MATHEMATICAL MODELS FOR DESCRIPTION OF SOLUTION-DIFFUSION PERTRACTION OF BENZOIC ACID

Piotr SZCZEPAŃSKI, Stanisław KOTER

Nicolaus Copernicus University, Faculty of Chemistry
Gagarina Str. 7, 87-100 Toruń, Poland
e-mail: piotrs@chem.uni.torun.pl

1. INTRODUCTION

Liquid membranes (LM) are frequently used in the transport and separation of organic acids [1]. Mathematical modeling of LM processes has received considerable attention because of its ability to determine the physico-chemical parameters required for the interpretation of laboratory and pilot scale results or designing the pertraction processes. The model proposed by Makino et al. [2] can be used for this purpose. In this model, the reversibility of interfacial phenomena at the boundaries donor|LM and LM|acceptor phase was assumed. The finite volume of the membrane and the kinetics of partitioning was also taken into account.

The model of diffusive transport of carboxylic acid trough the agitated bulk liquid membrane is presented in this presentation. The model is based on the concentration polarization layers, scheme of which is depicted in Fig. 1. For such a system, the total diffusive flux of benzoic acid (HA), in the diffusion layer for both aqueous and organic solutions J_i, can be described by the equation:

$$J_i = -D_i \frac{dc_i}{dx} \qquad i = a,\ d,\ m \tag{1}$$

where D_i is the apparent diffusion coefficient of HA, *a, d, m* denote acceptor, donor, and membrane phase, respectively. Assuming temporary stationary conditions for each interface with *J, and D* = const, Eq. (1) can be expressed as:

$$J_i = -\frac{1}{l_{p,i}} D_i \left(c_{i,m} - c_{i,b}\right) = -k_i \left(c_{i,m} - c_{i,b}\right) \qquad i = a,\ d \tag{2a}$$

$$J_{m,i} = -\frac{1}{l_{p,m,i}} D_m \left(c_{m,b} - c_{m,i}\right) = -k_{m,i} \left(c_{m,b} - c_{m,i}\right) \tag{2b}$$

where l_p is the thickness of the diffusion layer, k is the mass-transfer coefficient.

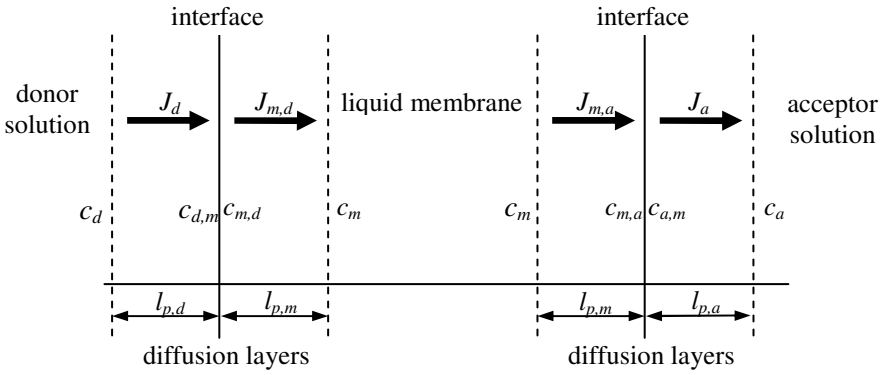

Fig. 1. Diffusion scheme at the boundary external solution|LM system.

Assuming further that the establishing of equilibrium is fast and the partition coefficient for undissociated HA is constant:

$$K_p \equiv [HA]_{m,i} / [HA]_{i,m} \tag{3}$$

consequently, the relation between the apparent partition coefficient HA at the boundaries, ($c_{m,i} / c_{i,m}$) is a function of concentrations, with two constants, i.e. the constant of dissociation and dimerization, which can be expressed as:

$$\frac{c_{m,i}}{c_{i,m}} = K_p \left(1 + 2K_p K_2 \left(c_{i,m} + K_a \right) - \frac{2\left(1 + 2K_p K_2 \left(2c_{i,m} + K_a\right)\right)}{1 + \sqrt{1 + 4c_{i,m} / K_a}} \right) \tag{4}$$

Because the accuracy of the experimental determination of K_p and K_2 is rather poor, it was proposed also to replace Eq. (4) by a simple linear dependence:

$$\frac{c_{m,i}}{c_{i,m}} = a_1 c_{i,m} \tag{5}$$

where a_1 is the adjusted parameter.

2. RESULTS

To verify the model derived, the pertraction of benzoic acid through an agitated bulk liquid membrane (ABLM) was carried out. In the experimental studies, six different solvents were used. Experimental results enable us to evaluate the model parameters (k, a_1, K_p, K_2) by minimizing the sum of squares using the simplex algorithm. The typical results of $c_i = \mathrm{f}(t)$ fitting, for the ABLM system with hexane as an organic phase, are shown in Fig. 2.

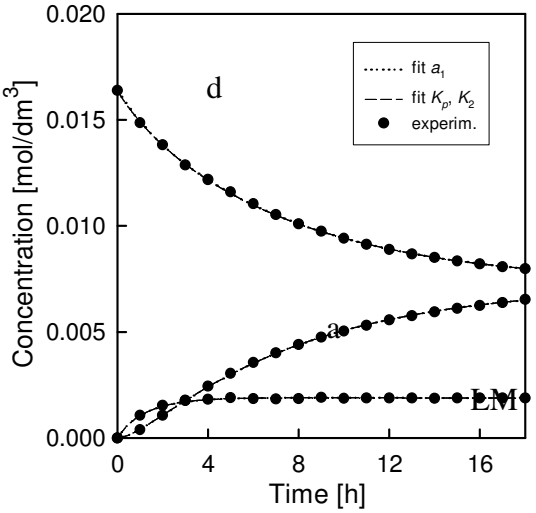

Fig. 2. Total concentration of solute in donor (d), acceptor (a) and LM phases vs. time; • – experimental data, dash line and dot line – models in which the partition of benzoic acid between aqueous and organic phases are described by the simple linear equation (1), and by the more exact expression (2), respectively.

3. CONCLUSION

The model of a diffusive transport of benzoic acid through an agitated bulk liquid membrane system, based on the concentration polarization layers, was developed and tested using the experimental results. The results indicate that $c = f(t)$ dependencies, calculated from the model in which Eq.(1) or (2) was applied, describe very well the experimental data and confirm its utility for a quantitative description of benzoic acid pertraction.

REFERENCES

[1] O. Kedem, L. Bromberg, A.M. Eyal, *Liquid–liquid extraction across ion-exchange membranes*, European Patent Application, EP 0574 717 A2; 18.05.93 (Cl. B01D11/04).
[2] K. Makino, H. Ohshima, T. Kondo, *Biophys. Chem.* 35 (1990) 85.