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A Theoretical Analysis of Solute Transport through a Membrane Bioreactor

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***Abstract*–** The current paper presents a theoretical analysis of the transport of solutes through a fixed-film membrane bioreactor (MBR), immobilised with an active biocatalyst. The dimensionless convection-diffusion equation with variable coefficients was solved analytically and numerically, for concentration profiles of the solutes through the MBR. The analytical solution makes use of regular perturbation, and accounts for radial-convective flow as well as axial diffusion of the substrate specie. The Michaelis-Menten (or Monod) rate equation was assumed for the sink term, and the perturbation was extended up to second-order. In the analytical solution only the first-order limit of the Michaelis-Menten equation was considered, hence the linearized equation was solved. In the numerical solution, however, this restriction was lifted. The solution of the non-linear, elliptic, partial differential equation was based on an implicit finite-difference method (FDM). An upwind scheme was employed for numerical stability. The resulting algebraic equations were solved simultaneously using the multi-variate Newton-Raphson iteration method. The solution allows for the evaluation of the effect on the concentration profiles of (i) the radial and axial convective velocity, (ii) the convective mass transfer rates, (iii) the reaction rates, (iv) the fraction retentate, and (v) the aspect ratio

***Keywords*:** Membrane bioreactor; Convection-diffusion equation; Implicit finite-difference; Upwind scheme; Multivariate Newton-Raphson; Regular perturbation

Nomenclature

B_m	coefficient of series solution, defined in text
c	substrate concentration (g dm^{-3})
c_0	substrate feed concentration (g dm^{-3})
$C = c/c_0$	dimensionless substrate concentration
D_{AB}	substrate diffusivity (m^2 s^{-1})
$f = u_1/u_0$	fraction retentate
h	step-size in the r-dimension (m)
i	grid point index in the r-dimension
j	grid point index in the z-dimension
$J_n(\lambda)$	Bessel function of order n of the first kind
K	step-size in the z-dimension (m)
K_m	saturation (or Michaelis) constant (g dm^{-3})
K_m^*	dimensionless Michaelis constant
L	membrane effective length (m)
$M(a,b,\theta)$	Kummer function of the first kind
$Pe_u = u_0 R_L/D_{AB}$	axial Peclet number
$Pe_v = v_0 R_L/D_{AB}$	radial Peclet number
r	radial spatial coordinate (m)
$R = r/R_1$	dimensionless radial spatial coordinate
R_L	membrane lumen radius (m)
u	axial velocity (m s^{-1})
u_0	feed axial velocity (m s^{-1})
$U = u/u_0$	dimensionless axial velocity
v	radial velocity (m s^{-1})
$V = v/v_0$	dimensionless radial velocity

V_M	maximum rate of reaction (g dm^{-3} s^{-1})
z	axial spatial coordinate (m)
$Z = z/L$	dimensionless axial spatial coordinate

Greek letters

α	coefficients of finite difference scheme, defined in text
$\beta = P_0 - P_2$	dimensionless transmembrane pressure
κ	dimensinless membrane hydraulic permeability
ϕ	Thiele modulus
$\varphi = R_1/L$	aspect ratio
λ_m	eigen values, m = 1, 2, …

1. Introduction

Membrane bioreactors (MBRs) are finding increasing use in the production of primary and secondary metabolites such as amino acids, antibiotics, anticancer drugs, tissue cells etc. (Giorno & Drioli, 2000; Charcosset, 2006; Stamatialis et al., 2008). This technology is favoured by recent trends towards environmentally-friendly technologies (Giorno & Drioli, 2000). The efficiency of MBRs is dependent mainly on the transport of solutes through the bioreactor, and this is influenced by biochemical, geometric, and hydrodynamic parameters (Charcosset, 2006; Curcio et al., 2006). This paper considers the solution of the convection-diffusion equation, for solute transport through a fixed-film MBR. This analysis is important for simulation of the performance (i.e. efficiency and effectiveness) of the bioreactor. The governing equation for mass transport of solutes through the bioreactor is the convection-diffusion equation, with Monod kinetics (Bird et al., 2002):

$$u\frac{\partial c}{\partial z} + v\frac{\partial c}{\partial r} = D_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + \frac{\partial^2 c}{\partial z^2}\right] - \frac{V_M c}{K_m + c} \tag{1}$$

Eq. (1) is made dimensionless by introducing the following variables:

$$U = \frac{u}{u_0};\quad V = \frac{v}{v_0};\quad C = \frac{c}{c_0};\quad \phi = \sqrt{\frac{V_M R_1^2}{c_0 D_{AB}}}\,K_m^* = \frac{K_m}{c_0};\quad Z = \frac{z}{L};\quad R = \frac{r}{R_1};\quad \varphi = \frac{R_1}{L} \tag{2}$$

Eq. (1) then becomes:

$$U^*\frac{\partial C}{\partial Z} + Pe_u\kappa\beta(2R - R^3)\frac{\partial C}{\partial R} = \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial C}{\partial R}\right) + \varphi^2\frac{\partial^2 C}{\partial Z^2}\right] - \frac{\phi^2 C}{K_m^* + C} \tag{3}$$

Where

$$U^* = -4Pe_u\kappa\beta\left[\frac{1}{(f-1)} + Z\right](1 - R^2)\ ,\ f \neq 1 \tag{4}$$

The fraction retentate, f, is defined as the ratio of the outlet to the inlet axial velocity (f = 0 for the dead-end mode and $f \sim 1$ for the closed-shell mode), β is the dimensionless transmembrane pressure. The corresponding boundary conditions are:

$$\begin{aligned} &B.C.1 \quad at\ Z = 0 \quad \forall R \quad C = 1 \\ &B.C.2 \quad at\ R = 0 \quad \forall Z \quad \frac{\partial C}{\partial R} = 0 \\ &B.C.3 \quad at\ R = 1 \quad \forall Z \quad \frac{\partial C}{\partial Z} = \frac{2}{\varphi Pe_u}\frac{\partial C}{\partial R} \end{aligned} \tag{5}$$

2. Analytical Models

The Graetz Problem (Graetz, 1883) is one of the oldest forced-convection problems, describing the steady-temperature distribution and rate of heat transfer in tube flow. The evaluation of Eq. (3) for concentration profiles in a tubular reactor is mathematical analogous to the Graetz problem (Bird et al., 2002). In the original Graetz problem however there is no reaction (or source) term, axial diffusion and radial convection is ignored. The assumption of negligible axial diffusion and radial convection is common in the majority of analytical models currently in use (Heath & Belfort, 1987; Nagy, 2012). Radial convective flows have been shown to significantly improve MBR efficiency (Curcio et al., 2006; Kelsey et al., 1990; Nagy, 2009). In the dead-end ultrafiltration mode, particularly, the assumption of negligible radial convective flow is not justifiable. Nagy (2009) investigated the effect of radial convective flows on the mass transfer rates of solutes through a biocatalytic membrane layer. Analytical solutions of Eq. (3) for the zero-order and first-order limits of the Monod equation were provided. This analysis, however, was restricted to the matrix/fiber region of the membrane and hence the radial velocity was assumed constant, and axial convective and diffusive flows were ignored. At axial Peclet numbers smaller than unity large concentration gradients exist in the membrane lumen, and ignoring axial diffusion is also not justified (Heath & Belfort, 1987; Godongwana et al., 2010).

The model proposed by Godongwana et al. (2010) follows the approach suggested by Davis (1973), *i.e.* writing the solution of Eq. (3) in terms of known functions. The model accounts for radial convective flow and axial diffusion, for the limiting case of first-order kinetics. In that model, Eq. (3) was solved by separation of variables and regular perturbation, resulting in the asymptotic expansion:

$$C\theta, x = m = 1\infty n = 0NBmFm\theta Tnx\kappa n \tag{6}$$

Making use of the following change of variables:

$$\xi = -\frac{2Pe_u\kappa\beta}{\varphi^2}\left[\frac{1}{(f-1)} + Z\right] \tag{7}$$

$$\theta = -\left(\frac{\varphi^2}{4Pe_u\kappa\beta}\right)\xi^2 \tag{8}$$

$$x = \lambda_m R \tag{9}$$

Where *F(θ)* in Eq. (6) is represented by the Kummer function (Abramowitz & Stegun, 1965):

$$F_m(\theta) = M\left[\frac{-\left(\lambda_m^2+\phi^2/K_m^*\right)}{4Pe_u\kappa\beta}, \frac{1}{2}, \theta\right] \tag{10}$$

The zero-order and first-order approximations of *T(x)* in Eq. (6) are, respectively:

$$T_0(x) = J_0(x) \tag{11}$$

And

$$T_1(x) = \sigma_1\left[\frac{(x)^2 J_2(x)}{3!!} + \sigma_2\frac{(x)^3 J_3(x)}{5!!} + \sigma_3\frac{(x)^4 J_4(x)}{7!!}\right] \tag{12}$$

3. Numerical Solution

A finite-difference representation of Eq. (3) is obtained by employing first-order upwind difference quotients for the first-order derivatives on the LHS and second-order central-differences for the second-order derivatives on the RHS:

$$\alpha_1 C_{i-1,j} + \left(\alpha_2 + \frac{\alpha_3}{K_m^* + C_{i.j}}\right) C_{i,j} + \alpha_4 C_{i+1,j} + \alpha_5 C_{i,j-1} + \alpha_6 C_{i,j+1} = 0 \tag{13}$$

Where

$$\alpha_1 = -\left[hPe_u \kappa\beta(2R - R^3) + 1 - \frac{h}{R}\right] \tag{14}$$

$$\alpha_2 = \left(\frac{h^2}{k}\right) U^* + hPe_u \kappa\beta(2R - R^3) + 2\varphi^2 \left(\frac{h^2}{k^2}\right) + 2 - \frac{h}{R} \tag{15}$$

$$\alpha_3 = h^2 \phi^2 \tag{16}$$

$$\alpha_4 = -1 \tag{17}$$

$$\alpha_5 = -h^2 \left(\frac{U^*}{k} + \frac{\varphi^2}{k^2}\right) \tag{18}$$

$$\alpha_6 = -\varphi^2 \left(\frac{h^2}{k^2}\right) \tag{19}$$

The solution domain is a regular 2-dimensional grid, and is sub-divided into *m*-intervals (of size *h*) in the *r*-dimension and *n*-intervals (of size *k*) in the *z*-dimension. The difference equation (13), including the boundary conditions, is solved by making use of the multivariate Newton-Rapshon iteration scheme:

$$\boldsymbol{C}_{(n+1)} = \boldsymbol{C}_n - \frac{\boldsymbol{F}(\boldsymbol{C}_n)}{\boldsymbol{J}_n} \tag{20}$$

Where $\boldsymbol{F}(\boldsymbol{C})$ is the residual Eq. (13), and $\boldsymbol{J}$ is the tridiagonal Jacobian matrix:

$$\boldsymbol{J} = \begin{bmatrix} D & B & 0 & & 0 & 0 & 0 \\ E & D & B & \cdots & 0 & 0 & 0 \\ 0 & E & D & & 0 & 0 & 0 \\ & \vdots & & \ddots & & \vdots & \\ 0 & 0 & 0 & & D & B & 0 \\ 0 & 0 & 0 & \cdots & E & D & B \\ 0 & 0 & 0 & & 0 & E & D \end{bmatrix} \tag{21}$$

The matrix elements *B*, *D*, and *E* are, respectively:

$$B = \alpha_4 + \alpha_5 \tag{22}$$

$$D = \alpha_2 + \alpha_3 \left[\frac{1}{K_m^* + C_{i.j}} + \frac{C_{i.j}}{\left(K_m^* + C_{i.j}\right)^2}\right] \tag{23}$$

$$E = \alpha_1 + \alpha_6 \tag{24}$$

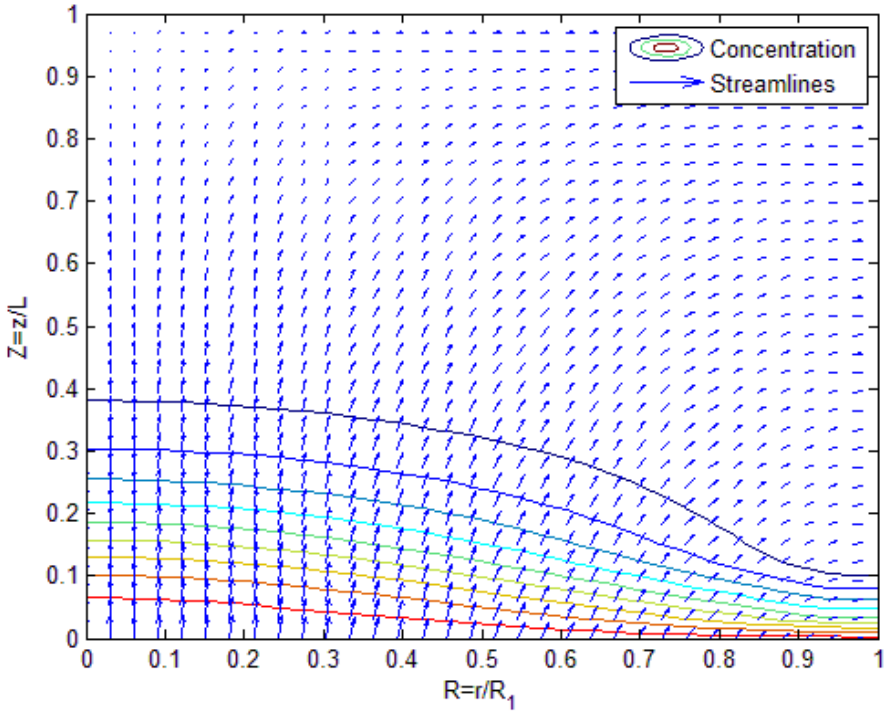
The Newton-Raphson iteration scheme was implemented on MATLAB R2014a. The algorithm begins with an initial guess of the solute concentration at each grid point; an initial guess of zero was used. Based on this guess, the residual column vector and the Jacobian matrix can be evaluated. The magnitude (Euclidean norm) of the quotient of the residual vector and Jacobian matrix, $d\boldsymbol{C}$, is evaluated. The iteration is repeated with new solute concentration guess values until the Euclidean norm is less than the prescribed tolerance.

4. Results

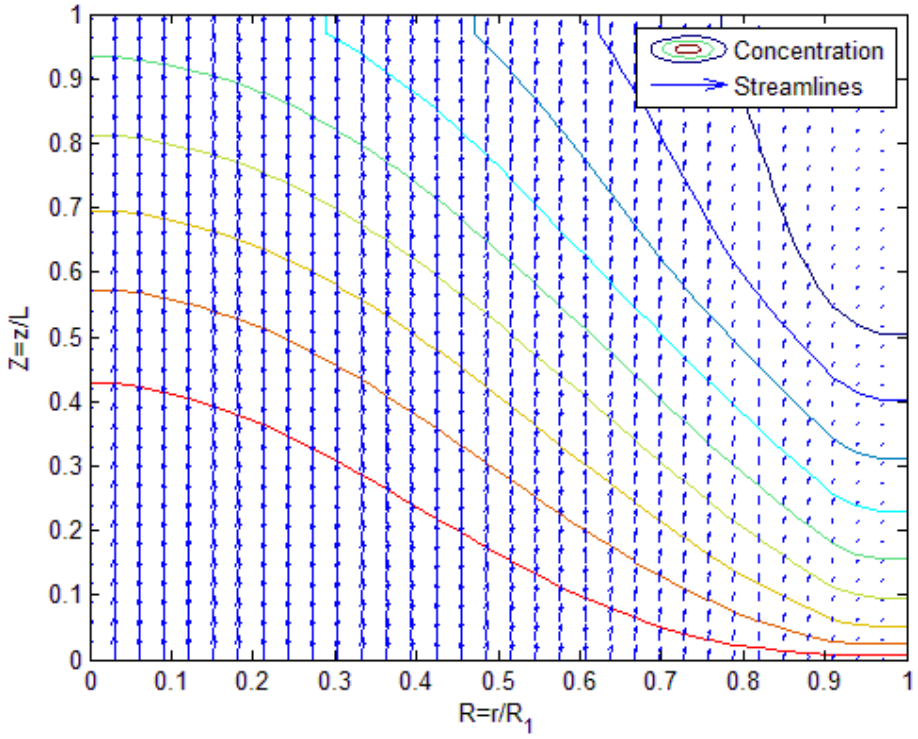
The implicit finite-difference scheme was shown to be unconditionally stable for the different values of *h* and *k*. The results are shown in Figure 1 for the parameter values listed in Table 1. Figure 1 illustrates the effect of the fraction retentate *f* on the solute concentration profiles. In the dead-end mode ($f = 0$) there is increased radial convective flow as shown by the streamlines in Figure 1a. This increased radial flow allows for more solute contact with the biofilm, and hence improved conversion, resulting in higher MBR efficiency. In this mode however the solute is limited to only the entrance half of the MBR as shown in Figure 1a. Increasing the fraction retentate to $f = 0.8$ allows for a uniform distribution of the solute (Figure 1b),however radial convective flow is significantly reduced. This result implies that an optimum *f* value should be sought for enhanced MBR efficiency. The developed finite-difference scheme also allows for the evaluation of the effect on the concentration profiles of the radial and axial convective velocity, the convective mass transfer rates, the reaction rates, and the aspect ratio. The sensitivity analysis of these parameters however has been omitted in the current paper.

In Figure 2a the FDM scheme is compared with the analytical model presented in Section 2 for the open-shell mode ($f = 0.8$). The analytical model predicts a linear decrease in the solute concentration inside the membrane lumen to 47% of the original concentration. This result is consistent, qualitatively, with the result of Heath and Belfort (1987) for the parameter values listed in Table 1. The FDM scheme predicts the same outlet concentration; however the decrease is gradual close to the entrance and rises with increasing length. The discrepancies between the two profiles arise from the assumption of first-order kinetics, assumed in developing the analytical solution. These two profiles suggest the open-mode is suitable for microbial growth since the substrate is not depleted inside the lumen. The rapid decline in the solute concentration in Figure 2b is due to increased radial convective flow in the dead-end mode.

This results in non-uniform microbial growth/tapering as observed by Godongwana et al. (2009) for the bacterium *Streptomyces coelicolor* on a ceramic membrane. This phenomenon can be reduced either by increasing the solute flowrate or increasing the fraction retentate *f*. The numerical scheme matches the analytical model approximately on a small interval close to the origin. The divergence again is attributed to the assumption of first-order kinetics.



(a)

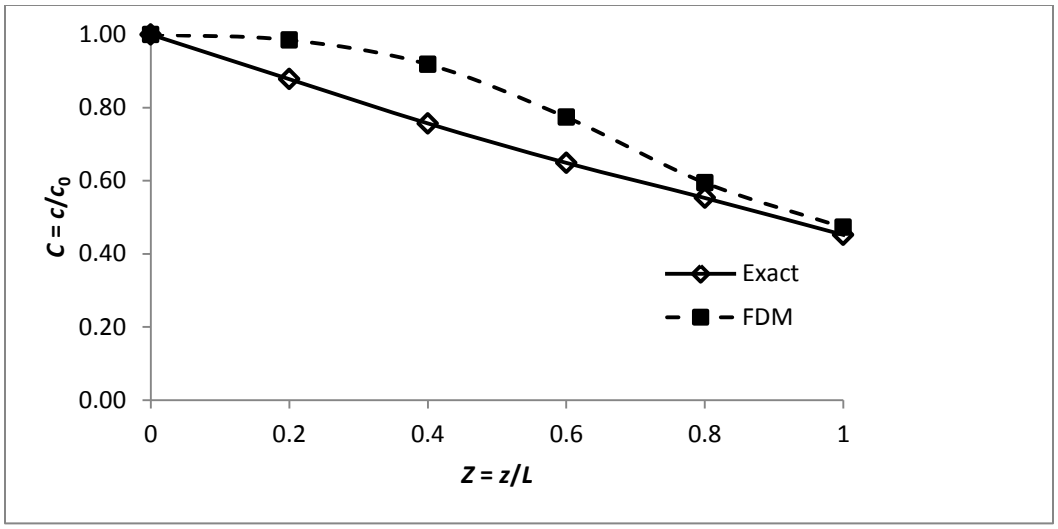


(b)

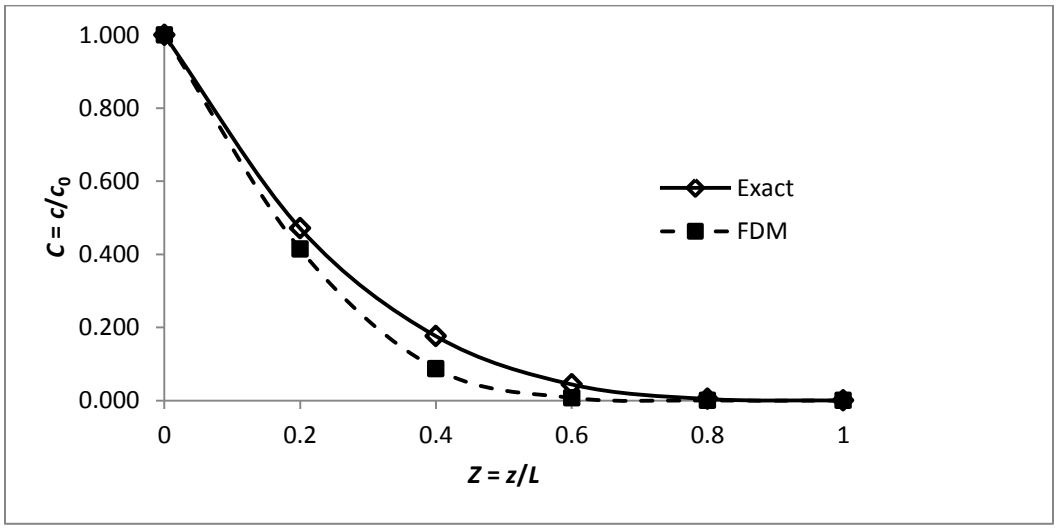
Fig. 1. Solute concentration profiles for $m = n = 64$ when (a) $f = 0$, and (b) $f = 0.8$ [for the parameter values listed in Table 1].

Table 1: Parameter values used to determine the concentration profile (Godongwana et al., 2010)

Model parameter	Symbol	Unit	Basic measured value
Membrane hydraulic permeability	k_m	m/Pas	3.82×10^{-11}
Membrane inner radius	R_1	m	1.30×10^{-4}
Effective membrane length	L	m	5.7×10^{-2}
Lumen-side entrance axial velocity	u_0	m s^{-1}	1.67×10^{-3}
Permeation velocity	v_0	m s^{-1}	1.91×10^{-7}
Lumen-side inlet hydrostatic pressure	p_0	Pa	106 325
Shell-side hydrostatic pressure	p_S	Pa	101 325
Glucose diffusivity	D_{AB}	m^2 s	1.0×10^{-10}
Glucose inlet concentration	c_0	g dm^{-3}	2.00
Kinetic constants	K_m / V_m	s^{-1}	0.10



(a)



(b)

Fig. 2. A comparison of the analytical versus the FDM solution for solute concentration profiles (a) $f = 0.8$, and (b) $f = 0$ [for the parameter values listed in Table 1].

5. Conclusion

A mathematical solution of the dimensionless convection-diffusion equation, with non-linear kinetics, was developed. The numerical scheme was performed using the Newton-Raphson method, and was shown to be unconditionally stable for different step-sizes (h and k). The analysis provides for evaluation of concentration profiles of solutes through a membrane bioreactor. The numerical solution was compared to a regular perturbation solution for two modes of operation, *i.e.* the dead-end mode and open-shell mode. In the dead-end mode the numerical results closely matched the perturbation solution. The assumption of linear kinetics, commonly used in literature models, was shown to result in inaccuracies in the open-shell mode. The numerical solution allows for the evaluation of the influence of the general operating parameters of a MBR on the concentration profiles. The fraction retentate (f) was shown to be an important optimisation parameter for improved MBR efficiency.

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References

Abramowitz M., Stegun I.A. (1965). "Handbook of Mathematical Functions," Dover.

Bird B.R., Stewart W.E., Lightfoot E.N. (2002). "Transport Phenomena 2nd edition," John Wiley.

Charcosset C. (2006). Membrane Processes in Biotechnology: An Overview, *Biotechnology Advances*, 24, 482-492.

Curcios S., Calabro V., Iorio G. (2006). A Theoretical and Experimental Analysis of a Membrane Bioreactor Performance in Recycle Configuration, *Journal of Membrane Science*, 273, 129-142.

Davis E.J. (1973). Exact Solutions for a Class of Heat and Mass Transfer Problems, *Canadian Journal of Chemical Engineering*, 51, 562-572.

Giorno L., Drioli E. (2000). Biocatalytic Membrane Reactors: Applications and Perspectives, *Tibtech*, 18, 339-349.

Godongwana B., De Jager D., Sheldon M.S., Edwards W. (2009). The Effect of Streptomyces Coelicolor Development on the Hydrodynamics of a Vertically Orientated Capillary Membrane Gradostat Reactor, *Journal of Membrane Science*, 333, 79-87.

Godongwana B., Solomons D., Sheldon M.S. (2010). A Solution of the Convective-Diffusion Equation for Solute Mass Transfer inside a Capillary Membrane Bioreactor, *International Journal of Chemical Engineering*.

Graetz L. (1883). Uber Die Warmeleitungsfahigkeit Von Flussigkeiten. Annalen Der Physik Und Chemie, 18, 79-94.

Heath C., Belfort G. (1987). Immobilization of Suspended Mammalian Cells: Analysis of Hollow Fiber and Microcapsule Bioreactors, *Advances in Biochemical Engineering/Biotechnology*, 34, 1-31.

Kelsey L.J., Pillarella M.R., Zydney A.L. (1990). Theoretical Analysis Of Convective Flow Profiles In A Hollow-Fiber Membrane Bioreactor, *Chemical Engineering Science*, 45, 3211-3220.

Nagy E. (2009). Basic Equations of Mass Transfer through Biocatalytic Membrane Layer, *Asia-Pacific Journal of Chemical Engineering*, 4, 270-278.

Nagy E. (2012). "Basic Equations of the Mass Transport Through a Membrane Layer," Elsevier.

Stamatialis D.F., Papenburg B.J., Giron M., Bettahalli S.N.M., Schmitmeier S., Wessling M. (2008). Medical Applications of Membranes: Drug Delivery, Artificial Organs and Tissue Engineering, *Journal of Membrane Science*, 308, 1-34.