Exercise 8C Liquid-Liquid Extraction

Course 28121: Chemical Unit Operations Laboratory

Team B

Harsh Maheshwari Aashish Kumar s186308@student.dtu.dk s190117@student.dtu.dk



Department of Chemical Engineering
Technical University of Denmark
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Abstract

In the experiment acetic acid (HAc) dissolved in a n-paraffin oil (C10-C13) which is the feed, is extracted into demineralised water , which is the solvent at room temperature in a mixer-settler extractor. The product streams are extract (water+acetic acid) and raffinate (paraffin oil+acetic acid). The distribution coefficient of HAc between the two phases is determined after equilibration for a longer period using the funnel test with contact time of 2.5 hours. In a mixer settler unit of volume 1.63 L, two stirring speeds of 303 rpm and 206 rpm were fixed and the HAc concentrations of the raffinate and extract were measured for W/O and O/W emulsions for each speed.

The distribution coefficient from the funnel test was calculated to be 135.06. The minimum volume of water to extract 99 % of water was 36.65ml. The mass balances for the system showed that the HAc concentration in the extract phase was more than that in the feed. For fixed flow of feed (paraffin oil + HAc) and solvent (water) the mass transfer of HAc and the values for mass transfer coefficients were determined for the two mixing speeds of 303 rpm and 206 rpm and for O/W as well as W/O conditions. Mass balances for every stationary condition shall verify the validity of the measurements. The experimental coefficients were inconsistent when compared to the one from the funnel test. The value of mass transfer coefficient for 303 rpm was calculated to be more than that for 206 rpm. The mass transfer coefficient for W/O emulsion was more than that for O/W emulsion at the same stirring speeds.

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LIST OF SYMBOLS

E Volumetric flowrate of the extract, L/s F Volumetric flowrate of the feed, L/s

k*a Distribution coefficient, 1/s

R Volumetric flowrate of the raffinate, L/s

 RT_{feed} Residence time of the feed, s

RT_{solvent} Residence time of the water phase, s

V Volume of the mixer-settler, L V_{aq} Volume of water phase, (ml) V_{oil} Volume of the oil phase, L V_{org} Volume of organic phase, (ml) V_{water} Volume of the water phase, L

 x^* Concentration of acetic acid in water phase at equilibrium

 x_E Concentration of acetic acid in the extract, mol x_F Concentration of acetic acid in the feed, mol Concentration of acetic acid in the raffinate, mol

y* Concentration of acetic acid in water phase at equilibrium

m Distribution coefficientO/W Oil in Water dispersionW/O Water in oil dispersion

Introduction

Liquid-liquid extraction is one of the separation technology used in industries. This process is quite different with distillation because it focuses on relative solubility of the species rather than volatility. Usually, extraction is more preferable than distillation for separation application that is not cost efficient and applicable for distillation. This process of liquid liquid extraction concerns the transfer of a solute from one liquid phase to another. It can take place using a mixer-settler unit in which the liquids are emulsified into each other. The mass transfer is dependent on the fluid flows and the mixing speed, which also controls the kind of emulsion (water-in-oil or oil-in water) being formed. If surface active agents are present the simple extraction can be very complicated due to difficulties in separating the emulsion into the two immiscible phases.

The aim of the experiment is to investigate the efficiency of the mixer settler which is dependent on many factors like the kind of emulsion, rotational speed of the stirrer, volume ratio between the two phases, etc. The plant comprises 4 glass vessels each 100 liter, pumps, stirrers and mixing unit.

Design and construction

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Figure 1: P&I Mixer Settler Diagram

The experimental setup shown in Figure 1 consists of 4 glass vessels each 100 liter: One for feed (F: Oil with HAc), one for solvent (S: Pure demineralised water), one for raffinate (R: Oil with reduced concentration of HAc) and one for extract (E: Water with HAc). From vessel F and S two piston pumps with variable drive transport the feed and solvent to the mixer-settler unit (figure 3), where the extraction takes place. The volume of the mixer-settler is 1.63 liter. On their way to the mixer the feed and solvent are passing measuring flasks, which are used for calibration of the pump speed. In the mixer is a stirrer with variable speed. The rotation of the stirrer can be measured using a hand operated tachometer. From the vigorously stirred part of the mixer a pipe allows sampling of the dispersed phase through V1; a conductivity sensor located at the same place is used for indication of the type of dispersion: O/W and W/O emulsion, where the former have a higher conductivity than the later.

The mixing and settling part of the extractor is separated by a perforated plate. In the settling part is a fixed overflow pipe, from where the extracted oil phase is running back to vessel R. Inside the settler the location of the boundary between the two phases can be adjusted by means of a level controller. Changing the location of the boundary between the phases may influence the ratio of the phases in the mixer and also the type of dispersion. The samples collected from V1 were allowed to settle to determine the phase ratio of the dispersions at different conditions. To analyze the composition of extract, raffinate, and feed, samples were collected from the valves V15, V16, and V4 respectively. The diagram for the mixer-settler setup has been presented above as Figure 1.

Results And Analysis

The distribution coefficient

1. Calculate the distribution coefficient from the funnel test. Based on this result and provided the coefficient is independent on the concentration, what would be the minimum volume of water (per unit volume of feed) needed to extract 99% of the acetic acid?

To determine the distribution ratio of HAc between the two phases, 50 ml of paraffin oil from the vessel F was mixed with 50 ml of demineralised water in a separating funnel and left undisturbed. After a contact time of 2.5 hours, the two phases were separated and the concentration of HAc in the two phases was determined by titration using 0.01 M NaOH. Data Obtained is in Table 1

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	Feed	Extract	Raffinate	
Volume of Solution (ml)	1	1	10	
Volume of 0.01 M NaOH (ml)	15.75	19.72	1.46	
Concentration	0.1575	0.1972	0.00146	

Table 1: Titration Results from the funnel test

We Know that 1 Mole of NaOH reacts completely with 1 mole of HAc thus,

Conc. NaOH * V olume Of NaOH = Conc. HAc * V olume Of Solution
$$Conc. HAc = \frac{Conc. NaOH * V olume Of NaOH}{V olume Of Solution}$$

Sample calculation for Feed:

Conc.
$$HAc = \frac{0.01 M * 15.75 * 10^{-3} L}{10^{-3} L}$$

Conc. $HAc = 0.1575 M$

Now the distribution coefficient is the ratio of the solution's total concentration in each phase Distribution coefficient (m) = $\frac{y^*}{x^*}$ where y* is the equilibrium concentration of HAc in the water phase and x* is the concentration of HAc in the oil phase. Substituting the values obtained from the funnel test, the value of distribution coefficient is obtained as:

Distribution coefficient =
$$m = \frac{0.1972}{0.00146} = 135.06$$

Thus Distribution Coefficient as found using funnel test is 135.06

Since the distribution coefficient is independent of concentration, the fraction of solute remaining in the oil phase after the extraction is given by the following relation obtained from Appendix $q_{org} = \frac{V_{org}}{m*V_{aq} + V_{org}}$

$$q_{org} = \frac{V_{org}}{m*V_{org}+V_{org}}$$

The minimum volume of water (per unit volume of feed) needed to extract 99 % of the acetic acid would have the value for q_{org} to be equal to 0.01. Substituting the values for m and q_{org} and solving for V_{aq} , the following is obtained:

$$0.01 = \frac{50ml}{(135.06)*V_{aq} + 50ml}$$
 thus, $V_{aq} = 36.65 \, ml$

Therefore, the volume of water required to extract 99% of the acetic acid is 36.65 ml. For the funnel test, 50 ml of water is used for extraction (Vaq = 50mL). The fraction of solute present in aqueous phase is then $q_{aq} = 1 - q_{org} = 1 - \frac{50ml}{135.06*50ml + 50ml} = 0.99265$.

Hence, the extraction efficiency is thus 99.265%.

Mass balances

2. Make mass balances for the transfer of HAc and calculate the rate of mass transfer and the mass transfer number K*a for the 4 operating conditions.

Mass balances for acetic acid are performed to verify the validity of the experimental values. Since the process of extraction is continuous, there is no accumulation of acetic acid in the system and there would be no generation either as it is involves no chemical reaction. Based on this, the equation for mass balance of HAc can be written as: Mass In = Mass Out, i.e

$$F * x_F = E * x_E + R * x_R$$

Where F, E, and R are the flow rates of the feed, extract, and raffinate phases respectively and x_F , x_R and x_E are the concentrations of acetic acid in the feed, raffinate, and extract respectively

The percentage in deviation in the input and the output values can be found as follows

% Deviation =
$$\frac{In - Out}{In} * 100$$

% Deviation = $\frac{F*x_F - (E*x_E + R*x_R)}{F*x_F} * 100$

Now since oil phase and water phase remain immiscible the feed flow rate is equal to the raffinate flow rate. Also in the beginning of the experiment we measured the time required to fill a 100 mL volume of feed and water.

$$F = \frac{100 \, ml}{0.412 \, sec} = 0.242 \, l/sec$$

$$E = \frac{100 \, ml}{0.412 \, sec} = 0.242 \, l/sec$$

Table 2 Verification of Mass Balances

Dispersion Type	Speed of Mixer	$F * x_F$	$E*x_E + R*x_R$	% Deviation
W/O	303 rpm	0.038115	0.05128	-34.54
O/W	303 rpm	0.038115	0.05145	-34.98
W/O	206 rpm	0.038115	0.05278	-38.47
O/W	206 rpm	0.038115	0.05171	-35.67

Since water and oil phases are insoluble in each other the mass transfer rate of HAc across the phase boundary can be calculated as

$$Mass\ Transfer = F(x_F - x_R)$$

Where F is the Feed flow rate, x_F is the concentration of HAc in feed, x_R is the concentration of HAc in raffinate. The validity of the equation is based on the assumption that the oil phase and water phase remain immiscible. i.e. the feed flow rate is equal to the raffinate flow rate.

Table 3: Concentrations obtained from the titrations for the four conditions

Dispersion Type	Speed	Feed	Extract	Raffinate	V_{oil} / V_{F}	V_{water} / V_{F}
W/O	303 rpm	0.1575	0.2108	0.0011	0.5	0.5
O/W	206 rpm	0.1575	0.2095	0.0031	0.4375	0.5625
W/O	303 rpm	0.1575	0.2135	0.0046	0.35	0.65
O/W	206 rpm	0.1575	0.2091	0.0046	0.2875	0.7125

Calculation of mass transfer coefficient

For W/O dispersion and speed of 303 rpm we have $Mass\ Transfer = 0.242 * (0.1575 - 0.0011) = 0.0378488\ mol/sec$

The mass transfer coefficient can then be obtained by equating the rate of mass transfer with this relation:

$$F(x_F - x_R) = K * a * V * (x_R - x_R^*)$$

where K = the mass transfer coefficient,

a = the area of the mass transfer per unit volume,

V = the volume of the extractor = 1.63 L,

 $x_R^* = \frac{y^*}{m}$ = the equilibrium concentration at the phase boundary, $x_R^* = \frac{y}{m}$ = the equilibrium concentration x_R^* can be determined by considering $y_E^* = y_E$ $K*a = \frac{0.0378488}{1.63*(0.0011 - \frac{0.2108}{13495})}$

$$K * a = \frac{0.0378488}{1.63*(0.0011 - \frac{0.2108}{134.95})}$$

The rate of mass transfer and the values for the mass transfer coefficients for the four operating conditions are presented in Table 4 as follows:

Table 4: The rates of mass transfer and the mass transfer coefficients

Dispersion Type	Speed	Mass Transfer (mol s^{-1})	Mass Transfer Coeff. (s ⁻¹)
W/O	303 rpm	0.03784	0.513
O/W	206 rpm	0.03736	0.255
W/O	303 rpm	0.03720	0.216
O/W	206 rpm	0.03700	0.103

Residence times

3. What is the residence time of feed and solvent in the mixer-settler extractor for the 4 operating conditions, under which the mass transfer is determined? Do you see any influence of the residence time/phase ratio on the mass transfer?

The total residence time is calculated from the initial determination of the flow rate where it took 0.412 sec to fill a volume of 100 ml. It was verified that both the feed and the solvent enter the mixer-settler at the same rate. Since the feed and the solvent enter the extractor at the same time, the total volume entering is 200 ml in 0.412 seconds. As the volume of the extractor is 1.63 L, the residence time for solvent is calculated as follows:

The volume ratios of the water and oil phases have been obtained by collecting 80 ml samples at different operating conditions and letting the settles in a beaker.

Calculations

For W/O dispersion and 303 rpm speed we have phase ratio p = 1:1

Volume of solvent (water) in the mixer settler region is $V_W = 1.63 * 0.5 l = 0.815 l$

Volume of feed in the mixer settler region is $V_F = 1.63 * 0.5 l = 0.815 l$

Also we know the net Inflow rate $netF = 2 * F = 2 * 0.242 \ l/sec = .484 \ l/sec$

Thus residence time for solvent $RT_{solvent} = \frac{V_W}{netF} = \frac{0.815 \, l}{2*0.242 \, l/sec} = 1.683 \, sec$ Thus residence time for feed $RT_{feed} = \frac{V_F}{netF} = \frac{0.815 \, l}{2*0.242 \, l/sec} = 1.683 \, sec$

The volume fractions of the oil and the water phases along with the respective calculated residence times at the four operating conditions are shown in Table given below:

Dispersion	Speed	V_{oil} / V_{F}	V water / V F	RT solvent	RT_{feed}
W/O	303 rpm	0.5	0.5	1.683 sec	1.683 sec
O/W	303 rpm	0.4375	0.5625	1.894 sec	1.473 sec
W/O	206 rpm	0.35	0.65	2.189 sec	1.178 sec
O/W	206 rpm	0.2875	0.7125	2.399 sec	0.968 sec

Table 5: Residence time calculations

It can be observed that the volume ratio of the the water phase increases with a decrease in the speed of the mixer. Consequently, the residence time of the water phase in the extractor increases with a decrease in the speed of the stirrer. At constant speed, the volume fraction of water is higher in the O/W dispersion when compared to the W/O dispersion. However, this difference between the two types of dispersions at the same speed is very less when compared to the difference between the same type of dispersion at different speeds. Hence it can be said that the speed of the stirrer has a huge impact on the volume ratios of the water and oil phases and also their respective residence times

Comparison of the distribution coefficients

4. Compare the experimental distribution coefficients with the one found from the funnel test.

The table below shows the experimental distribution coefficients and the one found from funnel test. The last column represents the deviation of experimental values from the funnel test

Table 6 : Comparison of distribution coefficients

Operating Conditions	Distribution Coefficient	% Deviation from Funnel Test
Funnel Test	134.95	0 %
W/O, 303 rpm	196.43	45.55 %
O/W, 303 rpm	68.45	-49.27 %
W/O, 206 rpm	46.48	-65.55 %
O/W, 206 rpm	45.66	-66.16 %

It is observed that the coefficients from the mixer-settler unit are much deviant (the minimum deviation value is 45.55%) from the distribution coefficient obtained from the funnel test and there is an inconsistency in the values. The error are so large probably because of error propagation from the titration of extract and raffinate. Also as the funnel test assumes that a state of equilibrium has been achieved between the two phases, the inconsistency might be explained by the possibility that a state of equilibrium might not have been achieved in the short stationary time of 20 minutes.

Triangular Phase Diagram

5. Make a principle sketch of a triangular phase diagram of the 3-component system at equilibrium taking into account, that water and HAc are completely miscible for all concentrations, water and oil are practically not miscible at all, and oil and HAc are only partially miscible.

The triangular phase diagram for ternary mixture of paraffin-water-acetic acid is shown in figure below. A triangular diagram gives a representation of the ternary liquid-liquid equilibrium data. Figure gives a very good representation of the equilibrium data with the assumption that paraffin oil and water are completely immiscible with each other while acetic acid is fully soluble in water and somewhat partially soluble in paraffin oil. So finally, water and acetic acid would be present in form of a single phase and a mixture of water and paraffin oil will form two distinct phases. Similarly, acetic acid and paraffin oil would split into two phases as acetic acid is only partially soluble in the oil.

Any point in the diagram corresponds to a ternary mixture. The mixtures present in the region above the curve form a single phase and the mixtures within the curve result in two phases. The curve corresponds to the equilibrium data. So by using the data at any point we can get the amount of solute in both phases.

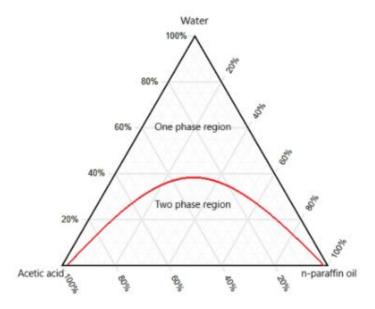


Figure 2: Ternary phase diagram for water-acetic acid-paraffin oil system

Analysis and Discrepancies in mass balances and rates of mass transfer

6. Comment on the mass balances and the differences in mass transfer between the W/O and O/W operating conditions for the two mixing rates.

The mass balances presented in Table 2 show that the mass exiting the system is more than mass entering the system. There might be error in calculating the feed concentration, as the mixing time of 10 minutes might not have been sufficient for the extraction of HAc in the demineralised water added to facilitate titration.

From Table 4 it can be observed that the rate of the mass transfer and the mass transfer coefficient are higher for higher speeds of stirring. This is in alignment with the theoretical expectations. It can additionally be observed that the rate of mass transfer for W/O dispersion is more or less higher than that of O/W dispersion. The reason can be attributed to as in the case of W/O emulsion, oil is the continuous phase and contains HAc which might facilitate a greater amount of mass transfer than in O/W emulsion, where oil is dispersed phase.

Discussion of assumptions made

7. In the calculation of K*a is it fair to assume, that $y_E^* = y_E$?

It is a closed system. The calculation of K*a is carried out based on the assumption that $y_E^* = y_E$. This is a reasonable assumption to make. The extraction of acetic acid from paraffin oil to water is being conducted in a closed system.

The calculation of K*a is done based on the concentration of the acetic acid obtained in the extract from the separation funnel. Since there is no external transfer of mass from the separation funnel. The concentration of the solute in the bulk of the two phases is assumed to be uniform due to perfect mixing. As the extraction of acetic acid continues, its concentration in the feed (raffinate) decreases which consequently increases in the solvent (extract). This continues until its concentration at the interface reaches an equilibrium. Since acetic acid is completely miscible in water, it can be assumed that its

concentration is uniform in the filmat the interface and in the bulk phase[3]. This process has been illustrated in Figure below

Figure 3: The evolution of the solute concentration in the vicinity of the interface in a closed system

Total extraction as a one-stage equilibrium process

8. Can we consider the total extraction as a one stage equilibrium process?

Yes, we can consider the total extraction as on stage equilibrium process as the distribution coefficient remains constant and does not vary with time as the concentration of HAc in aqueous phase and organic phase change from the initial value to its equilibrium value. In the experiment due to some measurement errors the distribution coefficient varied to a maximum error of 66 %, but the values in other operating conditions are better.

Uncertainty analysis

9. What is the uncertainty (quantified in numbers, not just words) on the determinations of distribution coefficient, phase ratio, HAc concentration and feed/solvent flow?

Uncertainty analysis is a technique that analyses a derived quantity, based on the uncertainties in the experimentally measured quantities that are used in some form of mathematical relationship to calculate that derived quantity, but to calculate uncertainty we should know the some certain value of the particular measurement, bur here we don't have that value, so we can't do the uncertainty analysis here.

$$Absolute\ Error = |v_A - v_E|$$
 $Percentage\ Error = \left| rac{v_A - v_E}{v_E}
ight| imes 100\%$ $v_A = approximate\ (measured)\ value$ $v_E = exact\ value$

Figure 4: Uncertainty Analysis

Conclusions

The process of liquid-liquid extraction was carried out for the extraction of acetic acid in paraffin oil into water. This was done both in a separation funnel and in a mixer-settler. The concentration of acetic acid in different oil phase and water phase samples was determined by titration of the samples with 0.01M of NaOH solution. The amount of acetic acid extracted by the solvent has been determined by considering its concentration difference in the feed and the raffinate. This method was adopted instead of directly considering the concentration of acetic acid in the extract obtained by titration as it resulted in concentrations higher than the feed which is an anomaly. This anomaly is probably due to error in titration of the feed. The feed which is an oil phase requires addition of water and stirring so that the acetic acid present in the feed gets extracted into water for titration and the stirring was done only for 10 minutes which might not have been long enough for all the acetic acid to get extracted into the water for titration. The percentage of acetic acid in the separating funnel was observed to be 99.265% when the separation funnel was left undisturbed for 2 hours and the ratio of solvent to feed was 1:1. To extract 99% of the acetic acid, the amount of solvent required was calculated to be 36.5ml for 50 ml feed i.e in a ratio of 0.733:1 with the feed.

The distribution coefficient at the different operating conditions was calculated. The separation funnel is considered to have reached equilibrium and hence the concentrations of acetic acid in the extract obtained from the separation funnel have been used to obtain the distribution coefficients at different operating conditions. The values of the distribution coefficient vary greatly from each other or from the value of the funnel test. The last operating condition (O/W at speed 206 rpm) however gives the maximum deviation of -66%. This could be attributed to errors in titration or improper washing of the beakers which might have had residues of the previous samples left. The process of extraction has been carried out for two different stirring speeds with two types of dispersions at each speed. During the last experiment, when the phase boundary was decreased to get the reading for the O/W emulsion for 206 rpm speed, the conductivity kept fluctuating between 0.8 and 1.1. It is plausible that this might have introduced errors in the measurements as well. The mass transfer rates for the four operational conditions were approximately the same and had a values of 0.37 mol/s. k × a values for 303 rpm were higher than that for 206 rpm indicating that mass transfer rate for higher agitations is higher. The mass balances show that the concentration of the extract is higher than that of the feed. The % deviations for the four readings are -34.54, -34.98, -38.47 and -35.67. This might have been because of insufficient stirring time before the titration of the feed which might have delivered lower concentration value than actual. As acetic acid forms an azeotrope with water, separation of acetic acid with water by distillation is very difficult. Another solvent might be required for further separation of water from acetic acid. Thus, retrieval of pure acetic acid might become more energy intensive as it would require further separation steps.

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Theory

The type of emulsion which is formed when a given pair of immiscible liquids is homogenized in absence of emulsifying agents depends on the relative volumes of the two phases. The higher the phase volume the more likely is a liquid to become the dispersion medium – the continuous phase. When water is added to a W/O dispersion, the dispersion will invert to an O/W at a certain (but unknown) water content. The opposite is true if we start with an O/W dispersion and add oil. The water ratios at inversion, Xw (volume fraction = volume of water/total volume) may depend on the mixing speed as is qualitatively shown in figure 5. Figure 6 shows the principle conditions around the oil-water interface in the equilibrium situation, i.e. after a certain period of contact time. When oil and water volumes first meet the acetic acid bulk concentration in the oil is much higher than in the solvent, and when the two phases leave the mixer-settler the actual concentrations are somewhere between the initial and the equilibrium values – dependent on the efficiency of extraction

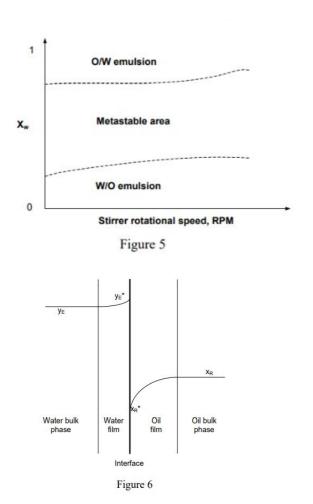


Figure 6: Oil-water phase boundary condition

The equilibrium distribution of HAc between oil and water is described by the coefficient of distribution m defined by:

 $m = \frac{V}{x^2}$ equation (1) where y* is the equilibrium concentration of HAc in the water phase and x* is the concentration of HAc in the oil phase. On contrary to what is normal for other separation processes x and y for 10 extraction both relates to liquid phases, in this case oil phase and water phase respectively. In addition x and y is not understood to be molar fractions; ordinary per weight or volume based concentrations are much more practical. The mass transfer rate of HAc across the phase boundary is

 $F(x_F - x_R)$ equation(2) where F is the feed flow, xF is the concentration of HAc in the feed and xR is the concentration in the raffinate. This equation is only valid because oil and water are practically immiscible, i.e. the feed flow equals the raffinate flow. This mass transfer is equal to the transport of HAc out of the oil phase given by:

 $K*a*V*(x_R-x_R^*)$ equation(3) where K is a mass transfer number, a is the area of mass transfer per unit volume, V is the extractor volume and xR* is the equilibrium concentration at the phase boundary (= yE*/m). From equation (2) and (3) K*a can be determined, considering

Appendix A

The extraction efficiency depends on the partitioning of the solute between the two phases when no secondary reactions are involved. In this case, the distribution ratio is equal to the partitioning coefficient.

$$m = k_D = \frac{[S_{aq}]}{[S_{org}]}$$

As the solute is initially present in the organic phase, the number of moles of solute present in the organic phase value is equal to the combined moles of solute present in the organic phase and that in the aqueous phase after extraction.

$$(moles S_{aq})_1 = (moles S_{orq})_0 - (moles S_{orq})_1$$

Where subscripts 0 and 1 refer to the system before and after the extraction respectively. The concentration in the organic phase is given as follows:

$$[S_{org}]_1 = \frac{(moles \, S_{org})_1}{V_{org}}$$

where V_{org} is the volume of the organic phase

The concentration of the aqueous phase is given as follows:

$$[S_{aq}]_1 = \frac{(moles \, S_{aq})_1}{V_{aq}}$$

where V_{aq} is the volume of the aqueous phase. From (18) and (20),

$$[S_{aq}]_1 = \frac{(moles\,S_{org})_0 - (moles\,S_{org})_1}{V_{aq}}$$

Thus, an expression for m can be obtained:

$$m = \frac{[S_{aq}]}{[S_{org}]} = \frac{\frac{(moles S_{org})_0 - (moles S_{org})_1}{V_{aq}}}{\frac{(moles S_{org})_1}{V_{org}}}$$

The fraction of solute remaining in the organic phase after extraction $(q_{org})_1$ can then be given by the ratio of the number of moles present in the aqueous phase and organic phase.

$$(q_{org})_1 = \frac{(moles S_{org})_1}{(moles S_{org})_0} = \frac{V_{org}}{mV_{aq} + V_{org}}$$