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ANALYSIS OF THE CONCENTRATION FIELD THROUGH THE INTEGRAL TRANSFORM TECHNIQUE FOR THE BIOCONVERSION OF SUGARS TO ETHANOL IN A PACKED BED BIOREACTOR

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Abstract. *Many processes in chemical and biochemical industries deal with mass transfer involving bioconversion in immobilized cell packed bed bioreactors. The evaluation of the concentration distribution in the reactor is extremely important to design and control the dynamic of the bioprocess, in this context it is necessary an accurate technique to predict reliable solutions which is valid within the reactor. The generalized integral transform technique (GITT) and the FDM-Gear approaches are utilized in the present work to solve the equation of conservation species related to the bioconversion of sugars to ethanol in a packed bed bioreactor. Therefore, computational codes were developed to analyze the parameters that influence the concentration distribution, and the present results were then compared with those previously reported in the literature for typical situations.*

Keywords*: Integral transform, bioconversion, bioreactor.*

1. INTRODUCTION

Continuous processes of bioconversion using immobilized cells present a great industrial interest, mainly due to the crescent interest in reducing equipment sizes and the operation costs. The use of immobilized cells provides a process of heterogeneous catalytic fermentation and the knowledge of the dynamics of the transport processes is important for its control and operation.

In the last years, some studies has been presented on the modeling and simulation of bioconversion of sugars to etanol in an immobilized cell packed bed bioreactor (Gupta and Chand, 1990; Soletti *et al.*, 1992). It has been observed that most of the studies of bioconversion deals with the process in steady state, a time that the mathematical treatment of the phenomenon is simplified if compared with unsteady state.

In a pioneering work, Gupta and Chand (1990) developed a theoretical and experimental study of the bioconversion of sugars to ethanol in a immobilized cell packed bed bioreator. In this work the authors presented a mathematical model to analyze the dynamic behavior resulting from perturbations in feed sugar concentration and feed flow rate. The partial diferential equations were numerically solved by the Crank-Nicolson method.

Soletti *et al.* (1992) using the Gupta and Chand model applied a polynomial approach to solve the related equations. Also the authors have made a dynamic approach for the production of etanol through the action of immobilized cells.

In present work, a new model is developed to study the bioconversion sugars in a bioreactor. This model differs from that considered for Gupta and Chand (1990) by the fact of presenting a partial differential equation for the product similar to one for the substrate. In the model of Gupta and Chand (1990) the calculation of the product concentration is taken by a direct relation with the substrate concentration. Therefore, the purpose of the

present study is also to solve the partial differential equations related to the new model applied to the bioconversion of sugars to ethanol in a packed bed bioreactor by employing the GITT approach (Cotta, 1993) and to establish reliable numerical results for the concentration field. In addition, another methodology by making use of the finite difference method in the spatial coordinate and the Gear's method in the time variable (FDM-Gear Approach) is employed in the solution of equations of the model.

2. MATHEMATICAL FORMULATION

The physical problem under picture in this work consists of an immobilized cell packed bed bioreactor, initially at the uniform substrate concentration S_i. For times t>0, the feed substrate concentration is givem by S_F, where a Danckwerts (1953) boundary condition is used. The rate of conversion of substrate to product was adopted to have a general order kinetic (n). The main hypotheses adopted in developing the present model are described by Gupta and Chand (1990). Then, the unsteady mass balance for the substrate and the product are given by:

$$\frac{\partial \Phi}{\partial \tau} = \frac{1}{Pe}\frac{\partial^2 \Phi}{\partial \eta^2} - \frac{\partial \Phi}{\partial \eta} - K\Phi^n, \qquad \text{in } \tau > 0, \quad 0 < \eta < 1 \tag{1.a}$$

$$\frac{\partial \theta}{\partial \tau} = \frac{1}{Pe}\frac{\partial^2 \theta}{\partial \eta^2} - \frac{\partial \theta}{\partial \eta} + \alpha_{ps} K\Phi^n, \qquad \text{in } \tau > 0, \quad 0 < \eta < 1 \tag{1.b}$$

Equations (1.a,b) are subject to the following initial and boundary conditions:

$$\Phi(\eta, \tau) = \Phi_i \quad \text{and} \quad \theta(\eta, \tau) = 0 \quad \text{for } \tau = 0, \quad 0 \le \eta \le 1 \tag{1.c,d}$$

$$-\frac{\partial \Phi}{\partial \eta} + Pe\Phi = Pe \quad \text{and} \quad \theta = 0 \quad \text{at } \eta = 0, \quad \tau > 0 \tag{1.e,f}$$

$$\frac{\partial \Phi}{\partial \eta} = 0 \quad \text{and} \quad \frac{\partial \theta}{\partial \eta} = 0 \quad \text{at } \eta = 1, \quad \tau > 0 \tag{1.g,h}$$

where in Eqs. (1) Φ and θ are the dimensionless substrate and product concentrations, respectively, Pe is the Peclet number, K is the dimensionless kinetic parameter, n is the order of reaction and α_{ps} is the product yield coefficient.

In Gupta and Chand (1990) the following relationship is used in the place of the partial differential equation (1.b):

$$\frac{\partial \theta}{\partial \tau} = \alpha_{ps}\left(-\frac{\partial \Phi}{\partial \tau}\right) \tag{2}$$

In the above formulation, the following dimensionless groups were employed:

$$\eta = z/L; \quad \tau = ut/L; \quad Pe = uL/D_c; \quad \Phi = S/S_F; \quad \theta = P/S_F; \quad \Phi_i = S_i/S_F; \quad K = (1-\varepsilon)kLS_F^{n-1}/\varepsilon u \tag{3.a-g}$$

where L is the length of the bioreactor, z is the longitudinal coordinate, S_i and S_F are the initial and feed concentrations, respectively, u is the linear velocity of the medium, D_c is the dispersion coefficient, k is the kinetic parameter and ε is the bioreactor porosity.

3. SOLUTION METHODOLOGY

3.1. The GITT Approach

Four approaches will be focused in the application of the Generalized Integral Transform Technique for the solution of the problem. The first approach consists in the application of GITT in the original problem without a filter to homogenize the boundary condition. The last three approaches present alternatives of filters to homogenize the boundary condition. The main objective in this analysis is to evaluate the influence of the filtering strategy in the convergence rate of the series solutions.

3.1.1 Formal Solution

In order to apply the generalized integral transform approach (Cotta, 1993) the appropriate eigenvalues problems are taken as:

- For the potential $\Phi(\eta,\tau)$:

$$\frac{d^2\Psi_i}{d\eta^2}+\mu_i{}^2\Psi_i=0,\quad \text{in } 0<\eta<1 \tag{4.a}$$

$$\frac{d\Psi_i}{d\eta}-Pe\Psi_i=0 \quad \text{at } \eta=0;\quad \frac{d\Psi_i}{d\eta}=0 \quad \text{at } \eta=1 \tag{4.b,c}$$

- For the potential $\theta(\eta,\tau)$:

$$\frac{d^2\Omega_\ell}{d\eta^2}+\beta_\ell{}^2\Omega_\ell=0,\quad \text{in } 0<\eta<1 \tag{5.a}$$

$$\Omega_\ell=0 \text{ at } \eta=0;\quad \frac{d\Omega_\ell}{d\eta}=0;\quad \text{at } \eta=1 \tag{5.b,c}$$

where the eigenfunctions, eigenvalues and norms are computed as

$$\Psi_i(\eta)=\mathrm{Cos}[\mu_i(1-\eta)];\ \ \mu_i\mathrm{Sin}(\mu_i)-Pe\mathrm{Cos}(\mu_i)=0;\ \ N_i=\frac{1}{2}\frac{\mu_i{}^2+Pe^2+Pe}{\mu_i{}^2+Pe^2};\ \ \widetilde{\Psi}_i=\Psi_i/\sqrt{N_i} \tag{6.a-d}$$

$$\Omega_\ell(\eta)=\mathrm{Sin}[\beta_\ell\eta];\ \ \beta_\ell=(2\ell-1)\pi/2;\ \ M_\ell=1/2;\ \ \widetilde{\Omega}_\ell=\Omega_\ell/\sqrt{M_\ell} \tag{7.a-d}$$

These eigenvalues problems allow the development of the following integral transform pairs:

$$\tilde{\Phi}_i(\tau)=\int_0^1\tilde{\Psi}_i(\eta)\Phi(\eta,\tau)d\eta \quad\Rightarrow\quad \Phi(\eta,\tau)=\sum_{i=1}^{N_\Phi}\tilde{\Psi}_i(\eta)\tilde{\Phi}_i(\tau) \tag{8.a,b}$$

$$\tilde{\theta}_\ell(\tau)=\int_0^1\tilde{\Omega}_\ell(\eta)\theta(\eta,\tau)d\eta \quad\Rightarrow\quad \theta(\eta,\tau)=\sum_{i=1}^{N_\theta}\tilde{\Omega}_\ell(\eta)\tilde{\theta}_\ell(\tau) \tag{9.a,b}$$

To perform the integral transformation, Eq. (1.a) should be multiplied by $\widetilde{\Psi}_i$ and Eq. (1.b) multiplied by $\widetilde{\Omega}_\ell$; after that they are integrated over the domain of solution [0,1]. Later, employing the inversion formulae, Eqs. (8.b) and (9.b), and boundary conditions, then the resultant transformed equations are written as:

$$\begin{cases}\dfrac{d\tilde{\Phi}_i}{d\tau}=\tilde{\Psi}_i(0)-\dfrac{\mu_i^2}{Pe}\tilde{\Phi}_i-\displaystyle\sum_{j=1}^{N_\Phi}A1_{ij}\tilde{\Phi}_j-KB1_i; \qquad \dfrac{d\tilde{\theta}_\ell}{d\tau}=-\dfrac{\beta_\ell^2}{Pe}\tilde{\theta}_\ell-\sum_{m=1}^{N_\theta}A2_{\ell m}\tilde{\theta}_m+\alpha_{ps}KB2_\ell \\ \tilde{\Phi}_i(0)=\Phi_i\tilde{C}_i; \qquad \tilde{\theta}_\ell(0)=0\end{cases} \tag{10.a-d}$$

where,

$$A1_{ij}=\int_0^1\widetilde{\Psi}_i(\eta)\frac{d\widetilde{\Psi}_j(\eta)}{d\eta}d\eta;\quad A2_{\ell m}=\int_0^1\widetilde{\Omega}_\ell(\eta)\frac{d\widetilde{\Omega}_m(\eta)}{d\eta}d\eta;\quad B1_i=\int_0^1\widetilde{\Psi}_i(\eta)\left(\Phi_H+\Phi_p\right)^n d\eta \tag{11.a-c}$$

$$B2_\ell=\int_0^1\widetilde{\Omega}_\ell(\eta)\left(\Phi_H+\Phi_p\right)^n d\eta;\quad \widetilde{C}_i=\int_0^1\widetilde{\Psi}_i(\eta)d\eta \tag{11.d,e}$$

In the case of the Gupta and Chand (1990) model, the integral transformation of Eq. (2) is given by:

$$\frac{d\tilde{\theta}_\ell}{d\tau}=-\alpha_{ps}\sum_{i=1}^{N_\Phi}D_{\ell i}\frac{d\tilde{\Phi}_i}{d\tau};\quad D_{\ell i}=\int_0^1\widetilde{\Omega}_\ell(\eta)\widetilde{\Psi}_i(\eta)d\eta \tag{12.a,b}$$

3.1.2 Filter Strategy I

In order to employ the GITT approach in its more efficient form, it is necessary to homogenize the boundary condition in the direction to be integral transformed, specifically the boundary condition at $\eta = 0$ to potential Φ, through a filtering process. This is accomplished by splitting up the analyzed potentials as:

$$\Phi(\eta,\tau) = \Phi_H(\eta,\tau) + \Phi_p(\eta)\,; \qquad \theta(\eta,\tau) = \theta_H(\eta,\tau) + \theta_p(\eta) \tag{13.a,b}$$

For simplicity, in order to avoid computationally involved mathematical expressions, the filters employed in the present analysis are the solutions of the linear steady-state version of the original problem, given by:

For the potential $\Phi_p(\eta)$:	**For the potential $\theta_p(\eta)$:**
$\dfrac{d^2\Phi_p}{d\eta^2} - Pe\dfrac{d\Phi_p}{d\eta} - PeK\Phi_p = 0\,,\quad \text{in } 0<\eta<1$ (14.a)	$\dfrac{d^2\theta_p}{d\eta^2} - Pe\dfrac{d\theta_p}{d\eta} - PeK\Phi_p = 0\,,\quad \text{in } 0<\eta<1$ (15.a)
$\dfrac{d\Phi_p}{d\eta} - Pe\Phi_p = -Pe \quad \text{at} \quad \eta = 0$ (14.b)	$\theta_p = 0 \quad \text{at} \quad \eta = 0$ (15.b)
$\dfrac{d\Phi_p}{d\eta} = 0 \quad \text{at} \quad \eta = 1$ (14.c)	$\dfrac{d\theta_p}{d\eta} = 0 \quad \text{at} \quad \eta = 1$ (15.c)

where the solution for the problems defined by Eqs. (14) and (15) are given by:

$$\Phi_p(\eta) = C_1 e^{W_1\eta} + C_2 e^{W_2\eta}\,; \quad \theta_p(\eta) = \alpha_{ps}KPe\left(A_1 e^{W_1\eta} + A_2 e^{W_2\eta}\right) + \frac{C_3}{Pe}e^{Pe\eta} + C_4 \tag{16.a,b}$$

$$C_1 = -PeW_2 e^{W_2}/\gamma\,; \quad C_2 = PeW_1 e^{W_1}/\gamma\,; \quad W_1 = \frac{Pe - \sqrt{Pe(4K+Pe)}}{2}\,; \quad W_2 = \frac{Pe + \sqrt{Pe(4K+Pe)}}{2} \tag{16.c-f}$$

$$\gamma = W_1 e^{W_1}(Pe - W_2) + W_2 e^{W_2}(W_1 - Pe)\,; \quad A_1 = C_1/\left[W_1(Pe - W_1)\right]\,; \quad A_2 = C_2/\left[W_2(Pe - W_2)\right] \tag{16.g-i}$$

$$C_3 = -\alpha_{ps}KPe\left(A_1 W_1 e^{W_1} + A_2 W_2 e^{W_2}\right)e^{-Pe}\,; \quad C_4 = -\alpha_{ps}KPe\left(A_1 + A_2\right) - \frac{C_3}{Pe} \tag{16.j,k}$$

Therefore, the governing equations for $\Phi_H(\eta,\,\tau)$ and $\theta_H(\eta,\tau)$ become:

$$\frac{\partial\Phi_H}{\partial\tau} = \frac{1}{Pe}\frac{\partial^2\Phi_H}{\partial\eta^2} - \frac{\partial\Phi_H}{\partial\eta} - K(\Phi_H + \Phi_p)^n + K\Phi_p\,, \qquad \text{in } \tau > 0,\quad 0<\eta<1 \tag{17.a}$$

$$\frac{\partial\theta_H}{\partial\tau} = \frac{1}{Pe}\frac{\partial^2\theta_H}{\partial\eta^2} - \frac{\partial\theta_H}{\partial\eta} + \alpha_{ps}K(\Phi_H + \Phi_p)^n - \alpha_{ps}K\Phi_p\,, \qquad \text{in } \tau > 0,\quad 0<\eta<1 \tag{17.b}$$

$$\Phi_H(\eta,\,\tau) = \Phi_i - \Phi_p(\eta) \quad \text{and} \quad \theta_H(\eta,\,\tau) = -\theta_p(\eta) \quad \text{for } \tau = 0,\quad 0 \le \eta \le 1 \tag{17.c,d}$$

$$-\frac{\partial\Phi_H}{\partial\eta} + Pe\Phi_H = 0 \quad \text{and} \quad \theta_H = 0 \quad \text{at} \quad \eta = 0,\quad \tau > 0 \tag{17.e,f}$$

$$\frac{\partial\Phi_H}{\partial\eta} = 0 \quad \text{and} \quad \frac{\partial\theta_H}{\partial\eta} = 0 \quad \text{at} \quad \eta = 1,\quad \tau > 0 \tag{17.g,h}$$

Following the basic steps of the GITT methodology, making use of the appropriate eigenvalues problems (4) and (5) and integral-transform pairs (8) and (9) results the following systems of ordinary differential equations:

$$\begin{cases} \dfrac{d\tilde{\Phi}_{H_i}}{d\tau} = -\dfrac{\mu_i^2}{Pe}\tilde{\Phi}_{H_i} - \displaystyle\sum_{j=1}^{N_\Phi} A1_{ij}\tilde{\Phi}_{H_j} - K\left(Bl_i - \tilde{f}_i\right); \quad \dfrac{d\tilde{\theta}_{H_\ell}}{d\tau} = -\dfrac{\beta_\ell^2}{Pe}\tilde{\theta}_{H_\ell} - \displaystyle\sum_{m=1}^{N_\theta} A2_{\ell m}\tilde{\theta}_{H_m} + \alpha_{ps}K\left(B2_\ell - \tilde{g}_\ell\right) \\ \tilde{\Phi}_{H_i}(0) = \Phi_i\tilde{C}_i - \tilde{f}_i; \qquad \tilde{\theta}_\ell(0) = -\tilde{h}_\ell \end{cases} \tag{18.a-d}$$

where $A1_{ij}$, $A2_{\ell m}$, $B1_i$, $B2_\ell$ and $\tilde{C}_i$ were defined by Eqs. (11), and the coefficients $\tilde{f}_i$, $\tilde{g}_\ell$ and $\tilde{h}_\ell$ are given by:

$$\tilde{f}_i = \int_0^1 \tilde{\Psi}_i(\eta)\Phi_p(\eta)d\eta, \qquad \tilde{g}_\ell = \int_0^1 \tilde{\Omega}_\ell(\eta)\Phi_p(\eta)d\eta, \qquad \tilde{h}_\ell = \int_0^1 \tilde{\Omega}_\ell(\eta)\theta_p(\eta)d\eta \tag{19.d-f}$$

3.1.3 Filter Strategy II

This is a particular case of the Filter Strategy I, where only the potential $\Phi(\eta,\tau)$ will be filtered in the form shown in Eqs. (13.a), (14) and (16.a). Then, the following problems for $\Phi_H(\eta, \tau)$ and $\theta(\eta,\tau)$ are given by:

$$\frac{\partial\Phi_H}{\partial\tau} = \frac{1}{Pe}\frac{\partial^2\Phi_H}{\partial\eta^2} - \frac{\partial\Phi_H}{\partial\eta} - K(\Phi_H + \Phi_p)^n + K\Phi_p, \qquad \text{in } \tau > 0, \quad 0 < \eta < 1 \tag{20.a}$$

$$\frac{\partial\theta}{\partial\tau} = \frac{1}{Pe}\frac{\partial^2\theta}{\partial\eta^2} - \frac{\partial\theta}{\partial\eta} + \alpha_{ps}K(\Phi_H + \Phi_p)^n, \qquad \text{in } \tau > 0, \quad 0 < \eta < 1 \tag{20.b}$$

$$\Phi_H(\eta, \tau) = \Phi_i - \Phi_p(\eta) \quad \text{and} \quad \theta(\eta, \tau) = 0 \quad \text{for } \tau = 0, \quad 0 \le \eta \le 1 \tag{20.c,d}$$

$$-\frac{\partial\Phi_H}{\partial\eta} + Pe\Phi_H = 0 \quad \text{and} \quad \theta = 0 \quad \text{at } \eta = 0, \quad \tau > 0 \tag{20.e,f}$$

$$\frac{\partial\Phi_H}{\partial\eta} = 0 \quad \text{and} \quad \frac{\partial\theta}{\partial\eta} = 0 \quad \text{at } \eta = 1, \quad \tau > 0 \tag{20.g,h}$$

Again, following the basic steps of the GITT approach, making use of the appropriate eigenvalues problems (4) and (5) and integral-transform pairs (8) and (9) results the following ordinary differential equations system:

$$\begin{cases} \dfrac{d\tilde{\Phi}_{H_i}}{d\tau} = -\dfrac{\mu_i^2}{Pe}\tilde{\Phi}_{H_i} - \displaystyle\sum_{j=1}^{N_\Phi} A1_{ij}\tilde{\Phi}_{H_j} - K\left(Bl_i - \tilde{f}_i\right); \quad \dfrac{d\tilde{\theta}_\ell}{d\tau} = -\dfrac{\beta_\ell^2}{Pe}\tilde{\theta}_\ell - \displaystyle\sum_{m=1}^{N_\theta} A2_{\ell m}\tilde{\theta}_m + \alpha_{ps}KB2_\ell \\ \tilde{\Phi}_{H_i}(0) = \Phi_i\tilde{C}_i - \tilde{f}_i; \quad \tilde{\theta}_\ell(0) = 0 \end{cases} \tag{21.a-d}$$

3.1.4 Filter Strategy III

Now, to employ the GITT approach, we homogenize the boundary condition (1.e) in the following form:

$$\Phi(\eta,\tau) = \Phi_H(\eta,\tau) + 1 \tag{22}$$

Making use of the eigenvalues problems and integral-transform pairs previously defined, results the following ODE system:

$$\begin{cases} \dfrac{d\tilde{\Phi}_{H_i}}{d\tau} = -\dfrac{\mu_i^2}{Pe}\tilde{\Phi}_{H_i} - \displaystyle\sum_{j=1}^{N_\Phi} A1_{ij}\tilde{\Phi}_{H_j} - KBl_i; \quad \dfrac{d\tilde{\theta}_\ell}{d\tau} = -\dfrac{\beta_\ell^2}{Pe}\tilde{\theta}_\ell - \displaystyle\sum_{m=1}^{N_\theta} A2_{\ell m}\tilde{\theta}_m + \alpha_{ps}KB2_\ell \\ \tilde{\Phi}_{H_i}(\tau = 0) = (\Phi_i - 1)\tilde{C}_i; \quad \tilde{\theta}_\ell(\tau = 0) = 0 \end{cases} \tag{23.a-d}$$

Therefore, the integral transformation process eliminates the longitudinal coordinate, η, and offers an ordinary differential system for the transformed potentials in the time variable. The infinity system should be truncated to sufficiently large finite orders, N_Φ and N_θ, in order to achieve numerical results to within a user prescribed accuracy target. This is attained through well-established subroutines for initial value problems such as DIVPAG from the IMSL package (IMSL, 1991). Once these transformed potentials have been numerically evaluated at any time, τ, the related potentials are analytically recovered by recalling their inversion formulae.

3.2. The Gear-FDM Approach

Now, following the idea of the Finite Difference Method (Ozisik, 1994), the discretization in the spatial variable is derived in accordance with following aproximations for first and second derivatives, over the mesh shown in Fig. (1):

$$\frac{\partial^2 F(x,\tau)}{\partial x^2} = \frac{F_{j+1}^{k+1} - 2F_j^{k+1} + F_{j-1}^{k+1}}{\Delta x^2}; \qquad \frac{\partial F(x,\tau)}{\partial x} = \frac{F_j^{k+1} - F_{j-1}^{k+1}}{\Delta x} \tag{24.a,b}$$

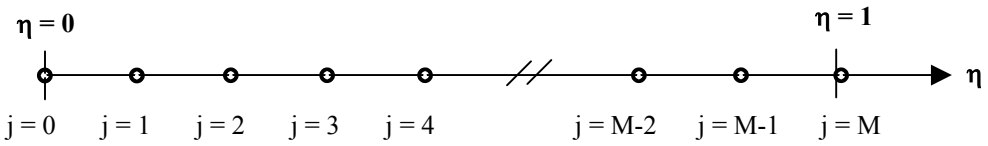

Figure 1. Scheme for the domain discretization.

Applying Eqs. (24.a,b) in Eqs. (1.a,b) for each internal point of the mesh and making use of the boundary conditions, the following ODE system results:

$$\begin{cases} \dfrac{d\Phi_j}{d\tau} = \dfrac{\delta_{\Phi_j}^{k+1}}{Pe\Delta\eta^2} - \dfrac{\Gamma_{\Phi_j}^{k+1}}{\Delta\eta} - K\left(\Phi_j^{k+1}\right)^n, \quad \dfrac{d\theta_j}{d\tau} = \dfrac{\delta_{\theta_j}^{k+1}}{Pe\Delta\eta^2} - \dfrac{\Gamma_{\theta_j}^{k+1}}{\Delta\eta} + \alpha_{ps} K\left(\Phi_j^{k+1}\right)^n; \quad j = 1,2,...,M\text{-}1 \\ \Phi_j(0) = \Phi_i; \qquad \theta_j(0) = 0 \end{cases} \tag{25.a-d}$$

where M is the number of the equal parts of mesh size ($\Delta\eta = 1/M$), k + 1 is the time level and δ^{k+1} and Γ^{k+1} are given by:

$$\delta_{\Phi_j}^{k+1} = \Phi_{j+1}^{k+1} - 2\Phi_j^{k+1} + \Phi_{j-1}^{k+1}; \quad \delta_{\theta_j}^{k+1} = \theta_{j+1}^{k+1} - 2\theta_j^{k+1} + \theta_{j-1}^{k+1} \tag{26.a,b}$$

$$\Gamma_{\Phi_j}^{k+1} = \Phi_j^{k+1} - \Phi_{j-1}^{k+1} \quad \Gamma_{\theta_j}^{k+1} = \theta_j^{k+1} - \theta_{j-1}^{k+1} \tag{26.c,d}$$

Equations (25.a,b) above, form a set of coupled first order ODEs subjected to the initial conditions given by Eqs. (25.c,d). For computational purposes, the domain is discretized at sufficiently large finite number of meshes M, which correspond to 2(M-1) ODEs. The ODE system of size 2(M-1) is computationally solved with the use of the subroutine DIVPAG from IMSL library (1991), where the ODE solver was employed with a required tolerance of 10^{-6}.

4. RESULTS AND DISCUSSION

Fortran codes were built and implemented on a Pentium IV 1.7 GHz computer imposing a relative error criterion of 10^{-6} for the subroutine DIVPAG (IMSL, 1991), i.e., an error control in the sixth significant digit for all potentials is searched. Results for the dimensionless substrate (Φ) and product (θ) potentials are illustrated, for various combinations of the dimensionless parameters Pe, K and n. Convergence behavior for $\Phi(1,\tau)$ and $\theta(1,\tau)$ are shown for different times. All figures presented here are illustrated with converged results.

Tables (1) and (2) present numerical values for a representative case, including all procedure of solution studied here for comparative purposes. These tables show a convergency analysis in the series solution with the several strategies adopted in the GITT approach and the mesh analysis convergency in the GEAR-FDM approach. The parameters analyzed were Pe = 10 and 100, n = 1 and K = 4. Also, are presented the results obtained by the solution methodologies (GITT and GEAR-FDM approaches) applied in the model proposed by Gupta and Chand (1990).

It can be observed that the formal solution in the GITT approach presents a very slow convergence rate, while the filter strategies shown to be more efficient and equivalent. In these tables, it can be verified that the filter strategies I, II and III converge in the fourth significant digit with less than 100 terms in the series, this provides a small computacional cost in the GITT approach. The effectiveness of the filtering strategies is quite noticeable from these tables.

An analysis of mesh convergence is accomplished in the GEAR-FDM approach, where it is observed that the most critical case needed a mesh with 400 to 500 points. In this case the computacional cost was also low. A comparison among the results obtained by the GITT and the GEAR-FDM approaches shows a excellent agreement. Also, the results obtained by Gupta and Chand (1990) model are presented, but only the results for the product present differences in relation to those obtained with the model proposed here.

Table 1. Convergence behavior of the exit concentration for Φ and θ with times τ = 0.1 and 0.8, and for Pe = 10, K = 4 and n = 1.

GITT Approach						**GEAR-FDM Approach**		
Φ(η = 1, τ = 0.1)								
NT	**F. S.** **	**Filter I** **	**Filter II** **	**Filter III****	**GITT**##	**M**	**FDM****	**FDM**##
10	0.6684	0.6703	0.6703	0.6703	0.6703	25	0.6703	0.6703
25	0.6707	0.6703	0.6703	0.6703	0.6703	50	0.6703	0.6703
50	0.6702	0.6703	0.6703	0.6703	0.6703	100	0.6703	0.6703
100	0.6703	0.6703	0.6703	0.6703	0.6703	200	0.6703	0.6703
200	0.6703	0.6703	0.6703	0.6703	0.6703	400	0.6703	0.6703
Φ(η = 1, τ = 0.8)								
10	0.0532	0.0610	0.0610	0.0611	0.0610	25	0.0674	0.0804
25	0.0585	0.0610	0.0610	0.0610	0.0610	50	0.0640	0.0640
50	0.0595	0.0610	0.0610	0.0610	0.0610	100	0.0625	0.0625
100	0.0603	0.0610	0.0610	0.0610	0.0610	200	0.0617	0.0617
200	0.0607	0.0610	0.0610	0.0610	0.0610	400	0.0614	0.0614
θ(η = 1, τ = 0.1)								
10	0.1617	0.1616	0.1615	0.1615	0.1590	25	0.1615	0.1615
25	0.1615	0.1615	0.1615	0.1615	0.1625	50	0.1615	0.1615
50	0.1615	0.1615	0.1615	0.1615	0.1610	100	0.1615	0.1615
100	0.1615	0.1615	0.1615	0.1615	0.1613	200	0.1615	0.1615
200	0.1615	0.1615	0.1615	0.1615	0.1614	400	0.1615	0.1615
θ(η = 1, τ = 0.8)								
10	0.3943	0.4187	0.4186	0.4187	0.4564	25	0.4129	0.4570
25	0.4077	0.4187	0.4187	0.4187	0.4616	50	0.4157	0.4586
50	0.4132	0.4187	0.4187	0.4187	0.4594	100	0.4172	0.4594
100	0.4160	0.4187	0.4187	0.4187	0.4597	200	0.4180	0.4597
200	0.4173	0.4187	0.4187	0.4187	0.4599	400	0.4184	0.4599

$NT = N_\Phi = N_\theta$; ** – Present Model; ## – Gupta and Chand (1990) Model; F.S. – Formal Solution.

In Table (2) the results for dimensionless substrate (Φ) and product (θ) concentrations are shown for Pe = 100, n = 1 and K = 4. It is observed that the results of the present model are close of the obtained by the Gupta and Chand (1990) model. Similar analysis is made in relation to the convergence rates for the methodologies used here. The same conclusions obtained in the analysis of Table (1) may be extended for the results of Table (2).

Figures (2) to (5) bring the influence of dimensionless parameters Pe, n an K in the exit concentration of the substract (Φ) and product (θ). A comparison among the results obtained with the model proposed in the present work and that one proposed by Gupta and Chand (1990) is shown in these figures. Such results, obtained by the two methodologies adopted here are shown as function of the time variable.

In Fig. (2) (for Pe = 10 and 100, n = 1 and K = 4) can be observed that the Peclet number has little influence in the exit concentrations for the substract and the product in the Gupta and Chand (1990) model. It is observed that, when the number of Peclet increases (i.e., Pe = 100) the results of both models become very close. However, for low values of Pe, it is noticed that the results of θ are smaller in the steady state. This can be explained by the fact of the present model to take into account the transport mechanisms during the process of conversion of substrate to product. This fact is not observed in the model of Gupta and Chand (1990), where there is a direct relationship with the conversion rate (see Eq. (2)). In this figure a perfect graphic agreement can be observed among the results obtained by the methodologies here employed.

Table 2. Convergence behavior of the exit concentration for Φ and θ with times τ = 0.1 and 0.8, and for Pe = 100, K = 4 and n = 1.

GITT Approach						GEAR-FDM Approach		
Φ(η = 1, τ = 0.1)								
NT	**F. S.** **	**Filter I** **	**Filter II** **	**Filter III****	**GITT**##	**M**	**FDM****	**FDM**##
10	0.6681	0.6699	0.6699	0.6700	0.6699	25	0.6703	0.6703
25	0.6704	0.6703	0.6703	0.6703	0.6703	50	0.6703	0.6703
50	0.6703	0.6703	0.6703	0.6703	0.6703	100	0.6703	0.6703
100	0.6703	0.6703	0.6703	0.6703	0.6703	200	0.6703	0.6703
200	0.6703	0.6703	0.6703	0.6703	0.6703	400	0.6703	0.6703
Φ(η = 1, τ = 0.8)								
10	0.0388	0.0413	0.0413	0.0414	0.0413	25	0.0469	0.0469
25	0.0398	0.0413	0.0413	0.0413	0.0413	50	0.0436	0.0436
50	0.0403	0.0413	0.0413	0.0413	0.0413	100	0.0423	0.0423
100	0.0407	0.0413	0.0413	0.0413	0.0413	200	0.0417	0.0417
200	0.0410	0.0413	0.0413	0.0413	0.0413	400	0.0415	0.0415
θ(η = 1, τ = 0.1)								
10	0.1612	0.1617	0.1617	0.1617	0.1610	25	0.1615	0.1615
25	0.1615	0.1615	0.1615	0.1615	0.1617	50	0.1615	0.1615
50	0.1615	0.1615	0.1615	0.1615	0.1614	100	0.1615	0.1615
100	0.1615	0.1615	0.1615	0.1615	0.1615	200	0.1615	0.1615
200	0.1615	0.1615	0.1615	0.1615	0.1615	400	0.1615	0.1615
θ(η = 1, τ = 0.8)								
10	0.4465	0.4686	0.4685	0.4685	0.4691	25	0.4635	0.4670
25	0.4544	0.4687	0.4687	0.4687	0.4700	50	0.4661	0.4686
50	0.4595	0.4687	0.4687	0.4687	0.4696	100	0.4674	0.4693
100	0.4635	0.4687	0.4687	0.4687	0.4697	200	0.4681	0.4695
200	0.4660	0.4687	0.4687	0.4687	0.4697	400	0.4684	0.4696

NT = $N_\Phi = N_\theta$; ** – Present Model; ## – Gupta and Chand (1990) Model; F.S. – Formal Solution.

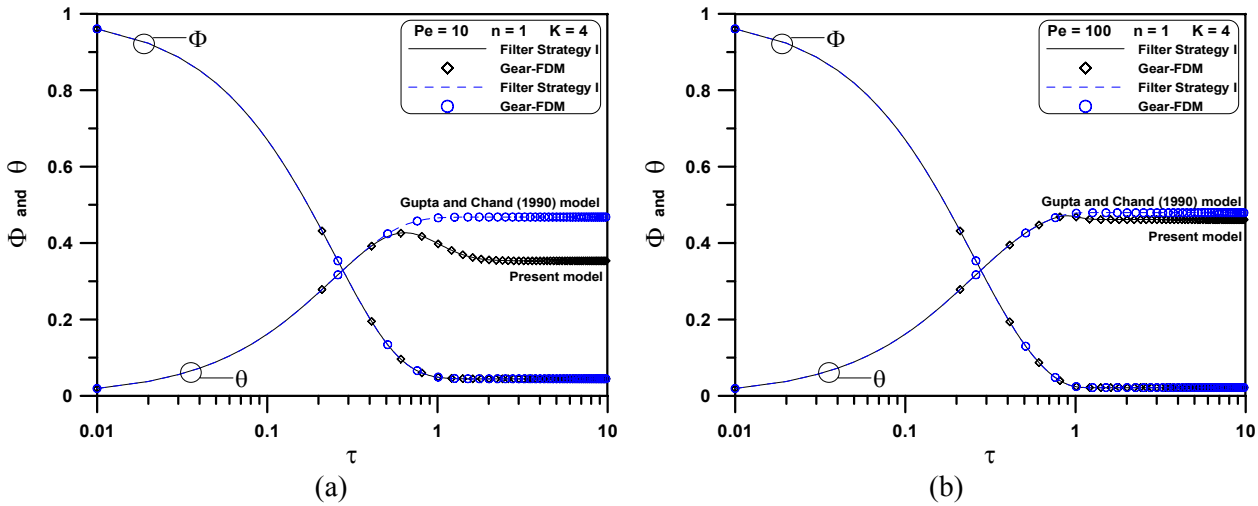

Figure 2. Exit concentration as function of the dimensionless time for Pe = 10 and 100, n = 1 and K = 4.

In Fig. (3) are presented similar results to those in Fig. (2) for Pe = 10 and 100, n = 2 and K = 4, the same observations can be applied for this case. However, making a comparison among these figures, it can be noticed the influence of the reaction order in the results. It is observed that as larger the order of reaction smaller will be the overall conversion rate of substrate to product.

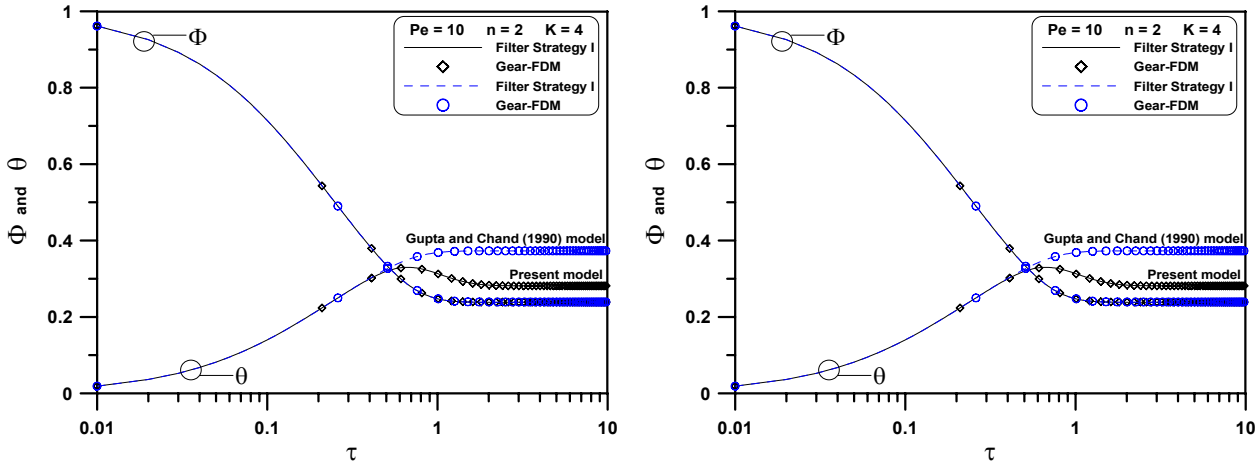

Figure 3. Exit concentration as function of the dimensionless time for Pe = 10 and 100, n = 2 and K = 4.

In Fig. (4) are presented the results for Pe = 10 and 100, n = 1 and K = 40. Again the same observations as those in Figs. (2) and (3) are valid here. However, it can be noticed that as the value of K increases, the overall conversion rate of substrate to product also increases.

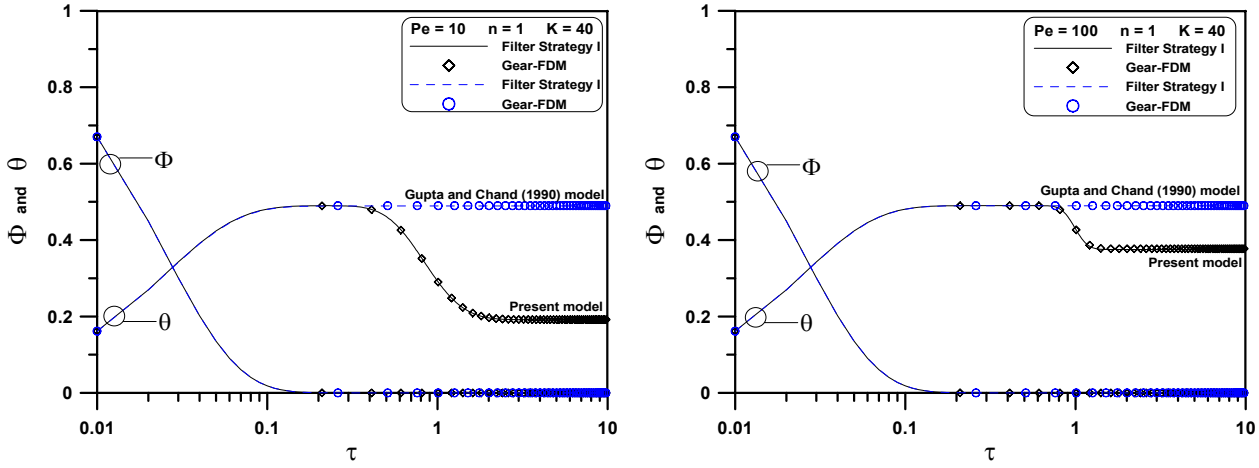

Figure 4. Exit concentration as function of the dimensionless time for Pe = 10 and 100, n = 1 and K = 40.

Figure (5) present results for Pe = 10 and 100, n = 2 and K = 40. Also, similar conclusions can be made for this case.

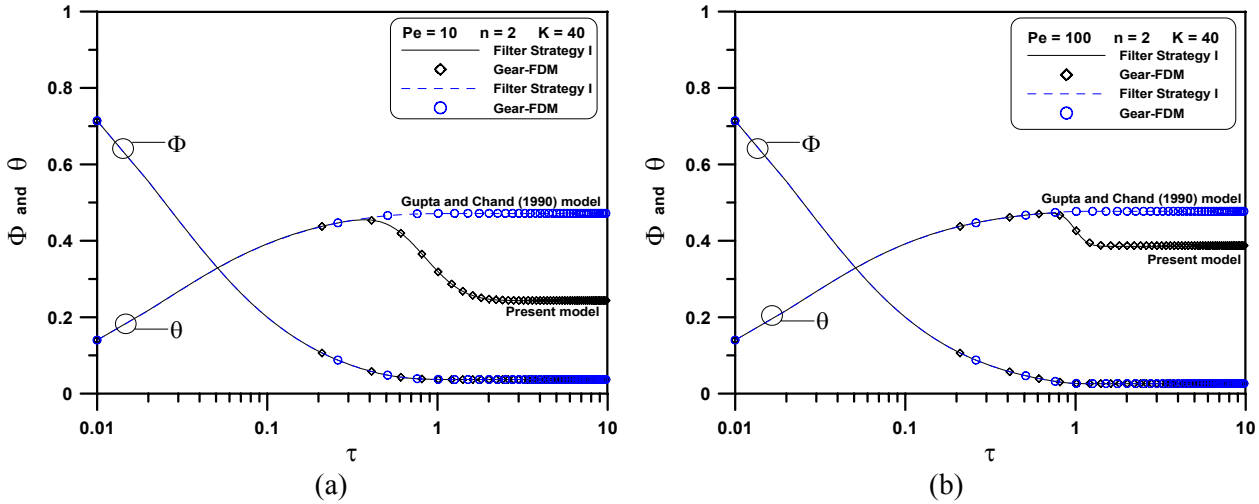

Figure 5. Exit concentration as function of the dimensionless time for Pe = 10 and 100, n = 2 and K = 40.

5. CONCLUSIONS

In this work a mathematical model was proposed to study the bioconversion sugar process in a fixed bed reactor of immobilized cells. With the objective of accomplishing critical comparisons, it was also used the model of Gupta and Chand (1990) in the present work. Two solution methodologies, the GITT and the GEAR-FDM approaches were employed to obtain the solutions of equations for the models analyzed. In the GITT approach four formulation were developed (i. e., Formal solution, Filter Strategies I to III), where the filtering techniques have presented excellent computational performances, enhancing the convergence rates of the resulting series. The GEAR-FDM approach, also, presented an excellent mesh convergences rates. In all methodologies utilized, the computational codes presented small CPU times. Results were presented for various dimensionless parameters, and comparisons between the two models and the two metodologies were also performed. The results of the two metodologies demonstrated excellent agreement and furnished direct validations of computational codes developed, as well as shown their consistencies.

6. ACKNOWLEDGEMENTS

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