SURVEY OF THEORETICAL APPROACHES TO MODELING PRESSURE-DRIVEN MEMBRANE PROCESSES (SUBMODELS FOR TRANSPORT IN PHASES)

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Contents

Summary

This chapter has considered approaches to modeling pressure-driven membrane processes accumulated in scientific literature. It covers submodels for hydraulic and mass transfer resistance in liquid phases, and also includes submodels for hydrodynamic and concentration fields and solutions describing phenomena of gel or cake accumulation on the membrane surface. Also discussed are transverse and axial subconstituents for velocity field in channels having symmetric and asymmetric configurations and various shapes (rectangular, cylindrical, etc.), and concentration submodels being received from reduced forms of convective diffusion equation. In particular, analytical and numerical solutions for concentration profiles in channels of various shapes are included. Approaches to modeling concentration field assuming concentration-dependent shear viscosity and shear-induced diffusivity are discussed. Finally, gel-polarization submodels and their modifications are covered. A submodel based on different assumptions and underlying premises is included and, in particular, approaches based on standard filtration theory, approaches considering lateral migration phenomena, stochastic approaches accounting individual trajectories and forces acting on the discrete particles are discussed.

Considered hydrodynamic, concentration and gel submodels are going to be conjoined and built into a comprehensive algorithm. A review of published literature indicates that there are some oversimplifications which are not justifiable in some particular cases. The field equations for any membrane process are decoupled and drastically reduced assuming symmetric, steady, unidirectional, isothermal, laminar dilute flow with shear independent viscosity and diffusivity having constant membrane properties and ignoring influence of entry and exit regions. In particular, there is no reliable correlation for quantitative estimation of concentration layer and gel behavior. Mass transfer correlations for membrane systems were predominantly borrowed from studies of flow in non-permeable channels.

1. Introduction

Modeling hydraulic and mass transfer resistances is one of the central tasks in calculation of pressure-driven membrane processes. The procedure of calculation is rather complicated and multivariable being influenced by many factors. Hydraulic and mass transfer resistances are closely linked with the configuration of related fields. A schematic diagram of longitudinal development of concentration and hydrodynamic profile is shown in Figure 1.

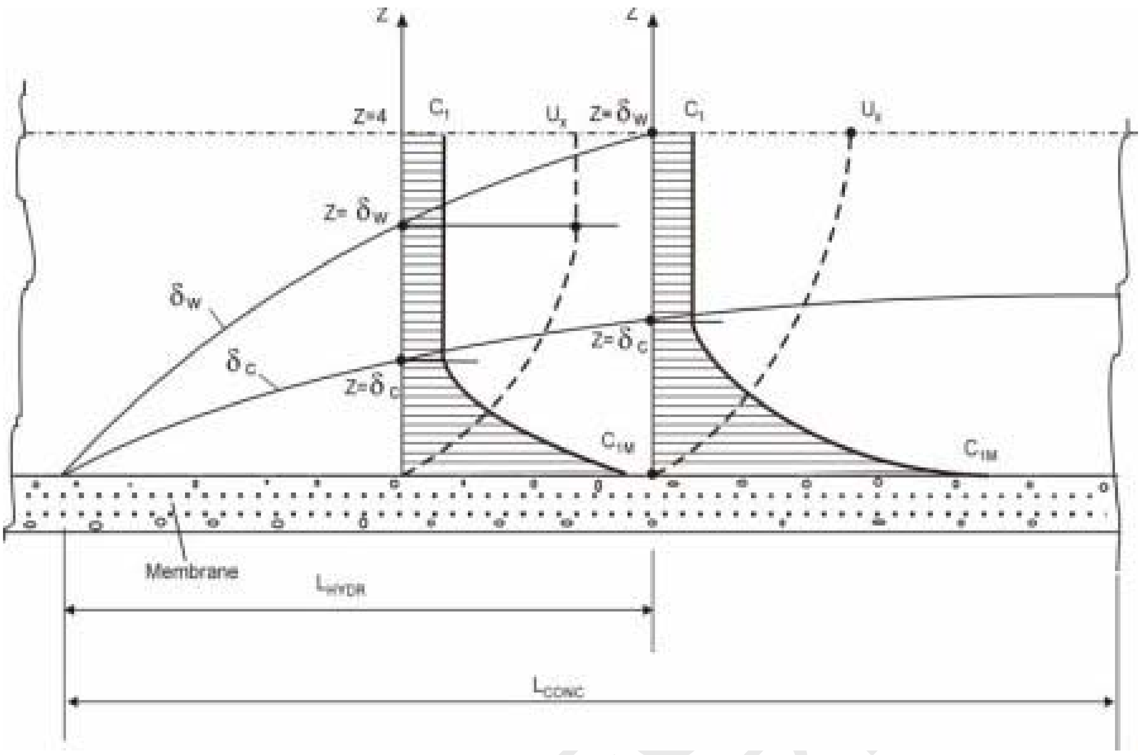

Figure 1. Schematic diagram of concentration and hydrodynamic profiles.

There is a plethora of approaches to modeling and various types of solutions, in particular, analytical and digital, exact and approximate ones. These operations are accompanied by concentration polarization and gel or cake accumulation.

These undesirable phenomena are caused by unbalanced transport between bulk and surface. As a consequence of all these negative factors the transmembrane fluxes in commercial plants are only 2-10 per cent of the transmembrane fluxes for pure water (Matthiasson and Sivik 1980).

Concentration and gel polarization submodels are going to be coupled and incorporated into a single algorithm, while equations describing transport within liquid phase have to be conjoined with those describing the growth of accumulated layer on the membrane surface (whether it is gel in the case of macromoleculars, or colloidal components, or cake, in the case of suspended systems).

Traditional approaches are based on equations of continuity, fluid motion and convection-diffusion equations which describe transport in liquid phases under isothermal conditions:

1. Continuity equation

$$\frac{\partial \rho}{\partial \tau} + \left(\nabla \cdot \rho \bar{u} \right) = 0 \qquad (1)$$

2. Fluid motion equation

$$\rho \frac{\partial}{\partial \tau}(\bar{u}) + \rho(\bar{u} \cdot \nabla)\bar{u} = -\nabla P + \rho g + \mu\left(\nabla^2 \bar{u}\right) \tag{2}$$

3. Convection-diffusion equation

$$\frac{\partial c}{\partial \tau} + (\bar{u} \cdot \nabla) c = (\nabla \cdot D \nabla c) - c(\nabla \cdot \bar{u}) \tag{3}$$

Where the last term on the right-hand side is zero for an incompressible fluid

Traditionally, the convection-diffusion equation is used as the principle equation where the axial and transverse velocity profiles are obtained either from prescribed functions or as a reduced form of the momentum equation.

The classification of approaches and solutions can be subdivided and differentiated in accordance with underlying physical premises, simplifying assumptions, underlying mathematical formulations, procedures and mathematical techniques being used.

There are different approaches to modeling concentration and hydrodynamic field namely: analytical and digital; exact and approximate.

The momentum-based set of equations (eqs 1-2) can be used to produce a mathematical description of the hydrodynamic field. The computed or assumed velocity field is then inserted into the convection-diffusion equation to obtain the dissolved species distribution.

In particular, approximation techniques were applied by Sherwood et al. 1965; Gill et al. 1965; Johnson and McCutchan 1972; Hung and Tien 1976; Leung and Probstein 1979, and a finite difference method was used by Brian 1965; Singh and Laurence 1979. This approach is only justified if transmembrane flux does not disturb the bulk flow.

2. Modeling Hydrodynamic Field

The conventional approach to modeling hydrodynamic field is based on a combination of the Navier-Stokes equations and continuity equation which describe the motion of a viscous, incompressible, Newtonian fluid under isothermal conditions. The continuity equation for three-dimensional, three-directional Newtonian flow can be written as (Gerhard et al. 1992)

$$\frac{\partial \rho}{\partial \tau} + \frac{\partial(\rho u_x)}{\partial x} + \frac{\partial(\rho u_y)}{\partial y} + \frac{\partial(\rho u_z)}{\partial x} = 0 \tag{4}$$

Navier-Stokes equations for three-dimensional, three-directional flow in rectangular coordinates were represented as (Gerhard et al. 1992)

X-component:

$$\rho\left(\frac{\partial u_X}{\partial \tau}+u_X\frac{\partial u_X}{\partial x}+u_Y\frac{\partial u_X}{\partial y}+u_Z\frac{\partial u_X}{\partial z}\right)=-\left(\frac{\partial P}{\partial x}\right)+\rho g_X+\mu\left(\frac{\partial^2 u_X}{\partial x^2}+\frac{\partial^2 u_X}{\partial y^2}+\frac{\partial^2 u_X}{\partial z^2}\right) \quad (5)$$

Y- component:

$$\rho\left(\frac{\partial u_Y}{\partial \tau}+u_X\frac{\partial u_Y}{\partial x}+u_Y\frac{\partial u_Y}{\partial y}+u_Z\frac{\partial u_Y}{\partial z}\right)=-\left(\frac{\partial P}{\partial x}\right)+\rho g_Y+\mu\left(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_Y}{\partial y^2}+\frac{\partial^2 u_Y}{\partial z^2}\right) \quad (6)$$

Z- component:

$$\rho\left(\frac{\partial u_Z}{\partial \tau}+u_X\frac{\partial u_Z}{\partial x}+u_Y\frac{\partial u_Z}{\partial y}+u_Z\frac{\partial u_Z}{\partial z}\right)=-\left(\frac{\partial P}{\partial x}\right)+\rho g_Z+\mu\left(\frac{\partial^2 u_Z}{\partial x^2}+\frac{\partial^2 u_Z}{\partial y^2}+\frac{\partial^2 u_Z}{\partial z^2}\right) \quad (7)$$

These equations can be transformed to other coordinates, such as cylindrical or spherical. No general analytical solution for the Navier-Stokes equations has been obtained.

The momentum-based set of equations can be used to derive a mathematical description of hydrodynamic field to incorporate into the convection-diffusion equation. A perturbation solution of a simplified equation of motion describing laminar flow between two porous plates (or in a porous tube) and constant wall velocity (permeate flux) was given by Berman (1953). Approximate solutions of problem-specific equations were reported by Gill et al. (1965) employing a series expansion, Kozinsky et al. (1970) using Bessel functions and Leung and Probstein (1979) resorting to the integral method. The "no slip" condition is usually invoked for the longitudinal velocity at the walls, however, Sparrow et al. (1972), Singh and Laurence (1979) and Kleinstreuer et al. (1982) investigated the effect of a thin moving layer in the porous walls.

Belfort and Nagata (1985) proposed a survey of literature sources related to analysis of flow in porous channel. Models proposed in this section will be subdivided in accordance with configuration of channel and underlying assumptions.

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