Registry No. H_2, 1333-74-0; Tetralin, 119-64-2; 2-methylnaphthalene, 91-57-6; *p*-cresol, 106-44-5; 4-picoline, 108-89-4; methyltetralin, 31291-71-1; naphthalene, 91-20-3; 2-methyltetralin, 3877-19-8.

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Received for review March 21, 1984. Accepted September 20, 1984. Contribution No. 266 from the thermodynamics research branch of the National Institute for Petroleum and Energy Research. The work upon which this research was based was sponsored by the Division of Coal Liquefaction Technology, Office of Fossil Energy, Department of Energy, and was conducted at what was formerly the Bartlesville Energy Technology Center, Department of Energy. This report was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency therefore, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

Supplementary Material Available: Two tables showing *Z*-series composition (Table VIII) and elemental analysis (Table IX) of SRC II heavy distillate 1009, three tables showing enthalpy of combustion results for samples 1007, 1008 and 1009 and the reconstituted whole crude (Tables X–XII), one table of crude distillation of blended coal liquid (Table XIII), and two tables of compositional and elemental analyses (Tables XIV and XV) of distillates from the blended coal liquid (8 pages). Ordering information is given on any current masthead page.

Diffusion Coefficient of Chlorine in Water at 25–60 °C

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The molecular diffusivity of chlorine in water was measured over the temperature range 25–60 °C and at atmospheric pressure by using a laminar jet apparatus. Experimental results are compared to values reported in the literature and with correlations. The diffusivity was found to vary from 1.38 × 10^{-5} cm^2/s at 25 °C to 3.11 × 10^{-5} cm^2/s at 60 °C.

Introduction

The purpose of this note is to report experimental values of the diffusion coefficient for chlorine in water measured over the temperature range 25–60 °C. A laminar liquid jet device was used in these experiments, and the experimental results are compared to values reported in the literature (Spalding (*1*), Ibrahim and Kuloor (*2*), Kramers et al. (*3*)) and with correlations (Wilke and Chang (*4*), Scheibel (*5*), Othmer and Thakar (*6*), Akgermann and Gainer (*7*)).

In this study we have followed Spalding (*1*) and used 0.1 N HCl rather than pure water in order to suppress the hydrolysis reaction

$$Cl_2(aq) + H_2O \rightleftarrows HOCl + H^+ + Cl^- \qquad (1)$$

It is necessary to suppress the hydrolysis reaction so that this reaction will not affect the rate of absorption and give a diffusion coefficient that is larger than the true value. For 0.1 N HCl at 25 °C, only 5.8% of the chlorine is hydrolyzed at equilibrium. Since the contact time in the jet device is short (less than 0.025 s) and the rate of hydrolysis is slow, the reaction has little effect on the rate of absorption. The addition of 0.35 wt % HCl to give a 0.1 N solution is expected to have little effect on the physical properties of the solution. For example, a falling-ball viscosimeter was used to measure the viscosity of the 0.1 N HCl solution and the viscosity was found to be 0.919 cP at 25 °C. This value may be compared to the pure-water viscosity of 0.890 cP at 25 °C. The viscosity is therefore only increased 3% by the addition of HCl. The Stokes–Einstein relation ($D\mu/T$ = a constant) normally overpredicts the effect of electrolytes on the diffusion coefficient and can be used to estimate a maximum effect on the diffusion coefficient by the addition of HCl. Thus, it is expected that the diffusion coefficient measured in this work for 0.1 N HCl is within 3% of the value for pure water.

Raimondi and Toor (*8*) did an extensive study on different jet designs and their characteristics. Using the CO_2–water system they found that jets formed by flow through thin, square-edged orifice plates produced absorption rate results closest to the theoretical values for rodlike flow and no interfacial resistance. In our work we have followed the results of Raimondi and Toor and have used a jet nozzle consisting of a square-edged orifice 5.1 × 10^{-4} m in diameter drilled in a 8.0 × 10^{-5} m thick stainless steel sheet. The face of the nozzle was coated with a thin layer of wax to prevent wetting.

For an ideal cylindrical jet the contact time for the liquid is given by

$$t = \pi d^2 l/4q \qquad (2)$$

Application of penetration theory to predict the rate of gas absorption with the contact time given by eq 2 gives

$$R = 4(Dql)^{1/2}C^{*} \qquad (3)$$

In eq 3 R, q, and l can be measured, and the gas solubility, C^{*}, is available from the literature. The diffusion coefficient, D, can thus be calculated from eq 3.

Experimental Apparatus and Procedure

A schematic drawing of the jet apparatus is shown in Figure 1. The temperature of the system is monitored by thermometers in the constant-temperature bath, in the jet chamber, and in the fluid stream.

The liquid feed is pumped through a rotameter and through a coil in the constant-temperature bath. It is then fed into a

0021-9568/85/1730-0189$01.50/0

Table I. Diffusivities of CO_2 in Water at 25 °C

$10^9 D_A$, m^2/s	ref	$10^9 D_A$, m^2/s	ref
1.92	*9*	1.98	*12*
2.00	*10*	1.98	this work
1.95	*11*		

Table II. Diffusivity of Cl_2 in Water

ref	T, °C	$10^5 D_A$, cm/s
this work	25	1.38
this work	35	1.63
this work	45	2.44
this work	60	3.11
1	25	1.48
2	25	1.40
3	25	1.42
3	35	1.81

glass slide tube. The height of the tube is adjusted by a screw mechanism which can vary the jet length from 0 to 0.20 m. The gas supply is fed through a rotameter and through a coil in the constant-temperature bath. It is then introduced into the jet chamber at the base of the jet near the receiver and is exhausted at the top of the chamber. The gas flows countercurrent to the liquid.

The jet chamber is made of a 0.25 m long, 0.044 m i.d. Plexiglas tube and is enclosed by the constant-temperature bath constructed from a 0.25 m long, 0.125 m i.d. Plexiglas tube.

The jet nozzle assembly attaches to a glass inlet tube by two O rings and six plastic screws. These screws also help to center the jet. The receiver is a capillary tube of 0.1×10^{-2} m i.d. fitted into a funnel-shaped base. A hole in the base allows draining of any liquid overflow. The jet is centered by manipulating the plastic screws on the nozzle assembly and by rotation of the glass tube. The jet is considered centered when all of its contents empty into the capillary tube with no overflow.

A leveling device consisting of a cup with an overflow drain is mounted on a pulley mechanism. This assembly allows very precise adjustments of the liquid level. If the level in the capillary tube is too low, gas entrainment occurs; if too high, then the liquid overflows. After changes in the liquid flow rate, the liquid level has to be readjusted. The length of the jet was measured by a cathetometer with an error of less than 0.5×10^{-4} m.

After the jet is flowing satisfactorily, the gas is turned on for enough time for the jet chamber and all the tubing to fill with the gas. Then the gas is turned off; the rate of gas absorption is found by measuring the amount of time needed for a soap film to travel through a certain volume.

All of the experiments were done under atmospheric pressure. The liquid flow rate varied between 20 and 60 mL/min and the exposure time varied approximately between 0.005 and 0.02 s.

Results

To test the experimental technique some initial experiments with carbon dioxide were carried out. The average value found for the diffusion coefficient of CO_2 in water at 25 °C is 1.98×10^{-9} m^2/s. This value shows good agreement with values available in the literature as shown in Table I.

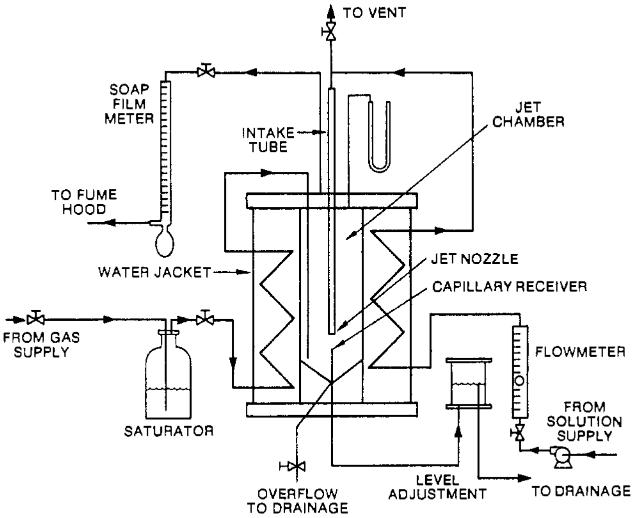

Figure 1. Schematic drawing of liquid jet apparatus.

The values obtained for the diffusion coefficient of chlorine in water are shown in Table II. Table II also compares the experimental values found in this work with those in the literature. Where data are available at 25 and 35 °C there is good agreement with the experimental results of this work.

The solubility of molecular chlorine in water (C^*), which is needed in order to calculate the diffusivity, was obtained from the data given in Perry et al. (*13*). The Henry's law coefficient for the 0.1 N HCl solutions used in this work was calculated by using the method recommended by Danckwerts (*14*)

$$\log (H/H^\circ) = hI \tag{4}$$

H° is the Henry's law constant for pure water, and I is the ionic strength of the solution defined as

$$I = \frac{1}{2}\sum_{i=1}^{n} c_i z_i^2 \tag{5}$$

h is composed of contributions from the negative ion, the positive ion, and from the gas itself.

$$h = h_- + h_+ + h_G \tag{6}$$

Danckwerts gives $h_-(Cl^-) = 0.021$ and $h_+(H^+) = 0$. h_G for chlorine is given as a function of temperature by Hikita et al. (*15*).

Table III compares the experimentally determined diffusivities with predicted values obtained from the correlations of Wilke and Chang (*4*), Scheibel (*5*), Othmer and Thakar (*6*), and Akgermann and Gainer (*7*). The percent deviation in Table III is defined as

$$\% \text{ devn} = 100[(\text{calculated} - \text{experimental})/\text{experimental}] \tag{7}$$

It is found that the correlation of Scheibel best predicts the experimental results.

Table III. Comparison of Diffusivity of Cl_2 in Water Obtained by Calculated and Experimental Methods

	$10^9 D$, m^2/s								
		Wilke–Chang		Scheibel		Othmer–Thaker		Akgermann–Gainer	
T, °C	exptl	calcd	% devn	calcd	% devn	calcd	% devn	calcd	% devn
25	1.38	1.72	24.6	1.31	-5.1	1.61	16.7	1.62	17.4
35	1.63	2.19	34.4	1.68	3.1	2.04	25.2	2.05	25.8
45	2.44	2.73	11.9	2.09	-14.3	2.50	2.5	2.52	3.3
60	3.11	3.63	16.7	2.78	-10.6	3.25	4.5	3.29	5.8
			21.9 (av)		-6.7 (av)		12.2 (av)		13.1 (av)

Glossary

C_i	ion concentration, kg mol/m^3
C^*	interfacial concentration of molecular chlorine, kg mol/m^3
d	jet diameter, m
D	diffusion coefficient, m^2/s
H°	Henry's law coefficient for pure water, Pa m^3/(kg mol)
H	Henry's law coefficient corrected for ions in solution, Pa m^3/(kg mol)
h, h_-, h_+, h_G	empirical parameters, m^3/(kg mol)
I	ion valence
l	jet length, m
q	liquid flow rate, m^3/s
t	contact time, s
π	3.141 59

Registry No. Cl_2, 7782-50-5.

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Received for review March 26, 1984. Accepted August 27, 1984.

Relative Viscosity and Density Data for Some Alkali Halides in Aqueous 20% Sucrose Solution at 25 °C

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Relative viscosity and density data are presented for seven alkali halides in aqueous 20% sucrose solution at 25 °C. The relative viscosities were fitted to the Jones–Dole equation. Corresponding data for aqueous solutions are also presented in most instances and the coefficients of the Jones–Dole equation compared where possible with literature values. *B* coefficients are shown to be additive properties of the constituent ions in aqueous 20% sucrose solution. Individual ionic *B* coefficients are assigned.

Introduction

For concentrations below 0.2 M, the dependence of the relative viscosity, η_r, of an electrolyte solution upon the molar concentration, C, of the electrolyte is generally in accordance with the Jones–Dole (*1*, *2*) equation

$$\eta_r = 1 + AC^{1/2} + BC \qquad (1)$$

The A coefficient of this equation is an index of ionic interactions. Falkenhagen (*3*) derived an explicit expression for A in terms of limiting ionic equivalent conductances λ and solvent properties. For a 1:1 electrolyte in a solvent of viscosity η_0 and dielectric constant ϵ_0, the expression reduces to

$$A = \frac{1.45}{\eta_0(2\epsilon_0 T)^{1/2}}\left[\frac{\lambda_1 + \lambda_2}{4\lambda_1\lambda_2} - \frac{(\lambda_1 - \lambda_2)^2}{(3 + 2^{1/2})\lambda_1\lambda_2(\lambda_1 + \lambda_2)}\right] \qquad (2)$$

where the subscripts 1 and 2 designate cation and anion, respectively.

Table I. Equivalent Conductances of Cesium Chloride Solutions in Aqueous 20% Sucrose at 25 °C

C	Λ, cm^2 Ω^{-1} g equiv^{-1}
0.002 313 8	92.579
0.010 528	89.865
0.016 607	88.587
0.020 629	87.918
0.040 881	85.446
0.054 490	84.313

If the influence of incomplete dissociation (or ion association) and the consequences of an approximation made in Falkenhagen's theory are neglected, the B coefficient may be regarded as an index of ion–solvent interaction.

Experimental Section

Relative viscosities were determined by using a flared-capillary viscometer described in a previous publication (*4*). For this viscometer kinetic energy corrections were unnecessary for water and 20% sucrose solution (*4*, *5*) and hence for the systems included in the present study. Thus, relative viscosities were calculated according to

$$\eta_r = \rho t/(\rho_0 t_0) \qquad (3)$$

where ρ represents density and t flow time. The subscript 0 refers to values for the solvent. The uncertainty in the measurements of flow times was about 0.01%. For the minimum of three consecutive flow times which were averaged for each solution the reproducibility was usually much better than 0.01%.

Densities were determined by using tare pycnometry. Three single-stemmed bulb pycnometers of approximately 30-cm^3 capacity were fabricated such that their masses were equal within 0.002 g and all contained the same volume of liquid (within 0.02 cm^3) when filled to a scratch mark on the stem of each. An accompanying tare of closely similar mass and shape

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