chemical engineering research and design 90 (2012) 1098–1104

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Research and Design

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

Modeling ultrafiltration of gelatin–water suspension by computational fluid dynamics

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ABSTRACT

In this paper, principles of computational fluid dynamics (CFD) are used to study ultrafiltration (UF) process. Model has been developed by a new technique in which permeation of solvent molecules is introduced to system via appropriate sink terms in conservation equations for computational domain. Experimental data and fittings are applied in model development. Model results have been compared for two and three-dimensional geometries. Finally a time step and mesh size independent model has been developed in two dimensions for modeling the permeation flux vs. filtration time in a gelatin–water UF system. Final model is able to predict steady-state permeation flux with relative error less than 2%. Accuracy of calculation is investigated through the comparison between mass imbalance and sum of local fluxes. Modeling results show that increase in cross flow velocity (CFV) and trans-membrane pressure (TMP) leads to increase in permeation flux but decrease in solute concentration and rejection of solute particles from membrane surface makes permeation flux increase.

Keywords: Ultrafiltration; Computational fluid dynamic; Concentration polarization; Permeation flux decline

1. Introduction

The widespread application of ultrafiltration (UF) in the industry has made the researchers and industrialists pay attention to the modeling of such processes. Inadequate knowledge of process mechanism and experimental data are examples of limitations in different types of modeling. White box modeling requires adequate knowledge of process mechanisms so it is possible to use white-box methods like computational fluid dynamics (CFD) approach for UF modeling as an almost well-known pressure driven membrane process. UF modeling can be classified in three groups: classical and empirical models, mathematical and CFD models and models based on artificial intelligence.

As empirical and classical models, Cheng and Wu (2001) developed a modified model to consider both effects of osmotic pressure and the boundary layer resistance on permeation flux. Paris et al. (2002) compared results of two-dimensional mathematical modeling with classical models like resistance in series and gel-polarization models. Mohammadi et al. (2005) used experimental data to calculate Lihan-Huang equation parameters and developed the model by adding third parameter for better adjustment between experimental data and model results for gelatin in water suspension. Sarkar et al. (2006) and Bhattacharjee et al. (2006) modeled UF of kraft black liquor with two irreversible thermodynamic methods, Spiegler–Kedem (SK) and Kedem–Katachalsky (KK). UF module of a rotating disk was also modeled in 2008. (Sarkar and Bhattacharjee, 2008).

Literature review of mathematical and CFD methods in modeling shows that in 1997, a circular channel was modeled via finite element method by coupling Navier–Stockes and Darcy equations (Nassehi, 1998). Huang and Morrissey (1999) used finite element method for modeling a rectangular

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Received 17 June 2011; Received in revised form 31 October 2011; Accepted 11 November 2011
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doi:10.1016/j.cherd.2011.11.010

Nomenclature

A	cell area (m^2)
C	concentration (kg/m^3)
D	diffusion coefficient (m^2/s)
J	local permeation flux ($10^{-3}\,m^3/m^2\,s$)
$\bar{J}$	average permeation flux ($10^{-3}\,m^3/m^2\,s$)
k	turbulent kinetic energy (m^2/s^2)
P	pressure (Pa)
Re	Reynolds number
S_m	mass balance source term ($kg/m^3\,s$)
S_s	species transport source term ($kg/m^3\,s$)
S_y	Y-momentum source term (N/m^3)
t	filtration time (s)
u	X-velocity (m/s)
v	Y-velocity (m/s)
w	Z-velocity (m/s)
V	cell volume (m^3)
V	permeate volume ($10^{-3}\,m^3$)
V_c	critical permeate volume or permeation volume after 60 s of process start-up ($10^{-3}\,m^3$)
$\rho u'v'$	tensor of Reynolds stresses (Pa)
y_g	gelatin mass fraction

Greek symbols

α, β and γ	model parameters reported in literature (Mohammadi et al., 2005)
ΔP	trans-membrane pressure (Pa)
ε	turbulent dissipation rate (m^2/s^3)
μ	viscosity (Pa s)
μ_t	turbulent viscosity (Pa s)
ρ	density (kg/m^3)
$C_{1\varepsilon}$	constant in the k–ε equations (equal to 1.44)
$C_{2\varepsilon}$	constant in the k–ε equations (equal to 1.92)
σ_k	constant in the k–ε equations (equal to 1.0)
σ_ε	constant in the k–ε equations (equal to 1.3)

channel. A staggered mesh procedure was also developed for modeling ultrafiltration process (Kumar and Upadhyay, 2000). Geraldes et al. (2002) modeled nanofiltration (NF) of NaCl by CFD technique. Pressure drop was modeled via CFD in a permeable channel and results were compared with Berman's equation (Karode, 2001). A hydrodynamic method was also used for modeling different symmetric and asymmetric commercial spacer arrangements (Karode and Kumar, 2001). CFD was used by Tarabara and Wiesner (2003) to model dead-end and cross-flow filtration. Some stationary regions were reported in dead-end processes which were determined as the reason of flux decline. Model with non-uniform meshing in adjacent of membrane was studied by Wiley and Fletcher (2003). Taha and Cui (2002) modeled turbulency creation in gas sparged tubular membranes. Staudacher et al. (2002) used CFD for modeling a gas and vapor permeation system, in the same year. Fluid permeation from membrane was introduced as sink terms in conservation equations. UF process modeling by variable physical properties of mixture (Wiley and Fletcher, 2002) and modeling UF of lysozyme (Magueijo et al., 2002) were published in 2002. Lipnizki et al. (2003) modeled a spiral wound module by CFD to investigate significant effect of spacer arrangement on pressure drop and mass transfer. In 2005, Ahmad et al. (2005) used Fluent and user defined functions in order to introduce membrane as boundary condition in a developed model. Microfiltration (MF) of deionized water was modeled by Rahimi et al. (2005) in simple and baffle-filled membrane channels. A review study showed that CFD applications in NF, UF, MF and reverse osmosis (RO) modeling has grown up to 2005 (Ghidossi et al., 2006). The main reason of the CFD application growth was introduced the development in processing power of computers. Dal-Cin et al. (2006) used CFD for modeling of one tubular membrane in order to simulate a module with five membrane channels then they compared the results with Bernoulli equation.

Staggered mesh technique was used in modeling a MF process (Pak et al., 2008). The model was able to predict the effect of Reynolds and Schmidt numbers on polarization boundary layer thickness. CFD was used to find the best arrangement of spacers in 12 available commercial spacer arrangements (Santos et al., 2007) and also to study the effect of geometrical specifications of spacer on mass transfer in a spiral wound membrane module (Shakaib et al., 2009).

Membrane was considered as porous medium and Darcy equation was used for flow modeling in membrane (Hanspal et al., 2009). One hollow fiber membrane was modeled in order to model a module with 50 hollow fiber membranes (Marcos et al., 2009). Liu et al. (2009) modeled a baffle-filled membrane tube and showed the central baffling is more effective than wall-baffling. Madaeni et al. (2010) used colored feed UF experiments to observe the deposition tendency of particles on membrane surface. Developed CFD model was used to investigate system's hydrodynamics. UF of protein solution was studied and it was shown that Because of low solute concentration, cake formation can be ignored in modeling (Schausberger et al., 2009).

Artificial intelligence methods of modeling which include genetic and neural network are also noticed by researchers. Razavi et al. (2003a, 2003b, 2004) used neural network for modeling the UF of milk and investigated the effects of temperature and trans-membrane pressure (TMP) on permeation flux and fouling resistances. Curcio et al. (2005, 2006), modeled UF of BSA via neural network in constant and variable pulsating condition. They also developed a gray-box model that used CFD technique for solving conservation equation and determination of adsorption behavior was made by a simple neural network (Curcio et al., 2009). Using genetic algorithm to optimize neural network modeling (Sahoo and Ray, 2006) and UF modeling of apple juice via four layer neural network (Gökmen et al., 2009) were also some of artificial intelligence modelings. Genetic algorithm and neural network were used for automation membrane back-wash (Strugholtz et al., 2008). Genetic programming was applied for a water treatment pilot plant (Hwang et al., 2009). Wei et al. (2009) modeled cross-flow membrane filtration of colloidal suspensions by a wavelet network approach.

Among several modeling methods, CFD by supplying detail information of flow characteristics all over the membrane channel (e.g. flow specification profiles), is the most beneficial procedure in membrane process studies so in this research, CFD approach is chosen as modeling method. A novel two-dimensional unsteady state and isothermal model which is tested to be independent of mesh and time step size is developed. In present study, in spite of similar studies, the effect of molecules permeation from membrane is mentioned in model as appropriate source and sink terms while previous studies involve permeation through membrane in boundary conditions or totally neglect it. This model is able to report flux-time behavior on membrane surface. Experimental data