

## Diffusion of Oxygen to Aqueous Surfactant Solutions

Saadet YAPAR, Sümer PEKER, Beno KURYEL  
*Ege University, Engineering Faculty, Chemical Engineering Department,  
35100 Bornova, İzmir-TURKEY*

Received 13.08.1998

### Abstract

In this work, the diffusion of oxygen in solutions of alkyl (C13-15) benzyldimethyl ammonium chloride (ABDAC), nonylphenol (9) ethoxylate (NP9EO) and their mixture was investigated. The variation of oxygen concentration in ABDAC solution was found to be linear. The deviation from the linearity observed in NP9EO solutions was attributed to the trapping of oxygen molecules in the interstices of the coils of ethoxylate chains. Apparent diffusion coefficients of oxygen in the solutions were calculated analytically and numerically. In surfactant solutions, the diffusion coefficients passed through a minimum. The rigidity of the monolayer was found to be the predominant effect in the reduction of the transfer rate.

**Key Words:** Diffusion of Oxygen, Surfactants, Monolayer, Marangoni Instability.

## Oksijenin Yüzey Aktif Madde Çözeltilerine Difüzyonu

### Özet

Bu çalışmada oksijenin alkil (C13-15) benzildimetil amonyum klorür (ABDAC) ve nonil fenol (9) etoksilat çözeltilerine difüzyonu incelendi. ABDAC çözeltilerinde oksijen konsantrasyonunun doğrusal olarak değiştiği gözlemlendi. NP9EO çözeltilerinde gözlenen doğrusallıktan sapma, oksijenin etoksilat zincirleri arasındaki boşluklarda hapsolmesi ile açıklandı. Oksijenin çözelti içindeki görünür difüzyon katsayısı analitik ve nümerik olarak hesaplandı. Difüzyon katsayısının bir minimumdan geçtiği ve transfer hızını azaltan asıl faktörün monolayer yapısı olduğu tespit edildi.

**Anahtar Sözcükler:** Oksijen Difüzyonu, Yüzey Aktif Madde, Monolayer, Marangoni Kararsızlığı.

### 1. Introduction

Diffusion of oxygen in surfactant solutions is of importance in biological processes such as wastewater treatment, fermentation, and production of bio-surfactants and in industrial applications such as in temporary corrosion prevention.

The presence of surfactants at the gas-liquid interface may cause a change in the mobility of the interface which in turn strongly depends on the existence of surface tension gradients. Under the effect of these gradients, the mobility of a surface can

be changed from complete stagnation to free motion. The pulling of the interface toward areas with higher tensions, Marangoni instability, can result in convection. The common effect of the Marangoni instability is the continuous renewal of the surface and therefore an increase in the rate of mass transfer (Thompson, 1970). Gibbs adsorption completely suppresses the Marangoni convection (Brian, 1971) and the result of this suppression is the formation of a resistance layer to flow and therefore a decrease in the rate of mass transfer (Sherwood, 1975). This effect may be

offset by a possible increase in the specific surface area (Zieminski, 1967).

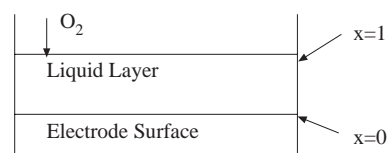
Retardation of mass transfer by surfactant monolayers was considered in terms of its overall effects in the literature. Work has been done to relate the interfacial behavior of surfactants to the rate of mass transfer. Lindland and Terjesen (1956) showed that the mass transfer from drops of carbon tetrachloride falling in water was reduced by 68 % with the addition of  $6.10^{-5}$  gram surfactant per 100 ml water. The mechanism by which the surfactant monolayer retards diffusion has been a controversial issue. Thompson (1970) investigated the diffusion of ammonia, and carbon and sulfur dioxides through surface films of long-chain alcohols. He could not detect any increase in mobility of the surface in the presence of surfactants and the reduction in interfacial mass transfer was attributed to the additional resistance formed by the monolayer. Brian (1971) indicated that the convection causes spontaneous emulsification in liquid-liquid extraction systems and the mass transfer rate is enhanced more than tenfold in gas-liquid systems. On the other hand, Davies (1972) showed the suppression of surface renewal by surface active agents to be mainly responsible for the reduction in the mass transfer rate.

Hüttinger and Schegk (1982) investigated the effect of anionic surface active agents on the degree of simultaneous dispersion and mass transfer in liquid-liquid extraction. On the grounds that surface rigidity is mainly responsible for the reduction in the mass transfer rate, they proposed destabilization of the interface to increase the mass transfer rate. Such destabilization could be brought about by a structural change in the monolayer, e.g., the use of an electrolyte to create the salting-out effect, spatial separation of surface active molecules by ions present in the subphase or forming a mixed monolayer of the surfactants having different hydrophile/lipophile group ratios.

In the literature cited above, the effect of surfactant monolayers on the rate of mass transfer was considered in terms of overall mass transfer coefficients or equivalent interfacial resistances. In this work, the effect of the monolayer is intended to be interpreted in terms of diffusion coefficients of oxygen in water and in the solutions of surfactants exhibiting various degrees of synergism as pairs (Yapar and Peker, 1994).

## 2. Description and Evaluation of Experimental Method

The measurement of concentration gradients in a diffusing system or the transfer of gas into or out of a liquid phase are the most widely used techniques to determine molecular diffusion coefficients of dissolved gases. The accurate measurement of the transport of very small quantities of gas and prevention of convection currents in the diffusion cell are major problems (Himmelblau, 1964). To overcome these problems, a Clark-type oxygen electrode was used in this work, which has higher accuracy. Goldstick (1970) showed that the electrode could be used to measure the diffusion coefficient. The experimental method used is based on the measurement of the changes in oxygen concentration at the bottom of the liquid layer.



Diffusion coefficients were calculated using the analytical and numerical solutions of the unsteady-state mass transfer equation given in Appendix A.

### Analytical Solution of Mass Transfer Equation

$$\theta = \frac{C^* - C}{C^* - C_0} = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \exp \left[ \frac{-D(2n+1)^2 \pi^2 t}{4l^2} \right] \cos \frac{(2n+1)\pi x}{2l} \quad (1)$$

Due to the existence of the monolayer, the equilibrium value of the oxygen concentration changes. For this reason, Eq. 1 was (Kuryel, 1976) rearranged.

The error introduced by taking only the first term of the series does not exceed  $\pm 0.3\%$  for  $\theta < 0.6$  and  $0 < x < 0.05l$  (Kuryel, 1976). Under these considerations Eq. 1 becomes

$$\theta = \frac{4}{\pi} \exp(-D\pi^2 t/4l^2) \quad (2)$$

If the time required for  $\theta = 0.1$  is  $t_1$ ,

$$0.1 = \frac{4}{\pi} \exp(-D\pi^2 t_1/4l^2) \quad (3)$$

for  $t=0$ ,  $\theta = 1$  for  $t=0$ ,  $q = 1$

$$1.0 = \frac{4}{\pi} \exp(-D\pi^2 0/4l^2) \quad (4)$$

Dividing Eq. 4 by 3 gives

$$D = \left( \frac{4l^2}{t_1\pi^2} \right) \ln 10 \quad (5)$$

and

$$\theta = \frac{4}{\pi} 10^{-t/t_1} \quad (6)$$

Equation 6 may be rearranged to give

$$C = A + \frac{4}{\pi} B 10^{-t/E} \quad (7)$$

where  $A=C^*$ ,  $B=(C_0-C^*)$  and  $E=t_1$ . The coefficients of Eq. 7, were found from the experimental data with non-linear regression and the diffusion coefficient from Eq. 5.

*Numerical Solution of Mass Transfer Equation*

An inherent handicap of this method is the imposition of the effects associated with the possible convection at the beginning of the experiment on the diffusion coefficient. To see the extent of the initial convection, the governing equation was solved numerically by using a Crank-Nicolson scheme. Details are given in Appendix A.

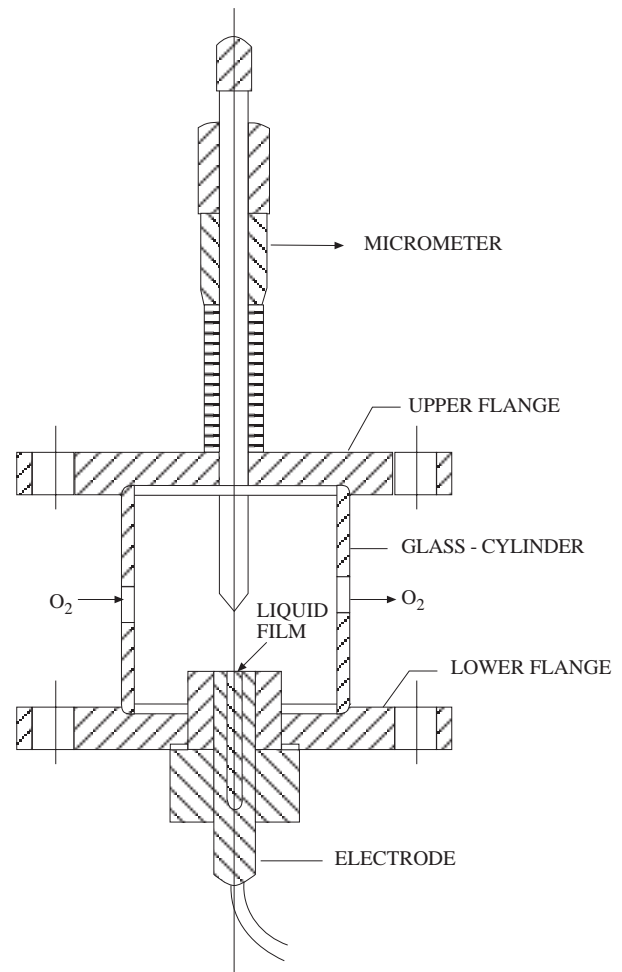
**3. Experimental**

The surfactants, nonylphenol(9) ethoxylate and alkylbenzyltrimethyl ammonium chloride were purchased from Gemsan A.Ş. Turkey. They were used as supplied.

The experiments were conducted in a diffusion cell, as shown in Figure 1. During the experiments, the temperature of the room was kept at 25°C. A Clark-type oxygen electrode was used to determine the oxygen concentration. The electrode was calibrated according to the method recommended by the manufacturer, before the measurements (Operating Instructions, Digital Oxygen Meter CG 867). After the calibration, it was inserted into the diffusion cell. The liquid film was formed by pouring a certain amount of solution into the cavity formed by winding a PTFE band 2.9 mm. in height around the electrode. The cell was covered and mounted between the upper and lower flanges. The film thickness was measured with a micrometer mounted on the upper flange at the beginning and at the end of the experiments.

After mounting the diffusion cell, measurements were done in groups by using air and/or oxygen as the gas phase. Both air and oxygen were saturated with water to prevent the evaporation of water from the solution. The aim of using two different media as

oxygen sources was to maintain a stepwise increase in the concentration difference between the gas and liquid phases. The step changes in concentration, in terms of gas and liquid phase concentrations, are given in Table 1. In the first group of experiments, the liquid phase was degassed by passing nitrogen at high volumetric flow rates (12-13 ml/s) through the headroom above the liquid layer until the concentration of oxygen in the liquid phase decreased to as near zero as feasible. The head room was cleaned of its N<sub>2</sub> content by passing air for a minute at maximum flow rate. Then the air flow rate was reduced to 1-2 ml/s and the change in the concentration of oxygen at the bottom of the liquid film with time was recorded.



**Figure 1.** Diffusion Cell.

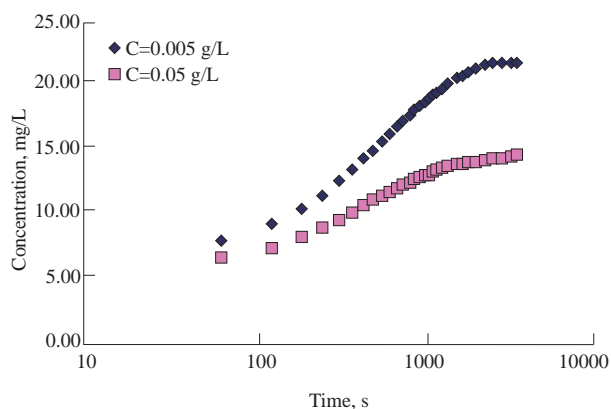
**Table 1.** Concentrations of Oxygen in Water Corresponding to Partial Pressure in the Gas Phase (  $T = 25^\circ\text{C}$  )

Gas Phase	Liquid Phase
$P_{O_2}$ (atm)	$C_{O_2}$ (mol/L). $10^4$
0.2	2.5
1.00	5.53

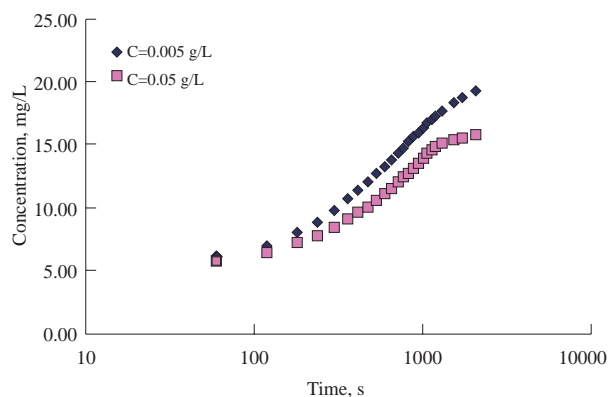
In the second group of experiments, the liquid phase was saturated with oxygen in air until the oxygen concentration in the liquid phase remained constant. After saturation, the same procedure was followed by using oxygen instead of air, to attain a stepwise increase in the driving force.

#### 4. Results and Discussion

The effect of the bulk concentrations of ABDAC and NP9EO on the variation of the  $O_2$  concentration at the bottom of the liquid film are given in Figures 2 and 3, respectively. The oxygen concentration at any time decreases with an increase in the concentration of NP9EO and ABDAC solutions, the decrease being greater in the case of ABDAC. After an initial retention period, a sharp increase in concentration is observed in NP9EO solutions. This increase is more gradual in ABDAC solutions.

**Figure 2.** Variation of Oxygen Concentration with ABDAC Bulk Concentration.

Retardation of oxygen transfer by the surfactant monolayer can be explained by plots of dimensionless concentration of oxygen  $\theta_s$  in the presence of surfactants drawn against  $\theta_w$  for clean surfaces. Such plots are given for solutions of ABDAC, NP9EO and their mixture in Figures 4, 5 and 6, respectively.

**Figure 3.** Variation of Oxygen Concentration with NP9EO Bulk Concentration.

The change of  $\theta_s$  in NP9EO solutions has a curvature whereas the plots of ABDAC are linear up  $\theta_w = 0.85$ . If the linearity could be attributed to the hydrophobic chain resistance (or resistance of the monolayer), the deviation from linearity would indicate the existence of another factor interfering with the transfer mechanism. A possible explanation for this behavior could be the "trapping" of oxygen molecules in the interstices of the coils of ethoxylate chains. The entrapping of water and oxygen molecules in the solution of polyoxyethylene surfactants was reported by Eini et al. (1976) and Infante et al. (1982). Depending on the molecular weight of the micelles, the polyoxyethylene surfactants form spherical, disk- or rod-shaped micelles (Schick, 1966). Tanford (1972) proposed that these micelles contain a hydrophobic core consisting of a hydrocarbon chain. Eini (1976) found that these micelles were heavily hydrated due to the formation of water-ether oxygen bonds and physically trapped water in the hydrophilic chains. Infante (1982) also attributed the high concentration of oxygen in micellar solutions of polyoxyethylene surfactants to the trapping of oxygen in the core of micelles. After the ethoxylate layer becomes saturated with  $O_2$ , all of the transfer is directed to the bulk.

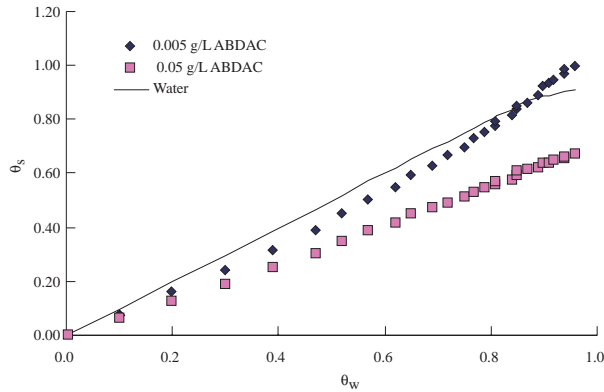
The behavior of the mixtures in Figure 6 is again linear as in the case of ABDAC.

#### The Variation of Apparent Diffusion Coefficient in Solutions

The model equations used in this work were checked by calculating the diffusion coefficient of oxygen in pure water. Janssen and Stroe (1993) pointed out the divergence of the diffusion coefficients given in the literature even when determined

under similar conditions. The values given in the literature range in between  $1.87 \times 10^{-5}$  and  $2.6 \times 10^{-5}$   $\text{cm}^2/\text{s}$  at  $25^\circ\text{C}$  (Himmelblau, 1964). In the present work, the diffusion coefficient of oxygen in pure water was determined to be  $1.74 \cdot 10^{-5}$  with the analytical solution and  $2.1 \cdot 10^{-5}$   $\text{cm}^2/\text{s}$  with the numerical solution of the model equation using the same experimental data. The difference between these two values may be the result of the convergency of the solutions.

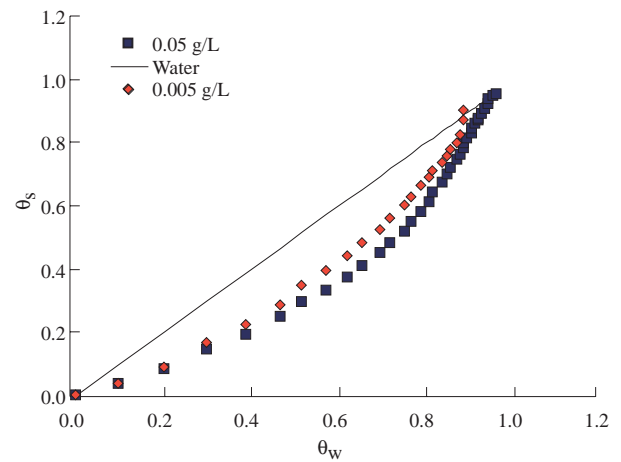
The variation of apparent diffusion coefficients with surfactant concentration in solutions saturated with the oxygen in air are calculated by using Equations 7 and 5 and given in Tables 2 and 3 for ABDAC and NP9EO, respectively. Examination of the tables reveals that the apparent diffusion coefficient of oxygen increases following an initial decrease with increasing surfactant concentration, passing through a minimum for both surfactants. Minimum diffusion coefficients are observed at  $8.1 \times 10^{-6}$  mol/L concentration in NP9EO and  $4.8 \times 10^{-5}$  mol/L in ABDAC. In the case of ABDAC, the increase appears near the critical micelle concentration (CMC) and for NP9EO, the increase starts well below the CMC. The critical micelle concentrations are  $5.44 \times 10^{-5}$  mol/L, and  $6.81 \times 10^{-5}$  mol/L, for ABDAC and NP9EO, respectively (Yapar and Peker, 1994).



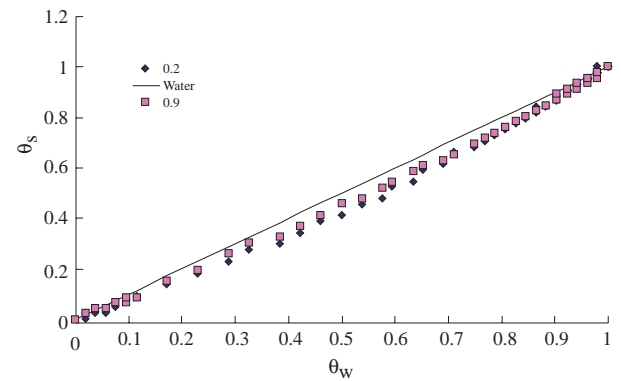
**Figure 4.** Variation of the Dimensionless Concentration of Oxygen in ABDAC Solutions.

Comparison of the tables shows that in spite of retention of oxygen in ethoxylate groups in the monolayer, the diffusion coefficients of oxygen in NP9EO solutions are higher than those of ABDAC. These high values may be attributed to the interfacial properties of NP9EO. Polyoxyethylene alkylphenols form gaseous films at the interface and polyoxyethylene chains penetrate the aqueous phase in

the form of coils (Schick, 1966). In addition to the type and structure of the film, the surface excess concentration of NP9EO is much lower than that of ABDAC. In a previous work, the surface excess concentrations were found to be  $2.64 \cdot 10^{-10}$  mol/ $\text{cm}^2$  and  $3.35 \cdot 10^{-10}$  mol/ $\text{cm}^2$  for NP9EO and ABDAC, respectively (Yapar and Peker, 1994). The corresponding areas occupied by a surfactant molecule are 62.8 and 49.5  $\text{A}^2/\text{molecule}$ . A comparison of these values reveals that the surface film formed by NP9EO molecules was more sparse than the surface film of ABDAC. If the surface can be considered analogous to a two-dimensional porous medium, corresponding tortuosity factor will be much lower and the mass transfer rate higher in the case of NP9EO.



**Figure 5.** Variation of the Dimensionless Concentration of Oxygen in NP9EO Solutions.



**Figure 6.** Variation of the Dimensionless Concentration of Oxygen in Mixtures.

**Table 2.** Apparent Diffusion Coefficient of Oxygen in ABDAC Solutions at 25°C)

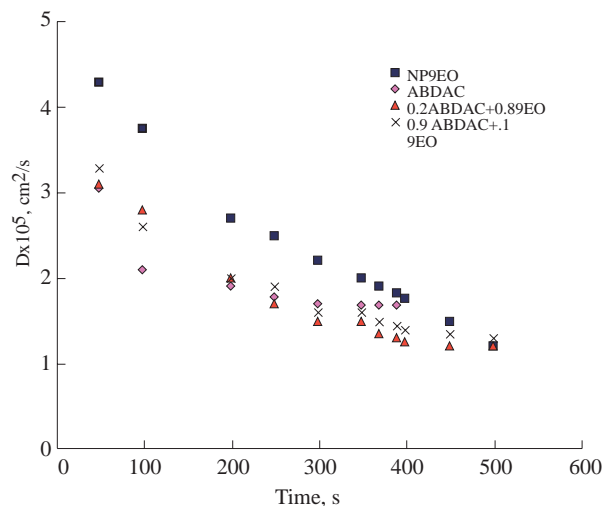
$C_{bulk}$ (mol/L)	$D \times 10^{-5}$ (cm <sup>2</sup> /s)
0	1.74
$2.7 \times 10^{-6}$	1.65
$4.8 \times 10^{-5}$	1.27
$5.4 \times 10^{-5}$	1.35
$8.2 \times 10^{-5}$	1.43

**Table 3.** Apparent Diffusion Coefficient of Oxygen in NP9EO Solutions at 25°C)

$C_{bulk}$ (mol/L)	$D \times 10^{-5}$ (cm <sup>2</sup> /s)
0	1.74
$8.1 \times 10^{-6}$	1.14
$1.6 \times 10^{-5}$	1.66
$3.2 \times 10^{-5}$	1.80
$6.5 \times 10^{-5}$	2.59

The variation of the numerically calculated diffusion coefficients with time are given in Figure 7. The diffusion coefficients of oxygen in ABDAC and in its mixtures show a sharp decrease initially, whereas, the decrease in NP9EO is much more gradual; that is, the effect of ABDAC is observed in the initial sharp decrease of diffusion coefficients. The reason for this behavior may be the formation of turbulence at the surface during the cleaning of the headroom. The mobility of the surface due to the turbulence has two consecutive effects. At the beginning, the monolayer is destroyed and it is mixed with the bulk of the solution. The result of this mixing is a change in the distribution of surfactants along the surface and the formation of surface tension gradients resulting in Marangoni instability. The magnitude of the initial value of diffusion coefficients reflects the mobility of the surface. After an initial period representing the mobility of the surface, the diffusion coefficients reach a constant value in the case of ABDAC. In the presence of ethoxylate the diffusion coefficients do not reach a constant value due to the existing Marangoni instability. Marangoni instabilities can be suppressed by removing the monomer diffusion gradients and a uniform surfactant distribution (Stebe,1993). When the adsorption kinetics and the decrease in the self-diffusion coefficients in dilute solutions of nonionic surfactants (Schick,1966 and Kato et al., 1993) are considered, it can be said that the restoration of the surface will take longer. This may be a plausible explanation for the gradual decrease in the diffusion coefficients of oxygen

in NP9EO solutions. The decrease in the diffusion coefficients is appreciable in pure NP9EO and is present to a lesser degree in its mixtures. Due to the higher diffusion rate of ABDAC in comparison with NP9EO, the surface can be restored rapidly in mixtures and therefore the decrease in the diffusion coefficients will be present to a lesser degree.

**Figure 7.** The Numerically Calculated Oxygen Diffusion Coefficients.

The synergism in this system is due to the interaction of ABDAC with NP9EO molecules through dispersion forces. It was shown in a previous paper (Yapar and Peker, 1994) that the ethoxylate chains wind up around the positively charged amine group of ABDAC. As this molecular complex is more spherical in shape, compaction of the surface monolayer becomes possible. The maximum interaction is observed at an ABDAC mol ratio of 0.2. The diffusion coefficients given in Figure 7 follow the same trend. The minimum diffusion coefficients are observed at maximum synergism.

#### 4. Conclusion

Both ABDAC and NP9EO monolayers and mixed monolayers form an additional resistance to mass transfer. The effect of ABDAC, in addition to forming an additional resistance layer, is to suppress small-scale surface motions. This rigid resistance film decreases the transfer rate at a constant ratio with respect to clean surfaces.

Ethoxylate groups in NP9EO retain part of the diffusing O<sub>2</sub> at the surface. The oxygen bridges could

possibly act to bind the ethoxylate groups lying randomly at the interface, opening up more room for diffusion of O<sub>2</sub>. The combined effect of O<sub>2</sub> retention in the monolayer and clearance of the interfacial film at the surface increases the apparent diffusion coefficient of O<sub>2</sub>. Synergism in the monolayer further decreases the diffusion coefficient due to the increased surface excess concentration and the rigidity of the resulting film.

## Notation

The following symbols are used in this paper:

$C$	=	Concentration of Oxygen
$C^*$	=	Equilibrium Concentration of Oxygen
$D$	=	Effective Diffusion Coefficient of Oxygen
$t$	=	Time
$\theta_s$	=	Dimensionless Concentration of Oxygen in the Presence of Surfactant
$\theta_w$	=	Dimensionless Concentration of Oxygen

## References

- Brian, P.L.T., "Effect of Gibbs Adsorption on Marangoni Instability", *AIChE Journal*, 17, 765-772, 1971.
- Davies, J.T., "Turbulence Phenomena at Free Surfaces", *AIChE Journal*, 18, 169-173, 1972.
- El Eini, D. I. D., Barry, B.W., and Rhodes, C. T., J., "Micellar Size, Shape and Hydration of Long-Chain Polyoxyethylene Nonionic Surfactants", *Colloid Interface Science*, 54, 348-351, 1976.
- Goldstick, T. K., "Oxygen Transport", 63924-Brozon (Gann: Physiology 1-ch.00-f.000-g.000), 257, 1970.
- Himmelblau, D. M., "Diffusion of Dissolved Gases in Liquids", *Chem. Rev.*, 64, 527, 1964.
- Hüttinger J.K., and Schegk, R.J., "Effect of Anionic Surfactants on Formation of Dispersion and Mass Transfer in the Liquid-Liquid System Water/Acetone/Toluene", *Ger. Chem. Eng.*, 5, 44-52, 1982.
- Infante, G.A., Caraballo, J., Irizarry, R., and Rodrigez, M., "Solubilization of Petroleum Oils by Micelle Forming Surfactants", in Mittal, K.L., Fendler, E.J. (Eds), *Solution Behavior of Surfactants*, 2, 921-931, 1982.
- Janssen, L. J.J., and Stroe van A.J., "Determination of the Diffusion Coefficient of Oxygen in Sodium Chloride Solutions with Transient Pulse Technique", *Analytica Chimica Acta*, 279, 213-219, 1993.
- Kato, T., Terao, T., Tsukada, M., and Seimiya, T., "Self-Diffusion Processes in Semidilute Solutions of Nonionic Surfactant (C<sub>16</sub>E<sub>7</sub>) Studied by Light Scattering and Pulsed-gradient Spin Echo Methods", 97, 3910-3917, 1993.
- Kuryel, B., Ph.D. Thesis, Ege University, Bornova, 1976.
- Lindland, K.P., and Terjesen, S.G., *Chem. Eng. Sci.*, 5, 1, 1956.
- Schick, M.J., Ed. *Nonionic Surfactants*, Marcel Dekker Inc. New York, 1966.
- Sherwood, T.K., Pigford, R.L., and Wilke, C.R., *Mass Transfer*, Wiley, New York, 1975.
- Stebe, K.J., and Maldarelli, C., "Remobilizing Surfactant Retarded Fluid Particle Interfaces", *J. Colloid and Interface Science*, 163, 177-189, 1994.
- Thompson, D.W., "Effect of Interfacial Mobility on Mass Transfer in Gas-Liquid Systems", *Ind. Eng. Chem. Fundam.*, 9, 243-248, 1970.
- Yapar, S., Ph. D. Thesis, Ege University, Bornova, 1992.
- Yapar, S., and Peker, S., "Synergistic Behavior of the Nonylphenol(9) Ethoxylate and Alkylbenzyltrimethylammonium Chloride Binary Mixture", *Ind. Eng. Chem. Res.*, 33, 2102-2106, 1994.

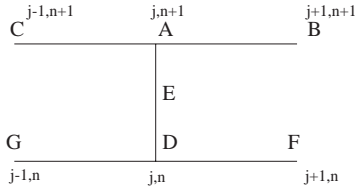
**APPENDIX A**

The mass transfer equation with boundary conditions,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \tag{1}$$

$$\begin{aligned} t=0 \quad 0 < x < 1 \quad C &= C_0 \\ t > 0 \quad x=1 \quad C &= C^* \\ t > 0 \quad x=0 \quad \frac{\partial C}{\partial x} &= 0 \end{aligned}$$

Crank-Nicolson scheme



$$\left(\frac{dC}{dt}\right)_E = \frac{C_{j,n+1} - C_{j,n}}{\Delta t} \tag{2}$$

$$\begin{aligned} \frac{d^2 C}{dx^2} &= \frac{1}{2} \left[ \left(\frac{d^2 C}{dx^2}\right)_A + \left(\frac{d^2 C}{dx^2}\right)_D \right] \\ \frac{d^2 C}{dx^2} &= \frac{1}{2} \left( \frac{C_{j-1,n+1} - 2C_{j,n+1} + C_{j+1,n+1}}{\Delta x^2} \right) \\ &\quad + \frac{1}{2} \left( \frac{C_{j-1,n} - 2C_{j,n} + C_{j+1,n}}{\Delta x^2} \right) \end{aligned} \tag{3}$$

By substituting 2 and 3 in 1, Equation 4 is found after slight re-arrangement.

$$C_{j,n+1} = \frac{F_{j,n} + \frac{M}{2(1+M)}}{(C_{j-1,n+1} + C_{j+1,n+1})} \tag{4}$$

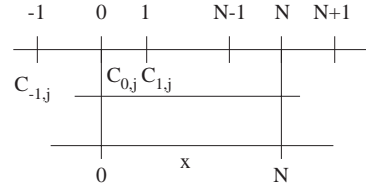
where,

$$F_{j,n} = \frac{1}{2(1+M)}(C_{j-1,n} + C_{j+1,n}) + \frac{1-M}{1+M}C_{j,n}$$

and

$$M = \frac{D\Delta t}{\Delta x^2}$$

Derivative Condition



By introducing a fictitious concentration  $C_{-1,j}$  at the external grid point, the condition becomes,

$$\frac{C_{1,j} - C_{-1,j}}{2\Delta x} = 0 \tag{5}$$

$$\frac{\partial C_{0,j}}{\partial T} = \frac{C_{-1,j} - 2C_{0,j} + C_{1,j}}{(\Delta x)^2} \tag{6}$$

Elimination of  $C_{-1,j}$  from 5 and 6 gives

$$\frac{\partial C_{0,j}}{\partial T} = \frac{2}{\Delta x} \left( \frac{C_{1,j} - C_{0,j}}{\Delta x} \right)$$

Crank-Nicolson formula is

$$C_{s,n+1} = \frac{C_{s,n} + M(C_{s-1,n+1} - C_{s,n})}{C_{s,n+1} + C_{s-1,n} - C_{s,n}} \tag{7}$$