Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Multi-scale modelling of OSN batch concentration with spiral-wound membrane modules using OSN Designer

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ARTICLE INFO

Article history:
Received 5 October 2015
Received in revised form 21 January 2016
Accepted 4 February 2016
Available online 11 February 2016

Keywords:
Batch concentration
Spiral-wound membrane module
Organic solvent nanofiltration
Multi-scale modelling
OSN Designer

ABSTRACT

Three commercial spiral-wound membrane modules of different sizes, from 1.8″ × 12″ to 4.0″ × 40″, are used to concentrate a solution of sucrose octaacetate in ethyl acetate under different operating conditions. A mathematical model to describe the batch concentration process is developed, based on a combination of the classical solution diffusion membrane transport model and the film theory, to account for the mass transfer effects. The model was implemented using the "OSN Designer" software tool. The membrane transport model parameters as well as all parameters in the pressure drop and mass transfer correlations for the spiral-wound modules were obtained from regression on a limited number of experimental data at steady state conditions. Excellent agreement was found between the experimental and multi-scale modelling performance data under various operating conditions. The results illustrate that the performance of a large scale batch concentration process with spiral-wound membrane modules can be predicted based on laboratory crossflow flat sheet test data when the fluid dynamics and mass transfer characteristics in the module, and the necessary channel geometry are known. In addition, the effects of concentration polarisation, pressure drop through feed and permeate channels, and thermodynamic non-ideality of the solution at large scale batch concentration are also investigated.

1. Introduction

Primarily, research activities in the field of organic solvent nanofiltration (OSN) have been focused on the development of new materials stable in organic solvents and harsh conditions, while industrial scale applications are still few. A fundamental understanding of the basic separation mechanism and a reliable modelling framework are crucial to bridge this gap, meet the growing needs and applications, and make the scale-up more efficient and economic [White, 2006]. In the development of a multi-scale mathematical model for an OSN process with spiral-wound membrane modules, the following problems have to be resolved: (i) selection of adequate membrane transport mechanism to describe the molecular transport across the membrane; (ii) knowledge of the fluid dynamics and mass transfer characteristics in the module;

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http://dx.doi.org/10.1016/j.cherd.2016.02.005
0263-8762/

Nomenclature

List of symbols

A	effective membrane area (m^2)
a	coefficient in friction coefficient correlation (dimensionless)
b	exponent of Reynolds number in friction coefficient correlation (dimensionless)
$C_{F,S,0}$	initial concentration of solute in feed ($mol\,m^{-3}$)
$C_{F,S,t}$	concentration of solute in feed at process time t ($mol\,m^{-3}$)
$C_{P,S,t}$	concentration of solute in permeate collection tank at process time t ($mol\,m^{-3}$)
d_h	hydraulic diameter (m)
f	friction coefficient (dimensionless)
J_i	molar permeate flux of species i ($mol\,m^{-2}\,s^{-1}$)
$J_{V,t}$	module flux at process time t ($m^3\,m^{-2}\,s^{-1}$)
k	mass transfer coefficient ($m\,s^{-1}$)
L	length of channel (m)
P	pressure (Pa)
$P_{m,i}$	permeability coefficient of species i ($mol\,m^{-2}\,s^{-1}$)
ΔP	pressure drop (Pa)
R	ideal gas constant ($Pa\,m^3\,mol^{-1}\,K^{-1}$)
Re	Reynolds number (dimensionless)
$Rej_{S,t}$	observed rejection of solute at process time t (%)
Sc	Schmidt number (dimensionless)
Sh	Sherwood number (dimensionless)
T	temperature (K)
$V_{F,t}$	solution volume in feed tank at process time t (m^3)
$V_{P,t}$	solution volume in permeate collection tank at process time t (m^3)
x_i	molar fraction of species i in solution (dimensionless)

Greek symbols

α	coefficient in Sherwood number correlation (dimensionless)
β	exponent of Reynolds number in Sherwood number correlation (dimensionless)
λ	exponent of Schmidt number in Sherwood number correlation (dimensionless)
ρ	density ($kg\,m^{-3}$)
v_i	molar volume of species i ($m^3\,mol^{-1}$)
γ_i	activity coefficient of species i (dimensionless)

Subscripts

F	feed solution or feed channel
FM	feed side membrane-liquid interface
P	permeate solution or permeate channel
t	process time t

Abbreviations

EA	ethyl acetate
OSN	organic solvent nanofiltration
SoA	sucrose octaacetate
UNIF-DMD	Dortmund modified UNIFAC method

(iii) availability of the thermodynamic and physical properties of the solutions under different operating conditions.

Marchetti and Livingston (2015) systematically compared different models (based on irreversible thermodynamics, pore-flow, solution-diffusion and hybrid approaches) using selected experimental data and concluded that the classical solution-diffusion model gives the best description of permeation through flexible chain glassy membranes and rubbery membranes, without overcomplicating (or overparameterising) the modelling procedure. Since the thin film composite membrane used in this study has a rubbery separating layer, the classical solution diffusion model was selected to describe the membrane transport.

Many studies [Schock and Miquel, 1987; Schwinge et al., 2000; Li et al., 2002; Fimbres-Weihs and Wiley, 2007; Koutsou et al., 2009] have been published on the fluid dynamics and mass transfer characteristics in spacer-filled channels, which mimic the channel of spiral-wound membrane modules, in aqueous solutions. Various dimensionless correlations for the friction coefficient and the Sherwood number were generated. However, from the point of view of process design, there is still lack of suitable correlations for OSN applications, due to the fact that the correlations derived from aqueous solutions may not be suitable for OSN applications where the Reynolds and Schmidt numbers can vary more significantly. Furthermore, the fluid dynamics and mass transfer characteristics are dependent on the spacer geometry which is usually confidential in commercial modules, and unknown for end users. Recently, Shi et al. (2015) proposed a procedure to generate correlations for characterising the fluid dynamics and mass transfer characteristics in spiral-wound membrane modules. Specifically, three correlations for describing the friction coefficients in both the feed and permeate channels and the Sherwood number in the feed channel for OSN applications were proposed.

The last stage in the development of a multi-scale process model is the availability of all required thermodynamic and physical properties of the solutions of interest, as a function of the operating conditions. Considering that the collection of thermodynamic and physical data for all the possible solute/solvent combinations by experiments would be prohibitively time consuming, it is useful to rely on a simulation tool to predict the values of these properties. Peshev and Livingston (2013) recently proposed a tool, "OSN Designer", which makes OSN unit operations available in process modelling environments such as Aspen Plus, HYSYS and ProSim Plus, to streamline OSN process design. The thermodynamic and physical properties of the solutions were obtained from the Aspen Properties Database or estimated using built-in models in the process modelling environment. This tool was validated using published experimental data under steady-state and batch conditions.

Some examples for application of OSN to concentration and purification in industrial applications have been published previously. For instance, OSN was applied to the recovery and purification of pharmaceuticals [Cao et al., 2001; Marchetti et al., 2013; Sun et al., 2014], solvent exchange [Sheth et al., 2003], separation of base chemicals [Werhan et al., 2012; Othman et al., 2010], purification and concentration of consumer chemicals [Vanneste et al., 2011; Tsibranska and Tylkowski, 2013], concentration and purification of specialty chemicals [Tsui and Cheryan, 2007], and homogeneous catalyst recycle [Van der Gryp et al., 2010]. These studies showed the feasibility of OSN technologies in different