THE DISTRIBUTION AND DISSOCIATION EQUILIBRIA OF PHASE-TRANSFER CATALYST TRICAPRYLMETHYLAMMONIUM CHLORIDE AND ITS AQUEOUS-PHASE MASS TRANSFER

Satoru ASAI, Hidemi NAKAMURA and Yousuke FURUICHI

Department of Chemical Engineering, University of Osaka Prefecture, Sakai 591

The distribution and dissociation equilibria of a representative phase-transfer catalyst, tricaprylmethylammonium chloride (Aliquat 336; Q^+Cl^-), were measured for the systems of *n*-butyl acetate–water, toluene–water, *n*-butyl acetate–aqueous NaCl solutions and toluene–aqueous NaOH solutions. The evaluated distribution coefficients of Q^+Cl^- and the OH^--substituted derivative (Q^+OH^-) were correlated as a function of the ionic concentrations in the aqueous phases. The dissociation constants of Q^+Cl^- and Q^+OH^- in the aqueous phase could be regarded as being identical.

The diffusivities of Q^+Cl^- in water and in *n*-butyl acetate, and the ionic diffusivity of Q^+ in the aqueous phase were measured. The aqueous-phase mass transfer of Q^+Cl^- could be quantitatively explained as that with an instantaneous reversible dissociation reaction.

Introduction

Heterogeneous liquid–liquid reactions with phase-transfer catalyst Q^+W^- such as a quaternary ammonium salt may consist of several steps, in principle: the dissolution of Q^+W^- into the aqueous phase, the formation of the relevant ion pairs Q^+X^- by ion exchange between Q^+W^- and X^-, which is originally present in the aqueous phase, the transfer of Q^+X^- into the organic phase, the main reaction between Q^+X^- and a reactant RY, which is originally present in the organic phase, and the transfer of reaction product Q^+Y^- into the aqueous phase to regenerate Q^+X^-. These cycles are repeated during the reaction process.

In previous studies of quite slow heterogeneous liquid–liquid reactions with phase-transfer catalyst,[4,10] the main reactions in the organic phase may be regarded as rate-determining. Consequently, only the values of the combined distribution and dissociation constants at infinite dilution or at a given ionic strength were reported for many ion pairs in terms of the concentrations of the relevant species in both phases. However, in the analysis of the overall reaction rates of relatively fast reactions, e.g., the alkaline hydrolysis of ester, such treatment is not always justified, and individual evaluations of the distribution coefficients and dissociation constants are required, as well as evaluations of the diffusivities of

the relevant species in both phases.

In this work, the dissociation constants of a representative phase-transfer catalyst, tricaprylmethylammonium chloride (Aliquat 336; Q^+Cl^-), and the OH^--substituted derivative Q^+OH^- in the aqueous phase, and the distribution coefficients between the organic and aqueous phases were determined. As the organic solvent, *n*-butyl acetate was mainly used in connection with the subsequent study of ester hydrolysis with Aliquat 336, which will demonstrate the importance of mass transfer on the overall reaction rates. Furthermore, the diffusivities of the catalyst Q^+Cl^- in both phases and the ionic diffusivity of Q^+ in the aqueous phase were measured. The mass transfer mechanism of the catalyst in the aqueous phase was also examined.

Aliquat 336 is also a representative extractant of metals such as Zn^{2+}, Cd^{2+} and Co^{2+}. Thus, the results of this study may also provide useful information for the analysis of such extraction processes.

1. Experimental

1.1 Distribution and dissociation equilibria

Aliquat 336 $(Q^+Cl^-)^*$ used is a commercial reagent

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* The analysis of Aliquat 336 was made according to the procedure of Lee and others[8]. The composition was as follows: methyltrioctylammonium chloride 16.9 wt%, methyldioctyldecylammonium chloride 36.5 wt%, methyloctyldidecylammonium chloide 27.5 wt%, methyltridecylammonium chloride 7.2 wt% and others 11.9 wt%; total quaternary ammonium chloride 88.1 wt%.

manufactured by General Mills, Inc. It was dissolved in n-butyl acetate (or in toluene in some runs) and was purified by washing several times with $1.0\,kmol/m^3$ NaCl or HCl aqueous solution. It was used without further purification. The resulting catalyst had a concentration of 0.04–$0.32\,kmol/m^3$. The other chemicals used were analytically pure reagent grade.

Using a shaker, $2.0 \times 10^{-5}\,m^3$ of each of these organic solutions was vigorously shaken at 298 K with the same volume of pure water, aqueous solutions of 0.5, 1.0 or $2.0\,kmol/m^3$ NaCl, or 0.2, 0.5 or $1.0\,kmol/m^3$ NaOH for about one hour. After attainment of equilibrium, the relevant ion concentrations in the aqueous phase were determined: Cl^- was analyzed by titration with a standard solution of $Hg(NO_3)_2$ using a mixed indicator of diphenylcarbazone, bromophenol blue and xylene cyanol.[5] The concentration of OH^- was determined by conventional neutralization titration with HCl using phenolphthalein as an indicator. The concentration of Q^+ was measured by means of an ultraviolet spectrophotometer (wavelength: 485 nm; absorptivity: $1.12 \times 10^6\,m^2/kmol$; precision: $10^{-5}\,kmol/m^3$), by which the concentration of the Q^+-orange II complex in chloroform is determined.[9] The concentration of Q^+Cl^- in the organic phase was directly measured by ultraviolet spectrophotometer (wavelength: 270 nm; absorptivity: $7.81 \times 10^2\,m^2/kmol$; precision: $10^{-3}\,kmol/m^3$).

The mass balance of the quaternary ammonium cation was in between 95 and 105%.

1.2 Mass transfer

The diffusivities of Q^+Cl^- in water and in n-butyl acetate were determined by using the conventional diaphragm cell. The ionic diffusivity of Q^+ in water was also evaluated from the diffusion experiments of dilute Q^+Cl^- in $3.0\,kmol/m^3$ aqueous NaCl solutions by means of the diaphragm cell.

The apparatus used in the experiments of mass transfer of Q^+Cl^- into the aqueous phase was of the same type of the agitated vessel with a flat interface as that used in a previous work.[1] The diameter of the agitated vessel was 0.083 m, yielding an interfacial area of $5.41 \times 10^{-3}\,m^2$ and a liquid volume of $4.30 \times 10^{-4}\,m^3$ for each phase. The upper phase consisted of n-butyl acetate dissolving Q^+Cl^- of 0.04–$0.24\,kmol/m^3$. The lower phase consisted of pure water or $3.0\,kmol/m^3$ aqueous NaCl solutions. The experiments were carried out at 298 K, and at agitation speeds of $2.5\,s^{-1}$ for each phase. Samples of $2.0 \times 10^{-6}\,m^3$ were taken from the lower aqueous phase at intervals of 3–10 min, and the concentrations of total chlorine $(Q^+Cl^- + Cl^-)$ were determined by titration with a standard aqueous solution of $Hg(NO_3)_2$ using the foregoing mixed indicator.

The mass transfer rates were evaluated from the variation of total chlorine concentration with time.

2. Analytical Procedure

2.1 Distribution and dissociation equilibria

The aggregation of the lipophilic catalyst Aliquat 336 in n-butyl acetate and toluene was assumed to be negligible, because the aggregation number for these water-saturated solvents may be regarded as being much less than 1.8 in view of previous studies,[3,11] which suggest that the aggregation of the quaternary ammonium salt in the organic phase decreases with increases in polarity and water content.

Aliquat 336 (Q^+Cl^-) in the organic phase dissolves slightly in the aqueous phase. Thus,

$$[Q^+Cl^-] = \alpha_1[\overline{Q^+Cl^-}] \qquad (1)$$

The dissolved Q^+Cl^- may dissociate according to:
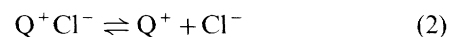
$$Q^+Cl^- \rightleftharpoons Q^+ + Cl^- \qquad (2)$$

giving rise to the following relationship:

$$K_1 = [Q^+][Cl^-]/[Q^+Cl^-] \qquad (3)$$

The mass balance of the quaternary ammonium cation Q^+ in both phases results in:

$$[\overline{Q^+}]_{obs} = [\overline{Q^+Cl^-}] \qquad (4)$$

$$[Q^+]_{obs} = [Q^+Cl^-] + [Q^+] \qquad (5)$$

When the original aqueous solution is pure water, Q^+ and Cl^- dissociate in equimolecular amounts, i.e., $[Q^+] = [Cl^-]$. Then, from Eqs. (1), (3)–(5), one obtains:

$$[Q^+]_{obs}/\sqrt{[\overline{Q^+}]_{obs}} = \alpha_{1w}\sqrt{[\overline{Q^+}]_{obs}} + \sqrt{\alpha_{1w}K_1} \qquad (6)$$

When the aqueous phase contains substantial amounts of NaCl, the equilibrium represented by Eq. (2) is shifted to the left-hand side, depressing the formation of Q^+. Since in this case $[Q^+] \simeq 0$, thus $[Q^+Cl^-] \simeq [Q^+]_{obs}$ from Eq. (5), the distribution equilibrium of Eq. (1) may be modified by using Eq. (4) as:

$$[Q^+]_{obs} = \alpha_1[\overline{Q^+}]_{obs} \qquad (7)$$

When the aqueous phase consists of the NaOH solution, part of the Q^+Cl^- dissolved in the aqueous phase may exchange Cl^- with OH^- to form Q^+OH^-, which is also one of the representative ion pairs in the phase-transfer catalytic reactions. Thus, in addition to the equilibria shown in Eq. (2), the following expression can be given:
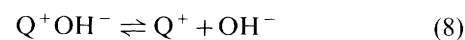
$$Q^+OH^- \rightleftharpoons Q^+ + OH^- \qquad (8)$$

The dissociation constant K_2 of Q^+OH^- is defined as:

$$K_2 = [Q^+][OH^-]/[Q^+OH^-] \qquad (9)$$

The Q^+OH^- formed in the aqueous phase distributes into the organic phase according to the

relation:

$$[Q^+OH^-] = \alpha_2 \overline{[Q^+OH^-]} \qquad (10)$$

When the volumes of both phases are assumed to be equal, from a mass balance of the relevant species in either or both phases,

$$\overline{[Q^+Cl^-]_0} = \overline{[Q^+Cl^-]} + [Q^+Cl^-] + [Cl^-] \qquad (11)$$

$$[NaOH]_0 = \overline{[Q^+QH^-]} + [Q^+OH^-] + [OH^-] \qquad (12)$$

$$[Cl^-]_{obs} = [Q^+Cl^-] + [Cl^-] \qquad (13)$$

$$[OH^-]_{obs} = [Q^+OH^-] + [OH^-] \qquad (14)$$

Using the observed equilibrium concentrations of the relevant species for the various initial concentrations, K_2 and α_2 were evaluated by the Simplex method from Eqs. (1), (3), (9)–(14) with the already evaluated values of α_1 and K_1.

2.2 Mass transfer

The mass transfer rate of Q^+Cl^- can be written as:

$$N_1 = \overline{k}_{L1}(\overline{[Q^+Cl^-]}_b - \overline{[Q^+Cl^-]}_i)$$

$$= \beta_1 k_{L1}([Q^+Cl^-]_i - [Q^+Cl^-]_b) \qquad (15)$$

When the effect of adsorption of Q^+Cl^- at the interface is negligible, and the dissociation reaction (2) of Q^+Cl^- in the aqueous phase is regarded as an instantaneous reversible reaction, the reaction factor β_1 of Q^+Cl^- may be given by the same expression as that for the hydrolysis of SO_2 in water. Hikita et al.[7] developed the approximate penetration theory solution of the reaction factor for the latter system by modifying the exact analytical solution based on the film theory, i.e., by replacing the diffusivity ratios appearing in the film theory solution by their square roots. However, in the present experimental conditions, in which an agitated vessel with a flat interface was used, the Lévêque model is preferable to the penetration theory.[6] Therefore, the diffusivity ratios in the film theory were replaced by their 2/3 power rather than the square roots. As a special case, if no other electrolytes are present in the aqueous phase in accordance with the present experimental condition, Q^+ and Cl^- have equal diffusivities and equal bulk concentrations. Then the general solution reduces to the following simple expression giving the reaction factor of the present system:

$$\beta_1 = 1 + \frac{(D_3/D_1)^{2/3}\sqrt{K_1}}{\sqrt{[Q^+Cl^-]_i} + \sqrt{[Q^+Cl^-]_b}} \qquad (16)$$

where

$$K_1 = [Q^+]_b[Cl^-]_b/[Q^+Cl^-]_b \qquad (17)$$

3. Physical Properties and Mass Transfer Coefficients

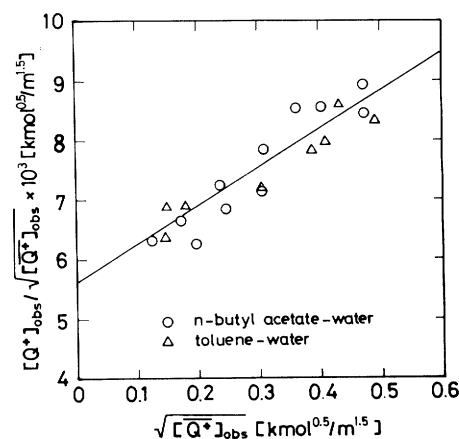The diffusivities of Q^+Cl^- in water and in n-butyl

Fig. 1. Equilibria of Q^+Cl^- for n-butyl acetate and toluene–water systems at 298 K

acetate, and the ionic diffusivity of Q^+ in water, were measured in this work, as discussed in the experimental section. The other relevant physical properties were measured or evaluated in the following manner:

Densities and viscosities were measured by the conventional procedure. Interfacial tensions were determined by the capillary method.

The mass transfer coefficients k_{L1} and $\overline{k}_{L1}$ in the aqueous and organic phases respectively were predicted from the correlation of Asai et al.[1]:

For the aqueous-phase mass transfer,

$$Sh = 0.0119 Sc^{1/3} Ca^{6/13}[\phi^4 Re^3 + \overline{Re}'^{8/3}]^{1/4} \qquad (18)$$

where

$$Sh = k_{L1}L/D_1, \quad Sc = \mu/\rho D_1, \quad Ca = gd^2\rho/\sigma,$$

$$Re = d^2 N\rho/\mu, \quad \overline{Re}' = d^2 \overline{N}\rho/\mu,$$

$$\phi = 1 \quad \text{for} \quad \overline{\mu}/\mu \leq 7.0;$$

$$\phi = (\overline{\mu}/7\mu)^{-1/5} \quad \text{for} \quad \overline{\mu}/\mu > 7.0 \qquad (19)$$

The mass transfer coefficient $\overline{k}_{L1}$ for the organic phase can be estimated by the replacement of k_{L1}, D_1, μ, ρ and N with the corresponding ones for the organic phase.

4. Results and Discussion

4.1 Distribution and dissociation equilibria

The experimental results of the combined distribution and dissociation equilibria of Q^+Cl^- at 298 K for the n-butyl acetate–water system are plotted in Fig. 1, in accordance with Eq. (6). A representative straight line was determined by the least-squares method. From the intercept and slope of the line, the values of the dissociation constant K_1 and the distribution coefficient α_{1w} were evaluated to be 0.0047 and 0.0064 kmol/m³ respectively. The data for the toluene–water system are also shown in Fig. 1. The dissociation constant K_1 pertains to the dissociation of Q^+Cl^- in water and therefore should be

independent of the kind of organic solvent. On the other hand, the distribution coefficient α_{1w} of Q^+Cl^- between the organic and water phases may be expected to vary with the kind of organic solvent. However, no meaningful distinction between the data for n-butyl acetate and those for toluene was found. This suggests that the relation of the distribution equilibrium of Q^+Cl^- for toluene is approximately the same as that for n-butyl acetate. This finding will be utilized later to predict the distribution of Q^+OH^- between n-butyl acetate and aqueous NaOH solution.

Figure 2 shows the distribution equilibria of Q^+Cl^- at 298 K for the system of n-butyl acetate–aqueous NaCl solutions with various ionic strengths. The distribution can be seen to be linear in the presence of large excess NaCl, as expected from Eq. (7). The distribution coefficients α_1 were evaluated from the slope of the respective straight lines to be 0.00418, 0.00309 and 0.00180 for ionic strengths of 0.5, 1.0 and 2.0 kmol/m^3.

Figure 3 presents the plot of α_1/α_{1w} against ionic strength I. The linear relationship suggests the usability of the correlation formula of Van Krevelen and Hoftijzer,[12] which was originally proposed for the correlation of gas solubility in single-electrolyte solutions. The resulting expression is:

$$\log(\alpha_1/\alpha_{1w}) = -0.294[\text{NaCl}] \qquad (20)$$

where $\alpha_{1w} = 0.0064$

From the value of the salting-out parameter, 0.294 m^3/kmol, the contribution of Q^+Cl^- is found to be 0.179 m^3/kmol at 298 K by using the contributions of Na^+ and Cl^- listed in the literature.[12]

The distribution and dissociation equilibria of Q^+OH^- cannot be measured when n-butyl acetate is used as the organic solvent, because n-butyl acetate reacts with OH^-. Therefore, toluene was used as the solvent for the measurements. **Figure 4** represents the experimental data of the distribution and dissociation equilibria of Q^+Cl^- at 298 K for the toluene–aqueous NaOH solutions system. The distribution coefficient and dissociation constant of Q^+Cl^- are required in order to obtain those of Q^+OH^- from the present data. Since both the n-butyl acetate–water and toluene–water systems were found in Fig. 1 to have approximately the same distribution coefficients α_{1w} of Q^+Cl^-*, the distribution coefficients α_1 of Q^+Cl^- for the present system were evaluated from the following expression:

$$\log(\alpha_1/\alpha_{1w}) = -(0.294[\text{NaCl}] + 0.334[\text{NaOH}]) \quad (21)$$

This equation is based on the formula of Danckwerts

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* When the aqueous solutions of Na_2SO_4 or CH_3COONa were used, the distribution of Q^+Cl^- was also found to be equal for n-butyl acetate and toluene.
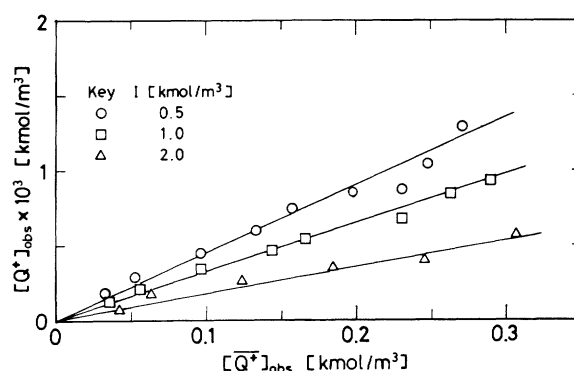

Fig. 2. Distribution equilibria of Q^+Cl^- for n-butyl acetate–aqueous NaCl solutions system at 298 K
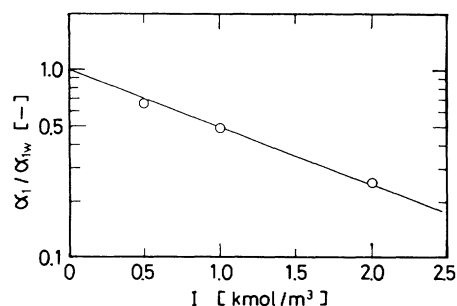

Fig. 3. Correlation of distribution coefficient of Q^+Cl^- between n-butyl acetate and aqueous NaCl solutions at 298 K
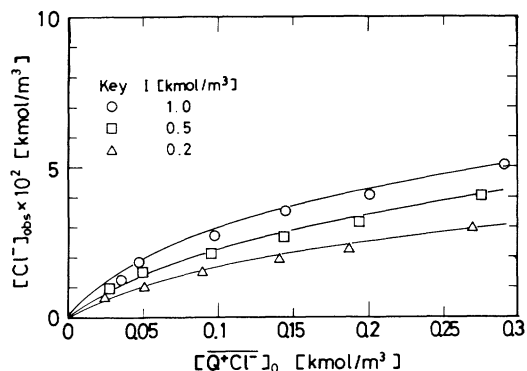

Fig. 4. Equilibria of Q^+Cl^- for toluene–aqueous NaOH solutions system at 298 K

and Gillham[2] giving the correlation of the gas solubility in the mixed-electrolyte solution. The value of the salting-out parameter for NaCl, 0.294 m^3/kmol, was taken from Eq. (20), and the value for NaOH was evaluated to be 0.334 m^3/kmol by allowing for the different contributions of Cl^- and OH^- to the salting-out parameter.[12] It was very difficult to determine the effect of the ionic strength on the dissociation constant K_1 of Q^+Cl^-, since the addition of NaCl and the other ions to adjust the ionic strength respectively depresses the dissociation of Q^+Cl^- and easily causes an exchange of the anions. Thus, assuming no dependence of the ionic strength, the dissociation constant K_1 was taken to be 0.0047

kmol/m^3, as determined in the equilibrium experiments for the n-butyl acetate–water system. The distribution coefficients α_2 and dissociation constants K_2 of Q^+OH^- were evaluated by fitting the experimental data in Fig. 4 with the theoretical predictions, as stated in 2.1. The estimated value of dissociation constant K_2 was independent of ionic strength, consistently with the assumption of no effect on K_1, and was identical with the value of K_1, yielding $K_2 = 0.0047$ kmol/m^3. The distribution coefficients obtained can be correlated by:

$$\log(\alpha_2/\alpha_{2w}) = -(0.261[\text{NaCl}] + 0.301[\text{NaOH}]) \quad (22)$$

where $\alpha_{2w} = 0.46$

The finding that α_2 can be correlated well by the type of correlation of Danckwerts and Gillham[2] also suggests the validity of the assumption of no dependence of K_1 on ionic strength. The solid lines in Fig. 4, showing the theoretical values, were drawn by using the evaluated values of α_2 and K_2. Good agreement may be seen from the figure.

4.2 Mass transfer

The diffusivity D_1 of Q^+Cl^- in water was measured at very low concentrations, so that the dissociation of Q^+Cl^- may be regarded as almost complete. The diffusivity 1.90×10^{-9} m^2/s measured at 298 K was in remarkable agreement with an error of only 2% from the predicted value from the Nernst-Planck equation by using the measured ionic diffusivity 1.71×10^{-9} m^2/s of Q^+ in water. This enables us to predict the aqueous-phase diffusivities of the other ion pairs with Q^+. On the other hand, the measured diffusivity $\bar{D}_1$ of Q^+Cl^- in n-butyl acetate was 3.60×10^{-9} m^2/s at 298 K. This value was about five times that estimated from the correlation of Wilke and Chang.[13]

First, the extraction experiment of Q^+Cl^- from n-butyl acetate containing 0.1 kmol/m^3 of Q^+Cl^- into the 3.0 kmol/m^3 aqueous NaCl solution was performed at 298 K in an agitated vessel with a flat interface, to examine the applicability of the correlation, Eq. (18), of the mass transfer coefficients. The NaCl concentration in the aqueous phase was high enough to depress the dissociation of Q^+Cl^-, so that the extraction of Q^+Cl^- may be regarded as a physical one. Mass transfer resistance in the organic phase was negligibly small. The measured aqueous-phase mass transfer coefficient k_{L1} was 2.1 times the value predicted from Eq. (18). However, it may be noted here that the correlation was obtained for liquids containing no surface-active agent. Aliquat 336 is a surface-active substance, and its existence in the liquid greatly reduces the interfacial tension. Various manners of application of Eq. (18) were tried. Consequently, a prediction using the fictitious interfacial tension, which is the value for the liquid
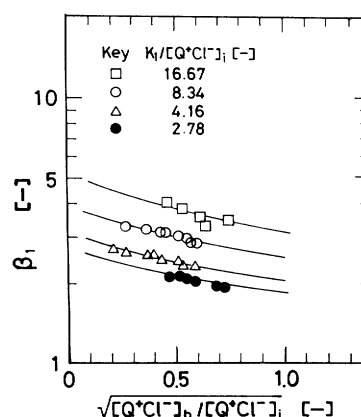

Fig. 5. Reaction factor of Q^+Cl^- for the extraction into water at 298 K

containing no Q^+Cl^-, was found to be in good agreement, within an error of 6.4%, with the measured aqueous-phase mass transfer coefficient. Similar experience was also gained in experiments on physical extraction of I_2 from the aqueous phase containing sodium dodecyl sulfate (SDS) into n-hexane, iso-butanol, or a mixture of 10 vol% n-hexane and 90 vol% paraffin oil, or of cyclohexanone into aqueous SDS solution. In these experiments also, it was found that the measured aqueous-phase mass transfer coefficients below the critical micelle concentration of SDS agreed well, within an error of 4.5%, with the predicted values from Eq. (18) by using a similar fictitious interfacial tension without SDS. Although we cannot give a clear explanation of this finding at the present stage, the use of such fictitious interfacial tension is likely to be appropriate.

The experimental results of extraction of Q^+Cl^- into water are shown in Fig. 5, as a plot of $\sqrt{[Q^+Cl^-]_b/[Q^+Cl^-]_i}$ vs. the reaction factors β_1 of Q^+Cl^- with a parameter $K_1/[Q^+Cl^-]_i$. The reaction factors were evaluated from Eq. (15) with the aqueous-phase mass transfer coefficients k_{L1} predicted from Eq. (18) using the fictitious interfacial tenion. In this case also, the organic-phase mass transfer resistance was negligible. The solid lines represent the theoretical predictions, Eq. (16). As shown in Fig. 5, the observed values of β_1 are in good agreement with the theoretical predictions. Thus, it can be seen that the adsorption resistance of Q^+Cl^- at the interface may be ignored, and the aqueous-phase mass transfer of Q^+Cl^- is accompanied by an instantaneous reversible dissociation reaction, of course indicating a similar mass transfer mechanism for the other ion pairs, such as Q^+OH^-. Furthermore, it may be noted that the values of the measured distribution coefficient and dissociation constant of Q^+Cl^- and of the relevant diffusivities are reasonable.

Conclusion

The distribution coefficients α_1 of Aliquat 336 (Q^+Cl^-) between n-butyl acetate (or toluene) and the aqueous solutions of NaCl and/or NaOH could be correlated by Eq. (21). The distribution coefficients α_2 of the OH^--substituted substance (Q^+Cl^-) for the same systems were correlated by Eq. (22). The dissociation constants K_1 of Q^+Cl^- and K_2 of Q^+OH^- in the aqueous phase could be regarded as being equal, giving $K_1 = K_2 = 0.0047\,\text{kmol/m}^3$.

The measured diffusivity of Q^+Cl^- in water ($1.90 \times 10^{-9}\,\text{m}^2/\text{s}$ at 298 K) was in good agreement with the estimated value from the Nernst-Planck equation using the measured ionic diffusivity of Q^+ ($1.71 \times 10^{-9}\,\text{m}^2/\text{s}$). However, the measured difiusivity of Q^+Cl^- in n-butyl acetate ($3.60 \times 10^{-9}\,\text{m}^2/\text{s}$ at 298 K) was much larger than the values predicted from the correlation of Wilke and Chang.[13]

The measured reaction factors β_1 of Q^+Cl^- in the water phase were in good agreement with the theoretical predictions shown by Eq. (16), clarifying that the aqueous-phase mass transfer of the catalyst is accompanied by an instantaneous reversible dissociation reaction, and proving the measured values of the distribution coefficient, dissociation constant and aqueous phase diffusivity of Q^+Cl^- to be reasonable.

Nomenclature

Ca	= capillary number	[—]
D	= diffusivity	[m²/s]
d	= diameter of stirrer blade	[m]
g	= gravitational constant	[m/s²]
I	= ionic strength of solution	[kmol/m³]
K	= dissociation constant	[kmol/m³]
k_L	= mass transfer coefficient	[m/s]
L	= diameter of vessel	[m]
N	= agitation speed	[1/s]
N_1	= mass transfer rate of Q^+Cl^-	[kmol/(m²·s)]
Re	= Reynolds number	[—]
Re'	= modified Reynolds number	[—]
Sc	= Schmidt number	[—]
Sh	= Sherwood number	[—]
α	= distribution coefficient	[—]
β	= reaction factor	[—]
μ	= viscosity	[Pa·s]
ρ	= density	[kg/m³]
σ	= interfacial tension	[N/m]
ϕ	= correction factor defined by Eq. (19)	[—]
[ ]	= concentration	[kmol/m³]

⟨Subscripts⟩

b	= bulk of liquid	
i	= interface	
obs	= observed	
w	= water	
0	= initial	
1	= Q^+Cl^-	
2	= Q^+OH^-	
3	= Q^+	

⟨Superscript⟩

—	= organic phase	

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