Environ. Sci. Technol. **1998**, *32,* 1433−1437

Henry's Law Constant for Trichloroethylene between 10 and 95 °C

GORM HERON,*,†
THOMAS H. CHRISTENSEN,† AND
CARL G. ENFIELD‡

Department of Environmental Science and Engineering,
Technical University of Denmark, Building 115,
DK-2800 Lyngby, Denmark, and National Risk Management
Research Laboratory, U.S. Environmental Protection Agency,
919 Kerr Research Drive, Ada, Oklahoma 74820

Experimental data on air−water partitioning of organic contaminants at temperatures above 40 °C is extremely scarce. We present Henry's law constants for trichloroethylene (TCE) in water between 10 and 95 °C determined using a modification of the Equilibrium Partitioning in Closed System (EPICS) procedure and calculated from vapor pressure and measured aqueous solubility data obtained by a column generator technique. The Henry's law constant for TCE increases by a factor of 20 between 10 and 95 °C, which is a dramatic change in volatility. Our results and a critical review of the thermodynamic equations suggest that the heat (enthalpy) of dissolution decreases with temperature and that Henry's law constants cannot be extrapolated to higher temperatures from the existing literature data. Heat of dissolution may be approximated by a linear function of temperature, leading to a simple equation for Henry's law constant $\ln k_H = A - B/T + C \ln T$ that fits the majority of the previously published experimental data. This equation is more precise than previously published equations, is valid for temperatures approaching 100 °C, and will assist in more accurate interpretation of Henry's law constant data for other chemicals of environmental concern.

Introduction

Partitioning of organic contaminants between the air phase (e.g., soil vapor) and the aqueous phase (e.g., groundwater or pore water) affects the spreading of contaminants in the environment and the performance of in-situ remediations. Henry's law constants express the equilibrium ratio of the gaseous to the aqueous phase concentrations. Henry's law constant data has been compiled for most environmentally important chemicals (*1*). However, data is generally available only for temperatures below 40 °C. Such data is relevant to the spreading and distribution of contaminants at ambient temperatures and for phase distribution during in-situ remediation and water treatment in the lower temperature range.

Thermally enhanced remediation has been proposed as a means of overcoming mass-transfer limitations during pump-and-treat, soil vapor extraction, and air sparging (*2*−*4*). The subsurface is heated by injecting hot water (*5*), hot air or steam (*6, 7*), electrical currents (*8, 9*), or a combination of the above (*10, 11*), potentially reaching temperatures close to 100 °C or even higher when radio frequency currents are injected (*12, 13*). This expands the need for Henry's law constant data to temperatures up to the boiling point of water. Apart from the recent work by Kolb et al. and Ettre et al. (*14, 15*), such data are currently not available in the literature for compounds such as chlorinated solvents or BTEX. For TCE, no value is given for temperatures above 50 °C.

In this study, we measure the Henry's law constant for trichloroethylene at temperatures from 10 to 95 °C. Our data are compared to previously published data on the temperature dependency of Henry's law constants. A critical examination of the theory behind the temperature dependency of Henry's law constants suggests that inadequate regression equations have been used, and more appropriate equations are proposed.

Thermodynamic Background

Henry's law constant is defined as the ratio of the gas phase concentration to the dissolved concentration at equilibrium. Two forms are typically used, one is the dimensionless Henry's constant H, the other (k_H) has the unit of atm·m^3/mol (*16*−*18*):

$$H = C_g/C_w \tag{1}$$

$$k_H = P_v/C_w \tag{2}$$

where C_g and C_w are gaseous and aqueous phase concentrations, respectively (mol/m^3). P_v is the vapor pressure (unit of atm). The two Henry's law constants are related by

$$k_H = HR_gT \tag{3}$$

where R_g is the natural gas constant and T is the temperature (in K). The derivation of the temperature dependence of H and k_H is not trivial. Two forms have been used most frequently:

$$\ln H = A - B/T \tag{4}$$

$$\ln k_H = A - B/T \tag{5}$$

However, knowing that k_H and H are related by eq 3, it appears that both eqs 4 and 5 cannot be true at the same time.

Derivation of Henry's law constants as a function of temperature is based on solution of the Clapeyron or Van't Hoff equation formulated for water−gas equilibrium using (*16*−*18*)

$$\mathrm{d}\ln k_H/\mathrm{d}T = \Delta H_{dis}/R_gT^2 \tag{6}$$

where ΔH_{dis} is the enthalpy (or heat) of dissolution of the gaseous contaminant into water. The heat of dissolution is given by the heat of vaporization (ΔH_{vap}) minus the excess heat of solution, ΔH_{sol} (*18*):

$$\Delta H_{dis} = \Delta H_{vap} - \Delta H_{sol} \tag{7}$$

For very narrow temperature intervals, the heat of dissolution may be assumed constant, and integration of eq 6 yields

$$\ln k_H = \ln k_H(T_o) - \Delta H_{dis}/R_g(1/T - 1/T_o) \tag{8}$$

---

* Corresponding author phone: 011-45-45251603; fax: 011-45-45932850; e-mail: thc@imt.dtu.dk.
† Technical University of Denmark.
‡ U.S. Environmental Protection Agency.

S0013-936X(97)00701-3 CCC: $15.00

TABLE 1. Regression Equations for Henry's Law Constant Based on Different Assumptions of Variation of Heat of Dissolution with Temperature[a]

assumption	ln k_H (atm·m^3/mol)	ln *H* (dimensionless *H*)
ΔH_{dis} = constant	$A - B/T$	$A - B/T - \ln T$
ΔH_{dis} = linear function in T	$A - B/T + C \ln T$	$A - B/T + C \ln T$
ΔH_{dis} = second-order polynomial in T	$A - B/T + C \ln T + DT$	$A - B/T + C \ln T + DT$

[a] The equations are derived by integration of the Clapeyron equation for k_H.

which is identical to eq 5 above. The correct equation in the dimensionless *H* is given by combining eqs 3 and 8:

$$\ln H = \ln k_H - \ln R_g T = \ln k_H(T_o) - \Delta H_{dis}/R_g(1/T - 1/T_o) - \ln R_g T \quad (9)$$

which has the form $\ln H = A - B/T - \ln T$ showing that eq 4 used by several authors (*14, 15, 19*−*22*) appears to be incorrect. When narrow intervals are considered, relative variations in the absolute temperature is limited (e.g, less than 7% between 10 and 30 °C). Therefore, the error introduced by ignoring the ln *T* term is small, which is the reason relatively good fits to experimental data have been achieved. However, when larger temperature intervals are considered, it becomes important to consider the importance of changes in the heat of dissolution and to evaluate the use the more accurate equations given in Table 1 and derived below.

For larger temperature intervals such as the one considered in this study, the heat of dissolution for TCE can be approximated more closely by a linear function ($\Delta H_{dis} = aT + b$). Equation 6 then reads

$$d \ln k_H/dT = (aT + b)/R_g T^2 \quad (10)$$

Simple integration gives

$$\ln (k_H/k_H(T_o)) = a/R_g \ln (T/T_o) - b/R_g(1/T - 1/T_o) \quad (11)$$

which simplifies into

$$\ln k_H = A - B/T + C \ln T \quad (12)$$

when a known value for a single temperature (T_o) is inserted. The function expressed in the dimensionless *H* is

$$\ln (H/H(T_o)) = a/R_g \ln (T/T_o) - b/R_g(1/T - 1/T_o) - \ln R_g T \quad (13)$$

which simplifies to eq 12, with a different value for *A* and *C*. Table 1 summarizes the equations, including the equations derived when the heat of dissolution is best approximated by a second-order polynomial in *T*, which would be true for compounds with strongly nonlinear behavior of ΔH_{dis} with temperature.

Materials and Methods

Henry's law constants for TCE were determined in the interval from 10 to 95 °C by the Equilibrium Partitioning In Closed Systems (EPICS) procedure previously used at much lower temperatures (*23*−*25*). At each temperature, six 25-mL serum bottles were used: three with 5 mL of distilled water and three with 15 mL of distilled water. Teflon-lined butyl rubber septa with crimp caps were used, and the bottles were placed upside down and heated to the desired temperature in a GC oven for 24 h. Then each bottle was turned, and the septum was penetrated by a thin needle, allowing for a pressure relief. A saturated TCE solution (200 μL with a concentration of 1265 mg/L, measured on a pentane extract) was injected into each bottle, and the needle was redrawn with the bottle upside down to prevent vapor losses. Incubation periods between 6 and 24 h were used before analysis, which by comparison was shown to be plenty of time to reach equilibrium (data not shown). The incubation pressure was close to 1 atm due to the puncture procedure, which was supported by the fact that the flexible septa stayed flat. Vapor losses were minimal since the septum was water covered. A gastight syringe (preheated at the actual temperature) equipped with a stop valve was used to sample 300 μL of the vapor, while the vial was still inside the oven. The sample was immediately injected into a gas chromatograph with a capillary column and FID detector. No condensation was observed inside the syringe. The dimensionless Henry's law constants were calculated for paired bottles (denoted 1 and 2) with different water volumes from

$$H = (C_{g1}V_{l1} - C_{g2}V_{l2})/(C_{g2}V_{g2} - C_{g1}V_{g1}) \quad (14)$$

where g and l denote gas and liquid, respectively, and *C* and *V* are concentration and volume. Henry's law constants were determined using the average of nine values calculated by pairing each of the three bottles with 5 mL of water with each of the three bottles with 15 mL of water. Henry's law constants given as k_H were calculated from the measured dimensionless *H* using eq 3 and the actual incubation temperature *T*. Standard deviation was calculated from the nine obtained values of *H*, assuming that the data were represented by a normal distribution function. Relatively high standard deviations were inevitable for temperatures above 70 °C, since the gas-phase concentrations measured in the bottles become more similar for *H* values above 1 (most of the organic compound is present in the gas phase; ref *25*).

Aqueous solubility for TCE at temperatures between 9 and 71 °C was determined by a column generator technique. A 20 cm long column (2 cm i.d.) was packed with clean medium-grained quartz sand, saturated with free phase TCE, flushed by three pore volumes of distilled water, and placed in a GC oven. The column had a homogeneous distribution of small TCE blobs trapped within the pores. Water presaturated with TCE at 23 °C was passed through the column at a flow rate of 1 mL/h, and the effluent water was sampled in triplicate for TCE using a gastight syringe (preheated at the actual temperature). The syringe was cooled in an ice bath for 20 s, and then the sample was extracted in pentane and analyzed by gas chromatography (capillary column and FID detector). Some condensation of TCE occurred when water sampled at the higher temperatures cooled, but the cloudy suspension in the syringe was easily pushed out and extracted. Between each measurement, the column was kept at a constant temperature for at least 2 h. This holding time was sufficient to bring the concentrations up to equilibrium, as seen by comparing to a 24 h holding time at 40 °C (data not shown). The highest temperature used was 71 °C, since the water−TCE mixture boils at 74 °C, leading to steam production and loss of water and TCE from the column.

TABLE 2. Review of Available Data on Temperature Dependency of Henry's Law Constant for Trichloroethylene

authors	method	temp interval (°C)	regression eq given by authors	corrected eq $\ln k_H = A - B/T$		ΔH_{dis} assumed constant (kJ/mol)	comment
				A	B		
Leighton & Calo (*39*)	BAS[a]	1–26.1	$\ln K_i = 21.89-4647/T$	11.54	4793	39.8	raw data recalcd[c]
Lincoff & Gossett (*23*)	EPICS[b]	10–30	$\ln k_H = 11.94-4929/T$			41.0	
Lincoff & Gossett (*23*)	BAS	10–30	$\ln k_H = 9.703-4308/T$			35.8	
Gossett (*25*)	EPICS	10–35	$\ln k_H = 11.37-4780/T$			39.7	
Munz & Roberts (*19*)	EPICS	10–30	$\log_{10} H = 6.026-1909/T$	10.15	4395	36.5	eq recalcd[d]
Ashworth et al. (*34*)	EPICS + BAS	10–30	$\ln k_H = 7.845-3702/T$			30.8	
Tancrede & Yanagisawa (*20*)	EPICS	25–47.2	$\log_{10} H = 6.664-2141/T$	11.65	4930	41.0	eq recalcd[e]
Tse et al. (*33*)	BAS	20–40	not given	9.74	4308	35.8	raw data calcd[f]
Robbins et al. (*40*)	EPICS	25–50	not given	7.20	3510	29.2	raw data calcd[f]
Dewulf et al. (*21*)	EPICS	2–25	$\ln H = 11.12-3648/T$	11.53	4857	40.4	raw data recalcd[g]
this study	EPICS	10–95	$\ln k_H = 7.99-3738/T$[h]			31.1	

[a] Batch air stripping. [b] Equilibrium partitioning in closed systems. [c] K_i data recalculated into k_H and linear regression made on $\ln k_H - 1/T$ plot. [d] $\ln k_H = \ln (HRT) = \ln RT + \ln 10 \times \log_{10} H$, assuming $T = 293$K. [e] $\ln k_H = \ln (HRT) = \ln RT + \ln 10 \times \log_{10} H$, assuming $T = 309$K. [f] Linear regression made after plotting $\ln k_H$ as function of $1/T$. [g] $\ln k_H = \ln (HRT) = \ln RT + \ln H$, assuming $T = 286.6$K. [h] Calculated from a linear fit to our experimental data given in Figure 4 (10–95 °C).

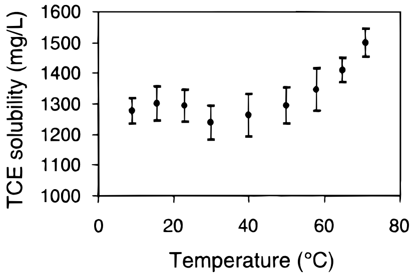

FIGURE 1. Aqueous solubility of trichloroethylene between 9 and 71 °C determined by a column generator technique. Error bars show value ± one standard deviation (σ_{n-1}) determined from triplicates.

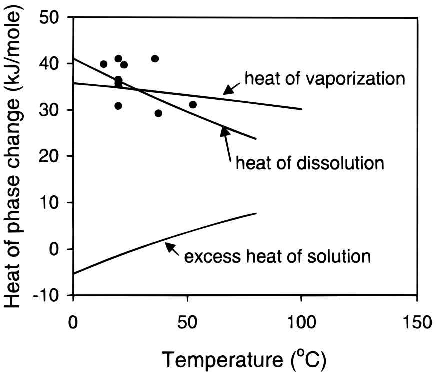

FIGURE 2. Heat of vaporization, excess heat of solution, and heat of dissolution as function of temperature for TCE. Aqueous solubility data (Figure 1) was used to derive the excess heat of solution. The Watson relation (*16*, *30*) and values given by Dean (*31*) and CRC (*32*) were used to derive the heat of vaporization. Inserted dots represent experimental values of heat of dissolution listed in Table 2, plotted at the average temperature of each interval used.

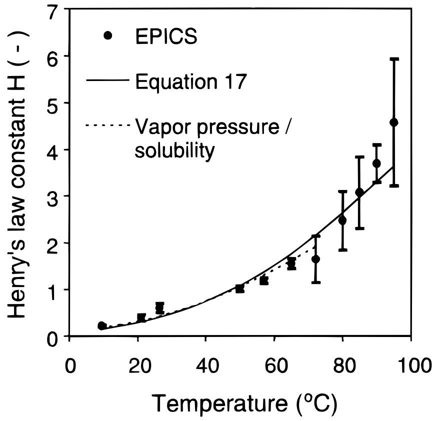

FIGURE 3. Dimensionless Henry's law constants for TCE determined by a modified EPICS procedure compared to calculations of vapor pressure divided by solubility and the curve predicted by using the linear approximation to the heat of dissolution data in Figure 2 (eq 17). Error bars show value ± one standard deviation (σ_{n-1}) determined from nine values for H.

Results and Discussion

The aqueous solubility of TCE increases from around 1300 to 1500 mg/L from 9 to 71 °C, with an apparent minimum around 30 °C (Figure 1). Only one other reference reports solubility data for TCE in this temperature range (*26*). However, the TCE data in this reference dates back to 1943 and reports values between 1050 (10 °C) and 1400 mg/L (80 °C). Recent work has shown that the absolute values given in this reference may easily be in error by 30% or more, exemplified by the data for tetrachloroethylene (*27, 28*) and a range of chemicals (*29*). Therefore, the older data will not be used here. Using the data in Figure 1, we calculated the excess heat of solution as the slope of the curve in a $\ln S - 1/T$ plot, where S denotes aqueous solubility (Figure 2). The excess heat of solution is negative below 30 °C and positive at higher temperatures (when the solubility increases with temperature). Heat of vaporization data was calculated using the Watson relation (*16, 30*) and literature values given at 25 and 87 °C (*31, 32*). The resulting heat of dissolution calculated from eq 7 varies by as much as 40% between 0 and 80 °C, showing that the assumptions behind eqs 4 and 5 are not valid in this larger temperature range. A good fit was obtained by the linear regression

$$\Delta H_{dis} = 40.68 - 0.217t \qquad \text{(kJ/mol)} \qquad (15)$$

Figure 3 shows the measured dimensionless Henry's law constant along with the curve predicted by inserting values into eq 13, including a value for H of 0.33 for 20 °C, calculated as the average of eight experimental values given by refs *1, 23, 24,* and *33–37*. The equation is presented below as eq 17. Also shown is H calculated directly by the following equation (*38*):

$$k_H(T) = P_{vap}(T)/S(T) \qquad (16)$$

where P_{vap} is the saturated vapor pressure of the chemical estimated by using Antoine's equation (*31*), and S is the aqueous solubility measured in this study. Strictly, the vapor pressure in eq 16 should be measured for an organic phase

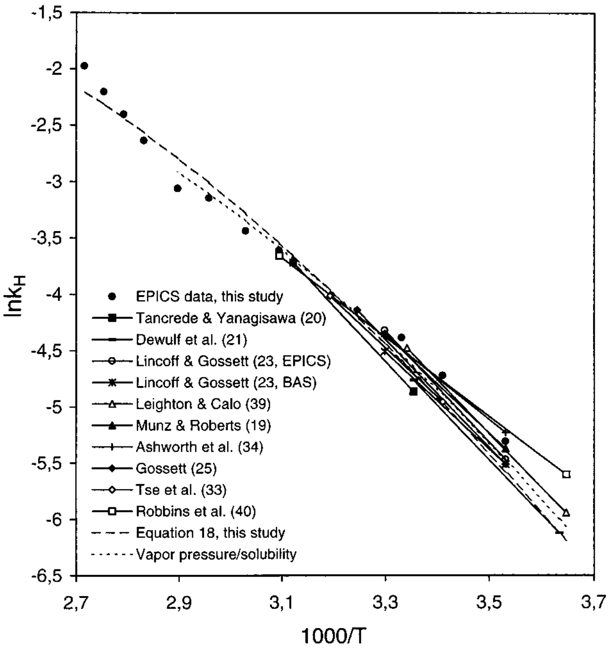

FIGURE 4. Natural logaritm of Henry's law constant for TCE plotted against 1000/*T* for all of the corrected regression equations listed in Table 2, calculations of vapor pressure divided by solubility, and the curve predicted by using the linear approximation to the heat of dissolution data in Figure 2 (eq 15). Our experimental values are given as dots.

saturated with water. However, such data are not available for TCE at the studied temperature range, and the error introduced by using the pure-compound vapor pressure is not great, since Stephenson (*28*) found water solubility in similar chlorinated solvents to be below 5 vol %. However, the error is greater at higher temperatures, since the solubility of water in most organics was found to increase with temperature. When using eq 16 at temperatures above 75 °C, the error may become significant.

Henry's law constant increases by a factor of 20 (from 0.2 to 4) between 10 and 95 °C. There is a reasonable fit between the experimental data and the predicted curve for temperatures below 80 °C, whereas the fit is less convincing for temperatures above 80 °C, where no solubility data are available and where the EPICS method becomes inaccurate since H increases above 3 (*25*).

Table 2 summarizes the previously published temperature dependency of TCE. So far, every study has assumed constant heat of dissolution in the studied temperature intervals. We took the liberty to calculate regression equations according to eq 5 for studies where such were not given (*33, 40*) or given as the less accurate eq 4 (*19*−*21, 39*). Then heat of dissolution was assumed constant in each studied interval and calculated from the slope of the fitted straight line in a $\ln k_H - 1/T$ plot (data not shown). This yielded values between 29 and 41 kJ/mol (Table 2; Figure 2). In summary, for each study the assumption of constant heat of dissolution seemed reasonable due to the narrow temperature intervals studied. When the data was looked at in total, a trend was observed indicating a decreasing heat of dissolution with temperature, in accordance with Figure 2.

To investigate the error introduced by assuming constant heat of dissolution, our experimental data was plotted as $\ln k_H$ as a function of $1000/T$ along with all the available literature data listed in Table 2 (Figure 4). Constant heat of dissolution would lead to a straight line in this plot. Our data alone plots relatively nicely on a line with the slope corresponding to a heat of dissolution of 31 kJ/mol as an average over the 10−95 °C interval (Table 2). However, including all the data reveals a tendency toward a downward curvature in the data, since the lines in the right side of the diagram tend to have a steeper slope, which corresponds to a higher ΔH_{dis}.

One cannot use the existing literature data for extrapolation to higher temperatures. If that was done, the slope of the lines in the lower right corner of Figure 4 would lead to very significant overestimation of k_H at higher temperatures (by a factor of at least 2). A reasonable fit can be achieved by either including a slight curvature in the fit (i.e., using the linear equation for heat of dissolution) or by using a linear fit in the $\ln k_H - 1000/T$ plot (eq 8), with a heat of dissolution value of 31 kJ/mol, which is significantly lower than the values derived at lower temperatures (Figure 2).

Curvature in similar $\ln k_H - 1000/T$ plots was observed in recent studies on toluene and chlorobenzene between 45 and 80 °C (*15*). We observed strong curvature when plotting data for tetrachloroethylene obtained from vapor pressure and solubility data, supporting the conclusions that heat of dissolution cannot be assumed constant in larger temperature intervals (data not shown).

On the basis of all of the above data, we suggest first using the linear equation for the variation in heat of dissolution of trichloroethylene. Considering our experimental data, the predicted curve, and the massive data material for temperatures below 50 °C, we recommend the following equations:

$$\ln H = 195.52 - 12540/T - 27.11 \ln T \qquad (17)$$

$$\ln k_{\mathrm{H}} = 186.10 - 12540/T - 26.11 \ln T \qquad (18)$$

As can be seen in Figures 3 and 4, the temperature effect on the Henry's law constant is very dramatic, and large effects on volatility can be expected during thermally enhanced remediation.

Acknowledgments

The U.S. Environmental Protection Agency through its Office of Research and Development funded a portion of the research described here under Cooperative Agreement CR 823908-01-0 entitled Joule Heating for DNAPL Remediation. It has not been subjected to Agency review and therefore does not necessarily reflect the views of the Agency, and no official endorsement should be inferred.

Literature Cited

(1) Mackay, D.; Shiu, W. Y. *J. Phys. Chem. Ref. Data* **1981**, *10*, 1175−1199.
(2) Udell, K. S. In *Annual Review of Heat Transfer*, Vol. 7; Chen, C.-L., Ed.; Hemisphere: New York, 1996; pp 333−405.
(3) Davis, E. L. *How heat can enhance in-situ soil and aquifer remediation: important chemical properties and guidance for choosing the appropriate technique*; EPA Issue Paper EPA/540/S-97/502; U.S. Environmental Protection Agency: Ada, OK, 1997.
(4) U.S. Environmental Protection Agency. *In Situ Remediation Technology Status Report: Thermal Enhancements*; Report EPA542-K-94-009; U.S. EPA: Ada, OK, 1994.
(5) Davis, E. L.; Lien, B. K. *Laboratory Study on the Use of Hot Water to Recover Light Oily Wastes from Sands*; Report EPA/600/R-93/021: U.S. Environmental Protection Agency, Ada, OK, 1993.
(6) Udell, K. S.; Stewart, L. D. *Field Study of In Situ Steam Injection and Vacuum Extraction for Recovery of Volatile Organic Solvents*; UCB−SEEHRL Report No. 89-2; University of California: Berkeley, CA, 1989.
(7) Clarke, A.; Wilson, D.; dePercin, D. P. In *Hazardous Waste Site Soil Remediation*; Wilson, D., Clarke, A., Eds.; Marcel Dekker: New York, 1994; pp 243−264.
(8) Buettner, H. M.; Daily, W. D. *J. Environ. Eng.* **1995**, *Aug*, 580−589.
(9) Gauglitz, P.; Roberts, J.; Bergsman, T.; Schalla, R.; Caley, S.; Schlender, M.; Heath, W.; Jarosch, T.; Miller, M.; Eddy-Dilek, C.; Moss, R.; Looney, B. *Six-phase soil heating for enhanced removal of contaminants: Volatile organic compounds in*

nonarid soils; Report PNL-10184, UC-406; Pacific Northwest Laboratory: CA, 1994.

(10) Newmark, R. L. Dynamic Underground Stripping Project Gasoline Spill Site Monitoring Team. *Demonstration of Dynamic Underground Stripping at the LLNL Gasoline Spill Site*; Dynamic Underground Stripping Project: LLNL Gasoline Spill Demonstration Report, Vol. UCRL-ID-116964, Vols. 1−4; Lawrence Livermore National Laboratory: Livermore, CA, 1994.

(11) Phelan, J.; Webb, S. *Thermal enhanced vapor extraction systems—design, application, performance prediction, including contaminant behavior*. In *Proceedings of the Thirty-Third Hanford Symposium on Health and the Environment: In Situ Remediation: Scientific Basis for Current and Future Technologies*; Gee, G., Wing, N., Eds. Battelle Press: Columbus, OH, 1994.

(12) Dev, H.; Bridges, J.; Sresty, G.; Enk, J.; Mshaiel, N.; Love, M. *Radio frequency enhanced decontamination of soils contaminated with halogenated hydrocarbons*; Report EPA/600/2-89/008; U.S. Environmental Protection Agency: 1989.

(13) Snow, R. H.; Sresty, G. C.; Conroy, C.; Collins, R. Test of Radio Frequency In Situ Heating for Treatment of Soil at Rocky Mountain Arsenal. In *Proceedings of Superfund 14 Conference and Exhibition*, November 30−Dec 1, 1993; pp 275−284.

(14) Kolb, B.; Welter, C.; Bichler, C. *Chromatographia* **1992**, *34*, 235−240.

(15) Ettre, L. S.; Welter, C.; Kolb, B. *Chromatographia* **1993**, *35*, 73−84.

(16) Reid, R.; Prausnitz, J.; Poling, B. *The Properties of Gases and Liquids*; McGraw-Hill Book Company: New York, 1987.

(17) Stumm, W., Morgan, J. J. *Aquatic Chemistry*; John Wiley: New York, 1981.

(18) Schwarzenbach, R.; Gschwend, P.; Imboden, D. In *Environmental Organic Chemistry*; John Wiley: New York, 1992; pp 76−108.

(19) Munz, C.; Roberts, P. *J. Am Water Works* Assoc. **1987**, *May*, 62−69.

(20) Tancrede, M. V.; Yanagisawa, Y. *J. Air Waste Manage. Assoc.* **1990,** *40*, 1658−1663.

(21) Dewulf, J.; Drijvers, D.; Van Langenhove, H. *Atmos. Environ.* **1995**, *29* (3), 323−331.

(22) Nirmalakhandan, N.; Brennan, R. A.; Speece, R. E. *Water Res.* **1997**, *31* (6), 1471−1481.

(23) Lincoff, A.; Gossett, J. In *Gas transfer at water surfaces*; Brutsaert, W., Jirka, G., Eds.; D. Reidel Publishing Company: Boston, 1984; pp 17−25.

(24) Garbarini, D.; Lion, L. *Environ. Sci. Technol.* **1985**, *19*, 1122−1128.

(25) Gossett, J. *Environ. Sci. Technol.* **1987**, *21*, 202−208.

(26) Horvath, A. *Halogenated Hydrocarbons. Solubility-Miscibility with Water*; Marcel Dekker: New York, 1982.

(27) Imhoff, P. T.; Frizzell, A.; Miller, C. T. *Environ. Sci. Technol.* **1997**, *31*, 1615−1622.

(28) Stephenson, R. M. *J. Chem. Eng. Data* **1992**, *37*, 80−95.

(29) Knauss, K. G.; Copenhaver, S. A. *Gechim. Cosmochim. Acta* **1995**, *59* (12), 2443−2448.

(30) Fishtine, S. H. *Hydrocarbon Process.* **1966**, *45*, 173−179.

(31) Dean, J. *Lange's Handbook of Chemistry*; McGraw-Hill Book Company: New York, 1985.

(32) *CRC Handbook of Chemistry and Physics*; The Chemical Rubber Company: Cleveland, OH, 1994.

(33) Tse, G.; Orbey, H.; Sandler, S. I. *Environ. Sci. Technol.* **1992**, *26*, 2017−2027.

(34) Ashworth, R.; Howe, G.; Mullins, M.; Rogers. *J. Hazard. Mater.*, **1988**, *18*, 25−36.

(35) Yurteri, C.; Ryan, D.; Callow, J.; Gurol, M. *J. Water Pollut. Control Fed.*, **1987**, *59*, 950−956.

(36) Grifoll, J.; Cohen, Y. *J. Hazard. Mater.* **1994**, *37*, 445−457.

(37) Munz, C.; Roberts, P. *Environ. Sci. Technol.* **1986**, *20*, 830−836.

(38) Meylan, W. M.; Howard, P. H. *Environ. Toxicol. Chem.* **1991**, *10*, 1283−1293.

(39) Leighton, D. J.; Calo, J. *J. Chem. Eng. Data* **1981**, *26*, 382−385.

(40) Robbins, G. A.; Wang, S.; Stuart, J. D. *Anal. Chem.* **1993**, *65*, 3113−3118.

Received for review August 6, 1997. Revised manuscript received January 23, 1998. Accepted February 17, 1998.

ES9707015