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An Alternative Model for Estimating Liquid Diffusion Coefficients Requiring No Viscosity Data

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AN ALTERNATIVE MODEL FOR ESTIMATING LIQUID DIFFUSION COEFFICIENTS REQUIRING NO VISCOSITY DATA

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Abstract

An equation, based on the free volume of a liquid solvent, was derived via dimensional analysis, to predict binary diffusion coefficients. The equation assumed that interaction between the solute and liquid solvent molecules followed a Lennard-Jones [6-12] potential. The equation was compared to other diffusivity equations and was found to give good results over the temperature range examined.

Introduction

The prediction of binary liquid diffusivities has a long and varied history. As early as 1905, the Stokes-Einstein equation was derived from a hydrodynamic model (1)--a large solute sphere diffusing in a solvent continuum.

$$D_{AB}=KT/(6\pi\mu_B R_A) \tag{1}$$

For definition of symbols, see the listing of notations.

In 1955, Wilke and Chang (2), also using a hydrodynamic model, derived the following semi-empirical expression:

$$D_{AB} = 7.4\times10^{-8}(X_B MW_B)^{1/2}T/(\mu_B V_A^{0.6}) \tag{2}$$

where, X_B is an association number of the solvent: 2.6 for water, 1.9 for methanol, 1.5 for ethanol, and 1.0 for unassociated solvents.

Starting in 1941, Eyring (3) and his co-workers (4) derived the following equation using absolute rate theory:

$$D_{AB} = [(KT)/(E_A\mu_B)]\ (N/V_B)^{1/3}\ \exp(E_{\mu B}-E_{D_{AB}}/RT) \tag{3}$$

This equation is based on a quasi-crystalline liquid structure model where the diffusing molecules "jump" through layers of solvent molecules. The geometric parameter, E_A, equals the number of nearest molecules, in a plane, around a central molecule. In using this equation, Eyring and co-workers assumed that $E_A = 6$ and that $E_{\mu B} = E_{D_{AB}}$ so that equation 3 reduced to:

$$D_{AB} = (KT/6\mu_B)(N/V_B)^{1/3} \tag{4}$$

Akgerman and Gainer (5) in 1972, building on Eyring's work, proposed the following equation:

$$D_{AB} = (KT/E_A\mu_B)\,(N/V_B)^{1/3}\,(MW_B/MW_A)^{1/2}\,\exp(E_{\mu B} - E_{D_{AB}}/RT) \tag{5}$$

In this equation, the geometric parameter is given by:

$$E_A = 6\,(V_A/V_B)^{1/6} \tag{6}$$

and, unlike Eyring, they did not assume that $E_{\mu B} = E_{D_{AB}}$.

Prediction of diffusion coefficients using equations based on a hydrodynamic model has been successful when the solute molecules are large and spherical, and the solvent molecules considerably smaller in size. The Eyring equation, based on an absolute rate model, has been found to predict diffusion coefficients too high by a factor of six. The Akgerman-Gainer equation has been found to give better values than the Eyring equation.

All the equations cited (Equations 1, 2, 3, and 5) utilize the solvent viscosity (a transport property) to calculate the diffusion coefficients (another transport property). Naturally, it was highly desirable to develop a model to calculate liquid diffusivities without using viscosity. In 1959, Cohen and Turnbull (6) derived the following relationship between the self diffusion coefficient in a model liquid of "hard spheres" and the "free volume" of the liquid:

$$D = A \exp\left[\frac{-\gamma V^*}{V_F}\right] \tag{7}$$

They theorized that the liquid free volume (V_F) redistributed itself leading to the formation of "holes" sufficiently large (V^*) for diffusion to occur. The use of equation 7 requires the estimation of V_F, V^*, and the constants A and γ which depend on the geometry and size of the liquid molecules.

The concept of relating liquid free volume to diffusivity is an interesting one, but modeling the interaction of the liquid molecules using a hard sphere potential (which incorporates only a repulsive force) apparently leads to the necessity of using a "hole" volume. The purpose of this work was to investigate the possibility of formulating a diffusivity equation based on the liquid free volume where the molecules interact according to the more realistic Lennard-Jones [6-12] potential. The use of the Lennard-Jones [6-12] potential (which incorporates both repulsive and attractive forces) should eliminate the need for the "hole" volume. An equation capable of predicting both self and binary diffusivities was sought.

Formulation of Free Volume Equation

The initial formulation of the diffusivity equation assumed that diffusion coefficients should depend on the temperature and free volume of the liquid solvent.

$$D_{AB} = f(T, V_{FB}) \tag{8}$$

The diffusion of solute molecules through solvent molecules also depends on the interaction between the molecules and the molecular size and shape of the molecules. In this case, the molecular interaction was modeled using the Lennard-Jones [6-12] potential which has two associated parameters --a distance parameter (σ), and energy parameter (ϵ/K). For solute molecule A interacting with solvent molecule B, the following empirical combining laws were used (7):

$$\sigma_{AB} = \frac{1}{2}(\sigma_A + \sigma_B) \tag{9}$$

$$(\epsilon/K)_{AB} = [(\epsilon/K)_A(\epsilon/K)_B]^{1/2} \tag{10}$$

One can then calculate $\Omega_{D_{AB}}$ which is a dimensionless function of $T/(\epsilon/K)_{AB}$; $\Omega_{D_{AB}}$ is derived from the kinetic theory of Chapman and Enskog, and is a measure of the deviation of the Lennard-Jones molecules from rigid-sphere behavior: $\Omega_{D_{AB}} = 1$ for rigid spherical molecules. Values of σ, (ϵ/K), and $\Omega_{D_{AB}}$ have been tabulated. The empirical combining laws give good estimates for nonpolar molecular pairs.

The molecular size was taken into account by empirically averaging the molecular weights of the solute and solvent:

$$MW_{AB} = \frac{1}{2}(MW_A + MW_B) \tag{11}$$

Including the Lennard-Jones parameters and the average molecular weight into the initial diffusivity relation yields the following:

$$D_{AB} = f(T, V_{FB}, \sigma_{AB}, \Omega_{D_{AB}}, MW_{AB}) \tag{12}$$

Dimensional analysis was then used to derive the following dimensionally correct equation:

$$D_{AB} = G\left(\frac{RTV_{FB}}{MW_{AB}\sigma_{AB}}\right)^{1/2} \tag{13}$$

where G is a dimensionless function of $\Omega_{D_{AB}}$. At this point, G was determined empirically. This was done by correlating equation 13 with the experimental diffusivity value of argon diffusing in carbon tetrachloride at 298K. The argon-carbon tetrachloride system is considered to approach the ideal conditions of a Lennard-Jones [6-12] model--nonpolar, nonhydrogen bonded spherical molecules. Letting $G = \Omega_{D_{AB}}^{-2}$ (the simplest form for G was sought) correlated the experimental result well.

The functional form for G was derived for the temperature equal to 298K. For temperatures other than 298K the exponent of $\Omega_{D_{AB}}$ should change. Rather than manipulate the exponent, equation 13 was scaled by multiplying it by $(T/298)^n$. The value of n was found by correlating equation 13 to the experimental diffusivity value or argon diffusing in carbon tetrachloride at 273K. Letting n=3 resulted in a diffusivity value that deviated by less than 1% from the experimental value (5); this results in equation 13 having a $T^{3\frac{1}{2}}$ temperature dependence.

The liquid free volume may be calculated approximately by one of two methods. Glasstone and co-workers (3) derived the following equation for the calculation of liquid free volume:

$$V_F^{1/3} \approx \frac{\alpha RT}{\Delta H_{vapor}} \left(\frac{V_B}{N} \right)^{1/3} \tag{14}$$

where α is a geometric packing factor for the molecules of the liquid. It is equal to 2 for regular arrays of hard spheres. They also derived the following equation for the calculation of free volume:

$$\frac{U_{Liq}}{U_{vapor}} \approx \left(\frac{V}{V_F} \right)^{1/3} \tag{15}$$

where V is the volume of a molecule in the liquid given by:

$$V = \frac{MW_B}{(\rho_B N)} \tag{16}$$

U_{Liq} and U_{vapor} are the velocity of sound in the solvent liquid phase and in the solvent vapor phase, respectively. Velocity of sound data for several liquids was obtained from the CRC Handbook (8). Calculated free volumes, based on velocity for some liquids are:

V_F (benzene) = 4.07×10^{-25} cm^3 at 302.6K
V_F (carbon tetrachloride) = 4.43×10^{-25} cm^3 at 298K
V_F (water) = 6.75×10^{-25} cm^3 at 298K

The following example illustrates the use of equation 13 for the calculation of the diffusion coefficient for benzene, A, in carbon tetrachloride, B:

$R = 8.314 \cdot 10^7$ $(g\text{-}cm^2)/(sec^2\text{-}gmole\text{-}K)$

$MW_A = 78$ g/gmole $\qquad MW_B = 153.8$ g/gmole

$\sigma_A = 5.349*10^{-8}$ cm $\qquad \sigma_B = 5.947*10^{-8}$ cm

$(\epsilon/K)_A = 412.3$ K $\qquad (\epsilon/K)_B = 322.7$ K

$T = 298$ K

$V_{FB} = 4.43*10^{-25}$ cm^3

$MW_{AB} = 1/2\ (MW_A + MW_B) = 116$ g/gmole

$\sigma_{AB} = 1/2(\sigma_A + \sigma_B) = 5.648*10^{-8}$ cm

$(\epsilon/K)_{AB} = ((\epsilon/K)_A*(\epsilon/K)_B)^{1/2} = 364.8$ K

$T/(\epsilon/K)_{AB} = 0.82 \Rightarrow \Omega_{D(AB)} = 1.59$

$D_{AB} = 1/(59)^2*((8.314*10^7)*(298)/(116))^{1/2}*((4.43*10^{-25})/(5.648*10^{-8}))^{1/2}$

$D_{AB} = 1.62*10^{-5}$ cm^2/sec

Equation 13 overpredicted the experimental value by 5% (9).

Table 1 lists the experimentally determined binary diffusion coefficients for a number of substances dissolved in different organic liquids. The calculated values using equation 13 are also listed, as well as the % deviation from the experimental values (5, 9) (the quantities in parenthesis). The calculated values and % deviation are also given using the Stokes-Einstein (S.E.), the Wilke-Chang (W.C.), and the Eyring, and the Akgerman-Gainer (A.G.) equations.

The calculated free volume results differ from the experimental results by an overall absolute average value of 13%. The absolute average deviations for the other equations are 71% (S.E.), 21% (W.C.), 61% (Eyring), and 47% (A.G.). Comparing only the free volume results, note that the diffusivity values for CO_2 dissolved in C_2H_5OH and for N_2 dissolved in C_6H_6 have the greatest deviation from the experimental values (-58% and +27%, respectively.) These results are not surprising if one considers that equation 13

These results are not surprising if one considers that equation 13 incorporated Lennard-Jones parameters that are derived from a model that considered the interacting molecules to be nonpolar spheres with no hydrogen bonding.

This point was explored further by calculating the diffusion coefficients of several different solutes in water--a polar, hydrogen-bonding molecule. The calculations are tabulated in Table 2. Equation 13 predictions are very poor compared to the other four equations. The free-volume overall absolute average deviation from the experimental values is 173%, whereas the deviations for the other equations are 46% (S.E.), 9% (W.C.), 30% (Eyring), and 10% (A.G.). In order to improve on equation 13 predictions, it was decided to use a polar potential, the Stockmayer potential, for water.

The Stockmayer potential has three associated parameters--a distance (σ) and energy (ϵ/K) parameters (which are not equal numerically to the Lennard-Jones parameters), and a dimensionless polarity parameter (t^*) which is a function of the molecule's dipole moment. These three parameters have been tabulated for a number of polar molecules (10).

In order to incorporate the polarity parameter t^*, equation 13 was modified to the following:

$$D_{AB} = (1-t^*) \left(\frac{T}{298}\right)^3 \frac{1}{\Omega^2_{D_{AB}}} \left(\frac{RTV_{FB}}{MW_{AB}\sigma_{AB}}\right)^{1/2} \tag{17}$$

The following example illustrates the use of equation 17:

Binary diffusion coefficient calculation for CO_2 (A) in water (B)

$MW_A = 44$ g/gmole
$MW_B = 18$ g/gmole
$\sigma_A = 3.94*10^{-8}$ cm
$\sigma_B = 2.52*10^{-8}$ cm

$(\epsilon/K)_A = 195$ K $\qquad\qquad (\epsilon/K)_B = 775$ K

$T = 298$ K

$V_{FB} = 6.75*10^{-25}$ cm^3

$t_B^* = 0.7$

$MW_{AB} = 31$ g/gmole

$\sigma_{AB} = 3.23*10^{-8}$ cm

$(\epsilon/K)_{AB} = 389$ K

$T/(\epsilon/K)_{AB} = 0.77 \rightarrow \Omega_{D(AB)} = 1.64$

$$D_{AB} = [(1-0.7)/(1.64)^2]*((8.314*10^7)*(298)/(31))^{1/2}*((6.75*10^{25})/(3.23*10^{-8}))^{1/2}$$

$D_{AB} = 1.44*10^{-5}$ cm^2/sec

Experimental value = $1.91*10^{-5}$ cm^2/sec (5)

Equation 17 underpredicted the experimental value by 25%.

Table 3 lists the free volume diffusion coefficients, for various solutes dissolved in water, using equation 17. Comparison with Table 2 shows that using the Stockmayer potential for water results in calculated diffusivity values (overall absolute average deviation of 28%) that are in better agreement with the reported experimental values. The diffusivity value was also calculated for CO_2 in ethanol (C_2H_5OH) using the Stockmayer parameters for ethanol. Comparison of Table 3 to Table 1 again shows that use of the Stockmayer parameters for ethanol results in a better prediction (-17% deviation compared to a -58% deviation.)

Equation 17 was finally used to calculate diffusivity values for CO_2 in ethanol and in water over a small temperature range. These values are tabulated in Tables 4 and 5. The calculated diffusivity values were also graphed against the experimental values and these results are shown in Figures 1 and 2.

For CO_2 in ethanol, equation 17 overpredicts diffusivity values from 10% to 17%, whereas the other four equations underpredict from 41% to 78%.

For CO_2 in water, equation 17 predictions are better than the Stokes-Einstein predictions and comparable to the Eyring predictions. Both the Wilke-Chang and Akgerman-Gainer equations gave better predictions than the free volume equation.

Conclusions

A new semi-empirical equation was formulated, via dimensional analysis, to predict both self and binary liquid diffusivities. The equation is based on the free volume of the liquid solvent and on the Lennard-Jones [6-12] molecular interaction between the solute and solvent molecules. Unlike other widely used diffusivity equations, equation 13 does not incorporate the liquid solvent viscosity (a transport property), and unlike equation 7, it does not need the "hole" volume. Equation 13 is able to predict both self and binary diffusivities with good results (over the temperature range considered) when compared with four other widely used diffusivity equations. This work also suggests that a similar equation may be derived to predict the viscosity of liquids.

REFERENCES

1. Bird, R.B.; Stewart, W.E.; and Lightfoot, E.N.: Transport Phenomena. Wiley, New York, 1960.
2. Wilke, C.R.; and Chang, P.: Correlation of Diffusion Coefficients in Dilute Solutions. AICHE J., vol. 1, no. 2, 1955, pp. 264-270.

3. Glasstone, S.; Laidler, K.J.; and Eyring, H.: Theory of Rate Processes. McGraw-Hill, New York, 1941.

4. Ree, T.S.; Ree, T.; and Eyringo, H.: Significant Structure Theory of Transport Phenomena. J. Phys. Chem., vol. 68, no. 11, 1964, pp. 3262-3267.

5. Akgerman, A.; and Gainer, J.L.: Predicting Gas-Liquid Diffusivities. J. Chem. Eng. Data, vol. 17, no. 3, 1972, pp. 372-377.

6. Cohen, M.H.; and Turnbull, D.: Moleculor transport in Liquids and Glasses. J. Chem. Phys., vol. 31, no. 5, 1959, pp. 1164-1169.

7. Hirschfelder, J.O.; Curtiss, C.F.; and Bird, R.B.: Molecular Theory of Gases and Liquids. Wiley, New York, 1964.

8. Lide, D.R.: CRC Handbook of Chemistry and Physics. Seventy-Third ed. CRC Press, Boca Raton, FL. 1993.

9. Hayduk, W.; and Buckley, W.D.: Effect of Molecular Size and Shape on Diffusivity in Dilute Liquid Solutions. Chem. Eng. Sci., vol. 27, no. 11, 1972, pp. 1997-2003.

10. Reid, R.C.; Prausritz, J.M.; and Poling, B.E.: The properties of Gases and Liquids. Fourth ed. McGraw-Hill, New York, 1987.

Notations

D	self diffusion coefficient
D_{AB}	diffusion coefficient of solute A and solvent B
E_A	number of B molecules around a central A molecule on the same plane
$E_{D(AB)}$	activation energy for diffusion
$E_{\mu B}$	activation energy for viscosity of solvent B
G	dimensionless function of $\Omega_{D_{AB}}$

ΔH_{vapor}	enthalpy of evaporation
K	Boltzman constant
MW_A	molecular weight of solute A
MW_B	molecular weight of solvent B
N	Avogadro's number
r	distance
R	universal gas constant
R_A	radius of solute A
T	absolute temperature
U_{Liq}	velocity of sound in solvent liquid phase
U_{vapor}	velocity of sound in solvent vapor phase
V_A	molar volume of solute A
V_B	molar volume of solvent B
V_{FB}	free volume of liquid B
V^*	hole volume
X_B	association number of solvent B
α	geometric packing factor
(ϵ/K)	Lennard-Jones energy parameter
σ	Lennard-Jones parameter distance
μ_B	viscosity of solvent B
ρ_B	density of solvent B
$\Omega_{D_{AB}}$	Lennard-Jones dimensionless function

TABLE 1

Solute A	Solvent B	Temp (K)	Exp'l D_{AB} x 10^5 (cm^2/sec)	Eq. 13 $D_{AB}x10^5$	S.E.	W.C.	Eyring	A.G.
CH_4	CCl_4	298	2.89	3.31 (-14)	1.07 (63)	3.96 (-37)	1.39 (52)	5.90 (-104)
CH_4	CCl_4	273	2.05	2.13 (-4)	0.68 (67)	2.46 (-20)	0.86 (58)	3.69 (-80)
C_6H_6	CCl_4	298	1.54	1.62 (-5)	-	-	-	-
Ar	CCl_4	298	3.63	3.79 (-4)	1.09 (70)	4.10 (-13)	1.38 (62)	4.54 (-25)
Ar	CCl_4	273	2.44	2.45 (0)	0.68 (72)	2.54 (-4)	0.88 (64)	2.88 (-18)
N_2	CCl_4	298	3.41	4.25 (-25)	1.06 (69)	3.82 (-12)	1.40 (59)	4.91 (-44)
N_2	CCl_4	273	2.44	2.77 (-14)	0.66 (73)	2.39 (2)	0.88 (64)	3.12 (-28)
O_2	CCl_4	298	3.71	3.70 (0)	1.15 (69)	4.34 (-17)	1.41 (62)	4.93 (-33)
CCl_4 (Self-diffusion)	CCl_4	298	1.41	1.55 (-10)	-	-	-	-
nC_6H_{14}	CCl_4	298	1.50	1.57 (-5)	-	-	-	-
CO_2	CCl_4	298	2.95	2.70 (8)	-	-	-	-
CO_2	C_2H_5OH	298	3.42	5.41 (-58)	0.86 (75)	2.05 (40)	1.37 (60)	1.81 (47)
N_2	C_6H_6	298	6.93	5.03 (27)	1.59 (77)	4.09 (41)	2.15 (69)	3.74 (46)

*Quantities in Parenthesis are % deviation

$$\% \text{ Deviation} = \left(\frac{\text{Exp'l value - calc. value}}{\text{exp'l value}} \right) \times 100$$

This definition used in Reference 5.

TABLE 2

Solute A	Solvent B	Temp. (K)	Exp'l D_{AB} x 10^5 (cm^2/sec)	Eq. 13 D_{AB} x 10^5	S.E.	W.C.	Eyring	A. G.
Cl_2	H_2O	298	1.45	2.92 (-101)	0.91 (37)	1.65 (-14)	2.44 (-68)	1.60 (-10)
SO_2	H_2O	298	1.94	2.98 (-54)	0.95 (51)	1.75 (10)	2.44 (-26)	1.71 (12)
O_2	H_2O	298	2.35	7.23 (-207)	1.15 (51)	2.44 (-4)	2.44 (-4)	2.42 (-3)
N_2	H_2O	298	2.01	9.28 (-362)	1.07 (47)	2.17 (-8)	2.45 (-22)	2.41 (-20)
CO_2	H_2O	298	1.91	4.61 (-141)	1.03 (46)	2.04 (-7)	2.45 (-28)	2.03 (-6)

*Lennard-Jones (6-12) potential used for water.

TABLE 3

Solute A	Solvent B	Temp (K)	Exp'l D_{AB} x 10^5 (cm^2/sec)	Eq. 17 D_{AB} x 10^5	S.E.	W.C.	Eyring	A.G.
Cl_2	H_2O	298	1.45	0.90 (38)	0.91 (37)	1.65 (-14)	2.44 (-68)	1.60 (-10)
SO_2	H_2O	298	1.94	1.63 (16)	0.95 (51)	1.75 (10)	2.44 (-26)	1.71 (12)
O_2	H_2O	298	2.35	2.24 (5)	1.15 (51)	2.44 (-4)	2.44 (-4)	2.42 (-3)
N_2	H_2O	298	2.01	2.78 (-38)	1.07 (47)	2.17 (-8)	2.45 (-22)	2.41 (-20)
CO_2	H_2O	298	1.91	1.44 (25)	1.03 (46)	2.04 (-7)	2.45 (-28)	2.03 (-6)
CO_2	C_2H_5OH	298	3.42	4.01 (-17)	0.86 (75)	2.05 (40)	1.37 (60)	1.81 (47)

*Stockmayer Potential used for water and for ethanol (C_2H_5OH)

TABLE 4

Solute A	Solvent B	Temp. (K)	Exp'l D_{AB} x10^5 (cm^2/sec)	Eq. 17 D_{AB} x 10^5	S.E.	W.C.	Eyring	A.G.
CO_2	C_2H_5OH	279.4	2.45	2.85 (-16)	0.56 (77)	1.35 (45)	0.91 (63)	1.23 (50)
CO_2	C_2H_5OH	283	2.78	3.05 (-10)	0.61 (78)	1.47 (47)	0.97 (65)	1.31 (53)
CO_2	C_2H_5OH	288	3.02	3.36 (-11)	0.70 (77)	1.63 (46)	1.09 (64)	1.48 (51)
CO_2	C_2H_5OH	298	3.42	4.01 (-17)	0.86 (75)	2.05 (40)	1.37 (60)	1.81 (47)
CO_2	C_2H_5OH	303	3.84	4.44 (-16)	0.96 (75)	2.27 (41)	1.50 (61)	2.04 (47)

*Stockmayer potential used for ethanol (C_2H_5OH).

TABLE 5

Solute A	Solvent B	Temp. (K)	Exp'l D_{AB} $\times 10^5$ (cm^2/sec)	Eq. 17 $D_{AB} \times 10^5$	S.E.	W. C.	Eyring	A.G.
CO_2	H_2O	2.83	1.25	1.09 (13)	0.68 (46)	1.33 (-6)	1.58 (-26)	1.34 (-7)
CO_2	H_2O	288	1.40	1.19 (15)	0.78 (44)	1.55 (-11)	1.85 (-32)	1.55 (-11)
CO_2	H_2O	293	1.70	1.30 (24)	0.90 (47)	1.80 (-6)	2.13 (-25)	1.80 (-6)
CO_2	H_2O	298	1.91	1.43 (25)	1.03 (46)	2.04 (-7)	2.43 (-27)	2.03 (-6)
CO_2	H_2O	303	2.27	1.56 (31)	1.20 (47)	2.32 (-2)	2.75 (-21)	2.29 (-1)
CO_2	H_2O	313	2.77	1.84 (33)	1.47 (47)	2.91 (-5)	3.46 (-25)	2.83 (-2)
CO_2	H_2O	323	3.24	2.18 (33)	1.81 (44)	3.60 (-11)	4.28 (-32)	3.47 (-7)
CO_2	H_2O	338	4.29	2.77 (35)	2.40 (44)	4.72 (-10)	5.62 (-31)	4.51 (-5)

*Stockmayer Potential used for water.

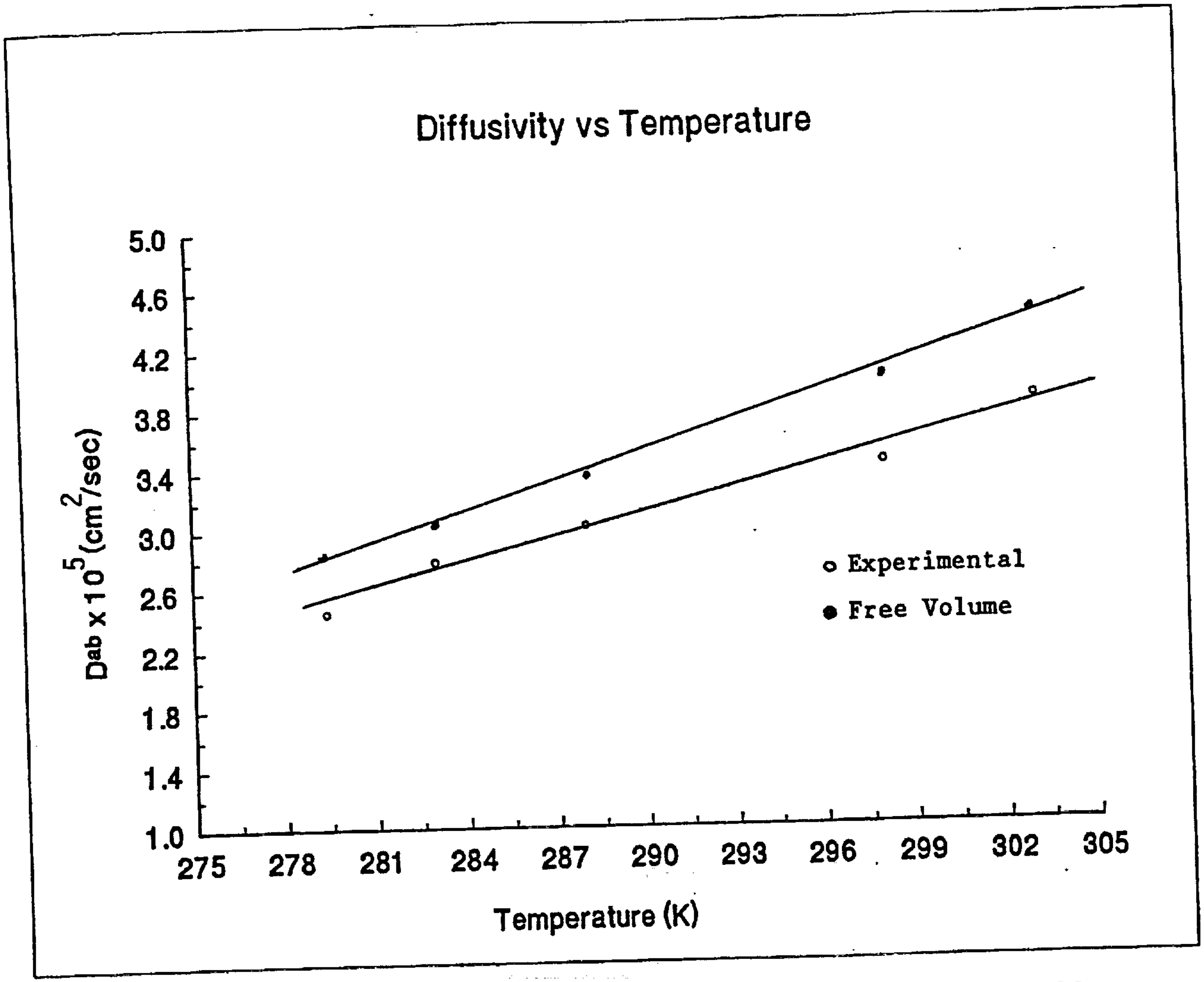

Figure 1. Comparison of Experimental and Free Volume Binary Liquid Diffusion Coefficients for the CO_2-Ethanol System

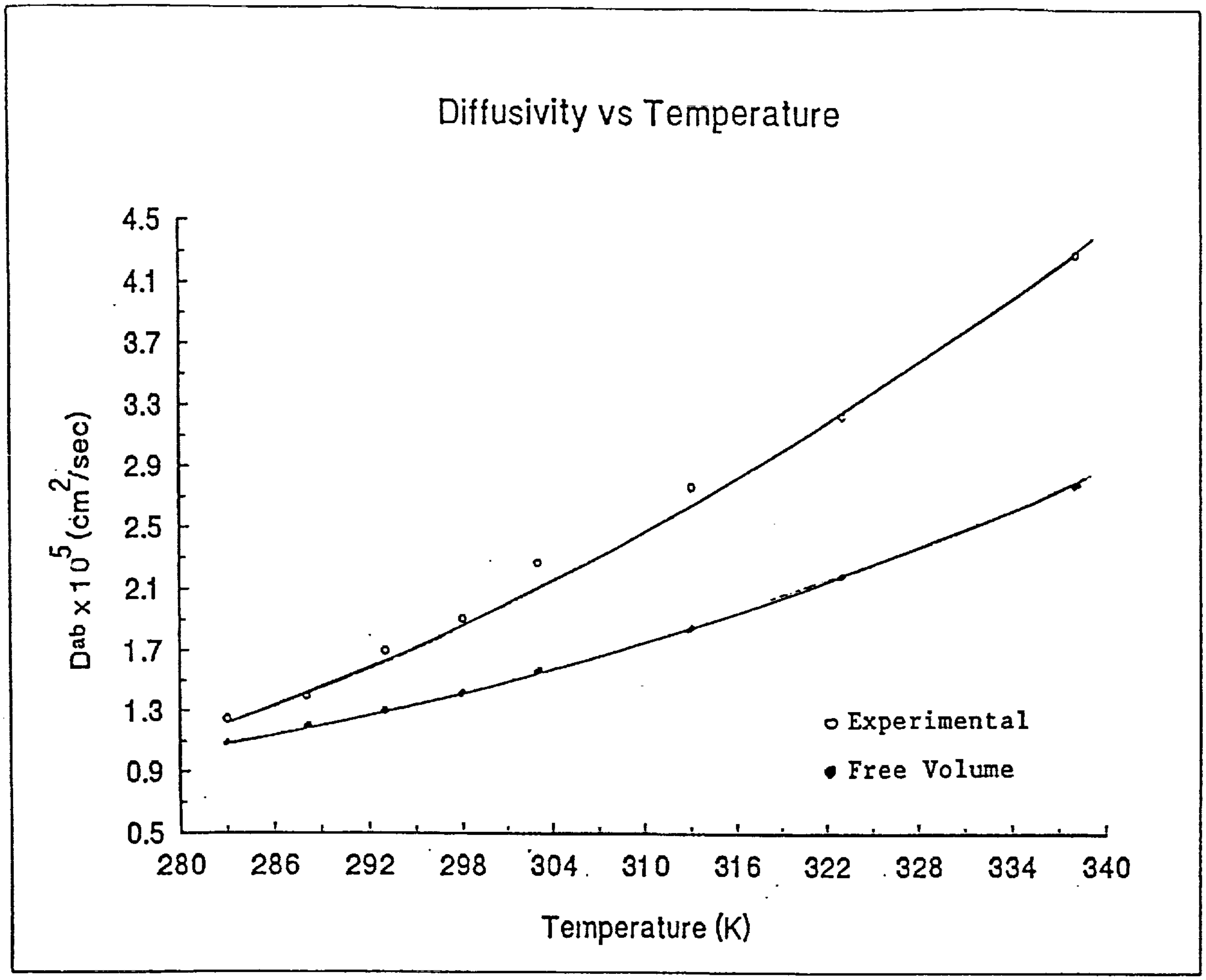

Figure 2. Comparison of Experimental and Free Volume Binary Liquid Diffusion Coefficients for the CO_2-Water System

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An equation, based on the free volume of a liquid solvent, was derived via dimensional analysis, to predict binary diffusion coefficients. The equation assumed that interaction between the solute and liquid solvent molecules followed a Lennard-Jones [6-12] potential. The equation was compared to other diffusivity equations and was found to give good results over the temperature range examined.

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