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CFD modeling of a transient hollow fiber ultrafiltration system for protein concentration

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ABSTRACT

A transient model based on the finite element method (CFD Comsol) to simulate numerically the flow (momentum equation) and the concentration (diffusion–convection equation) in an ultrafiltration unit is presented. The CFD model was developed by solving the 2D Navier–Stokes equation and the mass conservation equation for transient conditions. A resistance model was used to link the retained protein concentration, the feed and permeate velocity and the pressure at the membrane surface. The ultrafiltration unit consists of a hollow fiber module, a feed tank and a feed pump. In the hollow fiber module, the variable transmembrane pressure, a variable viscosity of the retentate and a polarization layer and a time variable cake occurring on the membrane are considered. Under laminar flow regime, the model allows for the predictions of the velocity fields, the pressure and the concentration along the membrane fiber. The model predictions for the transient permeate flux and the pressure profile in the fiber are compared to experimental data during the concentration of soy protein extracts in a hollow fiber module where total retention of the soy protein is achieved. The comparison shows that the proposed model fits well with the experiments and shows the interest to take into account the variation of resistance and the concentration dependant viscosity flux. The model shows that the transmembrane pressure is an important element on the polarization concentration profile and that a constant transmembrane pressure yields erroneous conclusion on the concentration polarization. The model alleviates some limitations on the polarization modeling avoiding the need to estimate the polarization thickness in the computation of the polarization resistance. The flexibility of the current model is only limited by the ability of the user to accurately define the variations of the properties of the system for industrial applications.

1. Introduction

Membrane technology has received considerable interest over the years for the concentration of soy proteins where proteins are retained by the membrane while the oligosaccharides and minerals are assumed to be removed through the membrane [16]. However, one limitation is the declining permeate flux with time as feed components accumulate on the membrane surface resulting in a polarization layer and possibly a cake formation and pore plugging. It is well known that these phenomena are related by the hydrodynamics of the system contributing to fouling. Accurate predictions of permeate flux and permeate quality are major tasks to design and evaluate membrane processes. To predict accurately the membrane operation and the transient behavior of the permeate flow, it is necessary to model the hydrodynamics and mass transfer phenomena that take place in the bulk solution and at the surface of the membrane.

In the context of membrane separation processes, the simulation approaches may use macroscopic or microscopic models. Most macroscopic models incorporate detailed resistance models such as pore-blocking resistance or cake resistance (Bolton et al. [1], Ho and Zydney [2]) while few microscopic models will include such resistance models. The macroscopic models consist of simplified global mass balance where permeate flux is related to the transmembrane pressure, global membrane resistance, viscosity and other average hydrodynamic parameters. In contrast, the microscopic models use the conservation equations that are solved with the help of numerical scheme either developed by authors (Damak et al. [3], Oxanrago et al. [4], Secchi et al. [5], Sulaiman et al. [6], Geraldes et al. [7], Pellerin et al. [8]), or by available commercial CFD tools (Ahmad et al. [9], Wiley and Fletcher [10], Bessiere et al. [11], Subramani et al. [12]). Broadly speaking, the mass diffusion equation is used but the momentum equation is not always completely solved. For example, Oxanrago et al. [4] used an asymptotic development of the Navier–Stokes equations. Such an approach introduces approximation on the radial velocity and consequently on the permeate flux. It also requires constant viscosity and diffusion although in reality the viscosity may change significantly for protein solutions. Recently,

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Bessiere et al. [11] developed a colloid dead-end filtration model in commercial CFD software taking into account variable diffusivity and viscosity. The microscopic approaches also differ with respect to the boundary conditions. Ahmad et al. [9], Lee et al. [13], Varol et al. [14] assume that the permeate velocity is constant along the fiber but the assumption is not realistic. Geraldes et al. [7] use experimental permeate velocity at different positions as boundary condition, but it is to be noted that the local permeate velocity flow may be quite difficult to measure. Bessiere et al. [11] assume that permeate velocity is variable along the fiber (depending on wall concentration and osmotic pressure) but constant with the time during the transient simulations. The relationship between the local permeate velocity and the different resistances is an important characteristic of the microscopic models. Wiley and Fletcher [10] assumes that the permeate velocity is independent of transmembrane pressure and the global resistance. Some authors consider the polarization layer. However, the definition of the polarization layer thickness is not uniform. Damak et al. [3] and Pak et al. [15] define the thickness of the polarization layer as the distance from the membrane surface to the position where the relative error between the wall concentration and the bulk concentration was inferior or equal to 10^{-3}. Geraldes et al. [7] define the polarization boundary layer thickness as the distance from the membrane surface at which the solute concentration exceeded by 5% the solute concentration in the bulk flow. Ahmad et al. [9] use the simple film theory to compute the thickness of the gel polarization layer but the film theory requires an estimate of the mass transfer coefficient and overestimates the thickness estimation.

Previous studies do not always include an experimental validation of the model (Damak et al. [3]) or may contain important gaps between the model predictions and the experimental data (Suleiman et al. [6]). The differences may come from the incomplete modeling of the resistance (Suleiman et al. [6]) or from some of the assumptions made, a constant viscosity (Secchi et al. [5]), a constant permeate velocity (Lee et al. [13]). Wiley and Fletcher [10] proved that the model predictions change significantly whether constant properties are assumed or if the properties are assumed to depend on the concentration. An accurate solution of the hydrodynamics and diffusion model is important because it enables the accurate computation of the radial velocity (the axial velocity follows closely the classical parabolic profile), the computation of the pressure related to the viscosity and the computation of the concentration. Due to the coupling of the mass and momentum equations, the CFD approach is relevant for solving such problems. Finally, the permeate flux is the important factor of the filtration process and an accurate prediction of the transient permeate flux should include the different fouling mechanisms. In this paper, we present a CFD modeling study for the analysis of the hydrodynamics and the mass transfer considerations in the bulk and at the membrane surface during the transient operation of the concentration of soy protein extracts by ultrafiltration operated at typical constant TMP conditions for soy protein concentration [29]. The concentration of soy protein extracts by cross-flow hollow fiber ultrafiltration is used to develop the model and to provide model predictions that are compared to experimental data. The experimental data enables the model validation.

2. Experimental

2.1. Experimental set-up

A high shear hollow fiber tangential flow membrane ultrafiltration unit was used (Fig. 1). Soy protein extracts were placed in a 2-L feed tank (1). During the filtration, the retentate was returned to the feed tank which agitated the feed solution resulting in homogenous mixing. A Moyno progressing cavity variable speed pump (2) with a

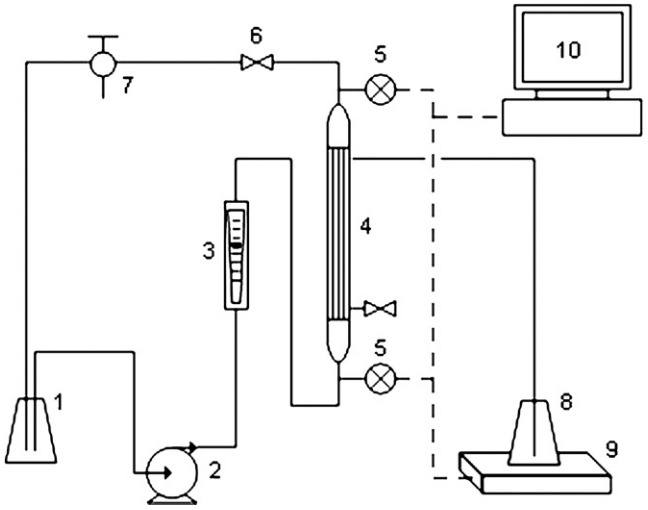

Fig. 1. Schematic diagram of the hollow fiber ultrafiltration experimental system: 1, feed tank; 2, pump; 3, flowmeter; 4, membrane; 5, pressure transducers; 6, pinch valve; 7, sampling valve; 8, permeate container; 9, balance; 10, PC/software.

fluid flow rate of 0–5.68 L/min (0–1.5 GPM) was used to provide high shear pulseless flow to the membrane module. A flow meter (Cole Parmer A-32477-04) was installed on the feed line (3) to measure the flow rate of the feed solution entering the membrane module. A hollow fiber ultrafiltration membrane cartridge (Amersham Biosciences UFP-100-E-4MA) was used (4). The membrane material was polysulphone with a 100-kDa molecular weight cut off. The module was 30 cm in length with 50 fibers of 1 mm inner diameter. The membrane surface area was 420 cm^2. The permeate was collected in a 2-L glass beaker (8) placed on an AdamLab AEP Top loader balance (Cole Parmer A-11700-92) which measured the mass of permeate collected with time enabling the determination of the permeate flux. The capacity of the balance was 2500 g with an accuracy of 0.001 g. Real time data acquisition was achieved via a data acquisition card (10) connected to a PC running Labview®. The data acquisition card was a USB based personal measurement device (Techmatron Instruments PMD-1208LS) which connected directly to the PC where Labview 6.1® was installed. Pressure transducers were placed on the feed (Cole Parmer 0–50 psig A-68075-16), retentate (Cole Parmer 0–50 psig A-68075-16) and permeate (Cole Parmer 0-25 psig A-68075-44) lines to measure the transmembrane pressure.

2.2. Experimental procedure

Soy protein extracts were provided by Agriculture and Agri-Food Canada (St-Hyacinthe, Canada) and produced according to Mondor et al. [17]. The extracts were produced by alkali extraction and had a final pH of 9. For the concentration experiments, the feed solution was prepared by reconstituting a given amount of the powdered extract in a given volume of Nanopure® water. The concentration studies were carried out at 25 °C and at the pH of extracts by drawing off the permeate to achieve a volume concentration ratio (VCR) of 3.5 defined as the ratio between the volume of the feed and the volume of the retentate. A shear rate of 8000 s^{-1} was employed corresponding to a 2.4-L/min feed flowrate (Q_{feed}). The global transmembrane pressure TMP, $TMP = ((P_{in} + P_{out})/2) - P_{Permeate}$, was maintained at 27580 Pa (4 psi) or 41370 Pa (6 psi). At the start of the experiment, the feed solution was circulated with the retentate valve completely open. Permeate flux measurements were taken by measuring the time it takes for 1 g of solution to permeate the membrane. Two permeate flux measurements were taken for every 25 g