



## Numerical analysis of dialysis with chemical reaction at steady state. Irreversible second-order reaction



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### ABSTRACT

In the present work, the effect of chemical reaction on the rate of dialysis is analysed. The attention is paid to an irreversible second-order chemical reaction at steady state. A simple scheme, in which component A is transported through the membrane by diffusion and reacts with component B diffusing in the opposite direction, is considered. The analogy between the solution-diffusion model in the membrane transport and mass transfer in gas-liquid systems described by the film theory, both accompanied by chemical reactions, is taken into consideration. A numerical solution scheme is presented and the effect of chemical reaction is evaluated in terms of the enhancement factor for a wide range of parameters. The analysis of limiting cases is carried out and the applicability of the existing approximate solutions for the mass transfer accompanied by chemical reaction is examined. An effort was made to develop new correlations for the enhancement factor in the case that no approximate solution is available in literature.

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### 1. Introduction

A number of industrial separation processes are based on polymeric membranes. Among them, dialysis belongs to the oldest membrane processes to be used on an industrial scale [1]. This process employs nonporous (dense) polymeric membranes. Mass transfer through such membranes is usually described by the solution-diffusion model [1–4]. According to this model, transported components dissolve in the membrane material and diffuse down a concentration gradient.

As the mass transfer is controlled by diffusion of components inside the membrane, the separation processes are generally very slow, especially in the cases of the separation of large molecules. The mass transfer rate can be increased by the addition of a component into a receiving solution, which chemically reacts with the component transported through the membrane. Typical examples involve neutralization dialysis of organic acids [5–7], recovery of phenol from industrial effluent streams [8–10] and dialysis enhanced by a complexation reaction of a stripping agent with the component transported [11].

Mass transfer processes accompanied by chemical reactions have received a lot of interest from researchers. Most attention has been paid to the mass transfer in gas-liquid systems accompanied

by a reaction in a liquid film [12]. Typical examples involve reactive absorption and reactive distillation. Several mass transfer theories are available in literature to describe the mass transfer accompanied by a chemical reaction in a liquid film, namely the Whitman's film theory, Higbie's penetration theory and Danckwert's surface renewal theory [12,13]. Analytical solutions to these mass transfer theories are available only for a limited number of special cases; therefore, numerical solution is often necessary. However, as this field has been under intensive research over many decades, a variety of approximate solutions have been proposed [14,15].

In the present work, the effect of an irreversible second-order chemical reaction on the rate of dialysis at steady state is analysed. The analogy between the dialysis described by the solution-diffusion model and mass transfer in gas-liquid systems described by the film theory, both accompanied by chemical reactions, is taken into consideration. The applicability of the existing approximate solutions for the mass transfer accompanied by chemical reaction is examined and new correlations are developed.

### 2. Theory

#### 2.1. General mathematical description

Transport of component A (e.g., acid) is assumed through a nonporous membrane from the source solution (compartment I) to the receiving solution (compartment II). Component A reacts with component B (e.g., base) diffusing in the opposite direction by an

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### Nomenclature

$Ai(\xi)$	Airy function of the first kind
$Bi(\xi)$	Airy function of the second kind
$c$	molar concentration, $\text{kmol m}^{-3}$
$C_1, C_2$	coefficients in Eq. (A.1), $\text{kmol m}^{-3}$
$d$	parameter in Eq. (B.1), dimensionless
$D$	diffusion coefficient, $\text{m}^2 \text{s}^{-1}$
$e_r$	relative error, %
$E$	enhancement factor, dimensionless
$E_i$	enhancement factor corresponding to instantaneous reaction, dimensionless
$E_1$	enhancement factor corresponding to excess of component B, dimensionless
$h$	integration step, m
$Ha$	Hatta number, dimensionless
$J$	molar flux, $\text{kmol m}^{-2} \text{s}^{-1}$
$k_2$	second-order reaction rate constant, $\text{m}^3 \text{kmol}^{-1} \text{s}^{-1}$
$n$	adjustable parameter in Eqs. (34), (52) and (54), dimensionless
$N$	number of grid points, dimensionless
$r^2$	coefficient of determination of simple linear regression, dimensionless
$t$	integration variable in Eqs. (A.2) and (A.3), dimensionless
$u$	parameter in Eq. (B.1), dimensionless
$v$	parameter in Eq. (B.1), dimensionless
$x$	spatial coordinate, m
$X$	dimensionless spatial coordinate, dimensionless
$z$	stoichiometric coefficient, dimensionless

### Greek letters

$\delta_M$	membrane thickness, $\mu\text{m}$
$\delta_M^*$	distance of reaction plane from left-hand side membrane boundary, $\mu\text{m}$
$\Psi$	partition coefficient, dimensionless
$\xi$	transformed spatial coordinate, dimensionless
$\Gamma$	gamma function

### Subscripts

A	component A
B	component B
M	membrane
REX	Richardson extrapolation

### Superscripts

I	source solution (compartment I)
II	receiving solution (compartment II)

irreversible second-order reaction



The concentration profiles of both components A and B are depicted schematically in Fig. 1. Considering the solution-diffusion model for the membrane transport, the one-dimensional steady-state differential mass balance can be formulated for both reacting components in the membrane as follows:

$$D_{AM} \frac{d^2 c_{AM}}{dx^2} - k_2 c_{AM} c_{BM} = 0 \quad (2)$$

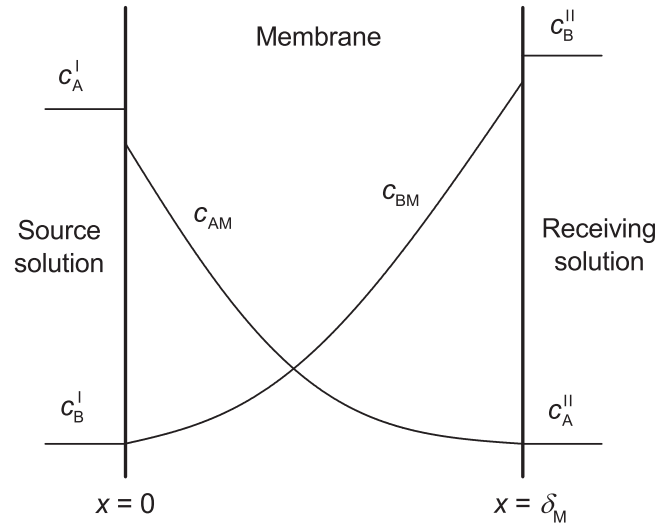


Fig. 1. Schematic representation of concentration profiles for dialysis with chemical reaction.

$$D_{BM} \frac{d^2 c_{BM}}{dx^2} - z k_2 c_{AM} c_{BM} = 0 \quad (3)$$

where  $D$  is the diffusion coefficient of the respective component,  $c$  is the molar concentration,  $x$  is the spatial coordinate,  $k_2$  is the second-order reaction rate constant and  $z$  is the stoichiometric coefficient. Subscripts A, B and M denote component A, component B and the membrane, respectively. The use of the one-dimensional mass balance implies that only local solutions are studied and concentration profiles of components A and B along the membrane are not considered in this paper.

Furthermore, the following assumptions are made:

- Well-mixed bulk liquids are present on both sides of the membrane; bulk liquids are in equilibrium with the membrane interface.
- Zero concentrations of components A and B in the receiving and source solutions are considered, respectively. This case is referred to as a fast reaction regime and is examined in this paper. As components A and B do not occur simultaneously outside the membrane, the chemical reaction is limited to the membrane only. In the case of a relatively slow reaction and relatively high mass transfer rates through the membrane, simultaneous presence of both components in the liquid bulk may occur, which implies that the bulk is not at equilibrium. This case is referred to as a slow reaction regime and requires rigorous mass balance over the respective liquid bulk to be used [14,16]. This case is not of interest in this paper.
- Mass transfer resistances in the liquid films on both sides of the membrane are considered negligible in order to avoid the necessity of solving the transport of both components in the membrane simultaneously with that in the liquid films.
- The system is isothermal; the effect of the reaction heat is neglected.
- Diffusion coefficients in the membrane are considered constant but generally unequal for both reacting components.

Provided that both components A and B are soluble in liquid phases on both sides of the membrane (Model 1), the boundary conditions for Eqs. (2) and (3) are as follows:

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