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MODIFIED RESISTANCE-IN-SERIES MODEL - DETERMINATION OF MEAN CONCENTRATION BY INTEGRAL TRANSFORMATION

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Abstract. *There are several mathematical models that describe permeate flow in membrane separation processes. Among these, the resistance-in-series model plays a prominent role. It takes into account membrane strength, concentration polarization, polarized layer and fouling to describe the permeate flow over time. In this work, an analysis of the modified resistance-in-series model was performed, in which the resistance by polarization of the concentration is defined as being directly proportional to the transmembrane pressure. The proportionality constant is given by the product of a specific coefficient of resistance – which is determined by means of experimental data – the thickness of the boundary layer of concentration and the mean concentration. Due to the inability to obtain experimentally the value of the average concentration within the boundary layer of concentration, its simulation is carried out from the conservation equation of the chemical species. Thus, the objective of the present work was to solve the chemical species conservation equation using GITT (Generalized Integral Transform Technique) and apply the modified resistance-in-series model to describe the permeate flow of a solution of dextran through a permeable tube under laminar flow. GITT provided satisfactory results for the mean concentration, verified by comparison with the permeate flow obtained by the resistance-in-series model with experimental results reported in the literature.*

Keywords: *Hybrid Methods, Permeate Flow, Polarization Resistance, Cross Flow*

1. INTRODUCTION

In the membrane separation processes (MSP), especially for ultrafiltration and microfiltration, there is an initial drop in permeate flow over time which is caused by phenomena that limit the transport of the solvent such as concentration polarization, polarized layer and fouling. The resistance in series model is a theoretical model that has been used to describe the phenomena of polarization and fouling and the permeate flux over time (Cheryan, 1998).

The Generalized Integral Transform Technique (GITT) is a hybrid method (numerical and analytical) which is very attractive for the treatment of multidimensional problems. Allied to this, the use of analytical filters, the choice of the most representative basis of the original problem and the use of symbolic manipulation platforms like (Cotta, 1993), contribute to the improvement of this technique. Development of hybrid techniques, which are able to assist in the understanding of the phenomena responsible for the permeate flow drop have been conducted (Venezuela *et. al.*, 2009; Kumar *et. al.*, 2010).

The objective of this work was to solve by hybrid methods (GITT), the conservation equation of chemical species in cylindrical coordinates to determine theoretical models that will assist the analysis of polarization phenomena responsible for permeate flow decreasing during the microfiltration process.

2. MATHEMATICAL MODEL

The permeate flow, *J*, varying with a pressure is:

$$J(\Delta p) = \frac{\Delta p}{\mu\left(R_m + R_f + \alpha_0 \delta \bar{c}\, \Delta p\right)}$$

For modeling purposes, a cylindrical membrane with fixed length *L*, radius R_0 and resistance R_m was considered. We assume that through it flows a dextran solution with velocity u_0, carrying a solute with initial concentration c_0, diffusivity *D*, viscosity μ, and transmembrane pressure Δp.

2.1 Determination of J_{lim}, *k and* δ

The thickness of the concentration boundary layer, δ, depends on the mass transport coefficient, *k*, which in turn depends on the permeate flow limit, J_{lim}. We have developed a methodology to obtain J_{lim}, which consists of a nonlinear expression with three unknown parameters, determined by nonlinear regression. Using the gel-polarization model along with the aforementioned experimental data, we can obtain the mass transfer coefficient *k* using a simple linear regression. From the stagnant film theory we evaluate the thickness of concentration boundary layer as δ = *D*/*k*.

2.2 Obtaining $\bar{c}$ via GITT

The mean concentration within the boundary layer, $\bar{c}$, can be modeled as the GITT solution of the chemical species conservation equation. *U* and *V* are the speed components of a laminar flow in a tube with permeable surface, with length *L* and radius R_0, whose dimensionless coordinates in cylindrical geometry are "*Z*" and "*R*" [3]. The regime is considered permanent of an incompressible and Newtonian fluid. Writing out the convective-diffusive equation and its boundary condition and entry in dimensionless form, we have, being $0 \le Z \le L/R_0$ e $0 < R \le 1$:

$$U\frac{\partial C}{\partial Z} + V\frac{\partial C}{\partial R} = \frac{2}{Pe}\frac{1}{R}\frac{\partial}{\partial r}\left(R\frac{\partial C}{\partial R}\right) \tag{1}$$

$$C(0,R) = 1, \qquad 0 \le R \le 1 \tag{2}$$

$$\frac{\partial C}{\partial R}(Z, R_{\min}) = 1, \qquad 0 \le Z \le L/R_0 \tag{3}$$

$$C(Z,1) = C_w = \frac{1}{\left(1 - \frac{\delta}{D}\right)\frac{\Delta p}{\mu \delta_m r_0}}, \qquad 0 \le Z \le L/R_0 \tag{4}$$

where *Pe*, δ_m and r_0, are respectively the Peclet number, membrane width and the mean pore radius.

Due to non-homogeneous boundary conditions given in Eqs. (3) and (4) we use a filter $F(R)$ and the potential function $C_H(Z, R)$ with the intention to re-write the problem in other one with homogeneous boundary conditions:

$$C(Z, R) = C_H(Z, R) + F(R), \qquad \text{i} = 1,2,3... \tag{5}$$

F is the solution of the initial value problem: $\partial^2 F/\partial^2 R = 0$, $F(R_{\min}) = 1$ and $F(1) = C_w$, $\text{R}_{\min} \ll 1$ e $R_{\min} \le R \le 1$. Thus,

$$F(R) = \left(\frac{1 - C_w}{ln(R_{\min})}\right) ln\, R + C_w .$$

Substituting Eq. (5) into Eqs. (1) through (4), we obtain:

$$U\frac{\partial C_H}{\partial Z}+V\frac{\partial C_H}{\partial R}=\frac{2}{Pe\ R}\ \frac{\partial}{\partial R}\left(R\frac{\partial C_H}{\partial R}\right)-V\frac{\partial F}{\partial R} \qquad (6)$$

where $0\le Z\le L/R_0$, $R_{\min}\le R\le 1$ and

$$C_H\left(0,R\right)=1 \qquad (7)$$

$$\frac{\partial C_H}{\partial R}\left(Z,R_{\min}\right)=0 \qquad (8)$$

$$C_H\left(Z,1\right)=0 \qquad (9)$$

The problem described by Eqs. (6) up to (9) has homogenous boundary conditions. Following the technique, the appropriate auxiliary problem (or problem of eigenvalue) is assumed as:

$$R\psi_i''(R)+\psi_i'(R)+\beta_i^2R\psi_i(R)=0,\ \psi_i\left(R_{\min}\right)=0 \text{ and } \psi_i(1)=0,\ i=1,2,3\ldots.$$

This Equation is the known Bessel's Equation, where β_i and ψ_i are, respectively, eigenvalues and eigenfunctions. The eigenvalue are obtained by:

$$\psi_i(R)=J_0\left(\beta_i R\right)Y_0\left(\beta_i\right)-J_0\left(\beta_i\right)Y_0\left(\beta_i R\right),$$

while the eigenvalues are obtained from equation:

$$J_0\left(\beta_i R_{\min}\right)Y_0\left(\beta_i\right)-J_0\left(\beta_i\right)Y_0\left(\beta_i R_{\min}\right)=0,$$

where J_0 and Y_0 are the Bessel functions of order zero of first and second kind, respectively. Eigenfunctions satisfy the following orthogonality property:

$$\int_{R_{\min}}^{1} R\psi_i\,\psi_j\,dR=\begin{cases}N_i, & i=j\\ 0, & i\neq j\end{cases},$$

with

$$N_i=\frac{2}{\pi^2}\frac{J_0^2\left(\beta_i R_{\min}\right)-J_0^2\left(\beta_i\right)}{\beta_i^2\,J_0^2\left(\beta_i R_{\min}\right)},$$

as per (Özisik, 1980).

The normalized eigenfunctions, or kernels, are defined by: $\tilde{\psi}_i(R)=\dfrac{\psi_i(R)}{N_i^{1/2}}$. We are now able to define the transform-inverse pair:

$$\overline{C}_i(Z)=\int_{R_{\min}}^{1} R\tilde{\psi}_i(R)C_H(Z,R)\,dR, \qquad \text{Transform}$$

$$C_H(Z,R)=\sum_{i=1}^{\infty}\tilde{\psi}_i(R)\overline{C}_i(Z), \qquad \text{Inversion formula}$$

Applying operator $\int_{R_{\min}}^{1} R\tilde{\psi}_i(R)\,dR$ on Eq. (6) and using the eigenvalue problem with the inversion formula we obtain, for *i* = 1,2,3...:

$$\sum_{j=1}^{\infty} A_{ij} U_2 \frac{d\bar{C}_i}{dZ} = \sum_{j=1}^{\infty}\left(-B_{ij} + \frac{\beta_j^2}{Pe}\delta_{ij}\right)\bar{C}_i - B1_i$$

where δ_{ij} is the kronecker delta.

The related coefficients are analytically determined by the following integrals:

$$A_{ij} = \int_{R_{\min}}^{1} RU_1\tilde{\psi}_i\tilde{\psi}_j dR \,,$$

$$B_{ij} = \int_{R_{\min}}^{1} RV\tilde{\psi}_i\tilde{\psi}_j' dR \,,$$

$$B1_i = \int_{R_{\min}}^{1} V\tilde{\psi}_i \, dR \,.$$

The transform results in the following initial condition for the infinite system of linear ordinary differential equations:

$$\bar{C}_i(0) = \int_{R_{\min}}^{1} R\tilde{\psi}_i\left(1 - F(R)\right)dR \,.$$

This system must be truncated to a convenient order N to allow the calculation of potentials $\bar{C}_i(Z)$. Together with the kernels $\tilde{\psi}_i(R)$ we can obtain $C_H(Z,R)$, from the inversion formula, and the filter $F(R)$, thus completing the dimensionless concentration profile $C(Z,R)$.

Finally, we can evaluate $\bar{c}$, $\bar{c} = c_0\bar{C}$, with

$$\bar{C} = \frac{R_0}{L}\int_0^1\int_0^{L/R_0} C(Z,R)\,dZdR \,.$$

2.3 Determination of α_0 and R_f .

In order to calculate the specific resistance, α_0, and the fouling resistance, R_f, we use:

$$\frac{\Delta p}{J_m \mu} = \left(\alpha_0 \delta \bar{c}\right)\Delta p + \left(R_m + R_f\right)$$

where J_m is the experimentally measured permeate flow. The slope, $\alpha_0\delta\bar{c}$, and the intercept, $R_m + R_f$, are determined by standard linear regression.

3. RESULTS AND DISCUSSION

The computational implementation of GITT was carried on the computer algebra system SAGe (Developers 2016; Pérez and Granger, 2007). Global convergence of the concentration profile was attained with a truncation of $N = 29$, considering a global relative error of 10^{-3}. The model properly reproduces the physical phenomena. Figure 1 summarizes the results for the concentration profile of one simulation setup.

Permeate flux results obtained with GITT, J_{GITT}, were compared with experimental data, J_{Exp}, and simulated data, J_Y, as reported by (Yeh *et. al.*, 2003). Table 1 shows that the relative differences $D_1 = \left|J_{GITT} - J_{Exp}\right| / J_{Exp}$ and $D_2 = \left|J_Y - J_{Exp}\right| / J_{Exp}$ are adequate.

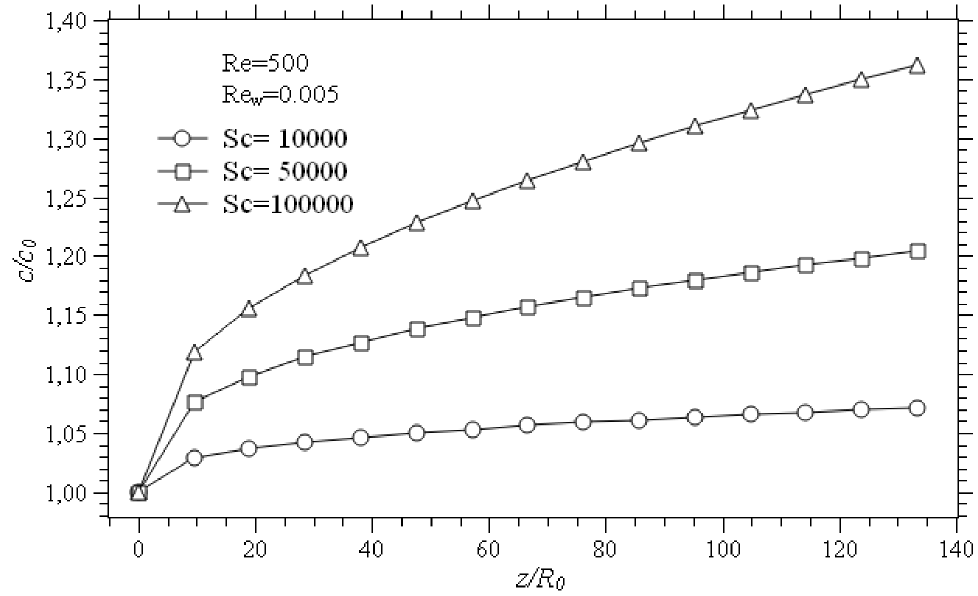

Figure 1. Schmidt's number effect over the concentration profile depending on the nondimensional axial position (z/R_0) near the permeable wall (R=0.98) for N=29, Re=500, Re_w=0.005 and R_0=3.0 10^{-3}m.

Table 1. Comparison amongst experimental and simulated data from [8] and the results obtained with the modified resistance in series model, depending on pressure, Δp For each case relative differences are also shown.

Δp $\left(10^{-5} Pa\right)$	u₀ (m/s)	$c_0 = 1.0 kg/m^3$			Rel. Diff.		$c_0 = 10.0 kg/m^3$			Rel. Diff.	
		J_{GITT}	J_{Exp}	J_Y	D_1 (%)	D_2 (%)	J_{GITT}	J_{Exp}	J_Y	D_1 (%)	D_2 (%)
0,45	0.051	3.327	3.331	4,433	0,1	24,9	2,087	2,092	2,163	0,2	3,3
0,65		4.150	4.225	4,922	1,8	14,2	2,354	2,328	2,355	1,1	1,1
0.95		4.881	4.838	5,131	0,9	5,7	2,529	2,512	2,527	0,7	0,6
1,15		5.165	5.078	5,311	1,7	4,4	2,586	2,551	2,597	1,4	1,8
1,35		5.359	5.311	5,131	0,9	3,5	2,621	2,636	2,653	0,6	0,7
0,45	0.102	3.694	3.682	4,493	0,3	18,0	2,281	2,252	2,338	1,3	3,7
0,65		4.741	4.861	5,201	2,5	6,5	2,558	2,590	2,554	1,3	1,4
0.95		5.723	5.767	5,875	0,8	1,8	2,735	2,738	2,723	0,1	0,5
1,15		6.126	6.114	6,215	0,2	1,6	2,792	2,782	2,799	0,4	0,6
1,35		6.411	6.391	6,459	0,3	1,1	2,827	2,825	2,859	0,1	1,2
0,45	0.153	3.688	3.623	4,977	1,8	27,2	2,481	2,487	2,653	0,2	6,3
0,65		4.871	4.919	5,705	0,9	13,8	2,877	2,864	2,919	0,4	1,9
0.95		6.102	6.175	6,469	1,2	4,5	3,148	3,148	3,138	0,1	0,3
1,15		6.653	6.745	6,869	1,4	1,8	3,237	3,206	3,250	1,0	1,4
1,35		7.057	7.012	7,113	0,6	1,4	3,294	3,277	3,317	0,5	1,2
0,45	0.204	4.135	4.044	5,446	2,2	25,7	2,753	2,788	3,081	1,2	9,5
0,65		5.505	5.633	6,384	2,3	11,8	3,293	3,345	3,423	1,6	2,3
0.95		6.940	7.041	7,323	1,4	3,8	3,696	3,683	3,715	0,4	0,9
1,15		7.572	7.617	7,772	0,6	2,0	3,834	3,831	3,834	0,1	0,1
1,35		8.038	8.024	8,106	0,2	1,0	3,922	3,887	3,940	0,9	1,4

J_{GITT}, J_{Exp}, J_Y $\left(10^6 m/s\right)$

4. CONCLUSIONS

Polarized concentration resistance was determined with the help of computational simulations of the mean concentration of solute within the boundary layer, via GITT. Next, permeate flux was calculated using the modified resistance-in-series model. Relative errors are satisfactory, when compared with the literature.

Thus, GITT can be regarded as an efficient tool to evaluate the permeate flow associated with microfiltration processes.

5. ACKNOWLEDGEMENTS

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