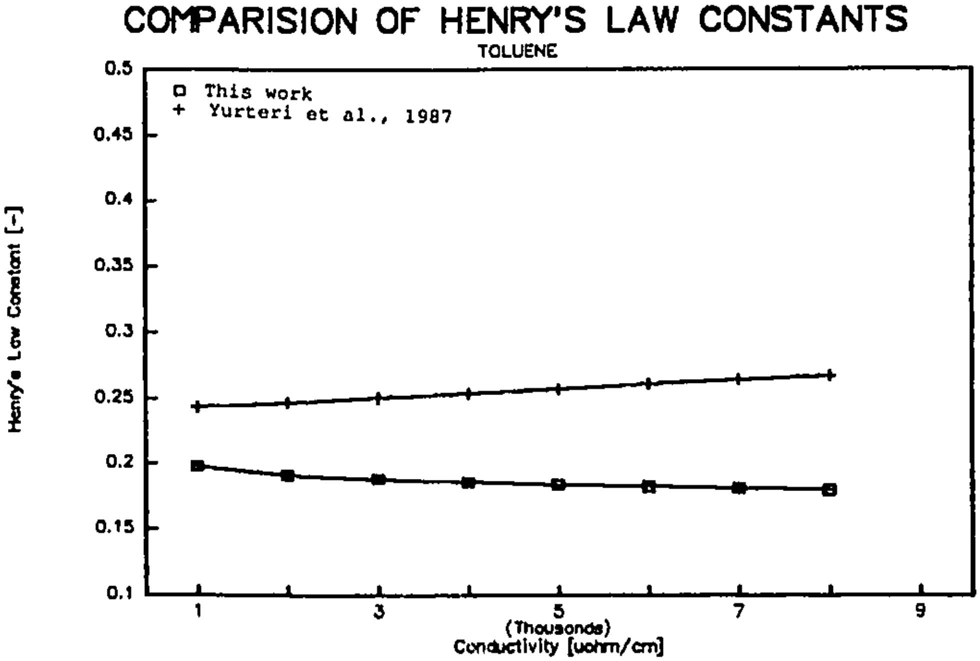


Figure 4.31 - Comparison of the Water Composition Dependency of Henry's Law Constants for $C_6H_5CH_3$

2. All studies employed a limited range of conductivity (e.g., 300 to 2300 µmho/cm for this study, 0 to 2000 µmho/cm for Nicholson, 1987 and 0 to 7500 µmho/cm for Yurteri, 1987).
3. The regression equations developed for all of the studies showed poor correlation and had a very lower coefficient of determination (e.g., average $R^2 = 0.41$ for Nicholson, 1987, 0.86 for Yurteri, 1987 and 0.507 for this study).
4. The effect of a complex mixture of VOC on the determination of H_C was not addressed by any of these studies.

4.1.5 Factorial Analysis of Henry's Law Constant Experiments

The factorial analysis for the Henry's Law constant experiments were conducted using the SAS general linear regression procedure. The linear model was developed to take into account the main and first order interaction effects of the two independent variables (i.e., conductivity and temperature) on the dependant variable (i.e., Henry's Law constant). The equation took the form

$$H_C = \beta_o + \beta_1 A + \beta_2 B + \beta_3 A*B + e \qquad (4.8)$$

where A = conductivity (µmho/cm)

B = temperature (^oC)

e = residual term representing the error between the predicted and observed H_C.

The least squares estimates of the β_i coefficients in the equation are presented in Appendix B on Figures B.1 to B.10 along with the analysis of variance of the fitted model for the variable. The analysis of variance was used to perform a test of significance on each of the estimated main and first order coefficients. The significance of each coefficient was tested by comparing the ratio

$$F = \frac{\text{mean square associated with the term}}{\text{residual mean square}} \qquad (4.9)$$

with the appropriate value of the F-distribution. For example, factor B of $C_6H_5CH_3$ has a ratio equal to

$$F = \frac{0.04871995}{0.00008315} = 585.90 \qquad (4.10)$$

The above value corresponds to a significance level of 0.02% using the F-distribution and therefore, would be considered highly significant. Table 4.1 summarizes the analysis of variance significance test results for the various VOC.

Compound	Significance Level (%)					
	Overall	A	B	A*A	B*B	A*B
$CH_2{=}CCl_2$	1.85	2.14	0.38	14.66	37.99	81.78
CH_3CHCl_2	0.01	3.03	0.01	14.12	2.51	30.36
$CHCl_3$	0.08	92.84	0.01	16.59	12.10	87.21
$ClCH_2CH_2Cl$	0.35	13.96	0.05	11.82	57.66	70.32
CH_3CCl_3	7.74	60.78	1.19	38.26	40.85	82.09
CCl_4	0.30	14.53	0.04	32.26	58.51	93.23
$CCl_2{=}CHCl$	0.12	23.77	0.02	13.10	10.13	80.52
C_6H_6	0.02	6.16	0.01	26.26	6.04	80.06
$CHBr_3$	7.10	15.79	1.20	94.40	74.73	39.10
$C_6H_5CH_3$	0.12	33.15	0.02	18.53	13.79	98.49
AVERAGE	1.77	26.62	0.29	28.00	31.43	74.32

* See Appendix B for full results.

Table 4.1 - Summary of Significance Test Results for H_C Experiments

The results indicate that the main effects (i.e., conductivity and temperature) are highly significant on the determination of H_C. The average significance level was 26.62% for factor A and 0.29% for factor B. Conductivity appears to have the greater effect on the highly volatile compounds such as $CH_2=CCl_2$ and CCl_4 and smaller effect on the less volatile compounds such as $ClCH_2CH_2Cl$ and $CHBr_3$. The significance testing also shows that temperature is the prime factor in determining H_C as indicated by its average significance level of 0.29%. It should be noted that a nonsignificant value for an estimated coefficient may occur because (Bacon 1970):

1. the term does not affect the dependant variable
2. the spacing of the levels of the factors was too narrow
3. the levels of the factors were near a conditional maximum.

In a factorial experiment it is not possible to identify which of these causes has produced the nonsignificant estimate. Therefore, it must be assumed that the range was chosen carefully and concluded that the nonsignificant estimate was a result of the factor itself.

To further assess the validity of the fitted model the individual residuals were studied to reveal any nonrandom tendencies in the data. The residual plots for $CH_2=CCl_2$ are shown on Figures 4.32 and 4.33 and no evidence of systematic behavior was detected indicating that the model represents the data adequately.

4.2 MASS TRANSFER COEFFICIENT EXPERIMENTS

The mass transfer experiments were performed to establish the effect of liquid and gas flow rates, conductivity and packing type on the air stripping of VOC and to evaluate the various mass transfer correlations available (e.g., Sherwood and Holloway, 1940, Shulman et al., 1955, Onda et al., 1968). The experiments were conducted using a 4-factor, 3-level fractional factorial design consisting of 27 runs (Bacon, 1970): liquid flow rate $2 < Q_L < 4$ L/min, gas

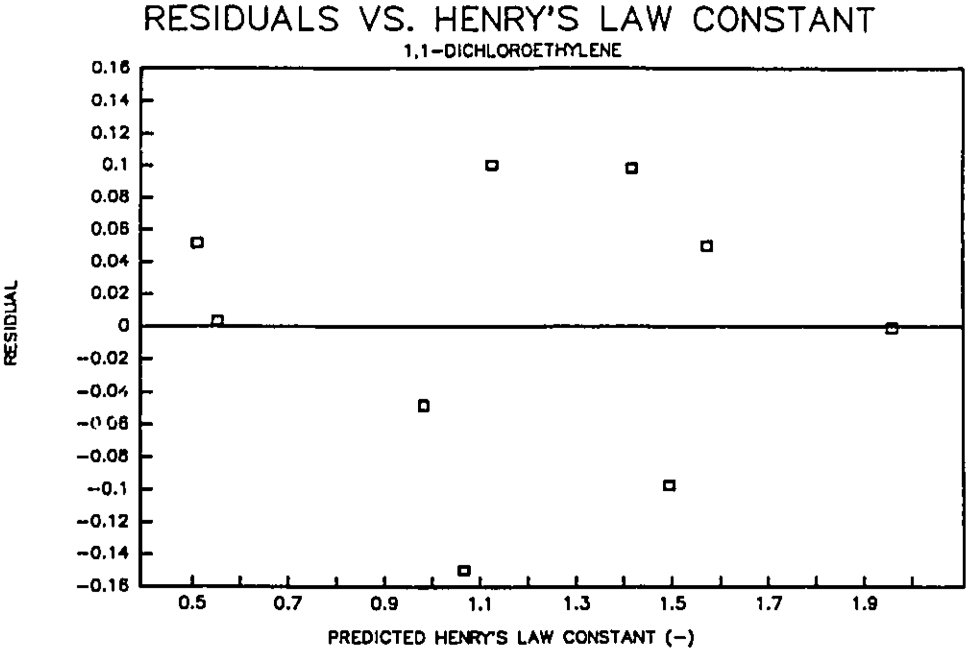


Figure 4.32 - Residuals verses H_C for $CH_2=CCl_2$

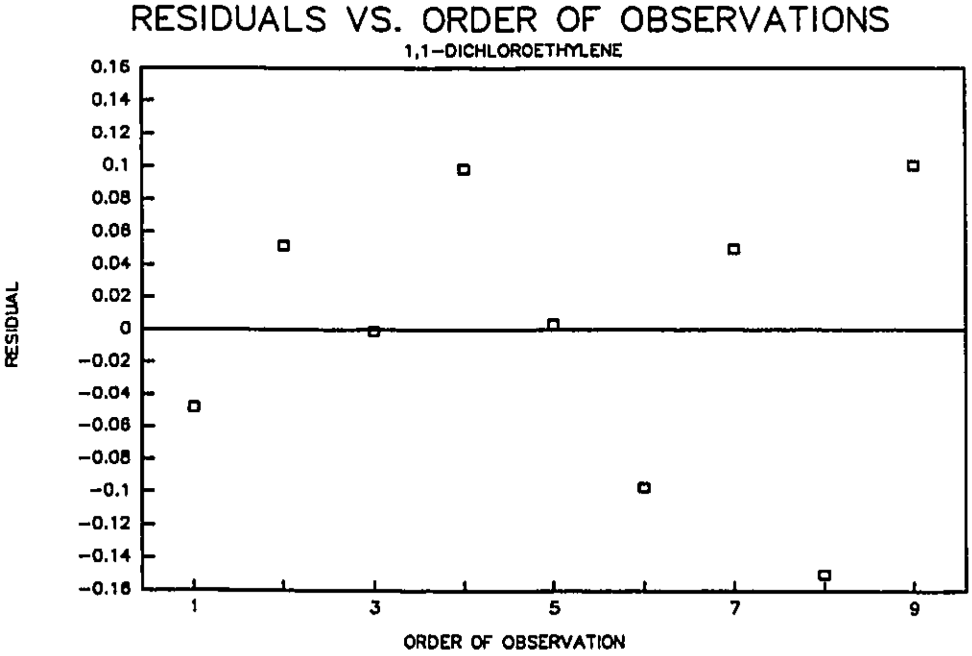


Figure 4.33 - Residuals verses Order of Observations for $CH_2=CCl_2$

flow rate $25 < Q_G < 75$ L/min, conductivity 300 µmho/cm < C < 2300 µmho/cm and packing type 6.4 mm Raschig rings (porosity 62%), 12.8 mm Raschig rings (64%) and 12.8 mm Intalox saddles (72%). The air and water temperatures were held constant at approximately 22°C ±1°C. The experiments were conducted in a random order and analyzed by the procedure developed by Lamarche, 1986 and Munz, 1985. The factorial analysis was performed by the SAS general linear regression computer package. The results of the experiments and regression analyses are given in Appendix E.

4.2.1 Assessment of Experimental Errors and Assumptions

Numerous possible sources of error are present both with the experimental and analytical procedures used, as well as with the data analysis method chosen. The possible errors include: measurement of liquid and gas flow rates, assumption of steady state conditions, column and pipe leaks, uneven liquid distribution, adsorption and desorption of organics to/from column materials, assumption of isothermic conditions, variation in GC analysis, losses from sampling syringes, sample injection errors and errors introduced by the use of constants. The errors will be discussed in detail below.

Measurements of the liquid, gas and VOC flow rates were monitored throughout the experiment to ensure that a constant flow rate was achieved. The liquid flow rate was monitored using a magnetic flowmeter attached to a strip recorder. The flow rate fluctuated throughout the experiment; however, the average flow rate remained constant. Gas and VOC flow rates were monitored by in-line rotometers and were monitored periodically throughout the experiment. The average flow rate remained constant during the run.

The assumption of steady state conditions is a basic assumption for the packed column design. The assumption of steady state was verified by the relatively stable VOC concentration throughout each of the experimental runs as indicated by a coefficient of variation < 10%.

Liquid and/or gas leaks from the column, piping, sample bags or pumps were not observed throughout the experimental runs. Measurements to confirm this observation however, were not made. To minimize any possible leaks that could occur all connections were clamped and/or sealed on the outside with sealant.

Liquid distribution throughout the column cross-section was observed to be relatively uniform however some channelling was observed in the 12.8 mm Raschig rings and Intalox saddles packings. Also the liquid distribution varied with changes in liquid and gas flow rates (i.e., more channeling at higher liquid flow rates). Roberts, 1982 noted that variations in liquid flow distribution is more critical in shorter columns. The measured liquid dispersion coefficient was generally in agreement or less than the predicted value for the column. The results of the tracer study will be presented later (Section 4.2.2).

The adsorption and desorption of VOC to the materials used in the column were not specifically investigated. However, Lamarche, 1986 and Munz, 1985 have studied the adsorption and desorption of VOC to teflon, tygon, glass, and plexiglass. They concluded that for the short term duration of the individual experiments, the effects would be minimal.

The assumption of isothermic conditions in the column was found to vary depending upon the temperature difference between the influent water temperature and the gas temperature. The average change in temperature between the influent and effluent liquid was approximately $0.6^{o}K$ (or approximately 0.2%). In the data analysis the average column temperature was used and therefore the effect should be insignificant.

Losses from the sampling syringes were investigated by Lamarche, 1986. Results from that study are reproduced in Appendix C. The losses in concentration over a 24 hour period ranged from 3 to 15%. This was considered to be insignificant for the approximate 6 to 8 hour analysis time.

The variation in the sample volume could directly affect the concentration measured by the GC. The actual volume of the sample injected into the GC by the sampling syringes was determined using a weighing technique. The precision of the injected sample volume was ± 1 to 3%. The results are shown in Appendix C.

Munz, 1985 determined that if the stripping factor, S was greater than 0.8 the variation in K_La would be approximately ± 5% due to the potential sources of error. Therefore, to minimize the effects of the errors, a stripping factor greater than 1.0 was desired. The minimum stripping factors for each of the VOC were all greater than 1.0 except for ClCH2CH2Cl and $CHBr_3$ ($H_C < 0.1$). The stripping factors for ClCH2CH2Cl ranged from 0.37 to 1.76 and for $CHBr_3$ ranged from 0.19 and 0.88. The errors associated with each of these compounds are more evident than with the other compounds and are noted in the analysis.

4.2.2 Evaluation of the Air Stripping of VOC

The results of the mass transfer experiments were evaluated initially in order to determine the effectiveness of air stripping as a method of removing VOC from a liquid-phase. A summary of the experimental results is presented on Table 4.2. The results indicate that air stripping would be an effective method of removing VOC from groundwater with an average removal rate of 84.3%. The removal rates for the VOC investigated ranged from 35.6% to 97.7% with the best results being found for the VOC with Henry's Law constants greater than 0.5.

Compound	Concentration (μg/L) Initial	Final	% Removal	H_C (at 20°C)
CH_2=CCl_2	8600.1	206.1	97.7	0.939
CH_3CHCl_2	3780.3	276.8	92.2	0.182
$CHCl_3$	4698.7	502.2	88.8	0.130
$ClCH_2CH_2Cl$	1199.9	472.0	60.5	0.043
CH_3CCl_3	2558.8	130.7	95.6	0.581
CCl_4	7578.6	225.0	96.9	1.078
CCl_2=CHCl	3593.2	186.8	94.5	0.290
C_6H_6	1925.4	145.3	92.1	0.180
$CHBr_3$	1163.7	738.2	35.6	0.022
$C_6H_5CH_3$	2312.7	176.1	92.1	0.190
AVERAGE	3741.1	309.9	84.3	

Table 4.2 - Summary of the Results of the Air Stripping Experiments

4.2.3 Packed Column Tracer Studies

The results of the packed column tracer studies are found in Appendix F. The methods used to calculate both the measured and predicted axial liquid dispersion coefficient are outlined in Sater and Levenspiel, 1966 and presented in Appendix F.

The dispersion number (D/uL) ranged from 0.0096 to 0.0545 (average 0.0275) for 6.4mm Raschig rings, 0.0111 to 0.3371 (average 0.0205) for 12.8 mm Raschig rings and 0.0257 to 0.0453 for 12.8 mm Intalox saddles (average 0.0339). The dispersion number would indicate an intermediate amount of dispersion (D/uL = 0.025) in the column. The design of a packed column assumes that the flow condition in the column is plug flow (i.e., D/uL = 0). The results indicate that the flow in the column was approximately plug flow. The channelling observed along the walls of the column was caused by the dispersion in the column, however, it would appear that this does not cause a significant change in the plug flow characteristics of the column.

The observed dispersion coefficient (D) was generally less than the predicted dispersion coefficient (D_{AL}). The differences may be due to the following factors: the flow condition range of the tracer study was different than that for which the correlation was developed (liquid flow rate: $2 < Q_L < 5$ L/min and gas flow rate: $50 < Q_G < 150$ L/min in this study compared to used in the Sater and Levenspiel, 1966 study); the packing bed used was approximately half the depth of the bed used for the correlation (packing depth: 1.829 m in this study compared to 3.14 m used in the Sater and Levenspiel study); and the packings used were not exactly the same as those used in the correlation (packing type: 6.4 and 12.8 mm Raschig rings and 12.8 mm Intalox saddles in this study compared to those used by Sater and Levenspiel). However, due to the reasonably close agreement between the two values, it would appear that the packing beds used in this study are similar to those used by Sater and Levenspiel.

The results indicate that the dispersion in the liquid-phase was notably increased with an increase in the liquid flow rate in the column but only slightly decreased with an increase in the gas flow rate. These findings agree with those found by Roberts, 1982. The findings show that the packed column and the experimental conditions were similar to those used in previous studies with respect to their axial dispersions and that the liquid flow in the column approximates the plug flow assumption used by the packed column design.

4.2.4 Evaluation of Mass Transfer Correlations

The mass transfer models investigated in this study were those of Sherwood and Holloway, 1940, Shulman et al., 1955 and Onda et al., 1968. These models were considered by Roberts, 1982 and Lamarche, 1986 to be potentially useful for predicting the mass transfer coefficient for the air stripping of VOC from water. For each packing, appropriate to the specific model, the observed and predicted mass transfer correlations were calculated according to the procedure and equations presented in Appendix E. The results are presented in Appendix E in Tables E.1 and E.4.

The models of Sherwood and Holloway and Shulman et al. could not be applied to the 6.4 mm Raschig rings and 12.8 mm Intalox saddles. The values for the constants used in the two models were only developed for the 12.8 mm Raschig rings. The Onda et al. model could be applied to all three packings as the constants required are readily available in the literature (Ludwig, 1979). The liquid and gas flow rates chosen were within the ranges for which the correlations were developed (Section 2.2.4).

The accuracy of the models to predict the mass transfer coefficients was evaluated by the linear regression of the two variables. The variables were logarithmicly transformed and regressed using the following relationship:

$$\mathrm{Log}_{10}\, K_L a_{PRED.} = A + B\, \mathrm{Log}_{10}\, K_L a_{OBS.} \qquad (4.8)$$

where A = regression intercept

B = regression slope fo the best fit line.

If perfect correlation existed then the predicted K_La value would equal the observed K_La value and Eq. 4.8 would become

$$\mathrm{Log}_{10}\, K_L a_{PRED.} = 0.0 + 1.0\, \mathrm{Log}_{10}\, K_L a_{OBS.} \qquad (4.9)$$

To evaluate the accuracy of the regression line to represent the above perfect correlation, the coefficient of determination (R^2) and standard error of the estimate (SEE) were used. The coefficient of determination is the ratio of the explained variation to the total variation and is an indication of how well the best fit line fits the observed data. It can be calculated by

$$R^2 = \frac{\Sigma\ (\text{Log } K_La_{PRED.} - K_La_{AVE})^2}{\Sigma\ (\text{Log } K_La_{OBS.} - K_La_{AVE})^2} \qquad (4.10)$$

where K_La_{AVE} = Average K_La observed value.

This ratio must lie between zero and one. If R^2 equals 1.0 then all the variation has been explained and the regression line is a perfect fit. While if R^2 equals zero then the regression line explains nothing. The standard error of the estimate is an estimate of the error associated with the predicted K_La value and is also known as the variance in the residuals. The value can be calculated by

$$SEE = \left[\frac{\Sigma\ (\text{log10 } K_La_{PRED.} - \text{Log10 } K_La_{OBS.})^2}{n - (k + 1)}\right]^{1/2} \qquad (4.11)$$

where n = number of observation of Y,
k = number of independent variables on which Y depends.

The results of the regression analysis are found in Appendix E in Tables E.5 to E.13. The predicted K_La and observed K_La values for each VOC are plotted on Figures 4.34 to 4.43.

The ability of the various mass transfer correlations (i.e., Sherwood and Holloway, Shulman et al. and Onda et al.) to predict the K_La of VOC of a range of volatilities (H_C) was evaluated by examining and comparing the following factors:

a) How well the best fit line approximates the perfect regression line (Eq. 4.9)
b) How well the best fit line is correlated to the data as indicated by the coefficient of determination (R^2)

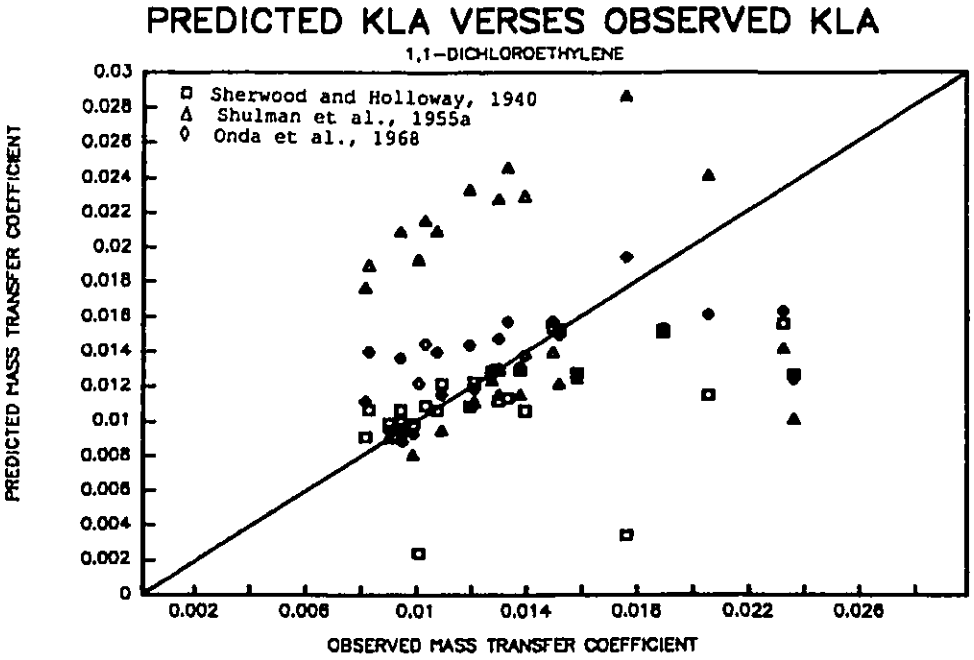


Figure 4.34 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for $CH_2{=}CCl_2$

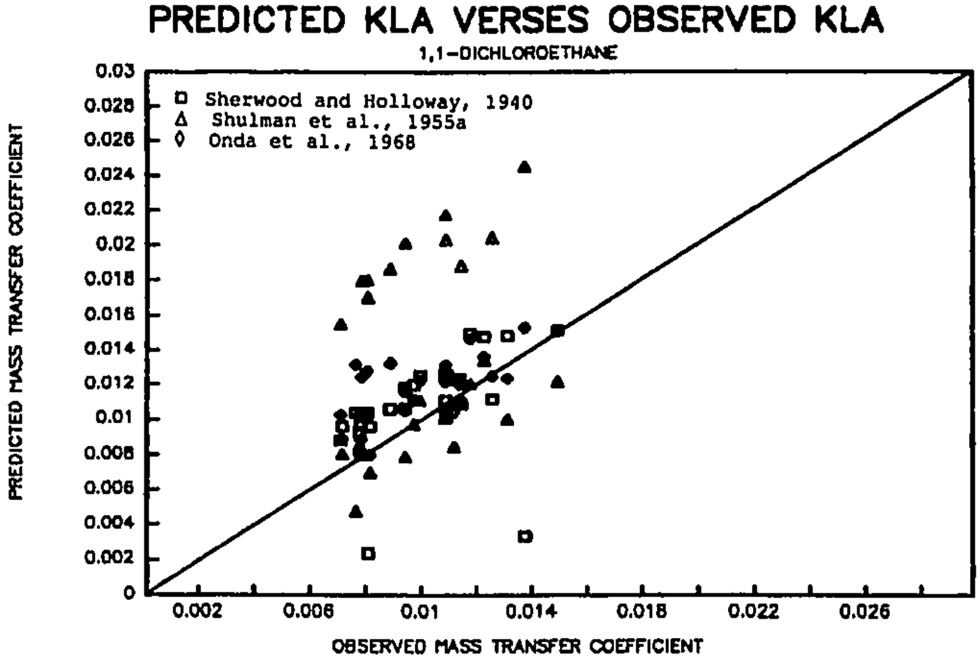


Figure 4.35 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for CH_3CHCl_2

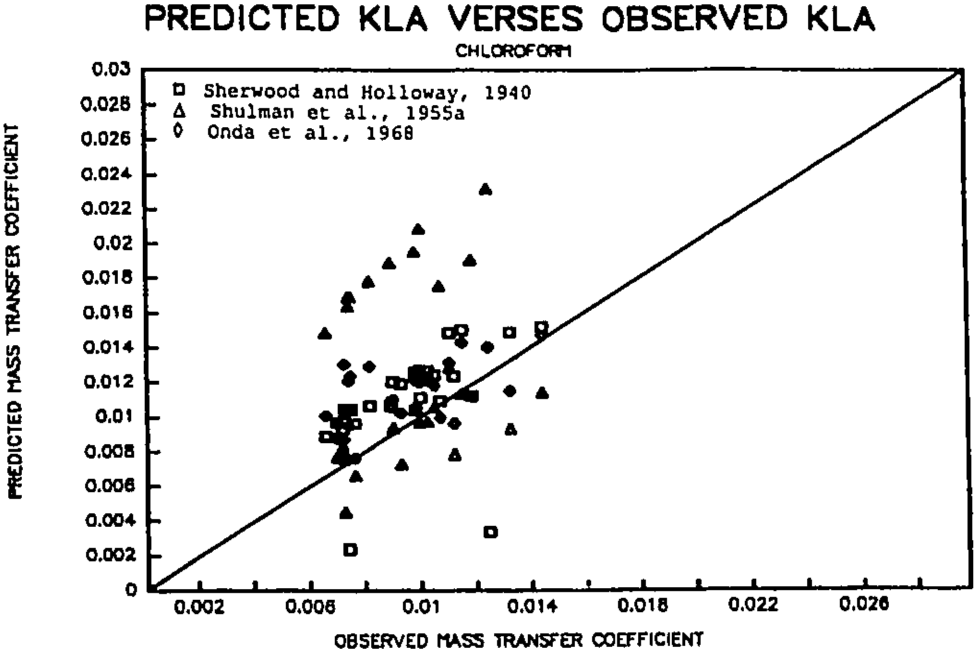


Figure 4.36 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for $CHCl_3$

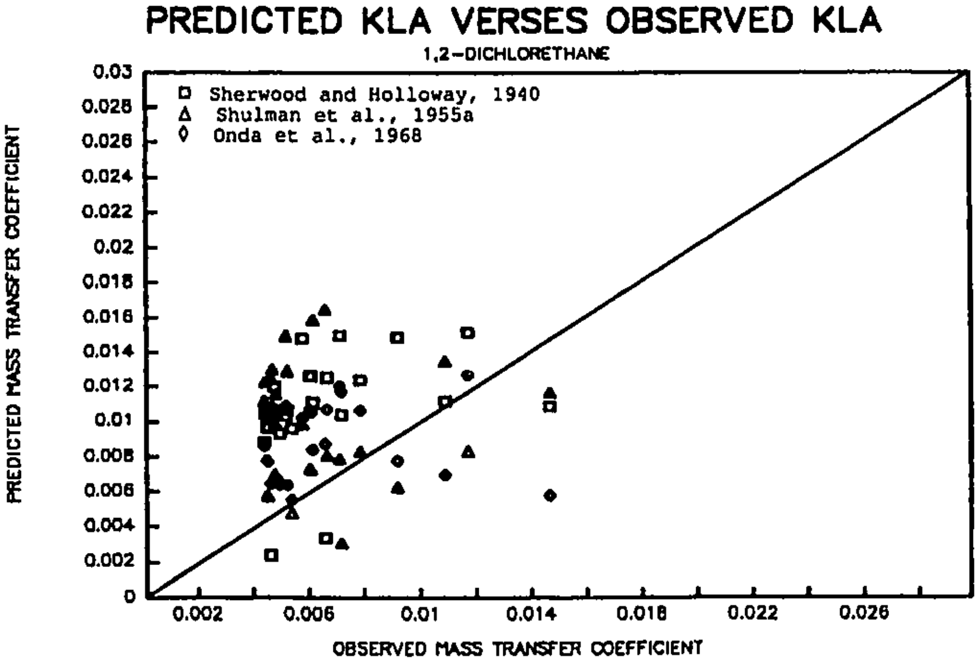


Figure 4.37 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for $ClCH_2CH_2Cl$

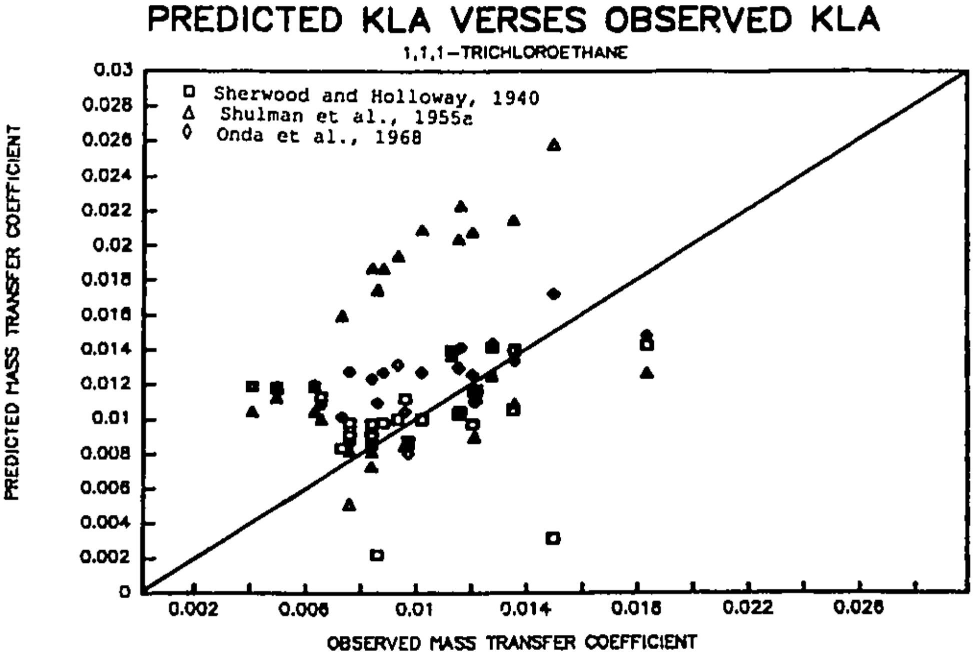


Figure 4.38 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for CH_3CCl_3

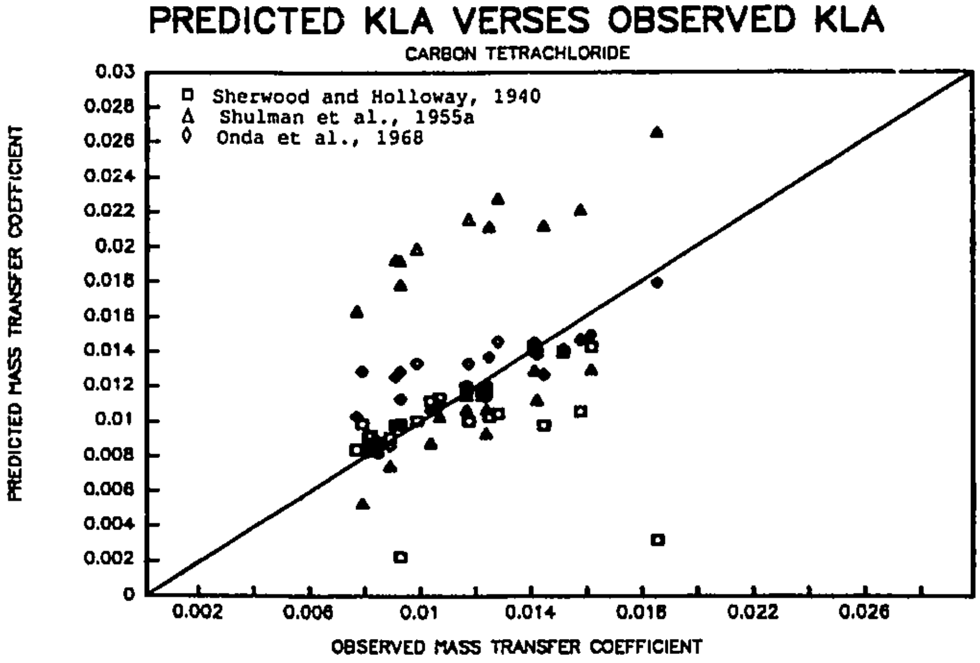
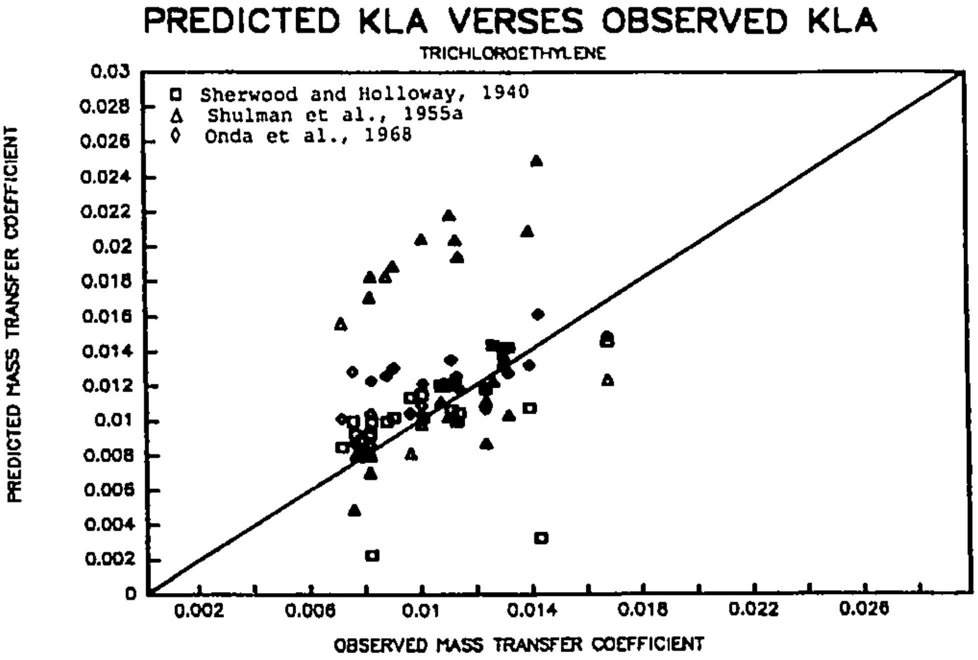
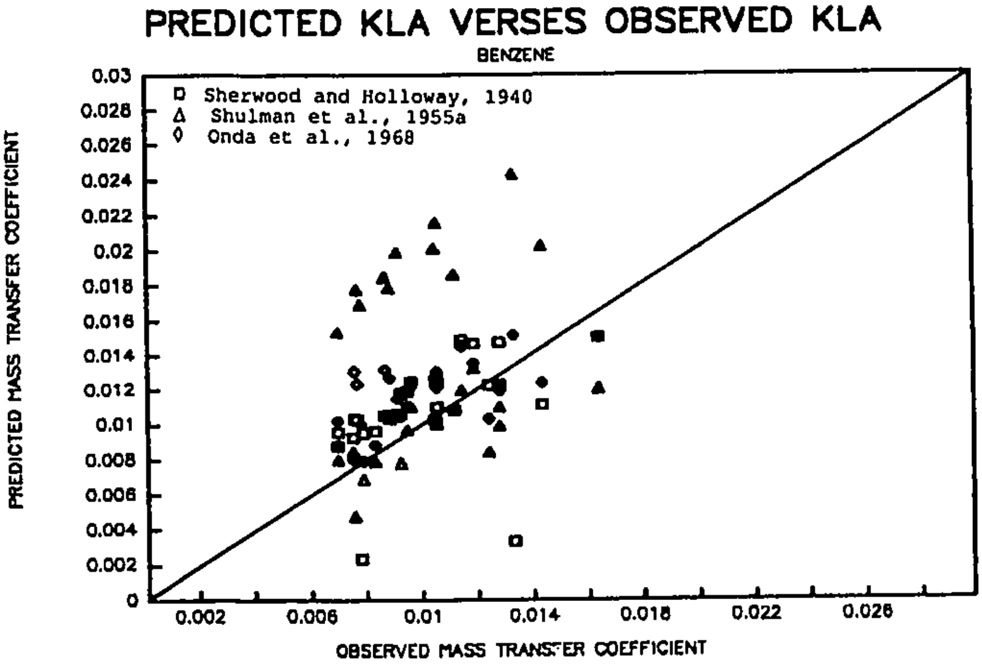


Figure 4.39 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for CCl_4


PREDICTED KLA VERSES OBSERVED KLA

TRICHLOROETHYLENE

Figure 4.40 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for $CCl_2=CHCl$


PREDICTED KLA VERSES OBSERVED KLA

BENZENE

Figure 4.41 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for C_6H_6

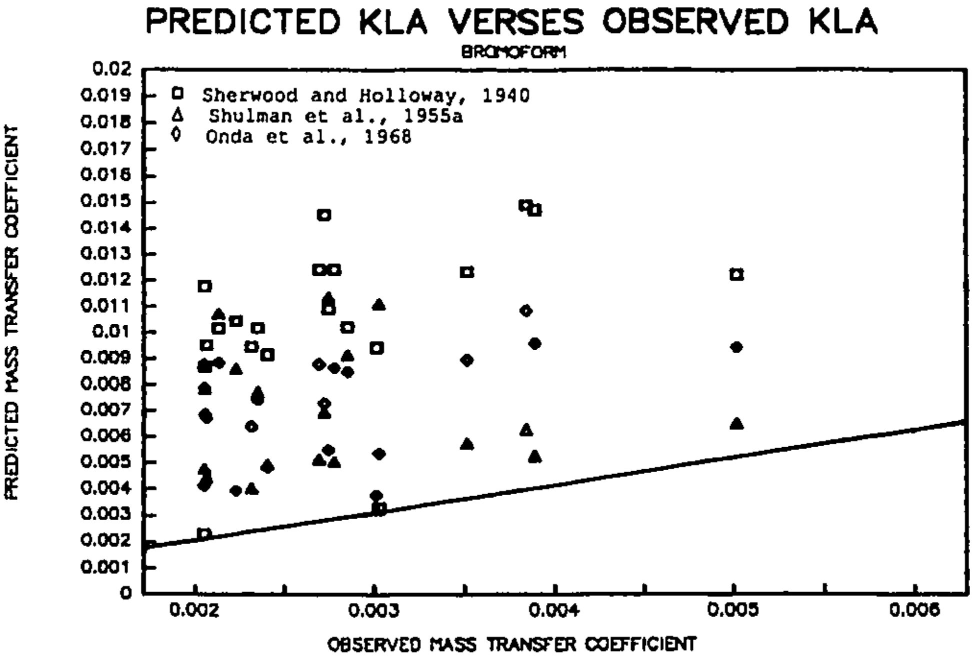


Figure 4.42 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for $CHBr_3$

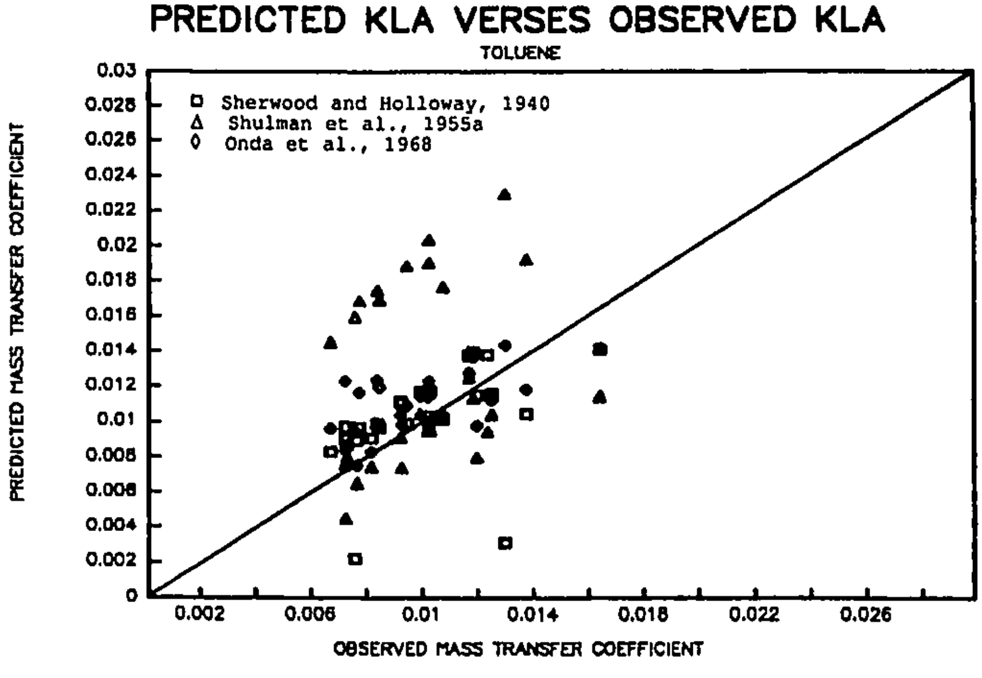


Figure 4.43 - Predicted Mass Transfer Coefficient verses Experimental Mass Transfer Coefficient for $C_6H_5CH_3$

c) How much of an error is included in the prediction of K_La as indicated by the standard error of Y estimate (SEE%).

The correlations are compared using the 12.8 mm Raschig rings packing since it was the only packing for which all the correlations were developed. The other packings used were only valid for the Onda et al. correlation and can only be used to compare the validity of this model to predict K_La for various packings.

As previously noted Eq. 4.9 represents the perfect correlation for the observed and predicted K_La. The results indicated that the Onda et al. correlation most closely represents the perfect regression line. Both the slope and the intercept of the lines are closer to the values expected by Eq. 4.9. The best fit lines for the correlation of Sherwood and Holloway tended to have a lower slope and higher intercept than that of the Onda et al. correlation for all VOC except $ClCH_2CH_2Cl$ and $CHBr_3$, the two lowest volatility VOC. This would seem to go against findings in past studies by Roberts et al., 1985, Munz, 1985 and Lamarche, 1986, who all showed that for low volatility compounds that Sherwood and Holloway would not be valid because of its basic assumption that the gas-phase resistance was zero. In the case of the Shulman et al. correlation, the slope and intercept of best fit lines were worse than both of the other correlations.

As stated earlier the coefficient of determination (R^2) indicates how well the regression line fits the observed data. An R^2 equal to 1.0 would mean that the line fits the data perfectly. The R^2 results for the 12.8 mm Raschig rings packing indicate that the regression lines developed for the Sherwood and Holloway correlation fit the data best as shown by the higher R^2 values. The R^2 value for the models tended to be greater than 0.8 for all compounds except the lower volatility compounds such as $ClCH_2CH_2Cl$ and $CHBr_3$

(i.e., 0.585 and 0.301, respectively). The R^2 values derived for the Onda et al. correlation were generally lower than those found for the Sherwood and Holloway correlation. Compounds such as $ClCH_2CH_2Cl$ and $CHBr_3$ displayed a very low correlation as indicated by the low R^2 values (i.e., 0.231 and 0.059, respectively).

The R^2 values calculated for the Shulman et al. correlation did not display as a high degree of correlation as the other two models. Generally the R^2 values were between 0.5 and 0.8 for all compounds except $ClCH_2CH_2Cl$ and $CHBr_3$ (i.e., 0.137 and 0.042, respectively). CH_3CCl_3 was poorly correlated for all models (i.e., average $R^2 = 0.103$).

The final parameter used to evaluate the performance of the various correlation was the SEE. As noted earlier the SEE is a measure of error associated with the prediction of the K_La value by the model. The Onda et al. correlation displayed the lowest SEE values for the VOC in general. However, the correlation of Shulman et al. predicted a lower SEE value than the Onda et al. correlation for the lower volatility compounds such as $ClCH_2CH_2Cl$ and $CHBr_3$. The Sherwood and Holloway correlation displayed a much higher SEE value than the other models except for the highly volatile compounds such as CCl_4. The SEE value for CCl_4 was similar to that of the Onda et al. model and thereby showing that the model could be used for the high volatility compounds. This conclusion was also noted by Munz, 1985 and Roberts et al., 1985.

The Onda et al. correlation was also applied to the 6.4 mm Raschig rings and 12.8 mm Intalox saddles packings even though these packings were not specifically used by Onda et al. to develop their correlation. The packing parameters (i.e., a_t and d_p) used in the correlation were readily available in the literature (Ludwig, 1979). The regression parameters of the best fit lines did not approach those of Eq. 4.9 and were significantly worse than those for the 12.8 mm Raschig rings packing. The slope was significantly lower than 1.0 and the intercept was not equal to zero. The results for the 6.4 mm Raschig rings packing also were not well correlated (i.e., $R^2 << 0.5$). The SEE value for all VOC were greater than 10% and significantly different from that of the 12.8 mm Raschig rings packing. The poor predictions were possibly due to the near flooding conditions present in the column. When applied to the 12.8 mm Intalox saddles packing, the Onda et al. correlation K_La values were as reliable as those of the 12.8 mm Raschig rings packing however, the results were considerably better than those for the 6.4 mm Raschig rings packing. The results regression lines had a slope and intercept lower than values (i.e., 1.0 and 0.0) for the 12.8 mm Raschig rings packing. The statistical parameters R^2 and SEE were also lower than the 12.8 mm Raschig rings packing. These results were also found by Lamarche, 1986 using the same setup and packing types.

In summary, it would appear than the results indicate that the Onda et al. correlation would be the best overall correlation to predict the mass transfer coefficient of VOC. However, for select compounds such as low volatility VOC, the Shulman et al. correlation may be used with better accuracy while with the higher volatility compounds the easier to apply Sherwood and Holloway correlation should predict values with as a high degree of accuracy as the Onda et al. model. It would also appear that the Onda et al. should not be blindly applied to any packing for which the packing data is available as considerable error may be introduced.

4.2.5 Effect of Water Composition on the Mass Transfer Coefficients

As previously noted the experiments were conducted at three different conductivity levels: 300; 1300; and 2300 µmho/cm. The experimentally measured values for the mass transfer coefficents were fitted to the following equation

$$\log_{10} KLa = B \log_{10} C + A \qquad (4.13)$$

where C is the conductivity in µmho/cm. Bias was removed by use of Finney's correction factor previously discussed.

Figures 4.44 to 4.53 show the conductivity dependence of the mass transfer coefficients of the VOC investigated. The solid line represents the best fit line for each of the VOC, according to Eq. 4.13. A summary of the experimental data can be found on Table E.14 in Appendix E.

The results of this study would suggest that the mass transfer coefficients decrease by approximately 3 to 5% with every 1000 µmho/cm change in conductivity. A literature search did not revealed a single author that studied the effect of water composition on the air stripping of volatile organics.

The small decrease in the mass transfer coefficient due to changes in conductivity found in this work may be a result of errors introduced due to:

1. The study employing a limited range of conductivity (i.e., 300 to 2300 µmho/cm)
2. The regression equations developed for all of the compounds showing poor correlation and having a very lower coefficient of determination (i.e., average $R^2 = 0.5$ for this study)
3. The effect of a complex mixture of VOC on the determination of H_C not being addressed by this study.

4.2.6 Factorial Analysis of Mass Transfer Coefficient Experiments

As previously noted the factorial analysis was carried out using the SAS general linear regression package. The model was designed on a four-factor, three-level fractional

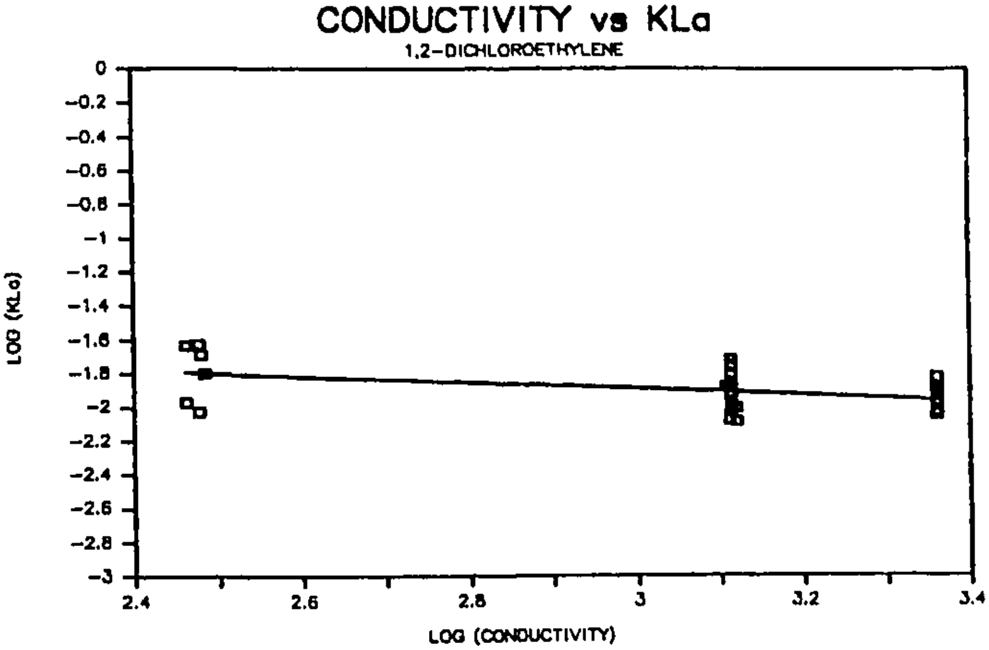


Figure 4.44 - Conductivity verses Experimental Mass Transfer Coefficient for $CH_2=CCl_2$

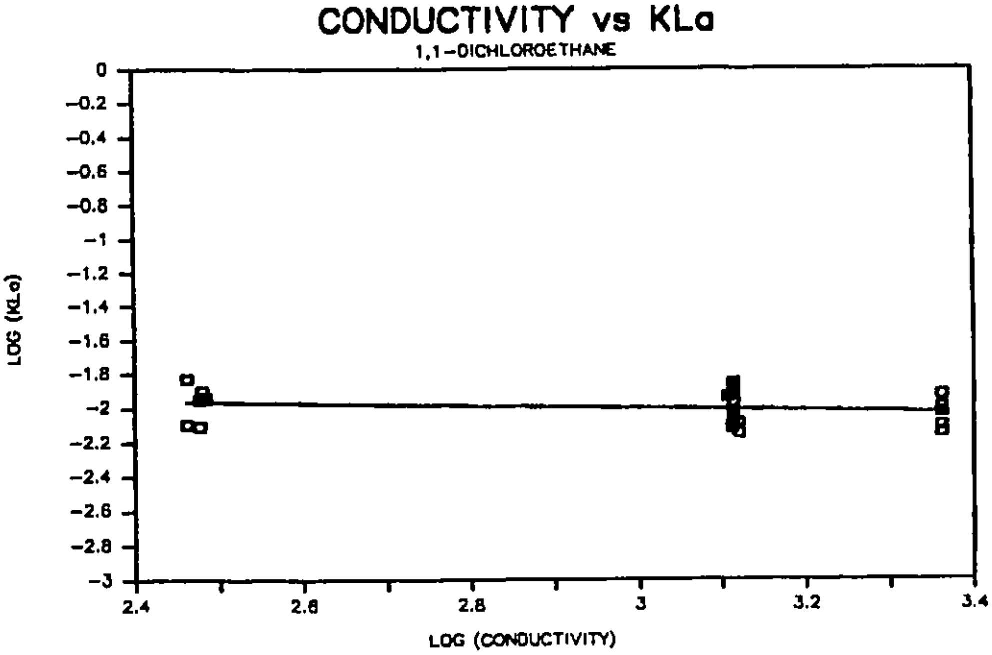


Figure 4.45 - Conductivity verses Experimental Mass Transfer Coefficient for CH_3CHCl_2

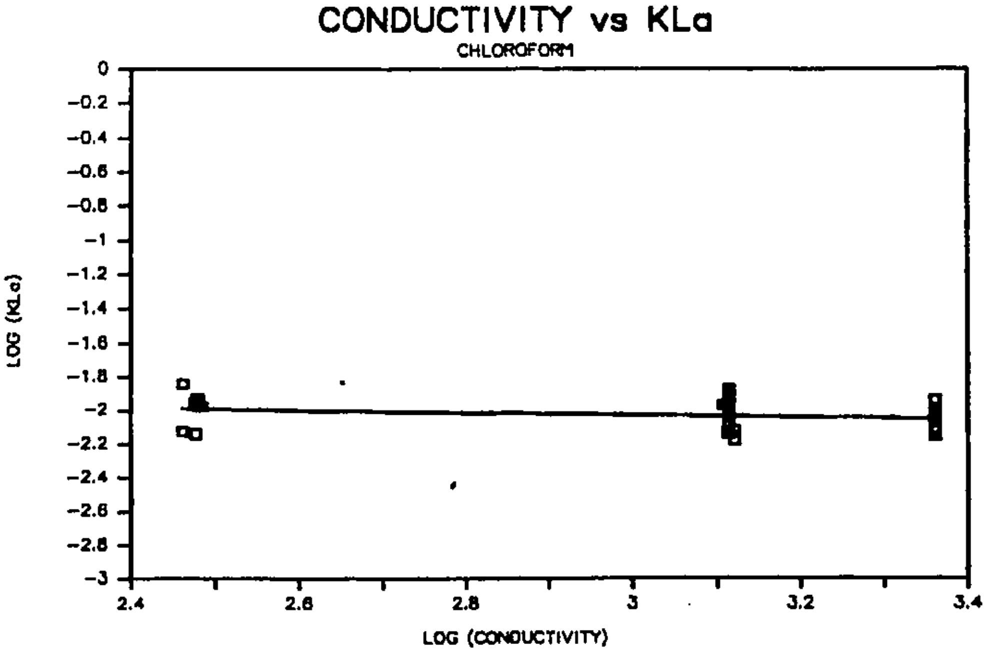


Figure 4.46 - Conductivity verses Experimental Mass Transfer Coefficient for $CHCl_3$

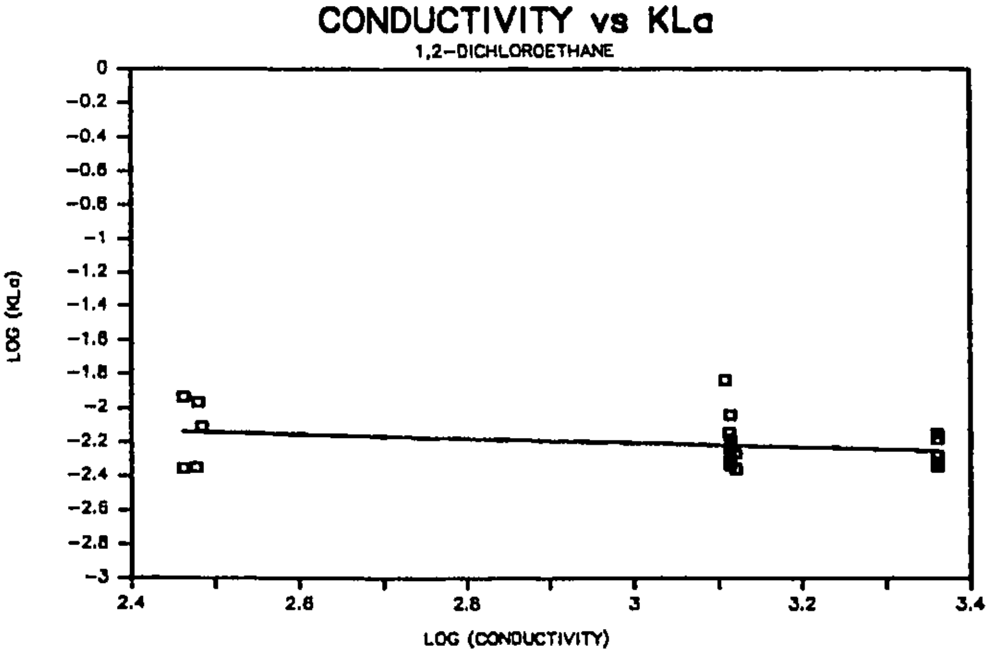


Figure 4.47 - Conductity verses Experimental Mass Transfer Coefficient for ClCH2CH2Cl

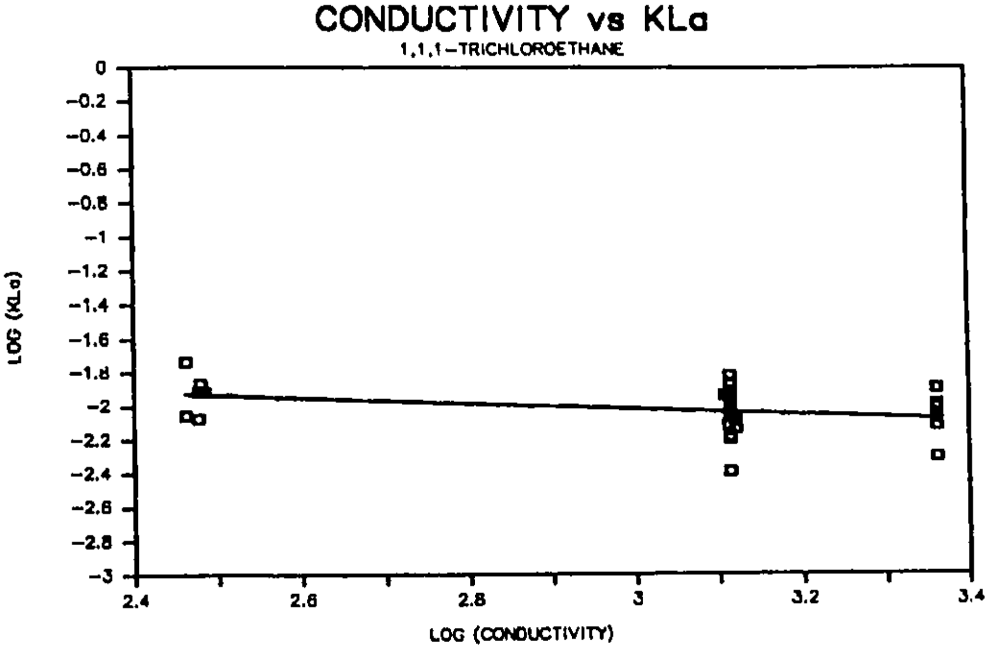


Figure 4.48 - Conductity verses Experimental Mass Transfer Coefficient for CH_3CCl_3

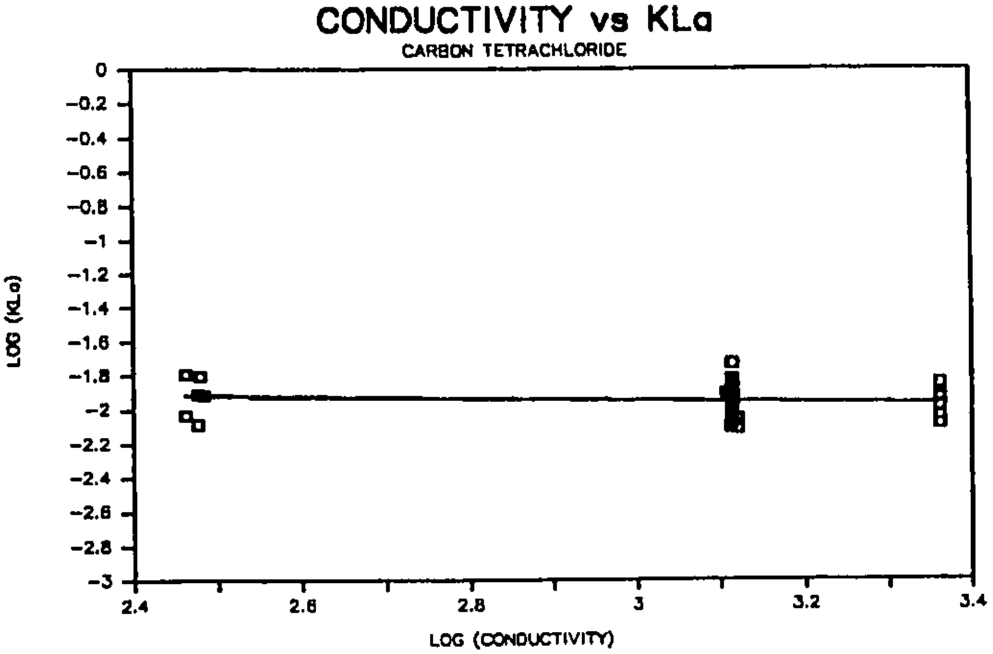


Figure 4.49 - Conductity verses Experimental Mass Transfer Coefficient for CCl_4

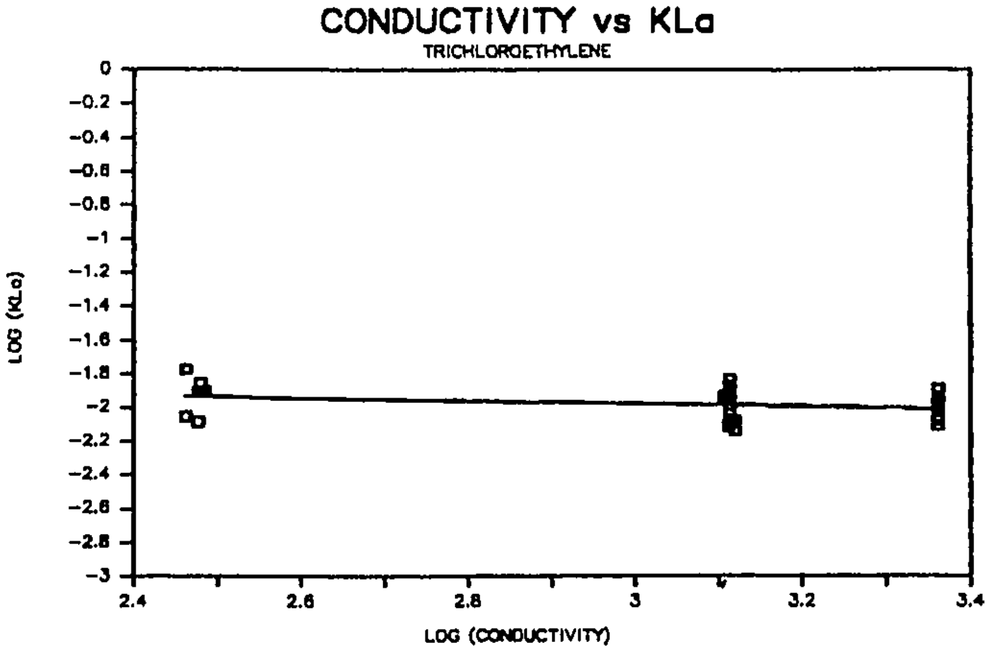


Figure 4.50 - Conductity verses Experimental Mass Transfer Coefficient for CCl2=CHCl

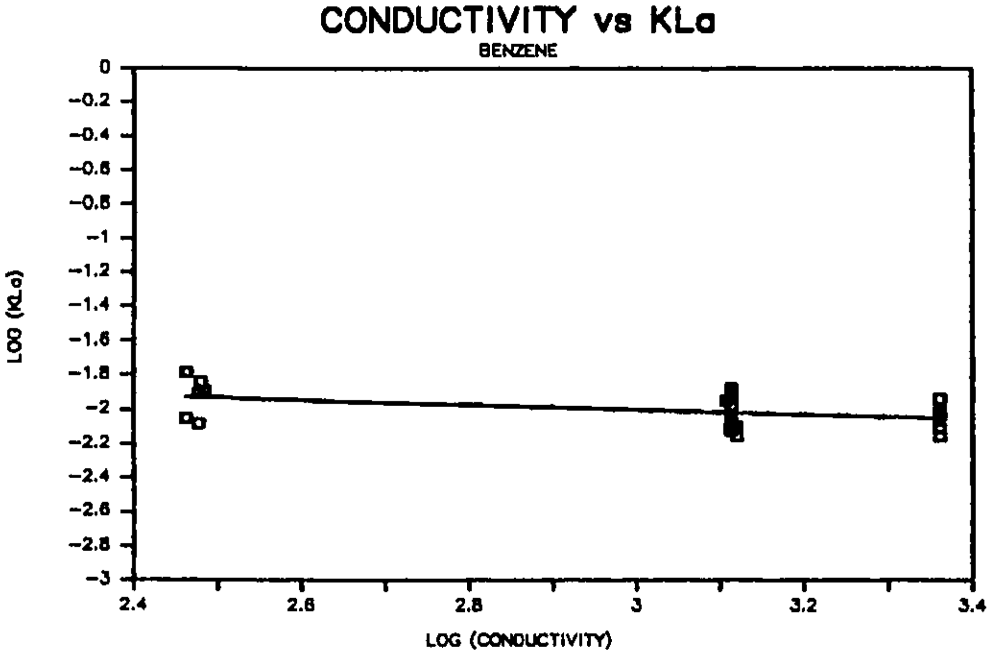


Figure 4.51 - Conductity verses Experimental Mass Transfer Coefficient for C_6H_6

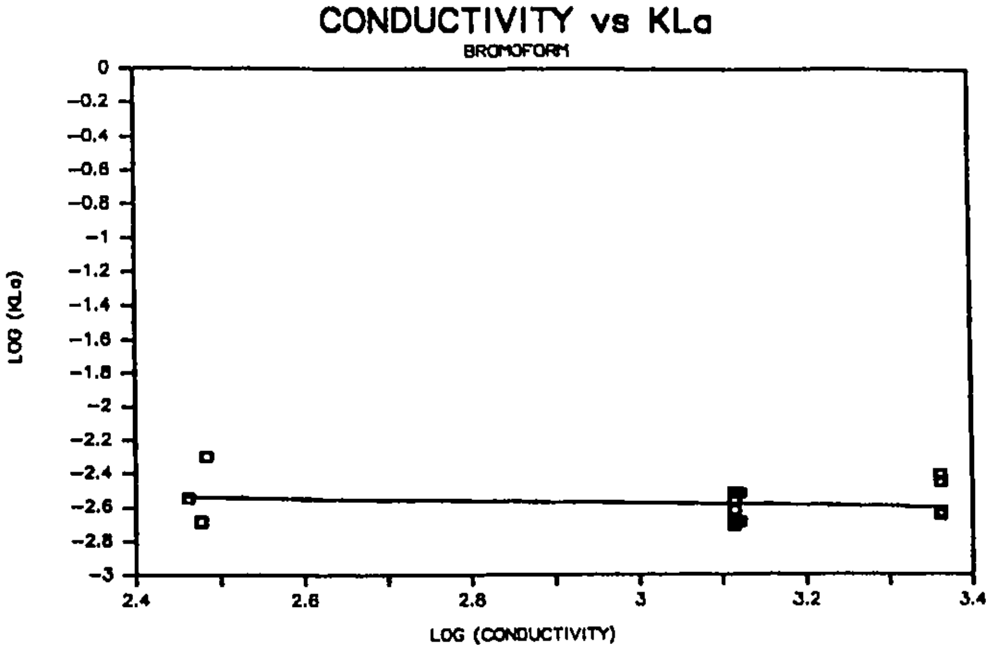


Figure 4.52 - Conductity verses Experimental Mass Transfer Coefficient for $CHBr_3$

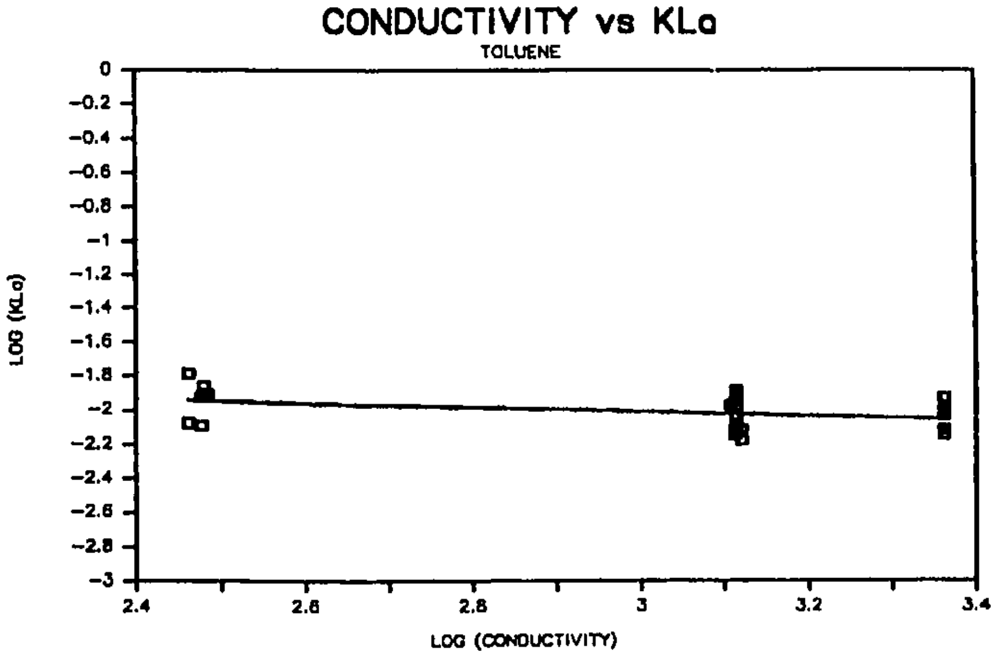


Figure 4.53 - Conductity verses Experimental Mass Transfer Coefficient for $C_6H_5CH_3$

factorial design. The linear model was developed to take into account the main and first order effects only. The equation took the form

$$\begin{aligned} K_La = {} & \beta_0 + \beta_1 A + \beta_2 B + \beta_3 C + \beta_4 D \\ & + \beta_5 A*B + \beta_6 A*C + \beta_7 A*D \\ & + \beta_8 B*C + \beta_9 B*D + \beta_{10} C*D + e \qquad (4.11) \end{aligned}$$

where A = liquid flow rate (L/min),

B = gas flow rate (L/min),

C = conductivity (µmho/cm),

D = packing porosity (%),

e = residual term representing the error between the predicted and observed K_La.

The least squares estimates of the β coefficients for the equations are presented in Appendix E on Figures E.1 to E.10 along with the analysis of variance of the fitted model for the variables. The procedure for evaluation of the Henry's Law constant experiments was also used here.

Table 4.2 summarizes the analysis of variance significance test results for the VOC. To assess the validity of the fitted model, the individual residuals were studied to reveal any nonrandom tendencies in the data. The residual plots for $CH_2=CCl_2$ are shown on Figures 4.54 and 4.55 and no evidence of systematic behavior was detected indicating that the model represents the data adequately.

Compound	Significance Level (%)				
	Overall	A	B	C	D
$CH_2=CCl_2$	0.01	0.01	4.06	0.01	0.01
CH_3CHCl_2	0.01	0.01	25.92	0.18	0.05
$CHCl_3$	0.01	0.01	80.96	0.59	0.12
$CLCH_2CH_2CL$	1.68	0.48	2.88	6.03	1.02
CH_3CCl_3	0.58	0.01	67.45	3.41	5.35
CCl_4	0.01	0.01	9.03	0.19	0.01
$CCl_2=CHCl$	0.01	0.01	10.22	0.02	0.04
C_6H_6	0.01	0.01	51.04	0.01	0.04
$CHBr_3$	51.01	13.53	34.44	50.62	84.00
$C_6H_5CH_3$	0.01	0.01	29.62	0.01	0.07
AVERAGE	0.26	0.06	31.56	1.16	0.75

* See Appendix E for complete results.

Table 4.3 - Summary of Significance Test Results for K_La Experiments

The results of the evaluation of the significance of the various main effects followed the results noted in the past studies. The following observations can be made concerning the results:

1. The R^2 for the models indicate that the best fit line is well correlated to the data (i.e., $R^2 > 0.9$) for all cases except 1,2-dichloroethane (0.7), 1,1,1-trichloroethane (0.64) and bromoform (0.34).
2. The range of significance levels for the various factors were: factor A 0.01% to 13.53% (average = 0.06%, bromoform not included), factor B 2.88% to 80.96% (average = 31.56%), factor C 0.01% to 50.56% (average = 1.16%, bromoform not included) and factor D 0.01% to 84.00% (average = 0.75%, bromoform not included).

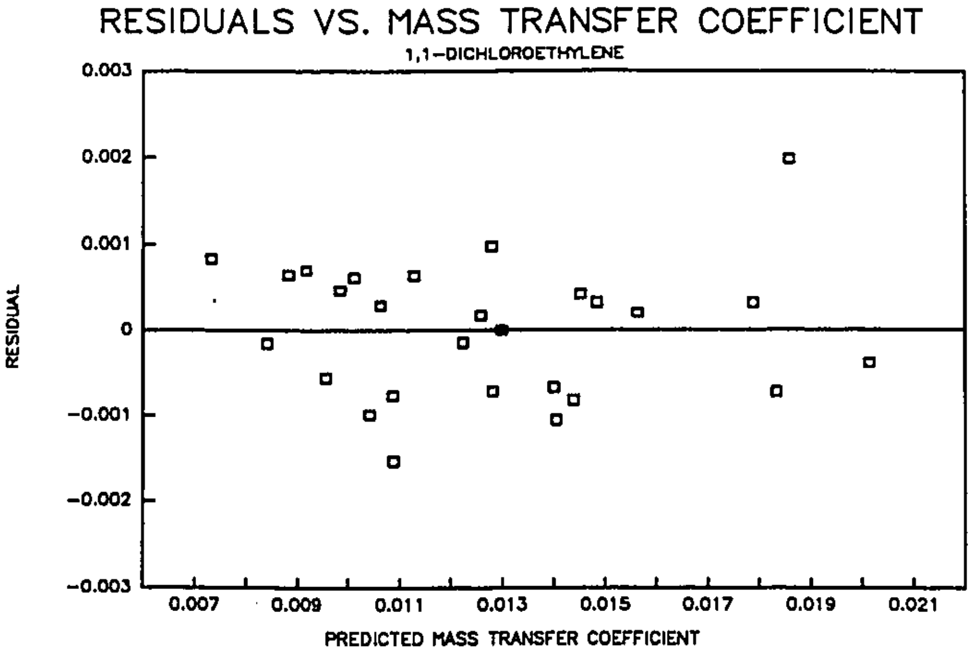


Figure 4.54 - Residuals verses K_La for $CH_2=CCl_2$

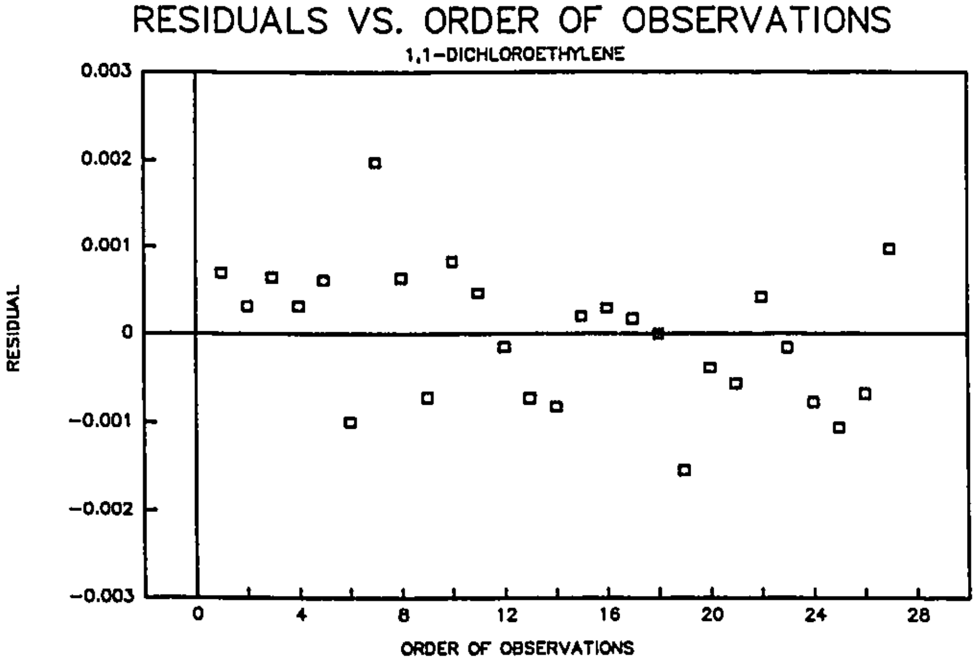


Figure 4.55 - Residuals verses Order of Observations for $CH_2=CCl_2$

3. Liquid flow rate appears to be highly significant for the determination of K_La. This would tend to agree with the findings of Onda et al., 1968 who found that the K_La dependency was approximately Q $L^{2/3}$. This was also confirmed by Munz, 1985.
4. Gas flow rate appeared to exhibit only a slight influence on K_La for the more volatile compounds while for the less volatile compounds there was a higher level of significance. This was also confirmed by Munz, 1985.
5. Conductivity would appear to be highly significant in the determination of K_La as indicated by the low average significance level (1.16%).
6. Packing porosity would also appear to be highly significant for the prediction of K_La (0.75%).

CHAPTER 5

CONCLUSION

5.0 SUMMARY

The occurrence of volatile synthetic organic compounds in our environment has increased significantly in recent years to a point where approximately one half of all water supplies are affected. The objective of this study was to examine the effect of water composition (i.e., conductivity) on the air stripping of VOC using a countercurrent packed column.

The Henry's Law constants were determined for various VOC of environmental significance: $CH_2{=}CCl_2$; CH_3CHCl_2; $CHCl_3$; $ClCH_2CH_2Cl$; CH_3CCl_3; CCl_4; $CCl_2{=}CHCl$; C_6H_6; $CHBr_3$; and $C_6H_5CH_3$. The experimental technique, introduced by McAuliffe, 1971 was used. The technique consisted of the multiple equilibration of an aqueous solution with the measurement of the liquid-phase VOC concentration. The Henry's Law constants were determined using a two-factor, three-level factorial design over a range of temperature ($10^oC < T < 30^oC$) and conductivity ($300\ \mu mho/cm < C < 2300\ \mu mho/cm$). The results of the experiments are presented in Appendix B.

The mass transfer experiments were performed to establish the effect of liquid and gas flow rates, conductivity and packing type on the air stripping of VOC and to evaluate the various mass transfer correlations available (i.e., Sherwood and Holloway, 1940, Shulman et al., 1955, Onda et al., 1968). The experiments were conducted using a four-factor, three-level fractional factorial design consisting of 27 runs (Bacon, 1970): liquid flow rate 2, 3, 4 L/min, gas flow rate 25, 50, 75 L/min, conductivity 300, 1300, 2300 mhos/cm and packing porosity, 6.4 mm Raschig rings (porosity

62%), 12.8 mm Raschig rings (64%) and 12.8 mm Intalox saddles (72%). The experiments were conducted in a random order and analyzed by the procedure developed by Lamarche, 1986 and Munz, 1985. The factorial analysis was performed by a SAS general linear regression analysis. The results of the experiments and regression analysis are shown in Appendix E.

5.1 CONCLUSIONS

The following conclusions can be made based on the research:

1. Henry's law constants for VOC increase approximately 30 to 40% with each 10°C increase in temperature.
2. Henry's law constants for VOC decrease approximately 5 to 15% with each 1000 µmho/cm increase in conductivity.
3. The SAS factorial analysis indicates that temperature is highly significant in determining the H_C of VOC (average = 0.29%). The analysis indicates that conductivity is not a significant factor in the determination of H_C for VOC (average = 26.62%).
4. The H_C approximation based on vapour pressure and solubility data would appear to be an adequate correlation if reliable data are available. The available data are limited for VOC.
5. The ME method for determining the H_C of VOC appears to be a reliable and accurate method ($R^2 > 0.99$).
6. Countercurrent packed column air strippers are an effective method to remove VOC from water. The fractional removal rate for most VOC in this study exceeded 95% and can be as high as 99% for column designs where the stripping factor is maintained above 1.0 and for optimal column dimensions and flow rates.

7. The overall mass transfer constant based on a liquid-phase driving force (K_La) can be predicted for VOC by air stripping with an accuracy of SEE < 10%.
8. The error in the K_La is significantly higher for VOC when the stripping factor is less than 1.0 (i.e., Bromoform, S_{AVG} = 0.5, SEE > ± 30% and 1,2-Dichloroethane, S_{AVG} = 0.7, SEE > ± 20%).
9. The error in the K_La for 1,1,1-Trichloroethane was significantly high than the other VOC. This was presumed to be due to the errors introduced because 1,1,1-Trichloroethane and Carbon Tetrachloride coelude together.
10. The Onda et al. correlation provides the best prediction for K_La with an average SEE = ± 3.7%. The correlations of Shulman et al. and Sherwood and Holloway were significantly worse than the Onda et al. model (i.e., SEE = ± 6.5% and SEE = ± 7.9%, respectively).
11. The Onda et al. correlation gave slightly better results, SEE = ± 3.6% (with Bromoform and 1,2-Dichloroethane omitted) when used with packings for which it was specifically developed (i.e., 12.8 mm Raschig rings). The SEE for the other two packings investigated (i.e., 6.4 mm Raschig rings and 12.8 mm Intalox saddles) were higher, SEE = ± 20.4% and SEE = ± 7.2%, respectively. This is also evidence in the Shulman et al. and Sherwood and Holloway correlations which were developed specifically for the 12.8 mm Raschig Ring packing (eg., SEE = ± 5.8% and SEE = ± 6.6%, respectively).
12. The correlation by Sherwood and Holloway, based on the assumption that the gas-phase resistance can be ignored, was effective in predicting the mass transfer coefficient for compounds where the H_C is greater then 0.1 (eg., Bromoform and 1,2-Dichloroethane), SEE = ± 3.8%.

13. K_La decreases approximately 3 to 5% with each 1000 μmho/cm increase in conductivity.
14. The SAS factorial analysis indicates that K_La of highly volatile VOC are significantly affected by the liquid flow rate and packing porosity (average 0.06 and 0.75%, respectively) and to a lesser extent by conductivity (average = 1.16%). The statistical analysis also indicated that the gas flow rate has no significance on the determination of K_La.

CHAPTER 6

RECOMMENDATIONS

6.0 RECOMMENDATIONS

The following recommendations can be drawn from this study:

1. Henry's law constants should be evaluated for VOC at temperatures greater than 30°C and lower than 10°C to evaluate the linearity of H_C over a wider temperature range than the 10 to 30°C range generally considered.
2. The need for research in the application of full-scale packed columns for the air stripping of VOC under practical operating conditions (i.e., gas and liquid flow rates), packing types and lower volatility compounds is indicated. The confirmation of the validity of the Onda et al. correlation under full-scale conditions should also be demonstrated.
3. Further research into the effect of higher temperatures on the air stripping of VOC of lower volatility is needed to provide a more economical design for these compounds.
4. With respect to the experimental procedure and packed column apparatus used in this study:

    a) The column should be redesigned to increase the diameter of the column from 100 mm to 200 mm such that the $d/d_p > 15$ as recommended by Treybal, 1980

b) The column should be redesigned so that the stripping factors for all compounds are greater than unity
c) The column should be redesigned into a single section of plexiglas rather than the 300 mm sections used in this study. This would eliminate the breaks in the packing which may affect the flow pattern of the liquid
d) Consideration should be given to automating the GC analysis by introducing a multi-head PAT concentrator. This will allow more than one experimental run to be completed in one day
e) A total mass balance should be made on the column to assess the column losses. This would require the analysis of the off-gas from the column

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APPENDIX A

CALIBRATION OF GC-DETECTOR RESPONSE

The Flame Ionization Detector (FID) had to be checked for its linearity or response as a function of concentration. Samples of known concentration and volume were injected into the GC through the PAT system and the output peaks were analyzed to determine the response factor, RF:

$$RF = \frac{A}{C.VS} \tag{A.1}$$

where A = peak area, C = sample concentration, and VS = sample volume. The data acquisition and peak integration was handled automatically by the Waters 820 computer data handling program. The RF values for a range of concentrations were analyzed and an empirical relationship between concentration and peak area was derived by a linear regression procedure. The detector rcesponse for the VOC studied is shown on Table A.1. The linearity of the detector was also checked at the end of the experiments to determine if there was any change in the detector over time. The results of the second linearity run is shown on Table A.2.

TABLE A.1 INITIAL LINEAR RESPONSE FACTORS FOR SOLUTES

Compound	Cond (µmho/cm)	Concentration vs Peak area	R^2
$CH_2=CCl_2$	300	C = -170.9 + 7.37E-3 * A	0.998
	1300	C = -97.49 + 9.64E-4 * A	0.995
	2300	C = -58.38 + 9.36E-4 * A	0.995
CH_3CHCl_2	300	C = -34.96 + 0.001 * A	0.999
	1300	C = 7.951 + 8.18E-4 * A	0.995
	2300	C = 63.18 + 7.93E-4 * A	0.993
$CHCl_3$	300	C = 0.9089 + 0.002715 * A	0.999
	1300	C = 47.26 + 0.002485 * A	0.995
	2300	C = 100.2 + 0.002474 * A	0.993
$ClCH_2CH_2Cl$	300	C = -27.54 + 8.24E-4 * A	0.999
	1300	C = 31.25 + 7.97E-4 * A	0.995
	2300	C = 82.40 + 7.85E-4 * A	0.992
CH_3CCl_3	300	C = -27.66 + 0.001336 * A	0.999
	1300	C = 2.895 + 0.001105 * A	0.994
	2300	C = 36.11 + 0.001138 * A	0.995
CCl_4	300	C = -29.18 + 0.0049 * A	0.998
	1300	C = 4.78 + 0.003982 * A	0.993
	2300	C = 17.77 + 0.004029 * A	0.996
$CCl_2=CHCl$	300	C = -63.95 + 0.001324 * A	0.999
	1300	C = 6.385 + 0.001104 * A	0.994
	2300	C = 26.71 + 0.001218 * A	0.995
C_6H_6	300	C = -24.05 + 2.70E-4 * A	0.999
	1300	C = 18.41 + 6.87E-4 * A	0.995
	2300	C = 21.24 + 2.21E-4 * A	0.994
$CHBr_3$	300	C = 126.7 + 0.00641 * A	0.999
	1300	C = 312.1 + 0.005875 * A	0.996
	2300	C = 363.8 + 0.00572 * A	0.991
$C_6H_5CH_3$	300	C = -52.76 + 2.63E-4 * A	0.999
	1300	C = 11.40 + 3.55E-4 * A	0.995
	2300	C = 13.36 + 2.43E-4 * A	0.994

Table A.2 FINAL LINEAR RESPONSE FACTORS FOR SOLUTES

Compound	Cond (µmho/cm)	Concentration vs Peak area	R^2
$CH_2=CCl_2$	300	C = 134.8 + 8.27E-4 * A	0.999
	1300	C = 173.8 + 8.35E-4 * A	0.995
	2300	C = 138.4 + 8.48E-4 * A	0.999
CH_3CHCl_2	300	C = 28.86 + 7.72E-4 * A	0.999
	1300	C = 50.04 + 7.49E-4 * A	0.998
	2300	C = 30.11 + 7.78E-4 * A	0.999
$CHCl_3$	300	C = 54.23 + 0.002414 * A	0.999
	1300	C = 65.39 + 0.0023 * A	0.998
	2300	C = 53.86 + 0.002398 * A	0.999
$ClCH_2CH_2Cl$	300	C = -6.513 + 7.78E-4 * A	0.999
	1300	C = 1.736 + 7.55E-4 * A	0.999
	2300	C = -6.568 + 7.84E-4 * A	0.999
CH_3CCL_3	300	C = 67.15 + 0.001021 * A	0.999
	1300	C = 58.27 + 0.001070 * A	0.998
	2300	C = 67.71 + 0.001029 * A	0.999
CCl_4	300	C = 185.4 + 0.003973 * A	0.999
	1300	C = 145.6 + 0.004075 * A	0.999
	2300	C = 183.9 + 0.003941 * A	0.999
$CCl_2=CHCl$	300	C = 33.72 + 0.001338 * A	0.999
	1300	C = 30.46 + 0.001224 * A	0.999
	2300	C = 33.66 + 0.001328 * A	0.999
C_6H_6	300	C = 3.983 + 2.27E-4 * A	0.999
	1300	C = 7.432 + 2.04E-4 * A	0.999
	2300	C = 3.945 + 2.24E-4 * A	0.999
$CHBr_3$	300	C = 397.5 + 0.007388 * A	0.999
	1300	C = 426.3 + 0.006987 * A	0.998
	2300	C = 393.0 + 0.007304 * A	0.999
$C_6H_5CH_3$	300	C = -17.21 + 2.75E-4 * A	0.999
	1300	C = -16.63 + 2.53E-4 * A	0.999
	2300	C = -17.20 + 2.75E-4 * A	0.999

All compounds exhibited a linear response over the concentration range tested. The R^2 values for the regressions are all greater than 0.99.

APPENDIX B

HENRY'S LAW CONSTANT RESULTS FROM INDIVIDUAL EXPERIMENTS

The results of the individual ME experiments are shown on Tables B.1 to B.10. The values for H_C were calculated by the following log-linear regression equation using 5 equilibration

$$\text{Log } C_{Li} = \text{Log } C_{Lo} - n \text{ Log } (1 + \frac{V_L}{V_G} H_C) \qquad (3.12)$$

The best fit linear regression equations obtained for log(H_C) vs 1/T and log(H_C) vs log(C) are shown on Tables B.11 and B.12. Also shown are the calculated R^2 values from the ME analysis for the best fit lines.

TABLE B.1 MEASURED H_C FOR 1,1-DICHLOROETHYLENE. TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (µmho/cm)	H_C (-)	R^2*
1	10	2300	0.566967	0.999
			0.557112	0.999
2	10	1300	0.558263	0.999
			0.54191	0.999
3	20	1300	1.007665	0.967
			1.053362	0.974
4	20	2300	0.923462	0.997
			0.908557	0.998
5	30	1300	1.445614	0.981
			1.512278	0.982
6	30	2300	1.512278	0.995
			1.518876	0.994
7	20	300	1.593966	0.999
			1.651008	0.993
8	30	300	1.936938	0.985
			1.980216	0.985
9	10	300	1.015485	0.963
			0.853442	0.982

TABLE B.2 MEASURED H_C FOR 1,1-DICHLOROETHANE. TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (µmho/cm)	H_C (-)	R^2*
1	10	2300	0.119428	0.997
			0.115938	0.999
2	10	1300	0.117713	0.999
			0.112927	0.999
3	20	1300	0.189839	0.999
			0.187008	0.998
4	20	2300	0.186208	0.999
			0.17906	0.999
5	30	1300	0.267689	0.971
			0.271896	0.996
6	30	2300	0.272907	0.999
			0.270445	0.999
7	20	300	0.191887	0.998
			0.195443	0.999
8	30	300	0.284197	0.999
			0.282303	0.999
9	10	300	0.12371	0.998
			0.120677	0.999

* As observed in the ME experiments.

TABLE B.3 MEASURED H_C FOR CHLOROFORM.
TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (°C)	Conductivity (μmho/cm)	H_C (-)	R^2*
1	10	2300	0.079922	0.995
			0.076862	0.997
2	10	1300	0.078828	0.998
			0.075411	0.999
3	20	1300	0.189839	0.999
			0.187008	0.998
4	20	2300	0.127768	0.999
			0.115812	0.999
5	30	1300	0.198239	0.998
			0.201805	0.994
6	30	2300	0.194989	0.999
			0.192328	0.999
7	20	300	0.125373	0.998
			0.127942	0.998
8	30	300	0.191501	0.999
			0.19038	0.999
9	10	300	0.078661	0.983
			0.076269	0.999

TABLE B.4 MEASURED H_C FOR 1,2-DICHLOROETHANE.
TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (°C)	Conductivity (μmho/cm)	H_C (-)	R^2*
1	10	2300	0.024328	0.99
			0.022775	0.982
2	10	1300	0.028011	0.981
			0.023616	0.998
3	20	1300	0.046642	0.997
			0.044456	0.997
4	20	2300	0.043312	0.998
			0.032931	0.984
5	30	1300	0.064218	0.996
			0.068315	0.984
6	30	2300	0.058092	0.999
			0.057267	0.997
7	20	300	0.043245	0.988
			0.044181	0.979
8	30	300	0.06352	0.995
			0.059754	0.997
9	10	300	0.026986	0.951
			0.029377	0.986

* As observed in the ME experiments.

TABLE B.5 MEASURED H_C FOR 1,1,1-TRICHLOROETHANE. TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (µmho/cm)	H_C (-)	R^2*
1	10	2300	0.331555	0.999
			0.32714	0.999
2	10	1300	0.331939	0.999
			0.321939	0.999
3	20	1300	0.543122	0.993
			0.551182	0.994
4	20	2300	0.541518	0.999
			0.521249	0.999
5	30	1300	1.022884	0.971
			1.075877	0.967
6	30	2300	0.827627	0.999
			0.825099	0.999
7	20	300	0.611889	0.998
			0.624517	0.999
8	30	300	0.927275	0.999
			0.916909	0.999
9	10	300	0.361484	0.998
			0.343497	0.999

TABLE B.6 MEASURED H_C FOR CARBON TETRACHLORIDE. TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (µmho/cm)	H_C (-)	R^2*
1	10	2300	0.573072	0.999
			0.565517	0.999
2	10	1300	0.5819	0.999
			0.562755	0.999
3	20	1300	1.163294	0.953
			1.2149	0.961
4	20	2300	1.079217	0.996
			1.0493	0.996
5	30	1300	1.686023	0.979
			1.81818	0.976
6	30	2300	1.874693	0.993
			1.904495	0.991
7	20	300	1.315295	0.992
			1.348116	0.994
8	30	300	1.958524	0.991
			1.993915	0.99
9	10	300	0.661415	0.995
			0.617752	0.996

* As observed in the ME experiments.

TABLE B.7 MEASURED H_C FOR TRICHLOROETHYLENE. TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (µmho/cm)	H_C (-)	R^2*
1	10	2300	0.181063	0.998
			0.18072	0.998
2	10	1300	0.183	0.999
			0.179193	0.999
3	20	1300	0.279174	0.999
			0.289356	0.996
4	20	2300	0.305203	0.999
			0.292564	0.999
5	30	1300	0.451271	0.997
			0.469017	0.997
6	30	2300	0.487193	0.999
			0.482281	0.999
7	20	300	0.332573	0.999
			0.340351	0.999
8	30	300	0.495842	0.999
			0.498771	0.999
9	10	300	0.188598	0.996
			0.182016	0.999

TABLE B.8 MEASURED H_C FOR BENZENE. TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (µmho/cm)	H_C (-)	R^2*
1	10	2300	0.116509	0.997
			0.114292	0.999
2	10	1300	0.118553	0.999
			0.114185	0.999
3	20	1300	0.185128	0.999
			0.18471	0.996
4	20	2300	0.183665	0.999
			0.171077	0.999
5	30	1300	0.260707	0.998
			0.266066	0.995
6	30	2300	0.270387	0.999
			0.267745	0.999
7	20	300	0.191047	0.998
			0.194515	0.999
8	30	300	0.278451	0.999
			0.277640	0.999
9	10	300	0.123578	0.991
			0.1204	0.999

* As observed in the ME experiments.

TABLE B.9 MEASURED H_C FOR BROMOFORM.
TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (μmho/cm)	H_C (-)	R^2*
1	10	2300	0.01612	0.967
			0.00903	0.973
2	10	1300	0.017118	0.972
			0.013099	0.96
3	20	1300	0.020127	0.967
			0.021257	0.985
4	20	2300	0.022999	0.971
			0.013433	0.962
5	30	1300	0.028749	0.981
			0.035261	0.926
6	30	2300	0.026607	0.987
			0.029545	0.991
7	20	300	0.03282	0.971
			0.030069	0.989
8	30	300	0.040545	0.935
			0.030001	0.983
9	10	300	0.010721	0.927
			0.012046	0.984

TABLE B.10 MEASURED H_C FOR TOLUENE.
TEMPERATURE AND WATER COMPOSITION EFFECTS.

Run	Temperature (^oC)	Conductivity (μmho/cm)	H_C (-)	R^2*
1	10	2300	0.11965	0.997
			0.117602	0.997
2	10	1300	0.122759	0.999
			0.119174	0.999
3	20	1300	0.190743	0.998
			0.193261	0.993
4	20	2300	0.198716	0.999
			0.186757	0.999
5	30	1300	0.280703	0.997
			0.289377	0.992
6	30	2300	0.308835	0.999
			0.305383	0.999
7	20	300	0.207035	0.997
			0.211815	0.999
8	30	300	0.310629	0.999
			0.312339	0.999
9	10	300	0.124932	0.992
			0.121817	0.999

* As observed in the ME experiments.

TABLE B.11 REGRESSION OF LOG (H_C) VS 1/T

Compound	C (μmho/cm)	Log (H_C) vs 1/T	R^2
$CH_2=CCl_2$	300	4.9117 - 1392.039 / T	0.911
	1300	5.9144 - 1741.485 / T	0.965
	2300	6.2697 - 1846.111 / T	0.999
CH_3CHCl_2	300	4.6266 - 1566.667 / T	0.998
	1300	4.6702 - 1585.135 / T	0.994
	2300	4.5778 - 1558.263 / T	0.998
$CHCl_3$	300	4.8328 - 1681.072 / T	0.998
	1300	5.1831 - 1778.506 / T	0.989
	2300	4.8376 - 1683.078 / T	0.992
$ClCH_2CH_2Cl$	300	3.6117 - 1459.494 / T	0.988
	1300	4.6579 - 1764.843 / T	0.971
	2300	4.2713 - 1669.192 / T	0.953
CH_3CCl_3	300	5.8948 - 1793.870 / T	0.992
	1300	7.1654 - 2168.768 / T	0.991
	2300	5.5712 - 1713.054 / T	0.999
CCl_4	300	7.2753 - 2107.960 / T	0.975
	1300	7.1597 - 2088.746 / T	0.973
	2300	7.6504 - 2234.101 / T	0.999
$CCl_2=CHCl$	300	5.7890 - 1842.097 / T	0.989
	1300	5.3835 - 1734.777 / T	0.997
	2300	5.7406 - 1835.055 / T	0.999
C_6H_6	300	4.5166 - 1535.524 / T	0.997
	1300	4.4530 - 1522.963 / T	0.995
	2300	4.6299 - 1575.989 / T	0.996
$CHBr_3$	300	5.5600 - 2106.483 / T	0.805
	1300	3.1193 - 1401.786 / T	0.898
	2300	3.6124 - 1567.592 / T	0.687
$C_6H_5CH_3$	300	5.1997 - 1726.726 / T	0.995
	1300	4.7275 - 1596.752 / T	0.998
	2300	5.3309 - 1770.945 / T	0.998

TABLE B.12 REGRESSION OF LOG (H_C) VS LOG (C)

Compound	Temp (°C)	Log (H_C) vs Log (C)	R^2
$CH_2{=}CCl_2$	10	0.6248 - 0.2698 * log (C)	0.868
	20	0.9162 - 0.2864 * log (C)	0.989
	30	0.6434 - 0.1466 * log (C)	0.747
CH_3CHCl_2	10	-0.8592 - 0.0227 * log (C)	0.447*
	20	0.6453 - 0.0269 * log (C)	0.706
	30	-0.4923 - 0.0230 * log (C)	0.790
$CHCl_3$	10	-1.1219 + 0.0040 * log (C)	0.029*
	20	-0.8763 - 0.0052 * log (C)	0.006*
	30	-0.7457 + 0.0118 * log (C)	0.244*
$ClCH_2CH_2Cl$	10	-1.3425 - 0.0827 * log (C)	0.577*
	20	-1.2195 - 0.0520 * log (C)	0.154*
	30	-1.1612 - 0.0162 * log (C)	0.050*
CH_3CCl_3	10	-0.3638 - 0.0369 * log (C)	0.680
	20	-0.0213 - 0.0761 * log (C)	0.953
	30	0.0443 - 0.0257 * log (C)	0.050*
CCl_4	10	-0.0464 - 0.0606 * log (C)	0.806
	20	0.3846 - 0.1036 * log (C)	0.913
	30	0.3733 - 0.0340 * log (C)	0.282*
$CCl_2{=}CHCl$	10	-0.7016 - 0.0125 * log (C)	0.436*
	20	-0.3073 - 0.0695 * log (C)	0.670
	30	-0.2569 - 0.0206 * log (C)	0.264*
C_6H_6	10	-0.8443 - 0.0282 * log (C)	0.731
	20	-0.6178 - 0.0386 * log (C)	0.678
	30	-0.5080 - 0.0203 * log (C)	0.559*
$CHBr_3$	10	-2.0775 + 0.0609 * log (C)	0.055*
	20	-0.7967 - 0.2851 * log (C)	0.705
	30	-1.2091 - 0.0982 * log (C)	0.356*
$C_6H_5CH_3$	10	-0.8633 - 0.0181 * log (C)	0.592*
	20	-0.5706 - 0.0446 * log (C)	0.735
	30	-0.4680 - 0.0176 * log (C)	0.141*

* $R^2 < 0.6$, and therefore, not a significant regression.

```
                                                   SAS                                  18:12 SUNDAY, FEBRUARY 19, 1989    1

                                     GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y
SOURCE                    DF        SUM OF SQUARES         MEAN SQUARE        F VALUE         PR > F        R-SQUARE          C.V.

MODEL                      5            1.41315682          0.36263136          18.39         0.0185        0.968406       11.8293

ERROR                      3            0.05915356          0.01971785                      ROOT MSE                      Y MEAN

CORRECTED TOTAL            8            1.67231038                                        0.14042027                  1.18705300

SOURCE                    DF           TYPE I SS         F VALUE       PR > F          DF       TYPE III SS       F VALUE       PR > F

A                          1          0.38603070           19.58       0.0214           1        0.11441333          5.80       0.0951
B                          1          1.33025672           67.45       0.0038           1        0.09467226          4.80       0.1161
A*A                        1          0.07482085            3.79       0.1466           1        0.07482085          3.79       0.1466
B*B                        1          0.02080331            1.06       0.3799           1        0.02080331          1.06       0.3799
A*B                        1          0.00124524            0.06       0.8178           1        0.00124524          0.06       0.8178

                                            T FOR H0:       PR > |T|         STD ERROR OF
PARAMETER                 ESTIMATE       PARAMETER=0                           ESTIMATE

INTERCEPT               0.38717242              0.93       0.4210           0.41723033
A                      -0.00072125             -2.41       0.0951           0.00029942
B                       0.09017515              2.19       0.1161           0.04115336
A*A                    1.93415E-07              1.95       0.1466           0.00000010
B*B                    -0.00030193             -1.03       0.3799           0.00029292
A*B                   -1.75440E-06             -0.25       0.8178           0.00000702

                          OBSERVED          PREDICTED               RESIDUAL       LOWER 95% CL        UPPER 95% CL
OBSERVATION                  VALUE              VALUE                                  FOR MEAN            FOR MEAN

          1             0.93646350         0.98267533            -0.04621183         0.58158151          1.38376915
          2             0.56193900         0.51056243             0.05137657         0.10956901          0.91175665
          3             1.95847700         1.95958400            -0.00110700         1.55659018          2.36077782
          4             1.51584700         1.41739550             0.09845150         1.01600168          1.81818932
          5             0.55008700         0.55325133            -0.00316433         0.22016105          0.88634162
          6             1.39759750         1.49497200            -0.09737450         1.16188171          1.82806229
          7             1.62248700         1.57316817             0.04931883         1.24007785          1.90625945
          8             0.90850850         1.05536767            -0.14685917         0.73277738          1.39875795
          9             1.22663950         1.12610017             0.10053933         0.79300988          1.45919045

              SUM OF RESIDUALS                                    0.00000000
              SUM OF SQUARED RESIDUALS                            0.05915356
              SUM OF SQUARED RESIDUALS - ERROR SS                 0.00000000
              PRESS STATISTIC                                     0.61307139
              FIRST ORDER AUTOCORRELATION                        -0.50556936
              DURBIN-WATSON D                                     2.60096474
```

Figure B.1 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for $CH_2=CCl_2$

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                                                       SAS                                    18:12 SUNDAY, FEBRUARY 19, 1989    1

                                          GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                 DF        SUM OF SQUARES        MEAN SQUARE       F VALUE          PR > F       R-SQUARE           C.V.

MODEL                   5            0.03705042         0.00741008        911.37          0.0001       0.999342         1.4710

ERROR                   3            0.00002439         0.00000813                       ROOT MSE                        Y MEAN

CORRECTED TOTAL         8            0.03707482                                        0.00285144                     0.19384861

SOURCE                 DF              TYPE I SS      F VALUE      PR > F        DF      TYPE III SS      F VALUE        PR > F

A                       1             0.00012254        15.07      0.0303         1       0.00002858         3.52        0.1575
B                       1             0.03674182      4518.20      0.0001         1       0.00025612        31.50        0.0112
A*A                     1             0.00003208         3.95      0.1412         1       0.00003208         3.95        0.1412
B*B                     1             0.00014151        17.40      0.0251         1       0.00014151        17.40        0.0251
A*B                     1             0.00001247         1.53      0.3036         1       0.00001247         1.53        0.3036

                                         T FOR H0:       PR > |T|            STD ERROR OF
PARAMETER                 ESTIMATE    PARAMETER=0                              ESTIMATE

INTERCEPT               0.07076224           8.35        0.0036              0.00847247
A                     -1.14603E-05          -1.88        0.1575              0.00000609
B                       0.00459026           5.61        0.0112              0.00081568
A*A                   4.00492E-09            1.99        0.1412              0.00000000
B*B                   8.41157E-05            4.17        0.0251              0.00002016
A*B                  -1.76547E-07           -1.24        0.3036              0.00000014

OBSERVATION               OBSERVED          PREDICTED            RESIDUAL          LOWER 95% CL         UPPER 95% CL
                             VALUE              VALUE                                 FOR MEAN             FOR MEAN

        1               0.12219350         0.12248718         -0.00029368           0.11434239           0.13063197
        2               0.19366500         0.19409506         -0.00043006           0.18733117           0.20085894
        3               0.28325000         0.28252626          0.00072374           0.27438147           0.29067106
        4               0.11532000         0.11572889         -0.00040889           0.10896501           0.12249277
        5               0.18842350         0.18557089          0.00285261           0.17880701           0.19233477
        6               0.26979250         0.27223622         -0.00244372           0.26547234           0.27900010
        7               0.11748300         0.11678043          0.00070257           0.10843564           0.12512522
        8               0.14263400         0.14505656         -0.00242256           0.17629267           0.19182044
        9               0.27167600         0.26995601          0.00171999           0.26181122           0.27810081

           SUM OF RESIDUALS                                    0.00000000
           SUM OF SQUARED RESIDUALS                            0.00002439
           SUM OF SQUARED RESIDUALS - ERROR SS                -0.00000000
           PRESS STATISTIC                                     0.00021036
           FIRST ORDER AUTOCORRELATION                        -0.66431094
           DURBIN-WATSON D                                     3.20300265
```

Figure B.2 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for CH_3CHCl_2

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                                              SAS                      18:12 SUNDAY, FEBRUARY 19, 1989     1

                                  GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE               DF      SUM OF SQUARES      MEAN SQUARE      F VALUE         PR > F        R-SQUARE          C.V.

MODEL                 5          0.02081724       0.00416345       159.40         0.0008        0.996250        3.8232

ERROR                 3          0.00007836       0.00002612                     ROOT MSE                        Y MEAN

CORRECTED TOTAL       8          0.02089560                                    0.00511078                    0.13367939

SOURCE               DF           TYPE I SS    F VALUE     PR > F        DF      TYPE III SS      F VALUE       PR > F

A                     1          0.00000025       0.01     0.9294         1       0.00005648         2.16       0.2378
B                     1          0.02060899     789.01     0.0001         1       0.00008477         3.25       0.1694
A*A                   1          0.00008676       3.32     0.1659         1       0.00008676         3.32       0.1659
B*B                   1          0.00012045       4.61     0.1210         1       0.00012045         4.61       0.1210
A*B                   1          0.00000080       0.03     0.8721         1       0.00000080         0.03       0.8721

                                        T FOR H0:     PR > |T|        STD ERROR OF
PARAMETER                 ESTIMATE     PARAMETER=0                      ESTIMATE

INTERCEPT               0.03702209            2.44       0.0927        0.01518564
A                     1.60254E-05            1.47       0.2379        0.00001090
B                       0.00239630            1.80       0.1694        0.00149783
A*A                  -6.51542E-09           -1.82       0.1659        0.00000090
B*B                   7.79558E-05            2.15       0.1210        0.00003614
A*B                   4.47750E-08            0.17       0.8721        0.00000026

OBSERVATION            OBSERVED          PREDICTED              RESIDUAL       LOWER 95% CL       UPPER 95% CL
                          VALUE              VALUE                               FOR MEAN           FOR MEAN

      1              0.07746509         0.07611495            0.00135014         0.06151653         0.09071319
      2              0.12665750         0.12651394            0.00014356         0.11439069         0.13863719
      3              0.19594050         0.19743409           -0.00149359         0.17783587         0.20703252
      4              0.07711955         0.08204983           -0.00493028         0.06992653         0.09417303
      5              0.13709790         0.13292551            0.00417239         0.12077336         0.14501986
      6              0.20002200         0.19926461            0.00075739         0.18714136         0.21138786
      7              0.07799200         0.07441186            0.00358014         0.06021353         0.08941019
      8              0.12179303         0.12610947           -0.00431644         0.11398319         0.13822969
      9              0.19355850         0.19282219            0.00073631         0.17832387         0.20752052

              SUM OF RESIDUALS                                      0.00000000
              SUM OF SQUARED RESIDUALS                              0.00007836
              SUM OF SQUARED RESIDUALS - ERROR SS                  -0.00000000
              PRESS STATISTIC                                       0.00076911
              FIRST ORDER AUTOCORRELATION                          -0.33166536
              DURBIN-WATSON D                                       2.63315132
```

Figure B.3 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for $CHCl_3$

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                                              SAS                              18:12 SUNDAY, FEBRUARY 19, 1989     1

                                    GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                  DF        SUM OF SQUARES        MEAN SQUARE        F VALUE         PR > F        R-SQUARE          C.V.

MODEL                    5            0.00195392         0.00039078          58.23         0.0035        0.989801        5.9933

ERROR                    3            0.00002013         0.00000671                      ROOT MSE                      Y MEAN

CORRECTED TOTAL          8            0.00197406                                       0.00259054                  0.04322367

SOURCE                  DF             TYPE I SS    F VALUE      PR > F          DF          TYPE III SS      F VALUE       PR > F

A                        1            0.00002673       3.99      0.1396           1           0.00001123         1.67       0.2864
B                        1            0.00189167     281.88      0.0005           1           0.00001812         2.70       0.1989
A*A                      1            0.00003166       4.72      0.1182           1           0.00003166         4.72       0.1182
B*B                      1            0.00000262       0.39      0.5766           1           0.00000262         0.39       0.5766
A*B                      1            0.00000118       0.18      0.7032           1           0.00000118         0.18       0.7032

                                         T FOR H0:     PR > |T|             STD ERROR OF
PARAMETER               ESTIMATE      PARAMETER=0                              ESTIMATE

INTERCEPT            0.01161140              1.51        0.2286              0.00769727
A                    7.14578E-06             1.29        0.2864              0.00000552
B                    0.00124753              1.64        0.1989              0.00075922
A*A                 -3.97433E-09            -2.17        0.1182              0.00000000
B*B                  1.14375E-05             0.62        0.5766              0.00001832
A*B                  5.41125E-08             0.42        0.7032              0.00000013

OBSERVATION          OBSERVED            PREDICTED              RESIDUAL           LOWER 95% CL        UPPER 95% CL
                        VALUE                VALUE                                    FOR MEAN            FOR MEAN

      1            0.02818150           0.02717879            0.00100271           0.01977922          0.03457837
      2            0.04371300           0.04324800            0.00046500           0.03710299          0.04939301
      3            0.06013700           0.06160471           -0.00146771           0.05420513          0.06900428
      4            0.02581350           0.02850150           -0.00268800           0.02235649          0.03464651
      5            0.04554900           0.04511383            0.00043517           0.03896882          0.05125885
      6            0.06626650           0.06401367            0.00225283           0.05786865          0.07015868
      7            0.02365150           0.02196621            0.00168529           0.01466663          0.02926578
      8            0.03812150           0.03902167           -0.00090017           0.03287665          0.04516668
      9            0.05767950           0.05846462           -0.00078512           0.05106505          0.06586420

                SUM OF RESIDUALS                                  0.00000000
                SUM OF SQUARED RESIDUALS                          0.00002013
                SUM OF SQUARED RESIDUALS - ERROR SS              -0.00000000
                PRESS STATISTIC                                   0.00024342
                FIRST ORDER AUTOCORRELATION                       0.32414829
                DURBIN-WATSON D                                   1.27114573
```

Figure B.4 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for $ClCH_2CH_2Cl$

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                                                   SAS                          18:12 SUNDAY, FEBRUARY 19, 1989    1

                                       GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                DF      SUM OF SQUARES        MEAN SQUARE      F VALUE         PR > F      R-SQUARE          C.V.

MODEL                  5          0.70028269         0.14005654         6.48         0.0774      0.915293       23.2564

ERROR                  3          0.06480882         0.02160294                    ROOT MSE                     Y MEAN

CORRECTED TOTAL        8          0.76509150                                     0.14697939                 0.63199550

SOURCE                DF           TYPE I SS    F VALUE     PR > F        DF      TYPE III SS      F VALUE      PR > F

A                      1          0.00705026       0.33     0.6078         1       0.01696959         0.79      0.4407
B                      1          0.64956905      30.07     0.0119         1       0.00024495         0.01      0.9219
A*A                    1          0.02249564       1.04     0.3826         1       0.02249564         1.04      0.3826
B*B                    1          0.01984988       0.92     0.4085         1       0.01984988         0.92      0.4085
A*B                    1          0.00131784       0.06     0.8209         1       0.00131784         0.06      0.8209

                                             T FOR H0:    PR > |T|          STD ERROR OF
PARAMETER                    ESTIMATE       PARAMETER=0                       ESTIMATE

INTERCEPT                  0.19495277              0.45     0.6857            0.43671942
A                          0.00027777              0.89     0.4407            0.00031340
B                         -0.00458695             -0.11     0.9219            0.04307566
A*A                     -1.05355E-07             -1.02     0.3826            0.00000010
B*B                        0.00099624              0.96     0.4085            0.00103930
A*B                     -1.81510E-06             -0.25     0.8209            0.00000735

OBSERVATION              OBSERVED          PREDICTED             RESIDUAL        LOWER 95% CL      UPPER 95% CL
                           VALUE             VALUE                                 FOR MEAN          FOR MEAN

      1                 0.35247250        0.31694833           0.03552417       -0.10288083        0.73677750
      2                 0.61820300        0.56450650           0.05369650        0.21585735        0.91315565
      3                 0.92209210        1.01131267          -0.08922057        0.59148350        1.43114183
      4                 0.32669700        0.40687617          -0.08017917        0.05822702        0.75552531
      5                 0.54715200        0.63628333          -0.08913133        0.28763419        0.98493248
      6                 1.23424900        1.06493850           0.16931050        0.71628935        1.41358765
      7                 0.32934750        0.28469250           0.04465500       -0.13513667        0.70452167
      8                 0.53138350        0.49594867           0.03543483        0.14729952        0.84459781
      9                 0.82636290        0.90645283          -0.08008993        0.48662367        1.32628200

          SUM OF RESIDUALS                                      0.00000000
          SUM OF SQUARED RESIDUALS                              0.06480882
          SUM OF SQUARED RESIDUALS - ERROR SS                  -0.00000000
          PRESS STATISTIC                                       0.70515423
          FIRST ORDER AUTOCORRELATION                           0.04059421
          DURBIN-WATSON D                                       1.80036555
```

Figure B.5 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for CH_3CCl_3

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                                              SAS                        16:13 SUNDAY, FEBRUARY 19, 1989    1

                                  GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                  DF       SUM OF SQUARES       MEAN SQUARE      F VALUE        PR > F       R-SQUARE         C.V.

MODEL                    5           2.49731626        0.49946325        63.74        0.0030       0.990675       7.2529

ERROR                    3           0.02350701        0.00783567                   ROOT MSE                      Y MEAN

CORRECTED TOTAL          8           2.52082328                                   0.08851933                  1.22046461

SOURCE                  DF          TYPE I SS     F VALUE      PR > F        DF        TYPE III SS      F VALUE      PR > F

A                        1         0.03001374        3.83      0.1453         1         0.01427779         1.82      0.2699
B                        1         2.45338976      313.11      0.0004         1         0.02819339         3.60      0.1541
A*A                      1         0.01093245        1.40      0.3226         1         0.01093245         1.40      0.3226
B*B                      1         0.00291335        0.37      0.5851         1         0.00291335         0.37      0.5851
A*B                      1         0.00006672        0.01      0.9323         1         0.00006672         0.01      0.9323

                                          T FOR H0:     PR > |T|          STD ERROR OF
PARAMETER                  ESTIMATE     PARAMETER=0                         ESTIMATE

INTERCEPT                0.22576414            0.86      0.4538            0.26301721
A                       -0.00025477           -1.35      0.2699            0.00018875
B                        0.04920953            1.90      0.1541            0.02594261
A*A                     7.33339E-08            1.18      0.3226            0.00000006
B*B                      0.00038166            0.61      0.5851            0.00062593
A*B                    -4.04412E-07           -0.09      0.9323            0.00000443

OBSERVATION                OBSERVED           PREDICTED             RESIDUAL         LOWER 95% CL         UPPER 95% CL
                             VALUE              VALUE                                  FOR MEAN             FOR MEAN

         1               0.63958350         0.68502260          -0.04543910          0.43217766          0.93786754
         2               1.33170560         1.29039199           0.04131361          1.08041560          1.50036818
         3               1.97621950         1.97209401           0.00412549          1.71924907          2.22493895
         4               0.57232750         0.54444589           0.02788161          0.33446960          0.75442218
         5               1.18909700         1.14573106           0.04336594          0.93575476          1.35570735
         6               1.75210150         1.82334906          -0.07124756          1.61337276          2.03332535
         7               0.56929450         0.55173701           0.01755749          0.29889207          0.80458195
         8               1.06425850         1.14893806          -0.08467956          0.93896176          1.35891435
         9               1.88959400         1.82247193           0.06712207          1.56962699          2.07531687

              SUM OF RESIDUALS                                     0.00000000
              SUM OF SQUARED RESIDUALS                             0.02350701
              SUM OF SQUARED RESIDUALS - ERROR SS                 -0.00000000
              PRESS STATISTIC                                      0.26647192
              FIRST ORDER AUTOCORRELATION                         -0.50597450
              DURBIN-WATSON D                                      2.73245438
```

Figure B.6 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for CCl_4

```
                                                      SAS                               18:13 SUNDAY, FEBRUARY 19, 1989   1

                                         GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y
SOURCE                  DF        SUM OF SQUARES          MEAN SQUARE        F VALUE          PR > F       R-SQUARE          C.V.

MODEL                    5            0.13621547           0.02724309         118.81          0.0012       0.994976        4.6847

ERROR                    3            0.00068787           0.00022929                        ROOT MSE                      Y MEAN

CORRECTED TOTAL          8            0.13690334                                           0.01514233                  0.32323267


SOURCE                  DF             TYPE I SS      F VALUE      PR > F          DF       TYPE III SS      F VALUE      PR > F

A                        1            0.00049619         2.16      0.2377           1        0.00085823         3.74      0.1485
B                        1            0.13347180       582.11      0.0002           1        0.00031028         1.35      0.3288
A*A                      1            0.00097649         4.26      0.1310           1        0.00097649         4.26      0.1310
B*B                      1            0.00125438         5.47      0.1013           1        0.00125438         5.47      0.1013
A*B                      1            0.00001663         0.07      0.8052           1        0.00001663         0.07      0.8052


                                          T FOR H0:      PR > |T|          STD ERROR OF
PARAMETER                  ESTIMATE     PARAMETER=0                          ESTIMATE

INTERCEPT               0.13754762            3.06      0.0551            0.04499236
A                     -6.24665E-05           -1.93      0.1485            0.00003229
B                       0.00511524            1.15      0.3288            0.00443780
A*A                    2.20952E-08            2.06      0.1310            0.00000001
B*B                     0.00025044            2.34      0.1013            0.00010707
A*B                   -2.03875E-07           -0.27      0.8052            0.00000076


OBSERVATION             OBSERVED          PREDICTED            RESIDUAL       LOWER 95% CL      UPPER 95% CL
                           VALUE              VALUE                             FOR MEAN          FOR MEAN

     1                0.18490700         0.19645242         -0.01154542        0.15280015        0.24010468
     2                0.33549200         0.32202600          0.01346600        0.28707695        0.35891505
     3                0.49730650         0.49922706         -0.00192056        0.45597482        0.54247935
     4                0.18109650         0.16770117          0.01339533        0.13179212        0.20362022
     5                0.28426494         0.29180600         -0.00754106        0.25588695        0.32772505
     6                0.46014400         0.46599833         -0.00585433        0.43007928        0.50191738
     7                0.18089250         0.18274242         -0.00184992        0.13949015        0.22599468
     8                0.29738350         0.30330850         -0.00592500        0.26588945        0.34072755
     9                0.48473700         0.47696208          0.00777492        0.43370982        0.52021435

          SUM OF RESIDUALS                                   0.00000000
          SUM OF SQUARED RESIDUALS                           0.00068787
          SUM OF SQUARED RESIDUALS - ERROR SS               -0.00000000
          PRESS STATISTIC                                    0.00777776
          FIRST ORDER AUTOCORRELATION                       -0.41897757
          DURBIN-WATSON D                                    2.55629458
```

Figure B.7 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for CCl_2=CHCl

```
                                                     SAS                         18:13 SUNDAY, FEBRUARY 19, 1989    1

                                           GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                  DF       SUM OF SQUARES       MEAN SQUARE       F VALUE        PR > F        R-SQUARE           C.V.

MODEL                    5           0.03512812        0.00702562        373.85        0.0002        0.998398         2.2692

ERROR                    3           0.00005638        0.00001879                    ROOT MSE                         Y MEAN

CORRECTED TOTAL          8           0.03518450                                    0.00433507                     0.19103639


SOURCE                  DF           TYPE I SS      F VALUE       PR > F        DF        TYPE III SS      F VALUE       PR > F

A                        1          0.00015994         8.51       0.0616         1         0.00004904         2.61       0.2046
B                        1          0.03476950      1850.10       0.0001         1         0.00019403        10.32       0.0488
A*A                      1          0.00003557         1.89       0.2626         1         0.00003557         1.89       0.2626
B*B                      1          0.00016269         8.66       0.0604         1         0.00016269         8.66       0.0604
A*B                      1          0.00000143         0.08       0.8006         1         0.00000143         0.08       0.8006

                                          T FOR H0:      PR > |T|          STD ERROR OF
PARAMETER                ESTIMATE       PARAMETER=0                          ESTIMATE

INTERCEPT              0.07532633              6.04        0.0089            0.01248077
A                    -1.47326E-05             -1.62        0.2046            0.00000924
B                      0.00409243              3.21        0.0488            0.00127049
A*A                  4.21733E-09               1.34        0.2626            0.00000000
B*B                  9.01303E-05               2.94        0.0604            0.00003065
A*B                 -5.97750E-08              -0.23        0.8006            0.00000022

OBSERVATION          OBSERVED           PREDICTED             RESIDUAL        LOWER 95% CL       UPPER 95% CL
                        VALUE               VALUE                               FOR MEAN           FOR MEAN

      1            0.12198900          0.12389053          -0.00190153        0.11150792         0.13627313
      2            0.19778100          0.19659244           0.00118856        0.19130925         0.20187564
      3            0.27804550          0.27733253           0.00071297        0.26494992         0.28971513
      4            0.11636900          0.11510794           0.00126106        0.10482475         0.12539114
      5            0.18491900          0.18221211           0.00270689        0.17192892         0.19249530
      6            0.26338710          0.26735444          -0.00396734        0.25707125         0.27763764
      7            0.11540050          0.11476003           0.00064047        0.10237742         0.12714263
      8            0.17737100          0.18126644          -0.00389544        0.17098325         0.19154964
      9            0.26906600          0.26581103           0.00325497        0.25342842         0.27819363

           SUM OF RESIDUALS                                     0.00000000
           SUM OF SQUARED RESIDUALS                             0.00005638
           SUM OF SQUARED RESIDUALS - ERROR SS                 -0.00000000
           PRESS STATISTIC                                      0.00060898
           FIRST ORDER AUTOCORRELATION                         -0.45330564
           DURBIN-WATSON D                                      2.65455295
```

Figure B.8 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for C_6H_6

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                                    SAS                                     18:16 SUNDAY, FEBRUARY 19, 1989   1

                               GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y
SOURCE              DF     SUM OF SQUARES       MEAN SQUARE      F VALUE       PR > F      R-SQUARE         C.V.
MODEL                5         0.00060958        0.00012192         6.93       0.0710      0.920329      18.4334
ERROR                3         0.00005277        0.00001759                    ROOT MSE                    Y MEAN
CORRECTED TOTAL      8         0.00066235                                    0.00419407                0.02275261

SOURCE              DF          TYPE I SS      F VALUE     PR > F        DF       TYPE III SS     F VALUE      PR > F
A                    1         0.00006166         3.51     0.1579         1        0.00000004        0.00      0.9671
B                    1         0.00052804        30.02     0.0120         1        0.00003092        1.76      0.2768
A*A                  1         0.00000010         0.01     0.9440         1        0.00000010        0.01      0.9440
B*B                  1         0.00000219         0.12     0.7473         1        0.00000219        0.12      0.7473
A*B                  1         0.00001759         1.00     0.3910         1        0.00001759        1.00      0.3910

                                        T FOR HO:    PR > |T|        STD ERROR OF
PARAMETER                  ESTIMATE    PARAMETER=0                      ESTIMATE

INTERCEPT               -0.00055455          -0.04     0.9673          0.01246193
A                       4.03550E-07           0.04     0.9671          0.00000894
B                        0.00162963           1.33     0.2768          0.00122917
A*A                     2.25167E-10           0.08     0.9440          0.00000000
B*B                    -1.04733E-05          -0.35     0.7473          0.00002966
A*B                    -2.09713E-07          -1.00     0.3910          0.00000021

OBSERVATION           OBSERVED          PREDICTED           RESIDUAL      LOWER 95% CL      UPPER 95% CL
                        VALUE              VALUE                            FOR MEAN          FOR MEAN

    1               0.01138350         0.01420626        -0.00282276        0.00222640        0.02618613
    2               0.03144410         0.02673149         0.00471261        0.01678315        0.03668063
    3               0.03527250         0.03716235        -0.00188985        0.02518228        0.04914272
    4               0.01510850         0.01287156         0.00223694        0.00292282        0.02282029
    5               0.02069200         0.02330006        -0.00260806        0.01335132        0.03324879
    6               0.03200500         0.03163369         0.00037111        0.02168515        0.04158263
    7               0.01257500         0.01198918         0.00058582        0.00000931        0.02396905
    8               0.01821600         0.02032056        -0.00210456        0.01037182        0.03025929
    9               0.02537600         0.02385726         0.00151874        0.01457740        0.03853713

          SUM OF RESIDUALS                                    0.00000000
          SUM OF SQUARED RESIDUALS                            0.00005277
          SUM OF SQUARED RESIDUALS - ERROR SS                 0.00000000
          PRESS STATISTIC                                     0.00057061
          FIRST ORDER AUTOCORRELATION                        -0.70967181
          DURBIN-WATSON D                                     3.22464178
```

Figure B.9 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for $CHBr_3$

```
                                                SAS                          18:16 SUNDAY, FEBRUARY 19, 1989    1

                                  GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE               DF       SUM OF SQUARES       MEAN SQUARE      F VALUE        PR > F        R-SQUARE         C.V.

MODEL                 5           0.04941110        0.00988222       118.84        0.0012        0.994977       4.4100

ERROR                 3           0.00024946        0.00008315                   ROOT MSE                       Y MEAN

CORRECTED TOTAL       8           0.04966057                                   0.00911857                   0.20677828

SOURCE               DF            TYPE I SS    F VALUE      PR > F        DF          TYPE III SS      F VALUE      PR > F

A                     1           0.00011104       1.34      0.3315         1           0.00024242         2.92      0.1863
B                     1           0.04871795     585.90      0.0002         1           0.00016926         2.04      0.2489
A*A                   1           0.00024388       2.93      0.1853         1           0.00024388         2.93      0.1853
B*B                   1           0.00033619       4.04      0.1379         1           0.00033619         4.04      0.1379
A*B                   1           0.00000003       0.00      0.9849         1           0.00000003         0.00      0.9849

                                          T FOR H0:      PR > |T|          STD ERROR OF
PARAMETER                 ESTIMATE       PARAMETER=0                         ESTIMATE

INTERCEPT               0.08690920              3.21       0.0490            0.02709488
A                   -3.31997E-05               -1.71       0.1863            0.00001944
B                       0.00381282              1.43       0.2489            0.00267249
A*A                  1.19427E-08                1.71       0.1853            0.00000001
B*B                     0.00012965              2.01       0.1379            0.00006449
A*B                  9.33750E-09                0.02       0.9849            0.00000046

OBSERVATION           OBSERVED           PREDICTED            RESIDUAL       LOWER 95% CL       UPPER 95% CL
                         VALUE               VALUE                              FOR MEAN           FOR MEAN

      1             0.12337450          0.12906526         -0.00569076         0.10301829         0.15511224
      2             0.20942500          0.20611772          0.00330728         0.18448688         0.22774856
      3             0.31148400          0.30910051          0.00238349         0.28305354         0.33514749
      4             0.12096650          0.11362722          0.00733926         0.09199638         0.13525806
      5             0.19224300          0.19077306          0.00146994         0.16914222         0.21240389
      6             0.28504000          0.29384922         -0.00880922         0.27221838         0.31548006
      7             0.11862600          0.12027451         -0.00164851         0.09422754         0.14632149
      8             0.19273650          0.19751372         -0.00477722         0.17588288         0.21914456
      9             0.30710900          0.30068325          0.00642574         0.27463629         0.32673024

            SUM OF RESIDUALS                                0.00000000
            SUM OF SQUARED RESIDUALS                        0.00024946
            SUM OF SQUARED RESIDUALS - ERROR SS            -0.00000000
            PRESS STATISTIC                                 0.00301816
            FIRST ORDER AUTOCORRELATION                    -0.01565565
            DURBIN-WATSON D                                 1.73597570
```

Figure B.10 - SAS General Linear Model Analysis of Henry's Law Constants Experiments for $C_6H_5CH_3$

APPENDIX C

EQUILIBRATION VESSEL AND SAMPLING SYRINGE LOSSES

The losses from the equilibration vessel were evaluated in this study by analyzing the syringe concentration change in the vessel over a 24 and 48 hour period. The 50 mL syringes were initially spiked with the VOC standard solution to give an initial concentration level of approximately 100 to 300 ug/L for each of the compounds. The concentration was determined at t = 0, 24 and 48 hours. The resulting concentrations are shown on Table C.1. The percent change in concentration was evaluated for each syringe. The overall loss ranged from 4.7 to 27.3% over the 48 hour period. Since the actual experiment lasts only 6 hours, the losses are considered to be insignificant during the experiment.

TABLE C.1 EQUILIBRATION VESSEL LOSSES

Syringe	Compound	Concentration (ug/L) t=0	 t=24	 t=48	%Change
1	CH_2=CCl_2	*	123.24	96.52	21.7
	CH_3CHCl_2	*	294.23	268.36	8.8
	$CHCl_3$	*	217.93	195.20	10.4
	$ClCH_2CH_2Cl$	*	236.08	216.85	8.1
	CH_3CCL_3	*	180.28	161.08	10.7
	CCl_4	*	253.80	205.69	18.9
	CCl_2=CHCl	*	153.24	135.93	11.3
	C_6H_6	*	114.76	105.72	7.9
	$CHBr_3$	*	**	**	**
	$C_6H_5CH_3$	*	180.97	164.84	8.9
2	CH_2=CCl_2	135.34	84.95	98.42	27.3
	CH_3CHCl_2	285.36	254.41	269.41	5.6
	$CHCl_3$	211.09	180.96	196.14	7.1
	$ClCH_2CH_2Cl$	228.14	203.07	217.34	4.7
	CH_3CCL_3	184.55	149.56	162.84	11.8
	CCl_4	258.44	190.84	206.45	20.1
	CCl_2=CHCl	159.46	123.88	135.81	14.8
	C_6H_6	111.22	95.84	104.65	5.9
	$CHBr_3$	**	**	**	**
	$C_6H_5CH_3$	182.27	151.40	165.16	9.4

* - Initial VOC concentration not available.
** - Bromoform concentration below detection limit.

The losses from the 5 and 10 mL sampling syringes were assessed previously by Lamarche, 1986. He determined that the losses ranged from 3 to 15% over the 24 hour period of the test. This was considered to be insignificant for the under 2 hour period for which the syringe are in use during the sampling.

APPENDIX D

PACKED COLUMN END EFFECTS

The packed column end effects (NNTU) were assessed by conducting mass transfer experiments for an empty column. The packing sections of the column were removed and the two end sections were connected. The end effects were evaluated for each VOC. Six end effects runs were conducted. The runs were selected randomly from the mass transfer runs set by the fractional factorial design. The NNTU/NTU for each run was determined and the average of the six runs was determined for each of the VOC and the final NTU of each of the mass transfer run was determined by

$$TNTU = NTU * \frac{NNTU}{NTU} \qquad (D.1)$$

The results are shown on Table D.1.

TABLE D.1 PACKED COLUMN END EFFECTS

Run	Temp	QL	QG	NNTU (first line)					NNTU/NTU (second line)				
	(C)	(L/min)	(L/min)	CH2-CCl2	CH3CHCl2	CHCl3	ClCH2CH2Cl	CHCCl3	CCl4	CCl2-CHCl	C6H6	CHBr3	C6H5CH3
3	21.9	2.006	75.096	0.265412	0.247724	0.236686	0.233274	0.246476	0.257417	0.248848	0.248597	0.244456	0.237019
				0.058764	0.066023	0.068032	0.094346	0.053125	0.063666	0.065592	0.068548	0.192243	0.067520
4	22.0	3.992	75.096	0.262505	0.243915	0.227329	0.172667	0.244576	0.238313	0.235112	0.239307	0.102462	0.226368
				0.058104	0.082311	0.085060	0.119790	0.090543	0.065776	0.075045	0.083554	0.142180	0.080548
13	21.9	2.995	25.185	0.285427	0.265964	0.250479	0.221683	0.269286	0.266318	0.265194	0.276806	0.214864	0.256584
				0.038045	0.073887	0.069344	*	0.069755	0.067577	0.066989	0.069351	*	0.066833
16	21.0	2.989	75.096	0.271078	0.235556	0.226534	0.199649	0.240325	0.249720	0.240107	0.230876	0.205059	0.228133
				0.066993	0.073604	0.071789	0.090396	0.152207	0.067245	0.069817	0.074786	0.165690	0.071773
17	22.0	1.999	50.620	0.234690	0.249759	0.237553	0.201097	0.231593	0.216861	0.236303	0.256886	0.148644	0.237279
				0.054578	0.069076	0.071005	0.093660	0.060336	0.057680	0.062498	0.066887	0.142189	0.063070
20	21.0	3.985	50.300	0.277539	0.236122	0.229547	0.235652	0.247971	0.254923	0.239191	0.235822	0.139583	0.230044
				0.078980	0.084157	0.083596	0.134370	0.082420	0.076461	0.079664	0.086687	0.137353	0.081811
	Average NNTU/NTU			0.063483	0.074843	0.074804	0.106512	0.071235	0.066400	0.069934	0.074968	0.155931	0.071925
	Standard Deviation			0.008751	0.006532	0.006851	0.017465	0.013761	0.005586	0.005825	0.007628	0.020673	0.007022

* - value for NTU in the mass transfer experiment not available.

APPENDIX E

PACKED COLUMN RESULTS FROM INDIVIDUAL EXPERIMENTS

The results of the individual experiments are summarized on Tables E.1 to E.4. The results for each compounds is given in the net number of transfer units according to Eq. 3.10 and the corresponding overall mass transfer coefficient (KLa). The results of the Sherwood and Holloway, Shulman et al., and Onda et al. mass transfer coefficient correlation calculations are shown on Tables E.5 to E.13.

The procedure used by Lamarche, 1986 was used to evaluate the mass transfer data. To show how the calculation were made the sample calculation for Run #1 and 1,1-Dichloroethylene are outlined below.

Mass Transfer Experiments:

Experimental Conditions:

Q_L = 1.9923 L/min
Q_G = 32.7037 L/min
T_G = 24.6 °C
T_{LI} = 21.7 °C
T_{LE} = 21.9 °C
T_{LB} = 24.2 °C
T_{CR} = 24.8 °C
PD_C = 35 mm
PD_R = 52 mm
P_B = 762.1 mm
Z = 1.829 m

C_{I1} = 9455.26 ug/L
C_{I2} = 9157.34 ug/L
C_{I3} = 9507.72 ug/L
C_{I4} = 9370.35 ug/L
C_{I5} = 9197.12 ug/L
C_{E1} = 106.64 ug/L
C_{E2} = 106.13 ug/L
C_{E3} = 100.2 ug/L
C_{E4} = 102.37 ug/L
C_{E5} = 106.47 ug/L

where C_{Li} = influent concentration
C_{Ei} = effluent concentration

Liquid Mass Flux:

$$T_L = (T_{LI} + T_{LE}) / 2$$
$$= 21.8 \ ^oC$$
$$\gamma_L = 1000 \ [1 - 1.9549 \ X \ 10^{-5} \ (T_L - 4)^{1.68}]$$
$$= 997.5349 \ kg/m^3$$
$$\gamma_M = 0.827 \ \gamma_L$$
$$= 824.4787 \ kg/m^3$$
$$L = Q_L \ \gamma_L \ / \ 0.008107$$
$$= 4.085709 \ kg/m^2/s$$

Gas Flow Rate:

$$P_{RA} = PD_R \ / \ 13.5694$$
$$= 3.832151 \ mm \ Hg$$
$$P_F = P_B + P_{RA}$$
$$= 765.9321 \ mm \ Hg$$
$$T_{CR} = 1.8 \ T_G + 32 + 460$$
$$= 536.28 \ ^oR$$
$$Q_{GC} = Q_G \ [\frac{530}{T_{CR}} \ X \ \frac{P_F}{760}]^{1/2}$$
$$= 0.000542 \ m^3/s$$
$$T_K = T_{CR} + 273.15$$
$$= 297.95 \ K$$
$$Q_G = Q_{GC} \ [\frac{760}{P_B} \ X \ \frac{T_K}{293.15}]$$
$$= 0.00055 \ m^3/s$$

Henry's Law Constant and Stripping Factor:

$$H_C = 10\text{^}[5.9144081 - 1741.485 \ / \ T_L] \ FCF$$
$$= 1.027566$$
$$S = H_C \ Q_G \ / \ Q_L$$
$$= 17.36235$$

Average VOC Concentrations:

$$C_I = \frac{\Sigma\ C_{LI}}{(n-1)} \qquad \text{and} \qquad C_E = \frac{\Sigma\ C_{LE}}{(n-1)}$$

$$= 9337.558 \text{ ug/L} \qquad\qquad = 104.362 \text{ ug/L}$$

Number of Transfer Units, Height of a Transfer Unit, and Mass Transfer Coefficient:

$$NTU = \frac{S}{(S - 1)}\ \text{Ln}\ \left[\frac{(\frac{C_I}{C_E})\ (S - 1) + 1}{S}\right]$$

$$= 4.707589$$

NNTU is used to account for the column end effects as determine in Appendix D.

$$NNTU = 0.063483\ NTU$$

$$= 0.298774$$

$$TNTU = NTU - NNTU$$

$$= 4.407589$$

$$HTU = Z\ /\ NNTU$$

$$= 0.414966$$

$$K_La = L\ /\ (\gamma_L\ HTU)$$

$$= 0.009870\ 1/s$$

Mass Transfer Correlation:

Density, Viscosity, Surface Tension, and Diffusion Coefficient:

$$\gamma_G = \frac{1.293}{1 + 0.00367\ T_{LB}}\ \frac{P_B}{760}$$

$$= 1.190811\ kg/m^3$$

$$\mu_L = [0.20319 + 1.5883\ \exp\ (\frac{-T_L^{0.9}}{22})]\ 10\text{-}3$$

$$= 0.000970\ kg/m/s$$

$$\mu_G = [1.71 + 0.005\ T_{LB}]\ 10^{-5}$$
$$= 0.000018\ \text{kg/m/s}$$
$$\phi_L = [(20987 - 92.613\ T_L)0.4348]\ 10^{-3}$$
$$= 0.072457\ \text{kg/s}^2$$
$$D_L = [\frac{13.46\ X\ 10^{-5}}{(1000\ \mu L)1.14\ (VB)0.589}]\ 10^{-4}$$
$$= 9.94\ X\ 10\text{-}10\ \text{m}^2/\text{s}$$
$$M_R = \frac{M_A + M_O}{M_A\ X\ M_O}$$
$$= 0.044834$$
$$D_G = [\frac{10^{-3}\ T_{LB}{}^{1.75}\ M_R{}^{1/2}}{(P_B\ /\ 760)\ (V_A{}^{1/3} + V_O{}^{1/3})^2}]$$
$$= 9.30\ X\ 10^{-6}\ \text{m}^2/\text{s}$$

Sherwood and Holloway, 1940:

$$Sc_L = \frac{\mu_L}{\gamma_L\ D_L}$$
$$= 977.9042$$
$$K_La = 10.764\ \alpha\ [\frac{0.3048\ L}{\mu_L}]^{1-n}\ S_{cL}{}^{0.5}$$
$$= 0.009825\ 1/\text{s}$$

Shulman et al., 1955:

$$\beta = 1.508\ d_S{}^{0.376}$$
$$= 0.336401$$
$$\phi_t = [\frac{(2.09\ X\ 10^{-6})\ \ (737.5\ L)^{\beta}}{dS^2}]$$
$$= 0.090396$$
$$\varepsilon = \varepsilon_D - \phi_t$$
$$= 0.539603$$
$$Re_{LD} = \frac{d_S\ L}{\mu_L}$$
$$= 77.91807$$

$$Re_{GD} = \frac{d_S\ G}{\mu_G}$$

$$= 81.66340$$

$$Sc_G = \frac{\mu_G}{\gamma_G\ D_G}$$

$$= 1.653832$$

$$a = d\ [\frac{808\ G}{\gamma_G^{0.5}}]^q\ L^h$$

$$= 27.73661\ m^2/m^3$$

$$k_L = 25.1\ Re_{LD}^{0.45}\ Sc_L^{0.5}\ D_L\ /\ d_S$$

$$= 0.000299\ m/s$$

$$k_G = 1.195\ (1-\varepsilon)^{0.36}\ Re_{GD}^{0.64}\ Sc_G^{0.33}\ D_G\ /\ d_S$$

$$= 0.008047\ m/s$$

$$K_La = [\frac{1}{k_La} + \frac{1}{H_C\ k_Ga}]^{-1}$$

$$= 0.008047\ 1/s$$

Onda et al., 1968:

$$Fr_L = \frac{L^2\ a_t}{\gamma_L^2\ g}$$

$$= 0.000695$$

$$Re_{LA} = \frac{L}{a_t\ \mu_L}$$

$$= 10.34837$$

$$Re_{GA} = \frac{G}{a_t\ \mu_G}$$

$$= 10.84579$$

$$We_L = \frac{L^2}{\gamma_L\ \sigma_L\ a_t}$$

$$= 0.000567$$

$$a_W = a_t\ [1 - \exp\ \{-1.45\ (\frac{\sigma_C}{\sigma_L})^{0.75} Re_{LA}^{0.1}\ Fr_L^{-0.05}\ We_L^{0.2}\ \}]$$

$$= 164.8684\ m^2/m^3$$

$$Re_{LW} = \frac{L}{a_W \, \mu_L}$$

$$= 25.54636$$

$$k_L = 0.0051 \, Re_{LW}^{2/3} \, Sc_L^{-0.5} \, (a_t \, d_P)^{0.4} \left(\frac{\gamma_L}{\mu_L \, g}\right)^{-1/3}$$

$$= 0.000057 \text{ m/s}$$

$$k_G = 5.23 \, Re_{GA}^{0.7} \, Sc_G^{1/3} \, (a_t \, d_P)^{-2} \, (a_t \, D_G)$$

$$= 0.004646 \text{ m/s}$$

$$K_La = \left[\frac{1}{k_La} + \frac{1}{H_C \, k_Ga}\right]^{-1}$$

$$= 0.009428 \text{ 1/s}$$

TABLE E.1 OBSERVED RESULTS OF MASS TRANSFER EXPERIMENTS

				TNTU (first line) KLa (1/min) (second line)									
Run	Temp (C)	QL (L/min)	QG (L/min)	CH2=CC12	CH3CHC12	CHC13	C1CH2CH2C1	CHCC13	CC14	CC12-CHC1	C6H6	CHBr3	C6H5CH3
1	21.8	1.99228	32.7037	4.407589	3.646757	3.416842	2.409009	3.740542	3.970435	3.661581	3.527566	1.346102	3.423830
				0.009870	0.008166	0.007651	0.005394	0.008376	0.008891	0.008199	0.007899	0.003014	0.007667
2	20.3	4.05568	33.5035	3.326040	2.878452	2.909370	2.011930	2.974708	3.114571	2.898666	2.802901	*	2.711124
				0.015162	0.013121	0.013262	0.009171	0.013560	0.014198	0.013214	0.012777	*	0.012359
3	20.0	1.99421	78.2951	4.229807	3.471223	3.218791	2.209174	4.331399	3.774749	3.528518	3.354725	1.073315	3.257846
				0.009481	0.007780	0.006588	0.004951	0.008263	0.008461	0.007909	0.007519	0.002405	0.007302
4	20.8	3.98229	78.2951	4.066567	2.741546	2.472547	1.287882	2.521827	3.382487	2.913844	2.649366	0.608277	2.608202
				0.018202	0.012271	0.011068	0.005764	0.011288	0.015140	0.013042	0.011859	0.002722	0.011674
5	21.0	2.90145	47.4209	3.291696	2.470006	2.301008	1.356030	2.696512	2.841978	2.705778	2.710241	0.875235	2.594170
				0.010735	0.008055	0.007504	0.004422	0.008794	0.009268	0.008824	0.008838	0.002854	0.008460
6	19.7	2.99599	48.7007	2.796047	2.332859	2.205984	1.423221	2.489631	2.698829	2.456762	2.280536	0.698105	2.298841
				0.009415	0.007856	0.007428	0.004792	0.008383	0.009088	0.008273	0.007679	0.002350	0.007741
7	21.0	2.99249	45.5013	6.111183	3.735316	3.528706	3.234511	4.014569	4.683701	4.151778	4.258304	*	4.086447
				0.020555	0.012564	0.011869	0.010879	0.013503	0.015754	0.013965	0.014323	*	0.013745
8	18.2	2.99449	57.8989	3.543356	2.801021	2.658264	1.551985	3.025826	3.486437	3.006496	2.711859	0.662246	2.804734
				0.011926	0.009427	0.008947	0.005223	0.010184	0.011734	0.010119	0.009127	0.002229	0.009440
9	20.2	2.15216	50.4603	3.371441	2.944656	2.729563	1.816240	3.027668	3.183824	2.970860	2.879288	0.850472	2.771695
				0.008155	0.007123	0.006603	0.004393	0.007324	0.007701	0.007186	0.006965	0.002057	0.006704
10	21.4	2.99349	50.3004	3.068074	2.639401	2.437579	1.391416	2.769512	2.934956	2.695661	2.577736	0.573160	2.489971
				0.010323	0.008880	0.008201	0.004681	0.009318	0.009875	0.009070	0.008673	0.001928	0.008378
11	21.8	2.02084	56.6992	4.435726	3.559359	3.265344	2.030437	3.775350	4.086479	3.622894	3.437315	0.903058	3.337200
				0.010075	0.008084	0.007417	0.004612	0.008575	0.009282	0.008229	0.007807	0.002051	0.007580
12	20.6	3.98628	56.6992	3.929135	3.069906	2.779616	1.469641	3.336730	4.135732	3.195934	2.966569	0.675956	2.899001
				0.017605	0.013755	0.012454	0.006584	0.014950	0.017136	0.014319	0.013292	0.003028	0.012989
13	21.1	2.99	32.7037	4.034908	3.330206	3.341888	**	3.604074	3.679233	3.681903	3.692140	*	3.563033
				0.013560	0.011192	0.011231	**	0.012112	0.012365	0.012374	0.012408	*	0.011974
14	21.3	2.99698	79.095	4.696376	3.376750	3.121759	2.329514	3.619616	3.625835	3.678668	3.793618	1.489148	3.713440
				0.015089	0.010401	0.009242	0.005507	0.011905	0.012155	0.011846	0.011501	0.002625	0.011280
15	18.7	2.99658	30.3041	3.239449	2.795993	2.766522	**	2.847126	3.075751	2.869440	2.740967	*	2.742972
				0.010910	0.009417	0.009317	**	0.009589	0.010359	0.009664	0.009231	*	0.009238

Table E.1 cont.

Table E.1 (cont.)

Run	Temp	QL	QG	TNTU (first line)					KLa (1/min) (second line)				
	(C)	(L/min)	(L/min)	CH2=CCl2	CH3CHCl2	CHCl3	ClCH2CH2Cl	CHCCl3	CCl4	CCl2=CHCl	C6H6	CHBr3	C6H5CH3
16	22.0	2.99399	78.2951	3.789475	2.960786	2.919507	1.973356	1.474078	3.466998	3.198565	2.855704	1.044625	2.949903
				0.012752	0.009963	0.009825	0.006640	0.004960	0.011667	0.010764	0.009610	0.003515	0.009927
17	20.7	2.08208	51.9001	3.990520	3.305720	3.080215	1.915000	3.337346	3.504927	3.483802	3.458189	0.857290	3.416944
				0.009339	0.007736	0.007208	0.004481	0.007810	0.008202	0.008153	0.008093	0.002006	0.007996
18	22.1	3.99227	55.0995	4.400831	3.323940	3.214857	2.605642	4.078635	3.599985	3.746975	3.647176	*	3.654768
				0.019748	0.014915	0.014426	0.011692	0.018302	0.016154	0.016814	0.016366	*	0.016400
19	21.5	2.01984	55.5794	3.968043	3.153939	3.079301	1.991461	3.345336	3.578289	3.382685	3.075955	1.019755	3.192314
				0.009008	0.007160	0.006991	0.004521	0.007595	0.008123	0.007679	0.006983	0.002315	0.007247
20	21.0	4.03654	55.8993	3.290924	2.595743	2.540477	1.566959	2.808827	3.112637	2.792513	2.516439	0.857771	2.609642
				0.014931	0.011777	0.011526	0.007109	0.012744	0.014122	0.012670	0.011417	0.003891	0.011840
21	20.5	2.95221	31.9038	2.492435	2.306773	2.195064	2.159090	2.290208	2.379408	2.287802	2.284350	*	2.180218
				0.008270	0.007654	0.007283	0.007164	0.007599	0.007895	0.007591	0.007580	*	0.007234
22	20.3	2.94947	71.8963	3.047110	3.287521	2.968057	1.558711	3.628580	2.653052	3.416446	3.158328	0.643080	3.093753
				0.010101	0.010899	0.009839	0.005167	0.012029	0.008795	0.011326	0.010470	0.002131	0.010256
23	19.5	2.99748	33.1836	3.854976	3.398760	3.184331	4.350448	3.420827	3.699740	3.385986	3.316235	*	3.190350
				0.012988	0.011451	0.010728	0.014657	0.011525	0.012465	0.011408	0.011173	*	0.010749
24	20.4	2.99698	78.615	3.954644	3.232187	2.975953	1.823865	3.442878	3.799146	3.309994	3.129106	0.815074	3.043720
				0.013321	0.010888	0.010025	0.006144	0.011597	0.012798	0.011150	0.010540	0.002745	0.010253
25	21.8	3.04076	55.2594	3.799607	3.174642	2.921686	1.777038	1.18967	3.409267	3.229220	3.080696	0.812417	2.992560
				0.012986	0.010850	0.009985	0.006073	0.004066	0.011652	0.011037	0.010529	0.002776	0.010228
26	22.4	2.99124	55.8993	4.094699	3.251610	3.052801	1.797665	1.877925	3.679713	3.351169	3.129611	0.801602	3.067669
				0.013767	0.010932	0.010264	0.006044	0.006314	0.012372	0.011267	0.010522	0.002695	0.010314
27	18.4	2.99074	55.8993	3.597153	2.893597	2.687051	1.416197	1.951158	3.178156	2.998544	2.815076	0.611009	2.740452
				0.012092	0.009727	0.009032	0.004760	0.006559	0.010683	0.010080	0.009463	0.002054	0.009212

* Could not be calculated because a negative logarithmic argument resulted in Eq. 2.58.

** Effluent concentration below GC detection limit.

TABLE E.2 SHERWOOD AND HOLLOWAY CORRELATION CALCULATIONS

Run	Temp	QL	QG	KLa (1/min)									
	(C)	(L/min)	(L/min)	CH2=CCl2	CH3CHCl2	CHCl3	ClCH2CH2Cl	CHCCl3	CCl4	CCl2=CHCl	C6H6	CHBr3	C6H5CH3
1	21.8	1.99228	32.7037	0.009825	0.009590	0.009629	0.009590	0.009037	0.009068	0.009217	0.009519	0.009419	0.008953
2	20.3	4.05568	33.5035	0.015185	0.014821	0.014883	0.014821	0.013967	0.014014	0.014245	0.014711	0.014557	0.013837
3	20.0	1.99421	78.2951	0.009531	0.009303	0.009341	0.009303	0.008766	0.008796	0.008941	0.009233	0.009137	0.008685
4	20.8	3.98229	78.2951	0.015137	0.014774	0.014835	0.014774	0.013923	0.013969	0.014199	0.014664	0.014510	0.013793
5	21.0	2.90145	47.4209					*					
6	19.7	2.99599	48.7007					*					
7	21.0	2.99249	45.5013					**					
8	18.2	2.99449	57.8989					**					
9	20.2	2.15216	50.4603					*					
10	21.4	2.99349	50.3004					*					
11	21.8	2.02084	56.6992					**					
12	20.6	3.98628	56.6992					**					
13	21.1	2.99	32.7037	0.012640	0.012337	0.012388	0.012337	0.011626	0.011665	0.011857	0.012246	0.012117	0.011518
14	21.3	2.99698	79.0950	0.012703	0.012398	0.012450	0.012398	0.011684	0.011723	0.011916	0.012306	0.012177	0.011575
15	18.7	2.99658	30.3041	0.012128	0.011838	0.011887	0.011838	0.011155	0.011193	0.011377	0.011750	0.011626	0.011051
16	22.0	2.99399	78.2951	0.012837	0.012529	0.012581	0.012529	0.011807	0.011847	0.012042	0.012436	0.012305	0.011697
17	20.7	2.08208	51.9001	0.009922	0.009684	0.009724	0.009684	0.009126	0.009157	0.009307	0.009612	0.009511	0.009041
18	22.1	3.99227	55.0995	0.015503	0.015132	0.015194	0.015132	0.014260	0.014308	0.014543	0.015019	0.014862	0.014177
19	21.5	2.01984	55.5794	0.009854	0.009618	0.009658	0.009618	0.009064	0.009094	0.009244	0.009547	0.009447	0.008979
20	21.0	4.03654	55.8993	0.015323	0.014956	0.015018	0.014956	0.014094	0.014142	0.014374	0.014845	0.014689	0.013963
21	20.5	2.95221	31.9038					*					
22	20.3	2.94947	71.8963					*					
23	19.5	2.99748	33.1836					**					
24	20.4	2.99698	78.6150					**					
25	21.8	3.04076	55.2594	0.012922	0.012613	0.012665	0.012613	0.011886	0.011926	0.012122	0.012519	0.012388	0.011775
26	22.4	2.99124	55.8993	0.012916	0.012607	0.012659	0.012607	0.011880	0.011920	0.012116	0.012513	0.012382	0.011770
27	18.4	2.99074	55.8993	0.012274	0.011980	0.012030	0.011980	0.011290	0.011328	0.011514	0.011891	0.011766	0.011184

* - Model not applicable to 6.4 mm Raschig rings.

** - Model not applicable to 12.8 mm Intalox saddles.

TABLE E.3 SHULMAN ET AL. CORRELATION CALCULATIONS

Run	Temp	QL	QG	KLa (1/min)									
	(C)	(L/min)	(L/min)	CH2=CCl2	CH3CHCl2	CHCl3	ClCH2CH2Cl	CHCCl3	CCl4	CCl2=CHCl	C6H6	CHBr3	C6H5CH3
1	21.8	1.99228	32.7037	0.008047	0.006947	0.006599	0.004776	0.007266	0.007458	0.007043	0.006873	0.003239	0.006507
2	20.3	4.05568	33.5035	0.012112	0.010029	0.009349	0.006254	0.010848	0.011239	0.010339	0.009917	0.004032	0.009402
3	20.0	1.99421	78.2951	0.009443	0.008539	0.008263	0.006602	0.008582	0.008735	0.008485	0.008460	0.004935	0.007988
4	20.8	3.98229	78.2951	0.015047	0.013377	0.012877	0.009864	0.013666	0.013935	0.013400	0.013234	0.006940	0.012513
5	21.0	2.90145	47.4209					*					
6	19.7	2.99599	48.7007					*					
7	21.0	7.99249	45.5013					**					
8	18.2	2.99449	57.8989					**					
9	20.2	2.15216	50.4603					*					
10	21.4	2.99349	50.3004					*					
11	21.8	2.02084	56.6992					**					
12	20.6	3.98628	56.6992					**					
13	21.1	2.99	32.7037	0.010115	0.008481	0.007837	0.005423	0.008979	0.009291	0.008708	0.008394	0.003920	0.007981
14	21.3	2.99698	79.0950	0.012441	0.011105	0.010594	0.008273	0.011212	0.011451	0.011104	0.011003	0.006492	0.010418
15	18.7	2.99658	30.3041	0.009477	0.007867	0.007248	0.004584	0.008437	0.008786	0.008130	0.007768	0.002909	0.007396
16	22.0	2.99399	78.2951	0.012411	0.011121	0.010662	0.008028	0.011228	0.011487	0.011130	0.011009	0.005745	0.010441
17	20.7	2.08208	51.9001	0.009034	0.007967	0.007550	0.005751	0.008117	0.008310	0.008005	0.007893	0.004409	0.007476
18	22.1	3.99227	55.0995	0.014091	0.012168	0.011415	0.008318	0.012603	0.012961	0.012347	0.012049	0.006270	0.011439
19	21.5	2.01984	55.5794	0.009025	0.008042	0.007686	0.005702	0.008155	0.008353	0.008067	0.007959	0.004033	0.007551
20	21.0	4.03654	55.8993	0.013942	0.012066	0.011362	0.007855	0.012523	0.012917	0.012263	0.011931	0.005268	0.011344
21	20.5	2.95221	31.9038					*					
22	20.3	2.94947	71.8963					*					
23	19.5	2.99748	33.1836					**					
24	20.4	2.99698	78.6150					**					
25	21.8	3.04076	55.2594	0.011529	0.010120	0.009680	0.007247	0.010438	0.010679	0.010188	0.010016	0.005059	0.009475
26	22.4	2.99124	55.8993	0.011530	0.010150	0.009726	0.007332	0.010446	0.010680	0.010208	0.010046	0.005135	0.009503
27	18.4	2.99074	55.8993	0.011109	0.009757	0.009337	0.006943	0.010064	0.010291	0.009820	0.009649	0.004766	0.009127

* - Model not applicable to 6.4 mm Raschig rings.

** - Model not applicable to 12.8 mm Intalox saddles.

TABLE E.4 ONDA ET AL. CORRELATION CALCULATIONS

Run	Temp	QL	QG					KLa (1/min)					
	(C)	(L/min)	(L/min)	CH2=CCl2	CH3CHCl2	CHCl3	ClCH2CH2Cl	CHCCl3	CCl4	CCl2=CHCl	C6H6	CHBr3	C6H5CH3
1	21.8	1.99228	32.7037	0.009249	0.008006	0.007614	0.005540	0.008355	0.008572	0.008108	0.007921	0.003775	0.007499
2	20.3	4.05568	33.5035	0.014908	0.012382	0.011557	0.007771	0.013360	0.013831	0.012749	0.012244	0.005030	0.011608
3	20.0	1.99421	78.2951	0.008817	0.008033	0.007801	0.006349	0.008023	0.008154	0.007957	0.007961	0.004835	0.007514
4	20.8	3.98229	78.2951	0.015279	0.013656	0.013176	0.010218	0.013887	0.014147	0.013649	0.013513	0.007275	0.012774
5	21.0	2.90145	47.4209	0.013950	0.012795	0.012388	0.010310	0.012652	0.012851	0.012643	0.012685	0.008481	0.011986
6	19.7	2.99599	48.7007	0.013566	0.012461	0.012090	0.009733	0.012332	0.012541	0.012320	0.012344	0.007417	0.011671
7	21.0	2.99249	45.5013	0.016029	0.012514	0.011187	0.006951	0.013971	0.014686	0.013225	0.012372	0.004726	0.011814
8	18.2	2.99449	57.8989	0.014358	0.011611	0.010563	0.006367	0.012711	0.013319	0.012129	0.011455	0.003931	0.010922
9	20.2	2.15216	50.4603	0.011103	0.010301	0.010093	0.008614	0.010136	0.010264	0.010125	0.010210	0.006869	0.009630
10	21.4	2.99349	50.3004	0.014394	0.013251	0.012940	0.010823	0.013125	0.013310	0.013070	0.013132	0.008435	0.012391
11	21.8	2.02084	56.6992	0.012160	0.010136	0.009493	0.006437	0.010919	0.011286	0.010428	0.010019	0.004150	0.009502
12	20.6	3.98628	56.6992	0.019351	0.015312	0.014033	0.008742	0.017202	0.017988	0.016078	0.015124	0.005365	0.014372
13	21.1	2.99	32.7037	0.012400	0.010425	0.009646	0.006706	0.011015	0.011392	0.010692	0.010319	0.004862	0.009810
14	21.3	2.99698	79.0950	0.012758	0.012046	0.011859	0.010657	0.011648	0.011763	0.011752	0.011949	0.009398	0.011267
15	18.7	2.99658	30.3041	0.011501	0.010540	0.010209	0.008156	0.010450	0.010631	0.010428	0.010440	0.006178	0.009868
16	22.0	2.99399	78.2951	0.012999	0.012286	0.012115	0.010694	0.011884	0.012009	0.011992	0.012182	0.008950	0.011495
17	20.7	2.08208	51.9001	0.009448	0.008880	0.008717	0.007736	0.008616	0.008709	0.008679	0.008808	0.006724	0.008307
18	22.1	3.99227	55.0995	0.016243	0.015105	0.014742	0.012696	0.014781	0.014972	0.014839	0.014978	0.010819	0.014142
19	21.5	2.01984	55.5794	0.009448	0.008912	0.008777	0.007693	0.008634	0.008729	0.008706	0.008836	0.006389	0.008338
20	21.0	4.03654	55.8993	0.015710	0.014631	0.014308	0.012027	0.014321	0.014519	0.014378	0.014500	0.009551	0.013699
21	20.5	2.95221	31.9038	0.013924	0.013170	0.013021	0.011729	0.012746	0.012863	0.012835	0.013062	0.009993	0.012306
22	20.3	2.94947	71.8963	0.013744	0.012820	0.012589	0.010896	0.012554	0.012702	0.012570	0.012711	0.008856	0.011984
23	19.5	2.99748	33.1836	0.014716	0.011076	0.009947	0.005779	0.012942	0.013699	0.011851	0.010934	0.003431	0.010406
24	20.4	2.99698	78.6150	0.015711	0.013154	0.012319	0.008401	0.014101	0.014573	0.013500	0.013008	0.005488	0.012329
25	21.8	3.04076	55.2594	0.013035	0.012211	0.012022	0.010541	0.011918	0.012046	0.011952	0.012106	0.008657	0.011413
26	22.4	2.99124	55.8993	0.013142	0.012321	0.012138	0.010671	0.012019	0.012145	0.012057	0.012215	0.008777	0.011516
27	18.4	2.99074	55.8993	0.011870	0.011142	0.010981	0.009648	0.010859	0.010969	0.010896	0.011044	0.007895	0.010410

TABLE E.5 PREDICTED LOG (K_La) VS EXPERIMENTAL LOG (K_La)
SHERWOOD AND HOLLOWAY MODEL
6.4 mm RASCHIG RINGS

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
CH_2=CCl_2 CH_3CHCl_2 $CHCl_3$ $ClCH_2CH_2Cl$ CH_3CCl_3 CCl_4 CCl_2=CHCl C_6H_6 $CHBr_3$ $C_6H_5CH_3$	(Model not applicable to this packing)		

TABLE E.6 PREDICTED LOG (K_La) VS EXPERIMENTAL LOG (K_La)
SHULMAN ET AL. MODEL - 6.4 mm RASCHIG RINGS

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
CH_2=CCl_2 CH_3CHCl_2 $CHCl_3$ $ClCH_2CH_2Cl$ CH_3CCl_3 CCl_4 CCl_2=CHCl C_6H_6 $CHBr_3$ $C_6H_5CH_3$	(Model not applicable to this packing)		

TABLE E.7 PREDICTED LOG (K_La) VS EXPERIMENTAL LOG (K_La)
ONDA ET AL. MODEL - 6.4 mm RASCHIG RINGS

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
CH_2=CCl_2	$-0.8101 + 0.5249 *$ Log $(K_La)_{obs}$	0.422	18.8
CH_3CHCl_2	$-1.2444 + 0.3181 *$ Log $(K_La)_{obs}$	0.256	21.9
$CHCl_3$	$-1.0709 + 0.4002 *$ Log $(K_La)_{obs}$	0.331	24.3
$ClCH_2CH_2Cl$	$-3.0623 - 0.4499 *$ Log $(K_La)_{obs}$	0.862	39.5
CH_3CCl_3	$-1.3917 + 0.2536 *$ Log $(K_La)_{obs}$	0.232	18.7
CCl_4	$-1.5598 + 0.1718 *$ Log $(K_La)_{obs}$	0.173	16.8
CCl_2=CHCl	$-1.2778 + 0.3076 *$ Log $(K_La)_{obs}$	0.245	19.2
C_6H_6	$-1.1283 + 0.3754 *$ Log $(K_La)_{obs}$	0.331	21.6
$CHBr_3$	$-1.7996 + 0.1127 *$ Log $(K_La)_{obs}$	0.026	71.3
$C_6H_5CH_3$	$-1.1745 + 0.3631 *$ Log $(K_La)_{obs}$	0.322	20.1

* No significant correlation ($R^2 < 0.1$)

TABLE E.8 PREDICTED LOG (K_La) VS EXPERIMENTAL LOG (K_La)
SHERWOOD AND HOLLOWAY MODEL
12.8 mm RASCHIG RINGS

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
$CH_2=CCl_2$	-0.8281 + 0.5716 * Log $(K_La)_{obs}$	0.814	5.7
CH_3CHCl_2	-0.3803 + 0.7718 * Log $(K_La)_{obs}$	0.905	8.2
$CHCl_3$	-0.4349 + 0.7359 * Log $(K_La)_{obs}$	0.900	10.6
$ClCH_2CH_2Cl$	-0.8002 + 0.5036 * Log $(K_La)_{obs}$	0.585	33.4
CH_3CCl_3	-1.6215 + 0.1570 * Log $(K_La)_{obs}$	0.138	18.9
CCl_4	-0.4925 + 0.7451 * Log $(K_La)_{obs}$	0.955	2.6
$CCl_2=CHCl$	-0.5407 + 0,7079 * Log $(K_La)_{obs}$	0.882	4.7
C_6H_6	-0.6425 + 0.6421 * Log $(K_La)_{obs}$	0.772	8.3
$CHBr_3$	-0.7408 + 0.4666 * Log $(K_La)_{obs}$	0.301	70.1
$C_6H_5CH_3$	-0.6259 + 0.6624 * Log $(K_La)_{obs}$	0.807	6.2

TABLE E.9 PREDICTED LOG (KLa) VS EXPERIMENTAL LOG (KLa)
SHULMAN ET AL. MODEL - 12.8 mm RASCHIG RINGS

Compound	Log (KLa)pred vs Log (KLa)obs	R^2	SEE%
$CH_2=CCl_2$	-0.7913 + 0.6166 * Log $(K_La)_{obs}$	0.794	8.7
CH_3CHCl_2	-0.6186 + 0.7010 * Log $(K_La)_{obs}$	0.599	3.8
$CHCl_3$	-0.8446 + 0.5929 * Log $(K_La)_{obs}$	0.451	4.9
$ClCH_2CH_2Cl$	-1.5817 + 0.2578 * Log $(K_La)_{obs}$	0.137	11.6
CH_3CCl_3	-1.7504 + 0.1219 * Log $(K_La)_{obs}$	0.069	16.7
CCl_4	-0.5343 + 0.7480 * Log $(K_La)_{obs}$	0.808	5.4
$CCl_2=CHCl$	-0.6682 + 0.6814 * Log $(K_La)_{obs}$	0.671	5.4
C_6H_6	-0.8652 + 0.5797 * Log $(K_La)_{obs}$	0.505	5.4
$CHBr_3$	-1.7547 + 0.2127 * Log $(K_La)_{obs}$	0.042	30.7
$C_6H_5CH_3$	-0.8163 + 0.6146 * Log $(K_La)_{obs}$	0.559	6.5

TABLE E.10 PREDICTED LOG(K_La) VS EXPERIMENTAL LOG(K_La)
ONDA ET AL. MODEL - 12.8 mm RASCHIG RINGS

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
$CH_2=CCl_2$	-0.6190 + 0.6860 * Log $(K_La)_{obs}$	0.838	4.8
CH_3CHCl_2	-0.2247 + 0.8679 * Log $(K_La)_{obs}$	0.806	4.2
$CHCl_3$	-0.3857 + 0.7855 * Log $(K_La)_{obs}$	0.696	5.4
$ClCH_2CH_2Cl$	-1.0796 + 0.4327 * Log $(K_La)_{obs}$	0.231	20.8
CH_3CCl_3	-1.6278 + 0.1597 * Log $(K_La)_{obs}$	0.103	18.0
CCl_4	-0.2326 + 0.8820 * Log $(K_La)_{obs}$	0.957	1.3
$CCl_2=CHCl$	-0.3320 + 0.8255 * Log $(K_La)_{obs}$	0.859	2.1
C_6H_6	-0.5122 + 0.7259 * Log $(K_La)_{obs}$	0.694	4.6
$CHBr_3$	-1.2365 + 0.3520 * Log $(K_La)_{obs}$	0.059	48.0
$C_6H_5CH_3$	-0.4542 + 0.7658 * Log $(K_La)_{obs}$	0.761	2.8

* No significant correlation ($R^2 < 0.1$)

TABLE E.11 PREDICTED LOG(K_La) VS EXPERIMENTAL LOG(K_La)
SHERWOOD AND HOLLOWAY MODEL
12.8 mm INTALOX SADDLES

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
$CH_2=CCl_2$	(Model not applicable to this packing)		
CH_3CHCl_2			
$CHCl_3$			
$ClCH_2CH_2Cl$			
CH_3CCl_3			
CCl_4			
$CCl_2=CHCl$			
C_6H_6			
$CHBr_3$			
$C_6H_5CH_3$			

TABLE E.12 PREDICTED LOG(K_La) VS EXPERIMENTAL LOG(K_La)
SHULMAN ET AL. MODEL
12.8 mm INTALOX SADDLES

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
$CH_2=CCl_2$	(Model not applicable to this packing)		
CH_3CHCl_2			
$CHCl_3$			
$ClCH_2CH_2Cl$			
CH_3CCl_3			
CCl_4			
$CCl_2=CHCl$			
C_6H_6			
$CHBr_3$			
$C_6H_5CH_3$			

TABLE E.13 PREDICTED LOG(K_La) VS EXPERIMENTAL LOG(K_La)
ONDA ET AL. MODEL - 12.8 mm INTALOX SADDLES

Compound	Log $(K_La)_{pred}$ vs Log $(K_La)_{obs}$	R^2	SEE%
$CH_2=CCl_2$	-0.9220 + 0.4650 * Log $(K_La)_{obs}$	0.636	8.2
CH_3CHCl_2	-0.7148 + 0.6105 * Log $(K_La)_{obs}$	0.670	7.0
$CHCl_3$	-0.8949 + 0.5298 * Log $(K_La)_{obs}$	0.492	6.9
$ClCH_2CH_2Cl$	-2.0135 + 0.0357 * Log $(K_La)_{obs}$	0.002	19.0
CH_3CCl_3	-0.4922 + 0.7106 * Log $(K_La)_{obs}$	0.880	8.8
CCl_4	-0.7029 + 0.6094 * Log $(K_La)_{obs}$	0.925	6.1
$CCl_2=CHCl$	-0.7074 + 0.6100 * Log $(K_La)_{obs}$	0.746	7.5
C_6H_6	-1.0215 + 0.4566 * Log $(K_La)_{obs}$	0.516	8.3
$CHBr_3$	-0.0646 + 0.8695 * Log $(K_La)_{obs}$	0.830	39.1
$C_6H_5CH_3$	-0.9489 + 0.5023 * Log $(K_La)_{obs}$	0.571	6.8

* No significant correlation ($R^2 < 0.1$)

TABLE E.14 REGRESSION OF $LOG_{10}(K_La)$ VS $LOG_{10}(C)$

Compound	$Log_{10}(K_La) = A + B\ Log_{10}(C)$	R^2
$CH_2=CCl_2$	$-1.34175 - 0.18298\ Log_{10}(C)$	0.198
CH_3CHCl_2	$-1.79315 - 0.06977\ Log_{10}(C)$	0.058
$CHCl_3$	$-1.82771 - 0.06679\ Log_{10}(C)$	0.051
$ClCH_2CH_2Cl$	$-1.82302 - 0.12766\ Log_{10}(C)$	0.074
CH_3CCl_3	$-1.52409 - 0.16486\ Log_{10}(C)$	0.129
CCl_4	$-1.79173 - 0.05155\ Log_{10}(C)$	0.024
$CCl_2=CHCl$	$-1.69538 - 0.09554\ Log_{10}(C)$	0.095
C_6H_6	$-1.58069 - 0.14005\ Log_{10}(C)$	0.198
$CHBr_3$	$-2.36815 - 0.06986\ Log_{10}(C)$	0.034
$C_6H_5CH_3$	$-1.63698 - 0.12386\ Log_{10}(C)$	0.155

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                                                   SAS                               18:25 SUNDAY, FEBRUARY 19, 1989     1

                                         GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                  DF          SUM OF SQUARES         MEAN SQUARE      F VALUE           PR > F        R-SQUARE          C.V.

MODEL                   14              0.00029476          0.00002105        16.07           0.0001        0.949370        9.0597

ERROR                   12              0.00001572          0.00000131                      ROOT MSE                        Y MEAN

CORRECTED TOTAL         26              0.00031048                                        0.00114454                    0.01263330

SOURCE                  DF                TYPE I SS      F VALUE      PR > F       DF        TYPE III SS      F VALUE      PR > F

A                        1               0.00016480       125.30      0.0001        1         0.00000000         0.00      0.9773
B                        1               0.00000690         5.26      0.0405        1         0.00000055         0.43      0.5239
C                        1               0.00003884        29.65      0.0001        1         0.00000865         6.60      0.0246
D                        1               0.00004763        35.40      0.0001        1         0.00000675         5.15      0.0424
A*A                      1               0.00000055         0.42      0.5295        1         0.00000001         0.01      0.9265
B*B                      1               0.00000011         0.08      0.7757        1         0.00000026         0.20      0.6630
C*C                      1               0.00000600         4.58      0.0536        1         0.00000311         2.37      0.1475
D*D                      1               0.00000306         2.34      0.1519        1         0.00000323         2.47      0.1422
A*B                      1               0.00000319         2.44      0.1440        1         0.00000356         2.71      0.1254
A*C                      1               0.00000605         4.52      0.0527        1         0.00000565         4.31      0.0600
A*D                      1               0.00000029         0.22      0.6478        1         0.00000039         0.29      0.5989
B*C                      1               0.00000002         0.01      0.9121        1         0.00000010         0.08      0.7779
B*D                      1               0.00000379         2.89      0.1146        1         0.00000165         1.26      0.2831
C*D                      1               0.00001269         9.68      0.0090        1         0.00001269         9.68      0.0090

                                              T FOR H0:        PR > |T|          STD ERROR OF
PARAMETER                   ESTIMATE         PARAMETER=0                           ESTIMATE

INTERCEPT                -0.05897570               -2.15          0.0527           0.02740300
A                         0.00014663                0.03          0.9773           0.00554685
B                         0.00013525                0.66          0.5239           0.00020601
C                        1.10901E-05                2.57          0.0246           0.00000432
D                         0.15704535                2.27          0.0424           0.06916921
A*A                      4.72213E-05                0.09          0.9265           0.00052541
B*B                     -4.27504E-07               -0.45          0.6630           0.00000096
C*C                      7.34275E-12                1.54          0.1475           0.00000000
D*D                      -0.08532733               -1.57          0.1422           0.05413025
A*B                      4.11537E-05                1.65          0.1254           0.00002479
A*C                     -1.23472E-06               -2.09          0.0600           0.00000058
A*D                       0.00393507                0.54          0.5989           0.00730195
B*C                      5.51236E-09                0.29          0.7779           0.00000002
B*D                      -0.00029555               -1.12          0.2831           0.00026302
C*D                     -1.81097E-05               -3.11          0.0090           0.00000582

OBSERVATION          OBSERVED          PREDICTED            RESIDUAL       LOWER 95% CL      UPPER 95% CL
                        VALUE             VALUE                              FOR MEAN          FOR MEAN

     1             0.00987200        0.00917262          0.00069936        0.00726062        0.01108461
     2             0.01526200        0.01494577          0.00031623        0.01295357        0.01693797
     3             0.00918100        0.00853329          0.00064771        0.00684524        0.01022134
     4             0.01800300        0.01768389          0.00031911        0.01588927        0.01947851
```

Figure E.1 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $CH_2=CCl_2$

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                                              SAS                        18:25 SUNDAY, FEBRUARY 19, 1989    2
                                  GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION        OBSERVED         PREDICTED          RESIDUAL       LOWER 95% CL     UPPER 95% CL
                     VALUE            VALUE                             FOR MEAN         FOR MEAN

      5          0.01073500       0.01011932        0.00061568       0.00826922       0.01196942
      6          0.00941500       0.01040605       -0.00099105       0.00852748       0.01228463
      7          0.02056500       0.01859257        0.00197243       0.01659621       0.02056893
      8          0.01192600       0.01128413        0.00064187       0.00931438       0.01325389
      9          0.01209200       0.01280997       -0.00071797       0.01141349       0.01420625
     10          0.00815500       0.00732563        0.00082937       0.00563952       0.00901173
     11          0.01032300       0.00985173        0.00047127       0.00864354       0.01105993
     12          0.01007500       0.01022440       -0.00014940       0.00807119       0.01237762
     13          0.01760500       0.01833398       -0.00072898       0.01629924       0.02036872
     14          0.01356000       0.01437372       -0.00081372       0.01261613       0.01614131
     15          0.01582000       0.01562383        0.00019617       0.01359723       0.01765044
     16          0.01091000       0.01061992        0.00029008       0.00867311       0.01256673
     17          0.01275200       0.01258026        0.00017174       0.01060645       0.01455407
     18          0.01298600       0.01298695       -0.00000095       0.01158951       0.01438439
     19          0.00933900       0.01087830       -0.00153930       0.00900646       0.01275014
     20          0.01974800       0.02013504       -0.00038704       0.01812582       0.02214425
     21          0.00900800       0.00956978       -0.00056178       0.00765289       0.01148667
     22          0.01493100       0.01451646        0.00041454       0.01250618       0.01652674
     23          0.00827000       0.00842811       -0.00015811       0.00671653       0.01013969
     24          0.01010100       0.01086816       -0.00076716       0.00907442       0.01266191
     25          0.01298800       0.01404763       -0.00105963       0.01211875       0.01597652
     26          0.01332100       0.01399728       -0.00067628       0.01199904       0.01599552
     27          0.01376700       0.01279530        0.00097170       0.01139908       0.01419153

          SUM OF RESIDUALS                              0.00000000
          SUM OF SQUARED RESIDUALS                      0.00001572
          SUM OF SQUARED RESIDUALS - ERROR SS           0.00000000
          PRESS STATISTIC                               0.00009150
          FIRST ORDER AUTOCORRELATION                   0.06074306
          DURBIN-WATSON D                               1.78733262
```

Figure E.1 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $CH_2=CCl_2$ (cont.)

```
                                                        SAS                                   18:25 SUNDAY, FEBRUARY 19, 1989    1

                                          GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y
SOURCE                 DF      SUM OF SQUARES      MEAN SQUARE      F VALUE        PR > F       R-SQUARE          C.V.

MODEL                  14          0.00011063       0.00000790        18.41        0.0001       0.955520        6.4417

ERROR                  12          0.00000515       0.00000043                   ROOT MSE                       Y MEAN

CORRECTED TOTAL        26          0.00011577                                  0.00065509                   0.01016952


SOURCE                 DF           TYPE I SS      F VALUE      PR > F      DF       TYPE III SS      F VALUE      PR > F

A                       1          0.00008274       192.40      0.0001       1        0.00000041         0.96      0.3465
B                       1          0.00000060         1.40      0.2592       1        0.00000214         5.00      0.0452
C                       1          0.00000686        15.98      0.0018       1        0.00000394         9.17      0.0105
D                       1          0.00000966        22.51      0.0005       1        0.00000182         4.23      0.0621
A*A                     1          0.00000001         0.01      0.9132       1        0.00000009         0.22      0.6504
B*B                     1          0.00000004         0.09      0.7716       1        0.00000000         0.00      0.9915
C*C                     1          0.00000000         0.01      0.9376       1        0.00000004         0.10      0.7557
D*D                     1          0.00000109         2.54      0.1366       1        0.00000061         1.42      0.2566
A*B                     1          0.00000006         0.13      0.7264       1        0.00000002         0.05      0.8207
A*C                     1          0.00000222         5.17      0.0421       1        0.00000206         4.80      0.0490
A*D                     1          0.00000012         0.27      0.6139       1        0.00000014         0.33      0.5753
B*C                     1          0.00000001         0.03      0.8752       1        0.00000000         0.00      0.9648
B*D                     1          0.00000405         9.43      0.0097       1        0.00000277         6.46      0.0259
C*D                     1          0.00000318         7.42      0.0185       1        0.00000319         7.42      0.0185


                                          T FOR H0:      PR > |T|        STD ERROR OF
PARAMETER                  ESTIMATE     PARAMETER=0                         ESTIMATE

INTERCEPT               -0.03864959           -2.42        0.0322          0.01597055
A                        0.00311105            0.98        0.3465          0.00317479
B                        0.00026355            2.24        0.0452          0.00011791
C                       7.48134E-06            3.03        0.0105          0.00000247
D                        0.08142477            2.06        0.0621          0.03958966
A*A                     -0.00013976           -0.46        0.6504          0.00030072
B*B                    -5.94449E-09           -0.01        0.9915          0.00000055
C*C                    -8.69750E-11           -0.32        0.7557          0.00000000
D*D                     -0.03690298           -1.19        0.2566          0.03098197
A*B                    -3.31354E-06           -0.23        0.8207          0.00001430
A*C                    -7.29736E-07           -2.19        0.0490          0.00000033
A*D                      0.00240725            0.58        0.5753          0.00417934
B*C                    -6.13356E-10           -0.05        0.9648          0.00000001
B*D                     -0.00038259           -2.54        0.0259          0.00015054
C*D                    -9.07371E-06           -2.72        0.0185          0.00000333

                           OBSERVED         PREDICTED                          LOWER 95% CL        UPPER 95% CL
OBSERVATION                   VALUE             VALUE          RESIDUAL            FOR MEAN            FOR MEAN

          1              0.00816600        0.00737507        0.00079093          0.00628072          0.00846942
          2              0.01312100        0.01300344        0.00011756          0.01186319          0.01414370
          3              0.00778000        0.00803851       -0.00025851          0.00690133          0.00917569
          4              0.01227100        0.01314808       -0.00087708          0.01200644          0.01428972
```

Figure E.2 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CH_3CHCl_2

```
                                              SAS                       18:25 SUNDAY, FEBRUARY 19, 1989   2
                               GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y
                                   PREDICTED                          LOWER 95% CL      UPPER 95% CL
OBSERVATION      OBSERVED VALUE    VALUE            RESIDUAL          FOR MEAN          FOR MEAN

       5          0.00805500       0.00849156      -0.00043656        0.00743264        0.00955049
       6          0.00941500       0.00913895       0.00027605        0.00806373        0.01021417
       7          0.01256400       0.01294864      -0.00038464        0.01181172        0.01408555
       8          0.00942700       0.00922701       0.00019999        0.00809960        0.01035442
       9          0.00712300       0.00700758       0.00011542        0.00604252        0.00797264
      10          0.00888000       0.00915241      -0.00027241        0.00846083        0.00984393
      11          0.00808400       0.00805503       0.00002897        0.00682262        0.00928744
      12          0.01375500       0.01378680      -0.00003180        0.01262220        0.01495141
      13          0.01119200       0.01081622       0.00037578        0.00980739        0.01182506
      14          0.01137500       0.01138272      -0.00000772        0.01022277        0.01254266
      15          0.00941700       0.00947974      -0.00006274        0.00836547        0.01059402
      16          0.00996300       0.00998088      -0.00001788        0.00885115        0.01111061
      17          0.00773600       0.00784228      -0.00010628        0.00677092        0.00891364
      18          0.01491500       0.01435300       0.00056200        0.01320301        0.01550300
      19          0.00716000       0.00773387      -0.00057387        0.00663672        0.00883102
      20          0.01177700       0.01160522       0.00017178        0.01045461        0.01275582
      21          0.00765400       0.00820556      -0.00055156        0.00722592        0.00918520
      22          0.01089200       0.01002294       0.00086906        0.00900327        0.01105660
      23          0.01145100       0.01179623      -0.00034523        0.01069221        0.01290025
      24          0.01088800       0.01035529       0.00053271        0.00921158        0.01149900
      25          0.01085000       0.01063092       0.00021908        0.00983108        0.01143076
      26          0.01093200       0.01049314       0.00043886        0.00969399        0.01129228
      27          0.00972700       0.01049861      -0.00077161        0.00969938        0.01129784

               SUM OF RESIDUALS                                0.00000000
               SUM OF SQUARED RESIDUALS                        0.00000515
               SUM OF SQUARED RESIDUALS - ERROR SS             0.00000000
               PRESS STATISTIC                                 0.00002764
               FIRST ORDER AUTOCORRELATION                    -0.25716143
               DURBIN-WATSON D                                 2.27723106
```

Figure E.2 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CH_3CHCl_2 (cont.)

```
                                                   SAS                                     18:25 SUNDAY, FEBRUARY 19, 1989    1

                                      GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y
SOURCE                 DF       SUM OF SQUARES      MEAN SQUARE      F VALUE         PR > F      R-SQUARE          C.V.

MODEL                  14           0.00011060       0.00000790        13.22         0.0001      0.939109        8.1156

ERROR                  12           0.00000717       0.00000060                    ROOT MSE                      Y MEAN

CORRECTED TOTAL        26           0.00011777                                   0.00077305                  0.00952548

SOURCE                 DF          TYPE I SS     F VALUE      PR > F      DF       TYPE III SS      F VALUE      PR > F

A                       1         0.00008243      137.93      0.0001       1        0.00000071         1.20      0.2958
B                       1         0.00000004        0.06      0.8096       1        0.00000124         2.08      0.1746
C                       1         0.00000665       11.13      0.0059       1        0.00000118         1.97      0.1859
D                       1         0.00001065       17.82      0.0012       1        0.00000386         6.46      0.0259
A*A                     1         0.00000008        0.14      0.7147       1        0.00000006         0.10      0.7569
B*B                     1         0.00000039        0.65      0.4365       1        0.00000010         0.16      0.6954
C*C                     1         0.00000049        0.82      0.3936       1        0.00000002         0.03      0.8576
D*D                     1         0.00000297        4.97      0.0456       1        0.00000210         3.52      0.0852
A*B                     1         0.00000031        0.51      0.4869       1        0.00000021         0.36      0.5607
A*C                     1         0.00000236        3.94      0.0704       1        0.00000234         3.91      0.0715
A*D                     1         0.00000003        0.06      0.8160       1        0.00000004         0.06      0.8034
B*C                     1         0.00000028        0.47      0.5056       1        0.00000032         0.53      0.4812
B*D                     1         0.00000291        4.89      0.0474       1        0.00000226         3.78      0.0758
C*D                     1         0.00000101        1.69      0.2181       1        0.00000101         1.69      0.2181

                                               T FOR H0:    PR > |T|          STD ERROR OF
PARAMETER                   ESTIMATE          PARAMETER=0                       ESTIMATE

INTERCEPT              -0.04553321               -2.54      0.0241           0.01894627
A                       0.00409501                1.09      0.2958           0.00374646
B                       0.00020073                1.44      0.1746           0.00013914
C                       4.04993E-06               1.40      0.1859           0.00000291
D                       0.11372395                2.54      0.0259           0.04471834
A*A                    -0.00011144               -0.31      0.7569           0.00035487
B*B                     2.53272E-07               0.40      0.6954           0.00000065
C*C                     5.91184E-11               0.18      0.8576           0.00000000
D*D                    -0.06459271               -1.83      0.0852           0.03656071
A*B                    -1.01003E-05              -0.60      0.5607           0.00001693
A*C                    -7.77335E-07              -1.99      0.0715           0.00000039
A*D                     0.00125521                0.25      0.8034           0.00473197
B*C                     1.15945E-08               0.73      0.4812           0.00000002
B*D                    -0.00034522               -1.94      0.0758           0.00017765
C*D                    -5.10940E-06              -1.30      0.2181           0.00000393

OBSERVATION              OBSERVED           PREDICTED          RESIDUAL        LOWER 95% CL     UPPER 95% CL
                            VALUE              VALUE                             FOR MEAN         FOR MEAN

      1                0.00795100         0.00734434        0.00060666       0.00575294       0.00893574
      2                0.01326200         0.01295185        0.00031015       0.01160528       0.01429743
      3                0.00658800         0.00737354       -0.00078559       0.00603082       0.00871637
      4                0.01105900         0.01215960       -0.00109160       0.01091239       0.01350690
```

Figure E.3 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $CHCl_3$

```
                                                    SAS                                   16:25 SUNDAY, FEBRUARY 19, 1989    2

                                      GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION          OBSERVED           PREDICTED           RESIDUAL         LOWER 95% CL      UPPER 95% CL
                       VALUE              VALUE                                FOR MEAN          FOR MEAN

     5             0.00750400         0.00818470         -0.00068070        0.00693510        0.00943430
     6             0.00742800         0.00796961         -0.00054161        0.00670077        0.00923844
     7             0.01186900         0.01195660         -0.00008760        0.01061497        0.01329823
     8             0.00874700         0.00871285          0.00003415        0.00718244        0.01024326
     9             0.00660300         0.00597613          0.00062687        0.00483730        0.00711497
    10             0.00820100         0.00821857         -0.00001757        0.00740252        0.00903461
    11             0.00741700         0.00728345          0.00013355        0.00582912        0.00873777
    12             0.01245400         0.01273110         -0.00027710        0.01135679        0.01410540
    13             0.01123100         0.01100665          0.00022435        0.00981616        0.01219714
    14             0.01051600         0.01035301          0.00016299        0.00898419        0.01172182
    15             0.00931700         0.00919539          0.00012161        0.00788046        0.01051031
    16             0.00982500         0.00957432          0.00025068        0.00824116        0.01090747
    17             0.00720800         0.00735765         -0.00014965        0.00609337        0.00862193
    18             0.01442600         0.01388432          0.00054168        0.01252726        0.01524139
    19             0.00699100         0.00731698         -0.00032598        0.00602227        0.00861168
    20             0.01152600         0.01107181          0.00045419        0.00971403        0.01242960
    21             0.00728300         0.00772768         -0.00044468        0.00657164        0.00888372
    22             0.00983900         0.00878132          0.00105768        0.00756978        0.00999285
    23             0.01072800         0.01122187         -0.00049387        0.00991906        0.01252468
    24             0.01002500         0.00933414          0.00069086        0.00798449        0.01068379
    25             0.00998500         0.00996233          0.00002267        0.00901847        0.01090619
    26             0.01026400         0.00981651          0.00044749        0.00887347        0.01075955
    27             0.00903200         0.00982165         -0.00078965        0.00887850        0.01076479

          SUM OF RESIDUALS                                0.00000000
          SUM OF SQUARED RESIDUALS                        0.00000717
          SUM OF SQUARED RESIDUALS - ERROR SS             0.00000000
          PRESS STATISTIC                                 0.00004125
          FIRST ORDER AUTOCORRELATION                    -0.04917257
          DURBIN-WATSON D                                 1.96007335
```

Figure E.3 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $CHCl_3$ (cont.)

```
                                         SAS                              18:26 SUNDAY, FEBRUARY 19, 1989     2
                             GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                DF       SUM OF SQUARES         MEAN SQUARE        F VALUE         PR > F      R-SQUARE          C.V.

MODEL                 14           0.00013576          0.00000970           3.98         0.0168      0.847985       23.9027

ERROR                 10           0.00002434          0.00000243                      ROOT MSE                      Y MEAN

CORRECTED TOTAL       24           0.00016010                                        0.00156003                  0.00652660

SOURCE                DF            TYPE I SS     F VALUE     PR > F     DF        TYPE III SS      F VALUE       PR > F

A                      1           0.00003151       12.98     0.0048      1         0.00000311         1.28       0.2844
B                      1           0.00001593        6.51     0.0290      1         0.00000060         0.24       0.6316
C                      1           0.00001091        4.48     0.0603      1         0.00000236         0.97       0.3481
D                      1           0.00002430        9.99     0.0102      1         0.00000133         0.55       0.4760
A*A                    1           0.00000271        1.12     0.3158      1         0.00000165         0.68       0.4294
B*B                    1           0.00001463        6.04     0.0338      1         0.00001909         7.84       0.0188
C*C                    1           0.00000536        2.20     0.1685      1         0.00000443         1.82       0.2070
D*D                    1           0.00000059        0.24     0.6366      1         0.00000000         0.00       0.9985
A*B                    1           0.00000260        1.07     0.3257      1         0.00000194         0.80       0.3927
A*C                    1           0.00000644        2.65     0.1349      1         0.00000617         2.53       0.1425
A*D                    1           0.00000000        0.00     0.9954      1         0.00000000         0.00       0.9973
B*C                    1           0.00000001        0.00     0.9454      1         0.00000000         0.00       0.9935
B*D                    1           0.00001785        7.34     0.0220      1         0.00001489         6.12       0.0329
C*D                    1           0.00000289        1.19     0.3019      1         0.00000288         1.19       0.3019

                                        T FOR H0:      PR > |T|        STD ERROR OF
PARAMETER               ESTIMATE      PARAMETER=0                        ESTIMATE

INTERCEPT            -0.04181695            -1.08        0.3044          0.03862880
A                     0.00859331             1.13        0.2844          0.00759684
B                     0.00014001             0.47        0.6316          0.00029525
C                    6.01446E-06             0.98        0.3481          0.00000610
D                     0.07244693             0.74        0.4760          0.09783057
A*A                  -0.00061567            -0.82        0.4294          0.00074752
B*B                  3.95047E-06             2.80        0.0188          0.00000141
C*C                  3.33435E-10             1.35        0.2070          0.00000000
D*D                   0.00014792             0.00        0.9985          0.07736504
A*B                 -3.04339E-05            -0.89        0.3927          0.00003407
A*C                 -1.25357E-06            -1.59        0.1425          0.00000077
A*D                  3.53374E-05             0.00        0.9973          0.00999815
B*C                  3.75437E-10             0.01        0.9935          0.00000005
B*D                  -0.00089012            -2.47        0.0329          0.00035909
C*D                 -8.65514E-06            -1.09        0.3019          0.00000795

OBSERVATION          OBSERVED        PREDICTED           RESIDUAL      LOWER 95% CL      UPPER 95% CL
                       VALUE            VALUE                             FOR MEAN          FOR MEAN

    1              0.00539400       0.00634142        -0.00094742        0.00352775        0.00915510
    2              0.00917100       0.01076450        -0.00159350        0.00789180        0.01363721
    3              0.00495100       0.00472614         0.00022492        0.00194294        0.00750942
    4              0.00576375       0.00649820        -0.00073445        0.00368235        0.00931405
```

Figure E.4 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $ClCH_2CH_2Cl$

```
                                                          SAS                              18:26 SUNDAY, FEBRUARY 19, 1989     3

                                           GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION          OBSERVED            PREDICTED            RESIDUAL         LOWER 95% CL       UPPER 95% CL
                       VALUE               VALUE                                 FOR MEAN           FOR MEAN

      5             0.00442200          0.00540975          -0.00098775         0.00266878         0.00815073
      6             0.00479200          0.00561384          -0.00082184         0.00280945         0.00841823
      7             0.01087900          0.01171242          -0.00083342         0.00877071         0.01465413
      8             0.00522300          0.00584778          -0.00062478         0.00301482         0.00868074
      9             0.00439300          0.00274251           0.00165049         0.00034493         0.00514008
     10             0.00468100          0.00463251           0.00004849         0.00291687         0.00634816
     11             0.00461200          0.00472165          -0.00010965         0.00159164         0.00785167
     12             0.00658400          0.00777571          -0.00119171         0.00488140         0.01067003
     13 *            .                  0.01095661            .                  0.00747833         0.01443489
     14             0.00784700          0.00804149          -0.00019449         0.00486666         0.01121632
     15 *            .                  0.01000231            .                  0.00565465         0.01434997
     16             0.00664000          0.00640428           0.00023572         0.00340154         0.00940703
     17             0.00448100          0.00447239           0.00000861         0.00178654         0.00715824
     18             0.01169200          0.00972647           0.00196553         0.00687361         0.01257932
     19             0.00452100          0.00492429          -0.00040329         0.00219107         0.00765751
     20             0.00710900          0.00547907           0.00162993         0.00262666         0.00833149
     21             0.00716400          0.00636998           0.00079402         0.00382730         0.00891265
     22             0.00516700          0.00585041          -0.00068341         0.00326302         0.00843780
     23             0.01455700          0.01258767           0.00196933         0.00964871         0.01552664
     24             0.00614400          0.00535376           0.00079024         0.00256468         0.00814284
     25             0.00607300          0.00577725           0.00029575         0.00382474         0.00772976
     26             0.00604400          0.00564223           0.00040177         0.00369233         0.00759213
     27             0.00476000          0.00564896          -0.00088896         0.00369876         0.00759916

* OBSERVATION WAS NOT USED IN THIS ANALYSIS

               SUM OF RESIDUALS                                  0.00000000
               SUM OF SQUARED RESIDUALS                          0.00002434
               SUM OF SQUARED RESIDUALS - ERROR SS               0.00000000
               PRESS STATISTIC                                   0.00019949
               FIRST ORDER AUTOCORRELATION                       0.10747391
               DURBIN-WATSON D                                   1.71569819
```

Figure E.4 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $ClCH_2CH_2Cl$ (cont.)

```
                                            SAS                         18:26 SUNDAY, FEBRUARY 19, 1989     1

                              GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                DF      SUM OF SQUARES       MEAN SQUARE      F VALUE      PR > F     R-SQUARE        C.V.

MODEL                 14          0.00024534        0.00001760         4.60      0.0058     0.843053     19.9795

ERROR                 12          0.00004586        0.00000382                 ROOT MSE                   Y MEAN

CORRECTED TOTAL       26          0.00029220                                 0.00195491               0.00978456


SOURCE                DF         TYPE I SS     F VALUE     PR > F     DF     TYPE III SS     F VALUE     PR > F

A                      1        0.00011580       30.56     0.0001      1      0.00000341        0.89     0.3635
B                      1        0.00000071        0.19     0.6745      1      0.00000034        0.09     0.7715
C                      1        0.00002185        5.72     0.0341      1      0.00000156        0.41     0.5351
D                      1        0.00001751        4.58     0.0535      1      0.00003235        8.47     0.0131
A*A                    1        0.00001113        2.91     0.1137      1      0.00003657        9.57     0.0093
B*B                    1        0.00000340        0.89     0.3639      1      0.00001569        4.11     0.0656
C*C                    1        0.00000553        1.45     0.2523      1      0.00001854        4.85     0.0479
D*D                    1        0.00003596        9.41     0.0098      1      0.00004056       10.61     0.0069
A*B                    1        0.00000146        0.38     0.5483      1      0.00000089        0.23     0.6396
A*C                    1        0.00001972        5.16     0.0423      1      0.00001857        4.86     0.0479
A*D                    1        0.00000002        0.00     0.9506      1      0.00000001        0.00     0.9591
B*C                    1        0.00000596        1.53     0.2392      1      0.00000591        1.55     0.2373
B*D                    1        0.00000620        1.62     0.2270      1      0.00000562        1.47     0.2494
C*D                    1        0.00000020        0.05     0.8236      1      0.00000020        0.05     0.8236


                                           T FOR H0:     PR > |T|     STD ERROR OF
PARAMETER                 ESTIMATE      PARAMETER=0                       ESTIMATE

INTERCEPT               0.11744075             2.46       0.0298        0.04765922
A                      -0.00894869            -0.94       0.3635        0.00947419
B                       0.00004553             0.30       0.7715        0.00015187
C                      4.73726E-06             0.64       0.5351        0.00000737
D                      -0.34373803            -2.91       0.0131        0.11814323
A*A                     0.00277634             3.09       0.0093        0.00089741
B*B                    3.31149E-06             2.03       0.0656        0.00000163
C*C                    1.74571E-09             2.20       0.0479        0.00000000
D*D                     0.30119189             3.26       0.0069        0.09245620
A*B                   -2.05643E-05            -0.48       0.6396        0.00004269
A*C                   -2.19142E-06            -2.20       0.0479        0.00000099
A*D                    -0.00065257            -0.05       0.9591        0.01247196
B*C                   -5.07774E-08            -1.24       0.2373        0.00000004
B*D                    -0.00054495            -1.21       0.2494        0.00044924
C*D                   -2.25479E-06            -0.23       0.8236        0.00000974


                          OBSERVED        PREDICTED                       LOWER 95% CL      UPPER 95% CL
OBSERVATION                  VALUE            VALUE          RESIDUAL         FOR MEAN          FOR MEAN

     1                  0.00837600       0.00670261        0.00167339       0.00343687        0.00996836
     2                  0.01356000       0.01458981       -0.00102981       0.01118707        0.01799255
     3                  0.00826300       0.00766271        0.00060029       0.00426705        0.01105837
     4                  0.01128800       0.01307743       -0.00178943       0.00957055        0.01648430
```

Figure E.5 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CH_3CCl_3

```
                                                     SAS                         18:26 SUNDAY, FEBRUARY 19, 1989    2

                                        GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION         OBSERVED         PREDICTED          RESIDUAL       LOWER 95% CL     UPPER 95% CL
                      VALUE            VALUE                             FOR MEAN         FOR MEAN

     5             0.00879400       0.01027244       -0.00147844       0.00711241       0.01343247
     6             0.00838300       0.00905522       -0.00067222       0.00584655       0.01226389
     7             0.01350300       0.01350752       -0.00000452       0.01011476       0.01690029
     8             0.01018400       0.00953257        0.00065143       0.00616817       0.01289697
     9             0.00732400       0.00724491        0.00007909       0.00436498       0.01012484
    10             0.00931800       0.00814570        0.00117230       0.00608206       0.01020934
    11             0.00857500       0.00912292       -0.00054792       0.00544516       0.01280068
    12             0.01495000       0.01546785       -0.00051785       0.01199245       0.01894325
    13             0.01211200       0.00966441        0.00244759       0.00665385       0.01267497
    14             0.01219300       0.01220881       -0.00001581       0.00874730       0.01567031
    15             0.00958900       0.00965596       -0.00006696       0.00633075       0.01298118
    16             0.00496000       0.00691139       -0.00195139       0.00354006       0.01028272
    17             0.00448100       0.00626783       -0.00178683       0.00307068       0.00946499
    18             0.01830200       0.01743373        0.00086827       0.01400193       0.02086554
    19             0.00759500       0.00789134       -0.00029634       0.00461723       0.01116545
    20             0.01274400       0.01042643        0.00231757       0.00699280       0.01386005
    21             0.00759900       0.00881802       -0.00121902       0.00589458       0.01174145
    22             0.01202900       0.00991071        0.00211829       0.00684694       0.01297449
    23             0.01152500       0.01262860       -0.00110360       0.00933400       0.01592321
    24             0.01159700       0.01007453        0.00152247       0.00666147       0.01348758
    25             0.00406600       0.00609575       -0.00202976       0.00370889       0.00848263
    26             0.00631400       0.00590079        0.00041321       0.00351599       0.00828558
    27             0.00655800       0.00591299        0.00064501       0.00352793       0.00829805

          SUM OF RESIDUALS                                0.00000000
          SUM OF SQUARED RESIDUALS                        0.00004586
          SUM OF SQUARED RESIDUALS - ERROR SS            -0.00000000
          PRESS STATISTIC                                 0.00025629
          FIRST ORDER AUTOCORRELATION                    -0.28916282
          DURBIN-WATSON D                                 2.50816537
```

Figure E.5 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CH_3CCl_3 (cont.)

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                                                  SAS                              18:26 SUNDAY, FEBRUARY 19, 1989     1

                                         GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                DF       SUM OF SQUARES        MEAN SQUARE     F VALUE         PR > F      R-SQUARE          C.V.

MODEL                 14           0.00018991         0.00001349       29.13         0.0001      0.971419        5.9866

ERROR                 12           0.00000556         0.00000046                   ROOT MSE                      Y MEAN

CORRECTED TOTAL       26           0.00019547                                    0.00068057                  0.01136819

SOURCE                DF          TYPE I SS      F VALUE      PR > F       DF       TYPE III SS      F VALUE      PR > F

A                      1         0.00012622       272.51      0.0001        1        0.00000016         0.35      0.5669
B                      1         0.00000157         3.39      0.0903        1        0.00000003         0.06      0.8127
C                      1         0.00000731        15.78      0.0019        1        0.00000233         5.03      0.0446
D                      1         0.00004393        94.85      0.0001        1        0.00000181         3.91      0.0713
A*A                    1         0.00000073         1.58      0.2320        1        0.00000009         0.20      0.6619
B*B                    1         0.00000021         0.46      0.5119        1        0.00000029         0.63      0.4421
C*C                    1         0.00000049         1.06      0.3240        1        0.00000015         0.32      0.5832
D*D                    1         0.00000093         2.00      0.1829        1        0.00000113         2.45      0.1436
A*B                    1         0.00000069         1.49      0.2451        1        0.00000066         1.43      0.2549
A*C                    1         0.00000136         2.93      0.1127        1        0.00000130         2.80      0.1203
A*D                    1         0.00000093         2.00      0.1828        1        0.00000100         2.17      0.1667
B*C                    1         0.00000052         1.13      0.3089        1        0.00000069         1.48      0.2475
B*D                    1         0.00000042         0.91      0.3575        1        0.00000009         0.20      0.6619
C*D                    1         0.00000360         7.76      0.0165        1        0.00000360         7.76      0.0165

                                         T FOR H0:    PR > |T|          STD ERROR OF
PARAMETER                ESTIMATE       PARAMETER=0                       ESTIMATE

INTERCEPT             -0.02231377             -1.42      0.1320          0.01559172
A                     -0.00194244             -0.59      0.5655          0.00329827
B                     2.93342E-05              0.24      0.8127          0.00012250
C                     5.75317E-05              2.24      0.0446          0.00002257
D                      0.08137983              1.98      0.0713          0.04112949
A*A                    0.00014005              0.45      0.5619          0.00031242
B*B                  -4.52201E-07             -0.79      0.4421          0.00000057
C*C                   1.07032E-10              0.55      0.5832          0.00000000
D*D                   -0.05030325             -1.56      0.1436          0.03218700
A*B                   1.77645E-05              1.20      0.2549          0.00001486
A*C                  -5.74827E-07             -1.67      0.1203          0.00000035
A*D                    0.00639147              1.47      0.1657          0.00434189
B*C                   1.72156E-08              1.22      0.2475          0.00000001
B*D                  -7.02145E-05             -0.45      0.5619          0.00015643
C*D                  -9.64035E-06             -2.79      0.0165          0.00000345

OBSERVATION            OBSERVED          PREDICTED           RESIDUAL      LOWER 95% CL      UPPER 95% CL
                          VALUE              VALUE                            FOR MEAN          FOR MEAN

      1              0.02389100         0.02345019         0.00044082        0.00731327        0.00959709
      2              0.01422800         0.01419421         0.00003379        0.01300961        0.01537881
      3              0.00846100         0.00815017         0.00031093        0.00696903        0.00933230
      4              0.01514000         0.01520953        -0.00006953        0.01402359        0.01639567
```

Figure E.6 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CCl_4

```
                                                   SAS                        18:26 SUNDAY, FEBRUARY 19, 1989    2

                                      GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION         OBSERVED          PREDICTED          RESIDUAL         LOWER 95% CL      UPPER 95% CL
                      VALUE             VALUE                               FOR MEAN          FOR MEAN

     5              0.00926800        0.00896256        0.00030544        0.00786245        0.01006267
     6              0.00908800        0.00938788       -0.00029988        0.00827084        0.01050492
     7              0.01575400        0.01520530        0.00054870        0.01402417        0.01638644
     8              0.01173400        0.01168369        0.00005031        0.01051243        0.01285494
     9              0.00770100        0.00720873        0.00049227        0.00620614        0.00821133
    10              0.00987500        0.00919034        0.00068466        0.00847192        0.00990876
    11              0.00982900        0.00957758        0.00025142        0.00829723        0.01085793
    12              0.01713600        0.01720967       -0.00007367        0.01599997        0.01841977
    13              0.01236500        0.01229658        0.00006842        0.01124851        0.01334466
    14              0.01221400        0.01200766        0.00020634        0.01080260        0.01321273
    15              0.01035900        0.01004686        0.00031214        0.00888925        0.01120448
    16              0.01166700        0.01144105        0.00022594        0.01026739        0.01261473
    17              0.00820200        0.00918579       -0.00098379        0.00807275        0.01029882
    18              0.01615400        0.01627941       -0.00012541        0.01508469        0.01747413
    19              0.00812300        0.00865907       -0.00053607        0.00751925        0.00979890
    20              0.01412200        0.01389386        0.00022814        0.01269851        0.01508922
    21              0.00789500        0.00854706       -0.00065206        0.00752932        0.00956480
    22              0.00879500        0.00932543       -0.00053043        0.00825883        0.01039203
    23              0.01246500        0.01297747       -0.00051247        0.01183052        0.01412443
    24              0.01279800        0.01306208       -0.00026408        0.01187389        0.01425028
    25              0.01165200        0.01170307       -0.00005107        0.01087212        0.01253402
    26              0.01237200        0.01154017        0.00083183        0.01070994        0.01237039
    27              0.01068300        0.01154528       -0.00086228        0.01071496        0.01237560

          SUM OF RESIDUALS                                  0.00000000
          SUM OF SQUARED RESIDUALS                          0.00000556
          SUM OF SQUARED RESIDUALS - ERROR SS               0.00000000
          PRESS STATISTIC                                   0.00002446
          FIRST ORDER AUTOCORRELATION                       0.01705456
          DURBIN-WATSON D                                   1.79714613
```

Figure E.6 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CCl_4 (cont.)

```
                                                                                       18:26 SUNDAY, FEBRUARY 19, 1989    1
                                                  SAS
                                    GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y
SOURCE               DF      SUM OF SQUARES      MEAN SQUARE      F VALUE        PR > F      R-SQUARE          C.V.
MODEL                14          0.00014947       0.00001061        18.32        0.0001      0.955296        7.1656
ERROR                12          0.00000695       0.00000058                   ROOT MSE                      Y MEAN
CORRECTED TOTAL      26          0.00015544                                  0.00076096                  0.01061970

SOURCE               DF           TYPE I SS      F VALUE     PR > F     DF      TYPE III SS      F VALUE     PR > F
A                     1          0.00010192       176.01     0.0001      1       0.00000034         0.58     0.4593
B                     1          0.00000181         3.13     0.1022      1       0.00000246         4.25     0.0615
C                     1          0.00001611        27.83     0.0002      1       0.00000147         2.54     0.1370
D                     1          0.00001367        23.60     0.0004      1       0.00000310         5.36     0.0391
A*A                   1          0.00000006         0.11     0.7504      1       0.00000003         0.05     0.8288
B*B                   1          0.00000000         0.00     0.9844      1       0.00000001         0.01     0.9251
C*C                   1          0.00000181         3.12     0.1028      1       0.00000072         1.25     0.2859
D*D                   1          0.00000221         3.82     0.0742      1       0.00000139         2.41     0.1468
A*B                   1          0.00000000         0.01     0.9327      1       0.00000003         0.05     0.8282
A*C                   1          0.00000413         7.13     0.0204      1       0.00000403         6.96     0.0216
A*D                   1          0.00000016         0.28     0.6069      1       0.00000018         0.31     0.5904
B*C                   1          0.00000019         0.32     0.5829      1       0.00000022         0.38     0.5497
B*D                   1          0.00000483         8.34     0.0136      1       0.00000376         6.50     0.0255
C*D                   1          0.00000159         2.73     0.1242      1       0.00000158         2.73     0.1242

                                         T FOR H0:      PR > |T|        STD ERROR OF
PARAMETER                ESTIMATE      PARAMETER=0                      ESTIMATE

INTERCEPT             -0.04542099          -2.45        0.0307          0.01855165
A                      0.00281951           0.76        0.4593          0.00368793
B                      0.00027843           2.05        0.0615          0.00013597
C                     4.57201E-05           1.59        0.1370          0.00002877
D                      0.10540537           2.32        0.0391          0.04548800
A*A                  -7.71319E-05          -0.22        0.8288          0.00034932
B*B                  -9.17555E-09          -0.10        0.9251          0.00000064
C*C                   3.54441E-10           1.12        0.2859          0.00000000
D*D                   -0.05543479          -1.55        0.1458          0.03578915
A*B                   3.54492E-06           0.22        0.8282          0.00001601
A*C                  -1.02135E-06          -2.64        0.0216          0.00000039
A*D                    0.00248507           0.55        0.5904          0.00455473
B*C                   9.74821E-09           0.62        0.5497          0.00000002
B*D                   -0.00044583          -2.55        0.0255          0.00017487
C*D                  -5.34725E-05          -1.05        0.1242          0.00005087

OBSERVATION        OBSERVED        PREDICTED          RESIDUAL      LOWER 95% CL     UPPER 95% CL
                     VALUE           VALUE                            FOR MEAN         FOR MEAN

     1            0.00819910      0.00746199        0.00073711      0.00619069       0.00873310
     2            0.01321400      0.01334095       -0.00012695      0.01201642       0.01466550
     3            0.00790900      0.00814844       -0.00023944      0.00682655       0.00947022
     4            0.01304170      0.01409705       -0.00105535      0.01277091       0.01542320
```

Figure E.7 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CCl_2=CHCl

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                                          SAS                          18:26 SUNDAY, FEBRUARY 19, 1989    2

                             GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION         OBSERVED          PREDICTED          RESIDUAL        LOWER 95% CL     UPPER 95% CL
                      VALUE             VALUE                             FOR MEAN         FOR MEAN

      5            0.00883800        0.00949844       -0.00066044      0.00826838       0.01072850
      6            0.00827300        0.00880610       -0.00053310      0.00755711       0.01005510
      7            0.01396500        0.01388586        0.00007914      0.01256521       0.01520652
      8            0.01011900        0.00993671        0.00018229      0.00862709       0.01124632
      9            0.00718600        0.00680524        0.00038076      0.00568421       0.00792627
     10            0.00907000        0.00908623       -0.00001623      0.00828295       0.00988952
     11            0.00822900        0.00814007        0.00008893      0.00670848       0.00957166
     12            0.01431900        0.01447667       -0.00015767      0.01312385       0.01582949
     13            0.01237400        0.01200570        0.00036830      0.01083382       0.01317758
     14            0.01239200        0.01242972       -0.00003772      0.01108231       0.01377713
     15            0.00966400        0.00939909        0.00026491      0.00810472       0.01069345
     16            0.01076400        0.01075759        0.00000641      0.00944528       0.01206990
     17            0.00815300        0.00856880       -0.00041580      0.00732428       0.00981331
     18            0.01681400        0.01613884        0.00067516      0.01480298       0.01747469
     19            0.00767900        0.00821881       -0.00053981      0.00694434       0.00949328
     20            0.01267000        0.01205954        0.00061046      0.01072298       0.01339610
     21            0.00759100        0.00787118       -0.00028018      0.00673322       0.00900915
     22            0.01132600        0.01021680        0.00110920      0.00902421       0.01140940
     23            0.01140800        0.01209057       -0.00068257      0.01080812       0.01337301
     24            0.01115000        0.01066012        0.00048988      0.00933157       0.01198867
     25            0.01103700        0.01097663        0.00006037      0.01004752       0.01190574
     26            0.01126700        0.01082301        0.00044399      0.00989472       0.01175131
     27            0.01008000        0.01083192       -0.00075192      0.00990352       0.01176032

          SUM OF RESIDUALS                                 0.00000000
          SUM OF SQUARED RESIDUALS                         0.00000695
          SUM OF SQUARED RESIDUALS - ERROR SS              0.00000000
          PRESS STATISTIC                                  0.00003948
          FIRST ORDER AUTOCORRELATION                     -0.23746488
          DURBIN-WATSON D                                  2.31537379
```

Figure E.7 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for CCl_2=CHCl (cont.)

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                                                 SAS                           16:29 SUNDAY, FEBRUARY 12, 1989    1

                                     GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                DF        SUM OF SQUARES        MEAN SQUARE       F VALUE          PR > F        R-SQUARE           C.V.

MODEL                 14            0.00014563         0.00001040         19.30          0.0001        0.957467         7.2372

ERROR                 12            0.00000647         0.00000054                      ROOT MSE                         Y MEAN

CORRECTED TOTAL       26            0.00015210                                       0.00073423                     0.01014526

SOURCE                DF           TYPE I SS      F VALUE      PR > F        DF           TYPE III SS      F VALUE      PR > F

A                      1          0.00008572       159.00      0.0001         1            0.00000057         1.06      0.3242
B                      1          0.00000025         0.46      0.5104         1            0.00000200         3.72      0.0779
C                      1          0.00003052        56.62      0.0001         1            0.00000202         3.74      0.0770
D                      1          0.00001303        24.18      0.0004         1            0.00000251         4.65      0.0520
A*A                    1          0.00000004         0.07      0.7956         1            0.00000018         0.33      0.5780
B*B                    1          0.00000010         0.19      0.6677         1            0.00000007         0.13      0.7254
C*C                    1          0.00000274         5.08      0.0436         1            0.00000153         2.83      0.1182
D*D                    1          0.00000167         3.11      0.1034         1            0.00000101         1.87      0.1964
A*B                    1          0.00000008         0.14      0.7118         1            0.00000003         0.05      0.8195
A*C                    1          0.00000442         8.19      0.0143         1            0.00000420         7.79      0.0163
A*D                    1          0.00000016         0.29      0.5977         1            0.00000018         0.34      0.5699
B*C                    1          0.00000001         0.01      0.9197         1            0.00000000         0.00      0.9852
B*D                    1          0.00000439         8.14      0.0145         1            0.00000319         5.89      0.0319
C*D                    1          0.00000250         4.64      0.0522         1            0.00000250         4.64      0.0522

                                                T FOR H0:     PR > |T|          STD ERROR OF
PARAMETER                  ESTIMATE        PARAMETER=0                           ESTIMATE

INTERCEPT             -0.04256373              -2.38       0.0345            0.01789996
A                      0.00365847               1.03       0.3242            0.00355834
B                      0.00025477               1.93       0.0779            0.00013215
C                    5.36557E-05                1.93       0.0770            0.00002777
D                      0.09523112               2.16       0.0520            0.04417250
A*A                   -0.00019275              -0.57       0.5780            0.00033705
B*B                  2.21752E-07                0.36       0.7254            0.00000061
C*C                  5.13273E-10                1.68       0.1182            0.00000000
D*D                   -0.04749652              -1.37       0.1964            0.03472491
A*B                 -3.73631E-06               -0.23       0.8195            0.00001603
A*C                 -1.04235E-06               -2.79       0.0163            0.00000037
A*D                    0.00274334               0.59       0.5699            0.00468425
B*C                 -2.93954E-10               -0.02       0.9852            0.00000002
B*D                   -0.00040951              -2.43       0.0319            0.00016873
C*D                 -8.04507E-06               -2.15       0.0522            0.00000373

OBSERVATION            OBSERVED           PREDICTED          RESIDUAL         LOWER 95% CL      UPPER 95% CL
                        VALUE               VALUE                               FOR MEAN          FOR MEAN

     1               0.00789900          0.00715541        0.00074359         0.00592855        0.00838197
     2               0.01277700          0.01282316       -0.00004616         0.01154515        0.01410116
     3               0.00751900          0.00778474       -0.00026576         0.00650943        0.00906013
     4               0.01185800          0.01287693       -0.00101893         0.01159637        0.01415749
```

Figure E.8 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for C_6H_6

```
                                                                              18:29 SUNDAY, FEBRUARY 19, 1989     2
                                                        SAS
                                          GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION         OBSERVED          PREDICTED           RESIDUAL        LOWER 95% CL      UPPER 95% CL
                      VALUE             VALUE                               FOR MEAN          FOR MEAN

     5             0.00883800        0.00948997         -0.00065197        0.00830312        0.01067682
     6             0.00767900        0.00828852         -0.00060952        0.00708340        0.00949363
     7             0.01432300        0.01411753          0.00020547        0.01284327        0.01539179
     8             0.00912700        0.00888510          0.00024190        0.00762149        0.01014871
     9             0.00696500        0.00644130          0.00052370        0.00535965        0.00752295
    10             0.00867300        0.00862350          0.00004950        0.00784844        0.00939857
    11             0.00780700        0.00773537          0.00007163        0.00635406        0.00911667
    12             0.01329200        0.01356100         -0.00026900        0.01225571        0.01486630
    13             0.01240800        0.01212163          0.00028637        0.01099092        0.01325235
    14             0.01277900        0.01260826          0.00017074        0.01130818        0.01390834
    15             0.00923100        0.00913702          0.00009398        0.00788813        0.01038592
    16             0.00961000        0.00956067          0.00004933        0.00829446        0.01082689
    17             0.00809300        0.00865919         -0.00056619        0.00745839        0.00985998
    18             0.01636600        0.01579831          0.00056769        0.01450938        0.01708723
    19             0.00698300        0.00746282         -0.00047982        0.00623312        0.00869252
    20             0.01141700        0.01072065          0.00069635        0.00943104        0.01201026
    21             0.00758000        0.00778295         -0.00020295        0.00668496        0.00888094
    22             0.01047000        0.00957876          0.00089124        0.00842806        0.01072946
    23             0.01117300        0.01180459         -0.00063159        0.01056720        0.01304199
    24             0.01054000        0.01015840          0.00038160        0.00887652        0.01144029
    25             0.01052900        0.01034754          0.00018146        0.00945107        0.01124401
    26             0.01052200        0.01019202          0.00032998        0.00929633        0.01108771
    27             0.00946300        0.01020561         -0.00074261        0.00930982        0.01110140

          SUM OF RESIDUALS                                  0.00000000
          SUM OF SQUARED RESIDUALS                          0.00000647
          SUM OF SQUARED RESIDUALS - ERROR SS               0.00000000
          PRESS STATISTIC                                   0.00003721
          FIRST ORDER AUTOCORRELATION                      -0.12884957
          DURBIN-WATSON D                                   2.08698134
```

Figure E.8 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for C_6H_6 (cont.)

```
                                              SAS                              18:29 SUNDAY, FEBRUARY 19, 1989    2

                                 GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                 DF      SUM OF SQUARES        MEAN SQUARE      F VALUE       PR > F      R-SQUARE          C.V.

MODEL                  14          0.00000919         0.00000059         1.07       0.5101      0.750337       27.4539

ERROR                   5          0.00000273         0.00000055                  ROOT MSE                      Y MEAN

CORRECTED TOTAL        19          0.00001092                                   0.00073826                  0.00268910


SOURCE                 DF           TYPE I SS      F VALUE      PR > F       DF      TYPE III SS     F VALUE      PR > F

A                       1          0.00000173         3.17      0.1333        1       0.00000009        0.17      0.6972
B                       1          0.00000059         1.09      0.3444        1       0.00000022        0.41      0.5511
C                       1          0.00000029         0.51      0.5062        1       0.00000000        0.00      0.9920
D                       1          0.00000002         0.05      0.8400        1       0.00000060        1.09      0.3433
A*A                     1          0.00000003         0.06      0.8146        1       0.00000001        0.01      0.9176
B*B                     1          0.00000174         3.19      0.1344        1       0.00000172        3.15      0.1361
C*C                     1          0.00000221         4.05      0.1002        1       0.00000154        2.82      0.1538
D*D                     1          0.00000053         0.97      0.3704        1       0.00000042        0.77      0.4216
A*B                     1          0.00000034         0.62      0.4670        1       0.00000030        0.54      0.4947
A*C                     1          0.00000013         0.23      0.6444        1       0.00000002        0.05      0.8390
A*D                     1          0.00000000         0.00      0.9[illegible]        1       0.00000001        0.02      0.8968
B*C                     1          0.00000055         1.01      0.3620        1       0.00000039        0.71      0.4379
B*D                     1          0.00000004         0.07      0.7953        1       0.00000005        0.08      0.7852
C*D                     1          0.00000001         0.01      0.9175        1       0.00000001        0.01      0.9175


                                              T FOR H0:    PR > |T|         STD ERROR OF
PARAMETER                   ESTIMATE        PARAMETER=0                       ESTIMATE

INTERCEPT                -0.01411057           -0.69       0.5206            0.02044325
A                         0.00182141            0.41       0.6972            0.00441793
B                        -0.00012292           -0.64       0.5511            0.00019247
C                        3.63755E-08            0.01       0.9920            0.00000343
D                         0.05113036            1.05       0.3433            0.04886322
A*A                     -4.52913E-05           -0.11       0.9176            0.00044414
B*B                      2.19322E-06            1.77       0.1361            0.00000124
C*C                      6.72739E-10            1.68       0.1538            0.00000000
D*D                      -0.03545939           -0.87       0.4216            0.04052731
A*B                     -2.07781E-05           -0.74       0.4947            0.00002809
A*C                     -1.25735E-07           -0.21       0.8390            0.00000059
A*D                       0.00071447            0.14       0.8968            0.00523792
B*C                     -2.19334E-08           -0.84       0.4379            0.00000003
B*D                     -8.51249E-05           -0.29       0.7852            0.00029943
C*D                     -5.33548E-07           -0.11       0.9175            0.00000583

OBSERVATION           OBSERVED           PREDICTED            RESIDUAL       LOWER 95% CL       UPPER 95% CL
                         VALUE               VALUE                            FOR MEAN           FOR MEAN

     1              0.00301400          0.00298438          0.00002962         0.00109796         0.00487079
     2 *                     .          0.00521130                   .        -0.00001895         0.01044154
     3              0.00240500          0.00282776         -0.00042276         0.00104113         0.00461439
     4              0.00272230          0.00321395         -0.00043595         0.00149030         0.00493760
```

Figure E.9 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $CHBr_3$

```
                                                    SAS                                   18:29 SUNDAY, FEBRUARY 19, 1989   3

                                       GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION        OBSERVED          PREDICTED           RESIDUAL         LOWER 95% CL      UPPER 95% CL
                     VALUE              VALUE                               FOR MEAN          FOR MEAN

     5            0.00285400         0.00277716         0.00007684       0.00096827        0.00458606
     6            0.00245000         0.00290694        -0.00045694       0.00111532        0.00469856
     7 *               .             0.00306554              .           -0.00110931        0.00844040
     8            0.00222900         0.00265612        -0.00042712       0.00087660        0.00443564
     9            0.00205700         0.00143147         0.00062553      -0.00022672        0.00308967
    10            0.00192900         0.00206929        -0.00014029       0.00098007        0.00315651
    11            0.00205100         0.00159546         0.00045554      -0.00018405        0.00337497
    12            0.00302800         0.00301781         0.00001019       0.00112616        0.00490946
    13 *               .             0.00454610              .            0.00021227        0.00887993
    14            0.00501600         0.00452852         0.00048748       0.00276138        0.00629565
    15 *               .             0.00549639              .            0.00168175        0.00931104
    16            0.00351500         0.00303809         0.00047691       0.00129127        0.00478491
    17            0.00200600         0.00256600        -0.00056000       0.00082882        0.00430318
    18 *               .             0.00413860              .            0.00021380        0.00806340
    19            0.00231500         0.00236633        -0.00005133       0.00061261        0.00412005
    20            0.00389100         0.00343365         0.00045735       0.00169151        0.00517579
    21 *               .             0.00348172              .            0.00043255        0.00653089
    22            0.00213100         0.00223613        -0.00010513       0.00061376        0.00385851
    23 *               .             0.00422140              .           -0.00045586        0.00889878
    24            0.00274500         0.00278362        -0.00003962       0.00106744        0.00449979
    25            0.00277600         0.00251958         0.00025642       0.00144738        0.00359179
    26            0.00269500         0.00246705         0.00022795       0.00140099        0.00353311
    27            0.00205400         0.00246870        -0.00041470       0.00140239        0.00353502

* OBSERVATION WAS NOT USED IN THIS ANALYSIS

             SUM OF RESIDUALS                                 0.00000000
             SUM OF SQUARED RESIDUALS                         0.00000273
             SUM OF SQUARED RESIDUALS - ERROR SS              0.00000900
             PRESS STATISTIC                                  0.00011474
             FIRST ORDER AUTOCORRELATION                     -0.07800199
             DURBIN-WATSON D                                  2.09257231
```

Figure E.9 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $CHBr_3$ (cont.)

```
                                                    SAS                         18:29 SUNDAY, FEBRUARY 19, 1989     1

                                     GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

SOURCE                  DF       SUM OF SQUARES       MEAN SQUARE      F VALUE        PR > F        R-SQUARE          C.V.

MODEL                   14           0.00013969        0.00000998        16.35        0.0001        0.950201        7.8276

ERROR                   12           0.00000732        0.00000061                   ROOT MSE                        Y MEAN

CORRECTED TOTAL         26           0.00014701                                   0.00078107                    0.00997837

SOURCE                  DF           TYPE I SS      F VALUE      PR > F       DF        TYPE III SS      F VALUE      PR > F

A                        1          0.00008680       142.28      0.0001        1         0.00000045         0.74      0.4064
B                        1          0.00000073         1.19      0.2962        1         0.00000217         3.56      0.0837
C                        1          0.00002160        35.40      0.0001        1         0.00000130         2.12      0.1708
D                        1          0.00001246        20.43      0.0007        1         0.00000292         4.79      0.0491
A*A                      1          0.00000000         0.00      0.9694        1         0.00000004         0.07      0.7940
B*B                      1          0.00000001         0.01      0.9241        1         0.00000001         0.01      0.9164
C*C                      1          0.00000541         8.87      0.0115        1         0.00000330         5.42      0.0393
D*D                      1          0.00000206         3.38      0.0908        1         0.00000128         2.10      0.1726
A*B                      1          0.00000003         0.04      0.8414        1         0.00000000         0.00      0.9509
A*C                      1          0.00000437         7.17      0.0201        1         0.00000419         6.87      0.0224
A*D                      1          0.00000011         0.17      0.6854        1         0.00000012         0.20      0.6612
B*C                      1          0.00000000         0.00      0.9652        1         0.00000000         0.00      0.9838
B*D                      1          0.00000420         6.88      0.0222        1         0.00000314         5.15      0.0425
C*D                      1          0.00000191         3.13      0.1025        1         0.00000191         3.13      0.1025

                                                T FOR H0:      PR > |T|          STD ERROR OF
PARAMETER                  ESTIMATE           PARAMETER=0                          ESTIMATE

INTERCEPT             -0.04453731                -2.34        0.0375             0.01904188
A                      0.00325695                 0.95        0.4064             0.00378534
B                      0.00026515                 1.89        0.0837             0.00014059
C                      4.29074E-06                1.46        0.1708             0.00000294
D                      0.10330131                 2.19        0.0491             0.04720322
A*A                   -9.57152E-05               -0.27        0.7940             0.00035855
B*B                    6.99334E-08                0.11        0.9164             0.00000065
C*C                    7.53115E-13                2.33        0.0393             0.00000000
D*D                   -0.05359039                -1.45        0.1726             0.03674016
A*B                   -1.07295E-06               -0.06        0.9509             0.00001705
A*C                   -1.04098E-06               -2.52        0.0224             0.00000040
A*D                    0.00223971                 0.45        0.6612             0.00498307
B*C                    3.35332E-10                0.02        0.9838             0.00000002
B*D                   -0.00040739                -2.27        0.0425             0.00017947
C*D                   -7.02135E-06               -1.77        0.1025             0.00000397

OBSERVATION            OBSERVED              PREDICTED           RESIDUAL         LOWER 95% CL      UPPER 95% CL
                         VALUE                 VALUE                                FOR MEAN          FOR MEAN

     1              0.00766700            0.00689998          0.00076702         0.00559517        0.00820478
     2              0.01235900            0.01248294         -0.00012394         0.01112340        0.01384248
     3              0.00730200            0.00757305         -0.00027105         0.00621594        0.00893036
     4              0.01157400            0.01271271         -0.00113871         0.01145152        0.01417389
```

Figure E.10 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $C_6H_5CH_3$

```
                                                    SAS                              18:29 SUNDAY, FEBRUARY 19, 1989   2

                                       GENERAL LINEAR MODELS PROCEDURE

DEPENDENT VARIABLE: Y

OBSERVATION          OBSERVED           PREDICTED          RESIDUAL         LOWER 95% CL       UPPER 95% CL
                      VALUE               VALUE                              FOR MEAN           FOR MEAN

       5            0.00846000          0.00926099       -0.00080099         0.00799843         0.01052356
       6            0.00774100          0.00837317       -0.00063217         0.00709117         0.00965517
       7            0.01374500          0.01361704        0.00012796         0.01226149         0.01497259
       8            0.00944000          0.00916959        0.00027041         0.00782537         0.01051381
       9            0.00670400          0.00617415        0.00052985         0.00502350         0.00732480
      10            0.00837800          0.00831981        0.00005819         0.00749530         0.00914432
      11            0.00758000          0.00754055        0.00003945         0.00607113         0.00900997
      12            0.01298900          0.01328854       -0.00029954         0.01189997         0.01467711
      13            0.01197400          0.01172112        0.00025288         0.01051828         0.01292397
      14            0.01250900          0.01234610        0.00016290         0.01096308         0.01372911
      15            0.00923800          0.00918053        0.00005747         0.00785197         0.01050909
      16            0.00992700          0.00983182        0.00009518         0.00848483         0.01117881
      17            0.00799600          0.00847555       -0.00047955         0.00719815         0.00975295
      18            0.01640000          0.01565355        0.00074645         0.01428240         0.01702470
      19            0.00724700          0.00779265       -0.00054565         0.00648451         0.00910080
      20            0.01184000          0.01109157        0.00074843         0.00971969         0.01246345
      21            0.00723400          0.00733360       -0.00009960         0.00616556         0.00850163
      22            0.01025600          0.00931128        0.00094472         0.00808718         0.01053539
      23            0.01074900          0.01130180       -0.00055280         0.00998546         0.01261813
      24            0.01025300          0.00983848        0.00041452         0.00847482         0.01120214
      25            0.01022800          0.01010378        0.00012422         0.00915013         0.01105744
      26            0.01031400          0.00995503        0.00035897         0.00900220         0.01090786
      27            0.00921200          0.00996603       -0.00075403         0.00901310         0.01091897

          SUM OF RESIDUALS                                0.00000000
          SUM OF SQUARED RESIDUALS                        0.00000732
          SUM OF SQUARED RESIDUALS - ERROR SS             0.00000000
          PRESS STATISTIC                                 0.00004313
          FIRST ORDER AUTOCORRELATION                    -0.07498232
          DURBIN-WATSON D                                 1.99193724
```

Figure E.10 - SAS General Linear Model Analysis of Mass Transfer Coefficient Experiments for $C_6H_5CH_3$ (cont.)

APPENDIX F

PACKED COLUMN TRACER STUDIES DATA

F.0 Objectives

The general objective of the tracer study was to evaluate the axial and longitudinal dispersion introduced by the packed column. The packed column design assumed that the flow through the column was ideal plug flow and therefore the studies secondary purpose was to show that the flow still approximates plug flow. The factors affecting the flow through the column are:

1. Packing Type (i.e., size, shape)
2. Liquid flow rate
3. Gas flow rate
4. Liquid properties (i.e., temperature, μ_L, γ_L)
5. Column dimensions (i.e, length, diameter).

The tracer study dealt with the variations in the first three factors. The final two factors were held constant.

F.1 Experimental Setup

The tracer study was conducted using a pulse input of fluorescent dye introduced 1000 mm upstream from the initial sampling port. The dye concentration was measured using two fluorometers; one at the inlet and one at the outlet to the column. The fluorometers were setup with flow through cells for continuous reading of the dye concentration passing the reading points. The water passing through the cells was pumped at a constant rate through both cells. Each fluorometer output was recorded on a strip recorder for later analysis.

F.2 Experimental Procedure

The following experimental factors were used to conduct the tracer study:

1. Tracer concentration: 10^3 ug/L,
2. Tracer volume: 20 mL,
3. Liquid flow rate: 0.5, 1.0, 2.0 L/min,
4. Gas flow rate: 90, 120, 150 L/min,
5. Packing type: 6.4 mm Raschig rings
   12.8 mm Raschig rings
   12.8 mm Intalox saddles.

The experimental design was based on a three-factor, three-level factorial design.

F.3 Results

The data from the input and output fluorometers where analyzed according to the procedure outlined by Levenspiel, 1972 and Sater and Levenspiel, 1966. The column was analyzed as a closed vessel. A closed vessel is defined as one in which fluid enters and leaves the column as plug flow and thus having a constant velocity profile. For the column and setup being studied this assumption was correct because firstly the mixing that occurred between injection point and the initial sampling point was observed to be minimal and insignificant. Secondly the mixing that occurred after the liquid exited the column was observed to occur only between the packing support plate at the bottom of the packing and the liquid pool at the bottom of the column. After that point it was assumed that plug flow was reestablished.

The mean and variance of the input and output concentration curves was determined by:

$$\bar{t} = \frac{\int_0^\infty t\ C\ dt}{\int_0^\infty C\ dt} \qquad (F.1)$$

$$= \frac{\Sigma\ t_i\ C_i\ t_i}{\Sigma\ C_i\ t_i} \qquad (F.2)$$

$$\bar{t} = \frac{\int_0^\infty t^2\ C\ dt}{\int_0^\infty C\ dt} - t^2 \qquad (F.3)$$

$$= \frac{\Sigma\ t_i{}^2\ C_i\ t_i}{\Sigma\ C_i\ t_i} - \bar{t}^2 \qquad (F.4)$$

For the closed vessel0 the dispersion number for the column was determined by

$$\sigma_\theta{}^2 = \frac{\sigma^2}{t^2} = 2\ \frac{D_L}{u\ L} - 2\ (\frac{D_L}{u\ L})\ \ (1 - e^{-u\ L/D_L}) \qquad (F.5)$$

The procedure used by Levenspiel was used to determine the dispersion coefficient (D_L/u L). Firstly, the second term on the right in Eq. F.5 was ignored and an initial estimate was determined. Secondly, the significance of the second term was evaluated by calculating the $\sigma_\theta{}^2$ term and comparing it with the experimental value initially used to determine D_L/u L. The results appear in Tables F.1 to F.3.

The correlation introduced by Sater and Levenspiel, 1966 for the local liquid-phase Peclét number, Pe_L was used to determine the predicted axial dispersion coefficient for the column:

$$Pe_L = \frac{u_L \ d_P}{D_{AL}} = 7.58 \ X \ 10^{-3} \ (\frac{d_P \ u_L \ \gamma_L}{\mu_L})^{0.703} \qquad (F.6)$$

The values for the DAL and the DL (experimental) were compared and may be seen in Tables F.1 to F.3.

TABLE F.1 - PACKED COLUMN TRACER STUDY
6.4 mm RASCHIG RINGS

			Input (first line) - Output (second line)						
					Average				
Run#	QL	QG	t (min)	σ2	t (min)	σ2	DL/uL	DL	DAL
1	2.0	50.0	0.2480	0.0033	0.2482	0.0030	0.0198	1.4883	6.9239
			0.2484	0.0028					
			1.4031	0.0638	1.5552	0.0706			
			1.7074	0.0774					
2	3.0	50.0	0.1664	0.0014	0.1774	0.0015	0.0545	6.1548	7.8099
			0.1884	0.0016					
			1.1422	0.0908	1.0184	0.0787			
			0.8946	0.0665					
3	5.0	50.0	0.1138	0.0015	0.1262	0.0013	0.0096	1.8126	9.0894
			0.1385	0.0010					
			0.6266	0.0049	0.6733	0.0070			
			0.7199	0.0092					
4	2.0	100.0	0.2432	0.0019	0.2453	0.0022	0.0262	1.9675	6.9239
			0.2475	0.0025					
			1.5612	0.0632	1.6546	0.1061			
			1.7480	0.1489					
5	3.0	100.0	0.1925	0.0016	0.1868	0.0016	0.1723	19.4472	7.8099
			0.1811	0.0017					
			1.3299	0.8557	1.3851	0.4966			
			1.4404	0.1374					
6	5.0	100.0				*			
7	2.0	150.0				*			
8	3.0	150.0				*			
9	5.0	150.0				*			

* - flooding, data not available.

TABLE F.2 - PACKED COLUMN TRACER STUDY
12.8 mm RASCHIG RINGS

Input (first line) - Output (second line)

					Average				
Run#	QL	QG	t (min)	σ2	t (min)	σ2	DL/uL	DL	DAL
1	2.0	50.0	0.3278	0.0083	0.3310	0.0103	0.3371	25.3636	6.9239
			0.3343	0.0123					
			1.4685	0.9956	1.3696	0.7376			
			1.2708	0.4796					
2	3.0	50.0	0.3138	0.0078	0.3122	0.0071	0.0255	2.8778	7.8099
			0.3106	0.0064					
			1.3555	0.0555	1.3548	0.0626			
			1.3542	0.0696					
3	5.0	50.0	0.2975	0.0074	0.3220	0.0091	0.0211	3.9600	9.0894
			0.3464	0.0107					
			1.3167	0.0537	1.3592	0.0544			
			1.4018	0.0550					
4	2.0	100.0	0.2228	0.0031	0.2324	0.0031	0.0279	2.0961	6.9239
			0.2420	0.0031					
			0.9295	0.0336	0.9531	0.0320			
			0.9767	0.0304					
5	3.0	100.0	0.2207	0.0027	0.2291	0.0028	0.0138	1.5540	7.8099
			0.2375	0.0028					
			0.9532	0.0189	0.9492	0.0170			
			0.9452	0.0151					
6	5.0	100.0	0.1444	0.0035	0.1850	0.0033	0.0234	4.3978	9.0894
			0.2256	0.0031					
			1.0381	0.0368	1.0071	0.0349			
			0.9761	0.0330					
7	2.0	150.0	0.1577	0.0018	0.1502	0.0014	0.0111	0.8344	6.9239
			0.1428	0.0011					
			0.6833	0.0054	0.6478	0.0069			
			0.6123	0.0084					
8	3.0	150.0	0.1672	0.0012	0.1511	0.0013	0.1036	11.6907	7.8099
			0.1350	0.0014					
			0.7300	0.0138	0.7030	0.0644			
			0.6760	0.1151					
9	5.0	150.0				*			

* - flooding, data not available.

TABLE F.3 - PACKED COLUMN TRACER STUDY
12.8 mm INTALOX SADDLES

Input (first line) - Output (second line)

Run#	QL	QG	t (min)	σ2	Average t (min)	Average σ2	DL/uL	DL	DAL
1	2.0	50.0	0.3279	0.0080	0.3138	0.0072	0.0380	2.8621	6.9239
			0.2998	0.0065					
			1.2279	0.0663	1.2067	0.0679			
			1.1854	0.0695					
2	3.0	50.0	0.3348	0.0076	0.3291	0.0068	0.0282	3.1806	7.8099
			0.3234	0.0060					
			1.1593	0.0441	1.1383	0.0437			
			1.1172	0.0433					
3	5.0	50.0	0.3247	0.0073	0.3331	0.0073	0.0429	8.0663	9.0894
			0.3414	0.0072					
			1.2487	0.0846	1.1993	0.0716			
			1.1500	0.0586					
4	2.0	100.0	0.2466	0.0034	0.2415	0.0036	0.0305	2.2924	6.9239
			0.2364	0.0038					
			1.0071	0.0336	0.9832	0.0371			
			0.9593	0.0405					
5	3.0	100.0	0.2393	0.0028	0.2541	0.0031	0.0405	4.5685	7.8099
			0.2689	0.0034					
			1.0058	0.0536	1.0060	0.0489			
			1.0062	0.0442					
6	5.0	100.0	0.2499	0.0027	0.2607	0.0028	0.0453	8.5284	9.0894
			0.2716	0.0028					
			1.0077	0.0658	0.9913	0.0512			
			0.9750	0.0365					
7	2.0	150.0	0.1819	0.0024	0.1813	0.0018	0.0257	1.9351	6.9239
			0.1808	0.0013					
			0.7158	0.0181	0.7211	0.0168			
			0.7265	0.0155					
8	3.0	150.0	0.1873	0.0017	0.1845	0.0016	0.0264	2.9763	7.8099
			0.1818	[illegible]					
			0.7123	0.0179	0.7104	0.0162			
			0.7086	0.0145					
9	5.0	150.0	0.1817	0.0029	0.1873	0.0024	0.0276	5.1986	9.0894
			0.1929	0.0019					
			0.7399	0.0226	0.7436	0.0195			
			0.7473	0.0164					

* - flooding, data not available.