Desalination 190 (2006) 267–276

DESALINATION

www.elsevier.com/locate/desal

Investigation of reverse osmosis on the basis of the Kedem–Katchalsky equations and mechanistic transport equations

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Received 30 May 2005; accepted 13 September 2005

Abstract

A comparative investigation was conducted into the operation of two descriptions of reverse osmosis. One of them was based on the equations of the Kedem–Katchalsky (KK) formalism, and the other on the reduced transport equations of the Kargols mechanistic formalism. It was demonstrated that if the former makes use of the correlation between KK transport parameters, i.e., the relation given by the formula $\omega = (1-\sigma^2)\bar{c}_s L_p$, the description becomes identical with the latter, as well as consistent with the expectation. This situation testifies to the fact that transport equations of both formalisms are mutually equivalent.

Keywords: Porous membranes; Reverse osmosis; KK equations; Mechanistic transport equations

1. Introduction

Transport processes of non-electrolytic substances across membranes can currently be investigated with the use of two transport formalisms: the thermodynamic formalism of Kedem–Katchalsky (KK) [1,2] and the equations of mechanistic transport formalism [3–7]. The equations of both these formalisms were applied to the investigation of reverse osmosis (RO). It is this process that has to be dealt with when the following condition is satisfied:

$$\Delta P > |-\sigma\Delta\Pi|$$

where ΔP is the mechanical pressure difference, σ is the reflection coefficient, and $\Delta\Pi$ is the osmotic pressure difference. The phenomenon of RO was described in 1997 [8] in an innovative way, based on practical KK equations:

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0011-9164/06/$– See front matter
doi:10.1016/j.desal.2005.09.007

$$J_v = L_p \Delta P - L_p \sigma \Delta \Pi \quad (1)$$

$$j_s = \omega \Delta \Pi + (1-\sigma)\overline{c}_s J_v \quad (2)$$

where J_v and j_s are flows; L_p, σ and ω are coefficients of filtration, reflection and permeability of the solute; and $\overline{c_s}$ is the mean concentration.

The starting point for this description is the relation [9]

$$C_0 = \frac{j_s}{J_v} \quad (3)$$

where C_0 is the permeate concentration (permeate being the solution obtained in the RO process). It is obvious here that at σ = 1, the permeate concentration should amount to $C_0 = 0$ (pure solvent).

Following the procedure of RO solving, as previously presented [8], we obtain (based on the above three equations and the Van't Hoff formula, $\Delta\Pi = RT(C_r - C_0)$, where R is the gas constant, T is the temperature, and C_r is the concentration of the feed, i.e., the input solution), the following expression:

$$C_0 = \frac{-L_p\left[\Delta P(1+\sigma) - 2\sigma RTC_r\right] - 2\omega RT +}{2L_p \sigma RT(1+\sigma)} \quad (4)$$

where

$$\Delta = \left\{L_p\left[\Delta P(1+\sigma) - 2\sigma RTC_r\right] + 2\omega RT\right\}^2 - 4L_p\sigma RT(1+\sigma)\left[L_p C_r((1-\sigma)\left(\sigma RTC_r - \Delta P\right) - 2\omega RTC_r\right]$$

The above expression, which in fact provides the solution to RO on the basis of the KK equations, represents the function

$$C_0 = f\left(L_p, \sigma, \omega, C_r, \Delta P, T\right) \quad (5)$$

A similar description of RO is presented here, but with the application of the equations of mechanistic transport formalism [3–7]. The need to do so results, as it were, from the fact that the KK equations were derived from a model of a membrane treated as a "black box". This means that in KK formalism, one does not go deeply into the microscopic structure of the membranes, whereas in research practice we mostly deal with membranes which have specific internal structures. These are mostly porous membranes, i.e., ones whose specific pores (channels) are capable of transporting the solvent and a variety of solutes. These membranes have been classified as homogeneous and heterogeneous in the literature [3–7]. This division assumes that a membrane is homogeneous if its pores do not differ in dimensions (cross-section radii), but a membrane whose pores do differ in dimensions is to be treated as heterogeneous.

At this point, we wish to stress that the equations of mechanistic formalism were derived on the basis of the model of a heterogeneous porous membrane. The final objective is a comparison of the description of RO made on the basis of the KK equations and the description of the self-same process with the application of mechanistic transport equations. Since mechanistic transport formalism has only been recently developed [3–5,7), detailed considerations are preceded with an outline of this formalism.

2. Outline of mechanistic formalism for membrane transport

In order to present the foundations of mechanistic formalism for membrane transport [3–7], considerations begin with the membrane system outlined in Fig. 1. In this system, the heterogeneous porous membrane M (whose pores differ in linear dimensions, i.e., cross-section radii) separates two compartments (A and B) containing non-electrolytic solutions of the same solute, with concentrations C_1 and C_2 ($C_1 < C_2$). These solutions are under hydrostatic pressures (P_1 and P_2) which satisfy the relation $P_1 < P_2$.