DESCRIPTION OF CARBOXYLIC ACIDS MEMBRANE TRANSPORT BY CHEMOMETRIC METHODS

Piotr SZCZEPAŃSKI

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

1. INTRODUCTION

The studies of quantitative structure-activity relationship (QSAR) and the quantitative structure - property relationships (QSPR) involve, various chemometric methods in which the chemical behaviour of a compound is correlated with its structure represented by the topological indices [1]. For example, QSPR methods were applied for the prediction of an octanol-water partition coefficient [2], a design of ligands for the separation of lanthanides and actinides [3] or prediction of pK_a of benzoic acids in different solvents [4]. In spite of the widespread use of the QSPR methods, only a few papers concerning the application of topological indices to describe the separation processes in membrane systems [5,6] are available. In this presentation, a study of quantitative structure-property relationships based on topological indices was applied for describing the mass transfer coefficients (or fluxes) of carboxylic acids in various membrane systems.

2. EXPERIMENTAL

The following experimental results were used in the formulation of flux or mass transfer characteristics vs. topological indices:

a) Permeation of acetic, propionic, lactic, oxalic, or tartaric acids through the polymeric anion-exchange membrane Neosepta AFN-7 [7],
b) Permeation of acetic, propionic, lactic, oxalic, or tartaric acids, through the bipolar polymer membrane Neosepta BP-1 [8],
c) Pertraction of benzoic acid through an agitated bulk liquid membrane where hexane, heptane, octane, nonane, decane, dodecane or cyclohexane were used as a liquid membrane phase,
d) Pertraction of acetic or propionic acids in a multimembrane hybrid system in which hexane, heptane, octane, decane, cyclohexane, or toluene were applied as the organic phase [9]

The details of experimental studies are described in referenced papers from which numerical data were reinterpreted herein.

3. RESULTS

For instance, the permeation of acetic, propionic, lactic, oxalic, and tartaric acids coefficients through the anion-exchange Neosepta AFN-7 membrane, were correlated with the average connectivity index (χ^{o}_{Av}) of carboxylic acids. The corresponding results presented in Fig.1 indicate that the dependence between mass the transfer coefficient k (cm/s) and connectivity index can be empirically described by the following relationship:.

$$k = - 2.05(\pm 0.26)\times 10^{-5} \cdot \chi^{1}_{A} + 1.32(\pm 0.14)\times 10^{-4}$$
$$r^2 = 0.954,\ S.D. = 3.71\times 10^{-7},\ F = 62 \qquad (1)$$

Other examples of the correlation between mass transfer coefficients of fluxes and selected topological indices are summarized in Tab. 1

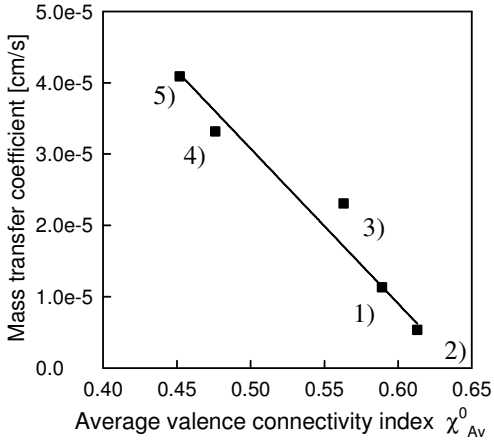

Fig. 1. Correlation between mass transfer coefficient (k) and average connectivity index χ^{0}_{Av} of carboxylic acids in permeation through the anion-exchange membrane Neosepta AFN-7: 1) acetic, 2) propionic, 3) lactic, 4) oxalic, and 5) tartaric acid.

Tab.1. Linear relationships between mass transfer coefficient (k, system a, b, c) or fluxes (J_{max}, system d) and topological indices of carboxylic acids or organic solvent (system c, d)

Membrane system	Topological index	Relationship	R^2
a)	3D MoRSE – 19 signal / weighted by Sanderson electronegativities (Mor19e)	$k = -5.65\times10^{-5}\times$ $\times$Mor19e$+1.87\times10^{-5}$	0.977
b)	Average connectivity index (χ^1_A)	$k = 6.03\times10^{-5}\cdot \chi^1_A -$ -2.95×10^{-5}	0.963
c) propionic acid	Average connectivity index (χ^5_A)	$k = 5.85\times10^{-5}\times$ $\times\chi^5_A+5.03\times10^{-6}$	0.874
d)	Reciprocal distance Radnič-type index (RDChi)	$J_{max}= -6.11\times10^{-10}\times$ $\times$RDChi$+3.13\times10^{-9}$	0.987

4. CONCLUSION

The relationships collected in Tab. 1, satisfactorily describe the mass transfer coefficients or fluxes as dependent on the selected topological indices.

The results demonstrated that the topological indices derived from the molecular structure of carboxylic acids (or solvents) can be correlated with the mass transfer coefficient (or fluxes) of carboxylic acids in various simple and complex multimembrane systems.

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