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Alternative pore hindrance factors: What one should be used for nanofiltration modelization?

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Abstract

In nanofiltration it is important for predictive purposes to obtain retentions and/or reflection coefficients from known sizes of the pores and the molecules of uncharged solutes. This correlation is also needed in order to model the mass transport of salts or other charged species. To complete these model and predictive needs, the hindrance factors have to be correlated with the ratio between the pore and the molecule sizes, λ. There are several correlations proposed in the literature. Moreover, the effect of the applied pressure was not accounted for in these correlations until recent revisions of the transport model. In some cases the action of the pore-wall friction has been also neglected.

Here we make a revision of these different assumptions on the hindrance factors, we discuss their effect on the transport and we show some conditions that a correct correlation should accomplish. It is shown that it is important to consider both the pressure and the pore-wall friction because the corresponding terms have important contributions to both retention and reflection. It is, nevertheless, less relevant an accurate choice of a relationship for the pore hindrance factors in terms of λ, as far as, both retention and reflection are mainly controlled by partitioning in the ranges where the different proposed correlations differ, what leads to the same transport predictions. In any case a theoretically correct correlation can be chosen attending to the conditions that the pore reflection must accomplish.

Keywords: Nanofiltration; Hindrance factors; Pressure effect; Pore-wall friction; Reflection coefficient

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1. Introduction

The transport equation

$$J_s = -\phi K_d D A_k \frac{\Delta c}{\Delta x} + \phi K_c J_V \bar{c} \quad (1)$$

gives the flux of an uncharged solute in terms of the diffusion coefficient, the volume flow, the average concentration and its gradient across the membrane and different coefficients (K_d and K_c). Where ϕ is the partitioning coefficient relating the concentration inside and outside the pores

$$\phi = \frac{c^i}{c} = (1-\lambda)^2 \quad (2)$$

This coefficient is sometimes called steric hindrance factor, and it is expressed in terms of $\lambda \equiv r_s/r_p$.

The K_d and K_c coefficients take into account the diffusive and convective hindrance due to other effects apart from partitioning and can be called pore hindrance factors. They can also be given in terms of the λ ratio. The effect of the friction forces between the solute molecules and the pore walls is usually included within these factors.

Actually there are many possible elections for the detailed expressions of both the pore hindrance factors. For predictive purposes both retention and reflection coefficient can be calculated for a given pore and molecule size. Both the points of view need an adequate election of the pore hindrance versus λ correlation. Thus an early question to be considered is which correlation to use. Here we give some criteria to be taken into account when answering this question in order to model the nanofiltration of uncharged molecules.

2. Pore hindrance factors

The pore hindrance factors, take into account the solute movement through the membrane pores where the transport is hindered due the restrictions of the movement of the solute molecules. Many alternative expressions have been proposed for these hindrance factors. All they are based on the analysis of the detailed fluid mechanics of particles moving through tubes or capillaries containing a still fluid.

A review of many of these calculations was presented by Deen [1]. After the seminal works of Ferry [2], Pappenheimer et al. [3], and Renkin [4], one of the first detailed study of such K_d and K_c functions of λ for wide range of λ ($0 < \lambda \leq 0.9$) was addressed by Haberman and Sayre [5], and afterwards used by Verniory et al. [6] and Nakao and Kimura [7]. They evaluated the factors as

$$K_d = \frac{1 - 2.105\lambda + 2.0865\lambda^3 - 1.7068\lambda^5 + 0.7260\lambda^6}{1 - 0.75857\lambda^5} \quad (3)$$

$$K_c = \frac{(1 + 2\lambda - \lambda^2)(1 - (2/3)\lambda^2 - 0.20217\lambda^5)}{1 - 0.75857\lambda^5} \quad (4)$$

Bohlin [8], derived similar equations.

A complete correlation ($0 < \lambda \leq 1$) was due to Bungay and Brenner [9]:

$$K_d = \frac{6\pi}{K_t} \quad (5)$$

and

$$K_c = (1 + 2\lambda - \lambda^2)\frac{K_s}{2K_t} \quad (6)$$

with

$$K_t = \frac{9}{4}\pi^2\sqrt{2}(1-\lambda_i)^{-5/2}\left(1 + \sum_{n=1}^{2} a_n (1-\lambda_i)^n\right) + \sum_{n=0}^{4} a_{n+3}\lambda_i^n \quad (7)$$

$$K_s = \frac{9}{4}\pi^2\sqrt{2}(1-\lambda_i)^{-5/2}\left(1 + \sum_{n=1}^{2} b_n (1-\lambda_i)^n\right) + \sum_{n=0}^{4} b_{n+3}\lambda_i^n \quad (8)$$