Nanofiltration Membrane Predictive Models

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Abstract

Literature models for nanofiltration (NF) are usually based either on a mechanism-independent approach, such as irreversible thermodynamics (IT), or depending on transport mechanism (hydrodynamic approach). Most current IT models are based on the work of Spiegler and Kedem. For the mechanistic models; it is divided into two categories: those based on the Space Charge (SC) model and Teorell-Meyer–Sievers (TMS) model. These approaches have been used in order to determine the ion transport mechanisms during separation process which is commonly governed by both of steric and charge effects.

Keywords: Nanofiltration membrane, Predictive models, Mechanism-independent, Mechanism dependent

1.0 Introduction

This paper briefly reviews nine NF predictive models including Space Charge (SC) model, Teorell-Meyer-Sievers (TMS) model, Electrostatic and Steric Hindrance (ES) model, Steric Hindrance Pore (SHP) model, Kedem Spiegler model (KSM), Adsorption-Amphoteric (ADS-AMF) model, Dielectric Exclusion (DE) model, Steric, Electric and Dielectric (SEDE) model and lastly Donnan Steric Pore model (DSPM). Each of the models has different approaches and assumptions for NF membrane characterization.

2.0 Space Charge (SC) Model

The Space Charge (SC) model, which was originally proposed by Osterle and co-workers in 1971, is a more realistic model to predict rejection performance of NF membranes, since the SC model assumes a straight capillary having charge on its surface. The basic equations of the SC model are the Poisson-Boltzmann equation for the radial distribution of electric potential and ion concentration, the Nernst-Planck equation for ion transport, and the Navier-Stokes equation for volumetric flow. According to Bowen et al. (2002), it has been mainly applied to describe electrokinetic phenomena of charged capillaries such as streaming potential and electric conductivity. The methods to predict rejection by the SC model are categorized into two approaches. One of those is the straightforward calculation for the SC model. Another approach is the analytical method (Wang et al., 1995).

3.0 Toerell-Meyer-Sievers (TMS) Model

Tsuru et al. (1991a; 1991b) stated that the Teorell-Meyer-Sievers (TMS) model has been successfully used in research employing ion-exchange membranes, and has been also applied to describe the rejection of charged reverse osmosis (RO) membranes and ultrafiltration (UF) membranes. The TMS model assumes uniform distribution of fixed charge; this model is not based on structural parameters such as pore radius. The mobile ion concentration and the electric potential vary with the direction of flow. This model simplifies mathematical analysis and gives an analytical equation of ionic transport. However, the range where the TMS model can be successfully applied is limited since one cannot assume uniform distribution of fixed charge, mobile ions and electric potential, especially for membranes with large pore radius.

4.0 Electrostatic and Steric-Hindrance (ES) Model

The Electrostatic and Steric-Hindrance (ES) model, describe the transport phenomena of charged solutes across a charged porous membrane by considering both the electrostatic and steric-hindrance effects, and verified the ES model in the permeation of a mixture of a tracer organic electrolyte (sodium benzenesulfonate) and a supporting salt (NaCl) through the four commercial NF membranes (Wang et al., 2006).

5.0 Steric-Hindrance Pore (SHP) Model

The Steric-Hindrance Pore (SHP) model to estimate the pore radius (r_p) and the ratio of membrane thickness to porosity (A_k/Δ_x) of UF membranes in terms of the membrane parameters obtained from permeation experiments of different neutral solutes. The pore radii of charged UF membranes were estimated from the SHP model to be a few nanometers as stated by Nakao (1986), which seems to be larger than those of NF membranes. The SHP model is applicable to the NF membranes which possess the pore radius larger than or equal to about 0.5 nm.

6.0 Kedem-Spiegler Model (KSM)

The Kedem-Spiegler Model (KSM) was observed to be able to predict lactose retention in the presence or absence of ions without providing any information about the membrane structure. KSM model is based on irreversible thermodynamics and it was firstly developed for RO membranes and for single solute non-electrolyte solutions (Kedem & Katchalsky, 1958). In this model the membrane is considered as a black box and it is characterized in terms of solute permeability and the reflection coefficient. The KSM model has been frequently used to describe the transport mechanism of ions through NF membranes and to calculate the retention of ions in single and mixed electrolyte solutions as mentioned by Koyoncu and Topacik (1995). The KSM parameters are solute permeability (P_s) and solute reflection coefficient (σ).

7.0. Adsorption-Amphoteric Model (ADS-AMF)

A simple rough version of the Adsorption-Amphoteric (ADS-AMF) model has been developed to describe the mechanism of charge formation in NF membranes (Bandini, 2005). The model introduced a site-representation of the membrane as the sum of hydrophobic as well as of hydrophilic groups, which can support charges derived from various chemical and physical mechanisms. The prevailing mechanisms in determining the volume membrane charge were considered as acid or base dissociation of the hydrophilic functional groups, counter-ion site binding on the dissociated hydrophilic groups and ionic competitive adsorption on the hydrophobic functional groups.

8.0 Dielectric Exclusion (DE) Model

The Dielectric Exclusion (DE) is also one type of membrane filtration's model. DE is phenomenon as an additional electrostatic partitioning effect. Yaroschuk (2000) believes that this phenomenon is due to a series of concomitant effects. The primary effect is caused by the difference existing between the dielectric constant of an aqueous solution and the corresponding value of the polymeric matrix. The secondary effect is due to the variations of the solvent dielectric properties inside the membrane pores, with respect to the external bulk values, which are caused by an alteration of the solvent structure when it is confined in small narrow pores.

9.0 Steric, Electric and Dielectric Exclusion (SEDE) Model

Another model that involved in membrane filtration is Steric, Electric and Dielectric Exclusion (SEDE) model. The SEDE model can be used to describe transport through pores of cylindrical or slit geometry and then used to assess the rejection rate of the membrane, the dielectric constant of the solution filling pores being the single adjustable parameter of the model. Szymczyk and Fievet (2005) stated that it is clearly shown that the dielectric exclusion cannot be neglected in the analysis of the filtration properties of NF membranes.

10.0 Donnan and Steric Pore Model (DSPM)

One model that is the focus of this paper was developed by Bowen et al. (1997). The so-called Donnan and Steric Pore Model (DSPM) is based on the extended Nernst-Planck equation and this equation has proven to be useful in describing the solute transport through NF membranes and to analyze retention properties of a variety of NF membranes (Bowen et al., 1997). DSPM has been shown to be successful in the prediction of NF performance in dye-salt diafiltration in previous study by Mohammad et al., 2007. Ion transport is described by the extended Nernst-Planck equation, modified to included hindered transport, with equilibrium partitioning due to a combination of electrical (Donnan) and sieving (steric) mechanisms. This model has been at least as successful as any other existing model in describing NF performance.

11.0 Conclusion

NF membrane predictive models are certainly vital in process performance prediction, hence, process design and optimization. The fundamental understanding of these models are crucial towards designing cost-performance effective membrane separation systems.

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