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INTEGRAL TRANSFORM ANALYSIS OF A SIMPLE ALCOHOLIC FERMENTATION MODEL

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Abstract. *This paper analyses the specific part of the production of beer, namely the fermentation process, by the use of a hybrid methodology based on the Generalized Integral Transform Technique (GITT). A non-linear partial differential equation arises from the one-dimensional mathematical model, which describes the temperature distribution, the concentration of biomass and substrate spatially in a cylindrical fermenter vessel. The third-kind (Robin) boundary condition is established on the wall of the vessel as a general formulation is provided, involving different test-cases based on the dimensionless quantity represented by the Biot number. The solution of the governing equations was carried out within the GITT framework, for a simplified version of the problem in which the reaction rate becomes independent of temperature. The convergence behavior of the solution was analyzed, showing that in general five converged digits can be obtained with 60 terms in the truncated series. Finally, illustrative results are presented showing the evolution of temperature and concentrations at different locations.*

Keywords: *GITT, fermentation, mathematical model*

NOMENCLATURE

c_p	mixture heat capacity, kJ/kg °C
h	outer convection heat transfer coefficient, W/(m^{2}K)
k	thermal conductivity of fermenting mixture, W/m^2 K
r	radius of fermenter vessel, m
A, B, C	integral coefficients
D	diameter of fermenter vessel, m
ΔH	heat of reaction, kJ/mol
K	Michaelis constant, mol/m^3
L_H	height of fermenter vessel, m
M, N	Norms
S	fermentable substrate concentration, mol/m^3
T	temperature, °C or K
V	volume of fermenting mixture, m^3
X	biomass (yeast) concentration, mol/m^3

Greek symbols

μ	specific growth rate of substrate, h^{-1}
μ_X	specific biomass growth rate, h^{-1}
ν	maximum reaction velocity, h^{-1}
ρ	mixture density, kg/m^3
γ, ω	eigenvalues
ϕ, ψ	eigenfunctions

Dimensionless quantities

τ	time
σ	substrate concentration
χ	biomass concentration
θ	temperature
η	radius of fermenter vessel
μ^*	normalized substrate growth rate
μ^*_χ	normalized biomass growth rate

I^*	inoculation rate
Y_{XS}	stoichiometric yield of biomass/substrate
Bi	Biot number
H^*	heat of reaction
κ_S^*	Michaelis constant for substrate
κ_X^*	Michaelis constant for biomass

Subscripts and superscripts

0	Initial
c	Cooling
i, j, k, l, m	integers
S	Fermentable Sugars
T	Temperature-dependent
X	Biomass
ref	Reference
$*$	Dimensionless quantity

Overscripts

$\bar{}$	transformed quantity

1. INTRODUCTION

Beer is a very popular beverage in the world, its origins is still uncharted, even though the process, production and industrialization is well-known. The composition of beer is mostly based on water, malted grains, hops and yeast; the two major steps of its manufacturing are the production of the wort, called mashing, and its fermentation. Specially in the fermentation part of the process, the use of the substrates are particularly based on maltose, glucose and maltotriose. Based on the higher concentration of maltose (Koljonen *et al.*, 1995), most models don't apply simplifications dealing with only that sugar. With that in mind, the focus of this work is to establish a methodology describing the fermentation process and simplifying most of the customary models present in the literature. This study relies on a hybrid analytical-numerical method as its tool of choice for a unique mathematical approach into the process.

In order to improve the quality of the beverage, some models based on experiments were proposed over the years, such as the kinetic model developed by Engasser *et al.* (1981) which was for the fermentation phase, taking into account the different fermentable sugars (maltose, glucose and maltotriose). Based on this model, Gee and Ramirez (1988), included the temperature effects in the kinetic rate expressions and added it as a state variable, the optimal controller was established during the fermentation, so the temperature can be maximized to achieve the higher final ethanol concentration. In 1994, Gee and Ramirez (1994) improved their model considering the temperature effects in the flavour and aroma compounds. Later, Hepworth *et al.* (2003), created a mathematical model to estimate yield coefficients for ethanol, higher alcohols, fermentable sugars and esters from the measures of CO_2. Recently, Liu *et al.* (2014), also adapted the Gee and Ramirez (1994) formulation for the Chinese rice wine due to the use of the same yeast (Saccharomyces cerevisiae) for ethanol production.

Most works involving fermentation models, regardless of being in beer production, generally apply numerical methods or/and experimental studies to discuss new optimization mechanisms in fermentation process. Brányik *et al.* (2004) established a comparison between the proposed kinetic model that estimates brewing yeast growth and spent grain particles with experimental results for continuous beer fermentation. Carrillo-Ureta *et al.* (2001) also based their work in both numerical and experimental approaches, where the beer fermentation model was implemented by the MATLAB software with parameters approximated by experimental data. Phisalaphong *et al.* (2006) also applied the MATLAB software to evaluate ethanol fermentation, where the influence of the temperature on kinetic parameters is investigated. As stated, the application of numerical methods in beer fermentation kinetics models are common; however, there is clear room for analytical and semi-analytical solutions. Hence, the application of hybrid analytical-numerical methods in beer fermentation models can be applied and presents itself as novelty, as their use was not yet found in the literature by the authors.

Even though there are many optimization and simulation studies, they lack how biomass and fermentable sugars behave in spatial coordinates inside the fermenter vessel. This paper deals with the theoretical formulation of brewing fermentation by the use of a hybrid methodology based on the Generalized Integral Transform Technique (Cotta, 1993).

2. PROBLEM FORMULATION

The employed problem formulation considers a modified version of the model presented by Gee and Ramirez (1994). The chemical reaction kinetics are simplified to consider a single species substrate fermentable S:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\mu\, X, \qquad \frac{\mathrm{d}X}{\mathrm{d}t} = \mu_X\, X, \tag{1}$$

where X is the biomass concentration (i.e. yeast), while μ and μ_X are the specific growth rate for substrate and biomass, respectively, which are defined as:

$$\mu = \frac{\nu\, S}{S + K_S}, \qquad \mu_X = \frac{Y_{XS}\, \mu\, K_X}{K_X + (X - X_o)^2}, \tag{2}$$

in which the quantities are taken from Gee and Ramirez (1994). Although a simplified chemical kinetics model is used, the heat transfer within the fermentation vessel includes local diffusion effects, such that all dependent variables can vary with position. An one-dimensional model is selected for representing the heat transfer within a cylindrical fermentation tank:

$$\rho\, c_p\, \frac{\partial T}{\partial t} = \frac{k}{r}\,\frac{\partial}{\partial r}\left(\frac{r \partial T}{\partial r}\right) + \Delta H\, \frac{\partial S}{\partial t}, \tag{3}$$

where ΔH is the heat released by the alcoholic fermentation reaction ($\Delta H = -226.3$ kJ/mol). The initial conditions are written as:

$$X(r,0) \,=\, X_0, \qquad S(r,0) \,=\, S_0, \qquad T(r,0) \,=\, T_0, \tag{4}$$

while the boundary conditions are given by:

$$|T(0,t)| < \infty, \qquad -k\,\frac{\partial T}{\partial r} = h\,(T - T_c), \quad \text{at} \quad r = D/2, \tag{5}$$

where X_0 represents the initial biomass concentration, S_0 the initial substrate concentration, T_0 the external temperature, k the thermal conductivity of the fermenting mixture (assumed constant), r the radius of the fermenter vessel, D the diameter of the fermenter vessel, and h is the convection heat transfer coefficient for the fluid outside the fermenter vessel. The normalization of the problem is carried out by defining the following dimensionless variables:

$$\tau = t\,\nu_{ref}, \qquad \sigma = \frac{S}{S_0}, \qquad \chi = \frac{X}{X_0}, \qquad \theta = \frac{T - T_0}{\Delta T}, \qquad \eta = \frac{2\,r}{D}, \tag{6}$$

such that the following normalized problem is obtained:

$$\frac{\partial \sigma}{\partial \tau} = -\mu^*\, I^*\, \chi, \tag{7a}$$

$$\frac{\partial \chi}{\partial \tau} = Y_{XS}\, \mu^*\, \mu_\chi^*\, \chi, \tag{7b}$$

$$\frac{\mathrm{Da}}{\mathrm{Le}}\, \frac{\partial \theta}{\partial \tau} = H^*\, \frac{\partial \sigma}{\partial \tau} + \frac{1}{\eta}\, \frac{\partial}{\partial \eta}\left(\eta\, \frac{\partial \theta}{\partial \eta}\right), \tag{7c}$$

$$\sigma(\eta,0) \,=\, 1, \qquad \chi(\eta,0) \,=\, 1, \qquad \theta(\eta,0) \,=\, 1, \tag{7d}$$

$$|\theta(0,\tau)| < \infty, \qquad -\frac{\partial \theta}{\partial \eta} = \mathrm{Bi}\, \theta \quad \text{at} \quad \eta = 1, \tag{7e}$$

where the characteristic dimensionless parameters are defined as:

$$H^* = \frac{\Delta H\, \nu_{ref}\, S_0}{k\, \Delta T}\left(\frac{D}{2}\right)^2, \qquad I^* = \frac{X_0}{S_0}, \qquad \kappa_S^* = \frac{K_S}{S_0}, \qquad \kappa_X^* = \frac{K_X}{X_0^2}, \tag{8}$$

$$\mathrm{Da} \,=\, \frac{\nu_{ref}\,(D/2)^2}{\mathcal{D}}, \qquad \mathrm{Le} \,=\, \frac{k}{\rho\, c_p\, \mathcal{D}}, \qquad \mathrm{Bi} \,=\, \frac{h\, D/2}{k}. \tag{9}$$

The parameters μ^* and μ_X^* are the normalized version of the reaction coefficients μ and μ_X, defined as:

$$\mu^* = \frac{\sigma}{\sigma + \kappa_S^*}, \qquad \mu_\chi^* = \frac{\kappa_X^*}{\kappa_X^* + (\chi - 1)^2}. \tag{10}$$

If the substrate and biomass concentration are relatively small, the coefficients μ^* and μ_X^* can be simplified using a Taylor Series expansion about $\sigma = 0$ and $\chi = 0$, and retaining the first-order term:

$$\mu^* \,\approx\, \sigma, \qquad \mu_\chi^* \,\approx\, 1, \tag{11}$$

such that equations (7a) and (7b) can be simplified to yield:

$$\frac{\partial \sigma}{\partial \tau} = -I^*\, \sigma\, \chi, \tag{12a}$$

$$\frac{\partial \chi}{\partial \tau} = Y_{XS}\, \sigma\, \chi. \tag{12b}$$

It is proposed the use of the Generalized Integral Transform Technique for solving the equation (7c). First of all, the transformation pairs must be defined:

$$\text{Transform} \implies \bar{\theta}_i(\tau) = \int_0^1 \theta(\eta,\tau)\,\psi_i(\eta)\,\eta\,\mathrm{d}\eta, \qquad \text{Inverse} \implies \theta(\eta,\tau) = \sum_{i=1}^{\infty} \frac{\bar{\theta}_i(\tau)\,\psi_i(\eta)}{N_i}, \tag{13a}$$

$$\text{Transform} \implies \bar{\sigma}_i(\tau) = \int_0^1 \sigma(\eta,\tau)\,\phi_i(\eta)\,\eta\,\mathrm{d}\eta, \qquad \text{Inverse} \implies \sigma(\eta,\tau) = \sum_{i=1}^{\infty} \frac{\bar{\sigma}_i(\tau)\,\phi_i(\eta)}{M_i}, \tag{13b}$$

$$\text{Transform} \implies \bar{\chi}_i(\tau) = \int_0^1 \chi(\eta,\tau)\,\phi_i(\eta)\,\eta\,\mathrm{d}\eta, \qquad \text{Inverse} \implies \chi(\eta,\tau) = \sum_{i=1}^{\infty} \frac{\bar{\chi}_i(\tau)\,\phi_i(\eta)}{M_i} \tag{13c}$$

where ψ_i and ϕ_i are orthogonal solutions of a Sturm-Liouville problem (eigenfuntions). Considering a cylindrical fermenter vessel and the only variation is in the radius direction, the one-dimensional Helmholtz problem is chosen for each eigenfunction:

$$\frac{\partial}{\partial\eta}\left(\eta\,\frac{\partial\psi_i}{\partial\eta}\right) + \gamma_i^2\,\psi_i\,\eta = 0, \tag{14}$$

$$\frac{\partial}{\partial\eta}\left(\eta\,\frac{\partial\phi_i}{\partial\eta}\right) + \omega_i^2\,\phi_i\,\eta = 0, \tag{15}$$

in which the boundary conditions are given by:

$$|\psi_i(0)| < \infty, \qquad -\frac{\partial\psi_i}{\partial\eta} = \mathrm{Bi}\,\psi_i, \quad \text{at} \quad \eta = 1, \tag{16a}$$

$$|\phi_i(0)| < \infty, \qquad \frac{\partial\phi_i}{\partial\eta} = 0, \quad \text{at} \quad \eta = 1, \tag{16b}$$

and ψ_i and ϕ_i can be described as infinite solutions of the Bessel equation:

$$\psi_i(\eta) = J_0(\gamma_i\,\eta), \tag{17}$$

$$\phi_0(\eta) = 1, \qquad \phi_i(\eta) = J_0(\omega_i\,\eta), \tag{18}$$

where ω_i and γ_i are the eigenvalues associated to ϕ_i and ψ_i, which are numerically calculated by the transcendental equations:

$$J_0(\gamma_i) = 0, \qquad \text{for} \quad \mathrm{Bi} \to \infty, \tag{19}$$

$$\frac{\mathrm{d}J_0(\gamma_i\,\eta)}{\mathrm{d}\eta} + \mathrm{Bi}\,J_0(\gamma_i\,\eta) = 0, \qquad \text{at} \quad \eta = 1, \tag{20}$$

$$J_1(\omega_i\,\eta) = 0. \tag{21}$$

Also, i is a positive integer, and the orthogonality properties and the norms can be written as:

$$\int_0^1 \psi_i\,\psi_j\,\eta\,\mathrm{d}\eta = \begin{cases} 0\ , & \text{for} \quad i \neq j \\ N_i\,, & \text{for} \quad i = j \end{cases}, \qquad N_i = \frac{1}{2}\Big(J_0^2(\gamma_i) + J_1^2(\gamma_i)\Big), \tag{22}$$

$$\int_0^1 \phi_i\,\phi_j\,\eta\,\mathrm{d}\eta = \begin{cases} 0\ , & \text{for} \quad i \neq j \\ M_i\,, & \text{for} \quad i = j \end{cases}, \qquad M_i = \frac{1}{2}\Big(J_0^2(\omega_i) + J_1^2(\omega_i)\Big). \tag{23}$$

To transform the normalized problem, it is necessary to multiply the three principal equations (7c, 12a, 12b) and the initial conditions (7d), by ψ_i for θ and ϕ_i for σ and χ and integrate within $0 \leq \eta \leq 1$, which leads to:

$$\frac{\mathrm{Da}}{\mathrm{Le}}\,\frac{\mathrm{d}\bar{\theta}_i}{\mathrm{d}\tau} = -\,I^*\,H^* \sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\sum_{l=0}^{\infty} B_{i,l}\,A^*_{l,j,k}\,\bar{\sigma}_j(\tau)\,\bar{\chi}_k(\tau) -\,\gamma_i^2\,\bar{\theta}_i, \tag{24}$$

$$\frac{\mathrm{d}\bar{\sigma}_i(\tau)}{\mathrm{d}\tau} = -\,I^* \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} A_{i,j,k}\,\bar{\sigma}_j(\tau)\,\bar{\chi}_k(\tau), \tag{25}$$

$$\frac{\mathrm{d}\bar{\chi}_i(\tau)}{\mathrm{d}\tau} = Y_{XS} \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} A_{i,j,k}\,\bar{\sigma}_j(\tau)\,\bar{\chi}_k(\tau), \tag{26}$$

$$A^*_{i,j,k} = \frac{1}{N_j}\,\frac{1}{N_k}\int_0^1 \phi_i(\eta)\,\phi_j(\eta)\,\phi_k(\eta)\,\eta\,\mathrm{d}\eta, \tag{27}$$

$$B_{i,j} \,=\, \frac{1}{M_j}\int_0^1 \psi_i\,\phi_j\,\eta\,\mathrm{d}\eta. \tag{28}$$

The initial conditions can be transformed as well:

$$\bar{\sigma}_i(0) = \bar{f}_\omega, \qquad \bar{\chi}_i(0) = \bar{f}_\omega, \qquad \bar{\theta}_i(0) = \,\bar{f}_\gamma, \tag{29}$$

where:

$$\int_0^1 \phi_i(\eta)\,\eta\,\mathrm{d}\eta = \bar{f}_\omega = \frac{J_1(\omega_i)}{\omega_i}, \qquad \int_0^1 \psi_i(\eta)\,\eta\,\mathrm{d}\eta = \bar{f}_\gamma = \frac{J_1(\gamma_i)}{\gamma_i}. \tag{30}$$

The system is then truncated in order to acquire the considered solution. The **NDSolve** function from *Mathematica* software (Wolfram, 2003) is then applied for the solution of the set of ordinary differential equations. A specific treatment is implemented with the Equation Simplification (Residual option) and the IDA package. Both are for partial differential equations systems that requires an implicit solver.

3. RESULTS AND DISCUSSION

Numerical results for the presented solution methodology are now presented. The results were calculated with $I^* = 1$, $H^* = -1$, $Y_{XS} = 1$, $\mathrm{Da} = 1$ and $\mathrm{Le} = 1$, for illustrative purposes. The first results are intended to verify the convergence behavior of the computational implementation. Table 1 presents values of the dimensionless temperature θ at different positions and different dimensionless times, calculated for an increasing truncation order. As can be seen from these results, the dimensionless temperatures yield a minimum of 5 fully converged digits for 60 terms. For $\mathrm{Bi} = 0.1$, for both considered positions, the convergence is achieved with 40 terms, while for $\mathrm{Bi} = 10$, at η = 0.1 the θ-values are fully converged using 40 terms, but for η = 0.9 only four converged-digits are seen at τ = 0.001 for 60 terms. Finally, for infinite Biot number values, fully converged temperature values are obtained with 50 terms near the fermenter wall, while near the center 40 terms gives a similar convergence. This implies that, for larger Biot numbers, the convergence is worse at the fermenter wall than at its center.

Table 1. Convergence Analysis of θ for different Bi values, at $\eta = 0.1$ and $\eta = 0.9$, for different τ-values

Bi = 0.1									
η = 0.1					η = 0.9				
	τ					τ			
imax	0.001	0.01	0.1	1	imax	0.001	0.01	0.1	1
1	1.00582	1.01451	1.10084	1.71411	1	0.99787	1.00649	1.09214	1.70056
5	0.94583	0.94597	1.07077	1.71105	5	1.08120	1.06708	1.10562	1.70226
10	0.93549	0.94451	1.07071	1.71102	10	1.06921	1.06692	1.10558	1.70225
20	0.93286	0.94450	1.07070	1.71102	20	1.06402	1.06690	1.10557	1.70224
30	0.93293	0.94451	1.07070	1.71102	30	1.06414	1.06690	1.10557	1.70224
40	0.93293	0.94450	1.07070	1.71102	40	1.06413	1.06690	1.10557	1.70224
50	0.93293	0.94450	1.07070	1.71102	50	1.06413	1.06690	1.10557	1.70224
60	0.93293	0.94450	1.07070	1.71102	60	1.06413	1.06690	1.10557	1.70224
Bi = 10									
η = 0.1					η = 0.9				
	τ					τ			
imax	0.001	0.01	0.1	1	imax	0.001	0.01	0.1	1
1	1.56644	1.50725	1.04728	0.16980	1	0.28918	0.27825	0.19334	0.03135
5	2.50970	1.89480	1.05426	0.17247	5	0.65049	0.39718	0.19863	0.03352
10	2.41495	1.89450	1.05396	0.17235	10	0.62765	0.39711	0.19856	0.03349
20	2.41679	1.89448	1.05394	0.17234	20	0.62803	0.39710	0.19855	0.03349
30	2.41679	1.89448	1.05394	0.17234	30	0.62803	0.39710	0.19855	0.03349
40	2.41680	1.89448	1.05394	0.17234	40	0.62803	0.39710	0.19855	0.03349
50	2.41680	1.89448	1.05394	0.17234	50	0.62802	0.39710	0.19855	0.03349
60	2.41680	1.89448	1.05394	0.17234	60	0.62803	0.39710	0.19855	0.03349
Bi = ∞									
η = 0.1					η = 0.9				
	τ					τ			
imax	0.001	0.01	0.1	1	imax	0.001	0.01	0.1	1
1	1.57137	1.50552	1.00495	0.15157	1	0.20770	0.19900	0.13283	0.02003
5	1.09903	1.01706	0.93513	0.14041	5	0.83084	0.49501	0.15292	0.02477
10	1.02714	1.01007	0.93476	0.14025	10	1.01368	0.50110	0.15359	0.02505
20	1.00033	1.00999	0.93468	0.14022	20	0.97363	0.50095	0.15345	0.02499
30	1.00101	1.01000	0.93469	0.14022	30	0.97428	0.50098	0.15348	0.02500
40	1.00100	1.01000	0.93469	0.14022	40	0.97427	0.50097	0.15346	0.02500
50	1.00100	1.01000	0.93469	0.14022	50	0.97427	0.50098	0.15347	0.02500
60	1.00100	1.01000	0.93469	0.14022	60	0.97427	0.50098	0.15347	0.02500

The next results are aimed at illustrating the evolution of the dimensionless temperature θ and concentrations (σ and χ) at different positions, for different values of the Biot number, as presented in figure 1. As can be seen, the fermentation itself its over by $\tau \approx 2$, as the substrate (σ) and biomass (χ) concentrations become constant for $\tau \approx 2$. The temperature (θ), however, decreases faster if the Biot number is higher, as seen for $\mathrm{Bi} \geq 1$. When the Biot number is zero there is no heat exchange, and thus θ grows while the reaction lasts and then becomes constant. If the Biot number is small as 10^{-2}, the heat exchange is small and θ slowly declines. When comparing the results at different positions, the behavion of the temperature is nearly the same for small Biot numbers (in fact, for zero Bi, the temperature is the same for any position, as the problem solution becomes independent of η). As the number of Biot increases, a larger temperature gradient develops, with the temperature near the vessel wall becoming considerably smaller than at the center, in reason of a more effective heat exchange.

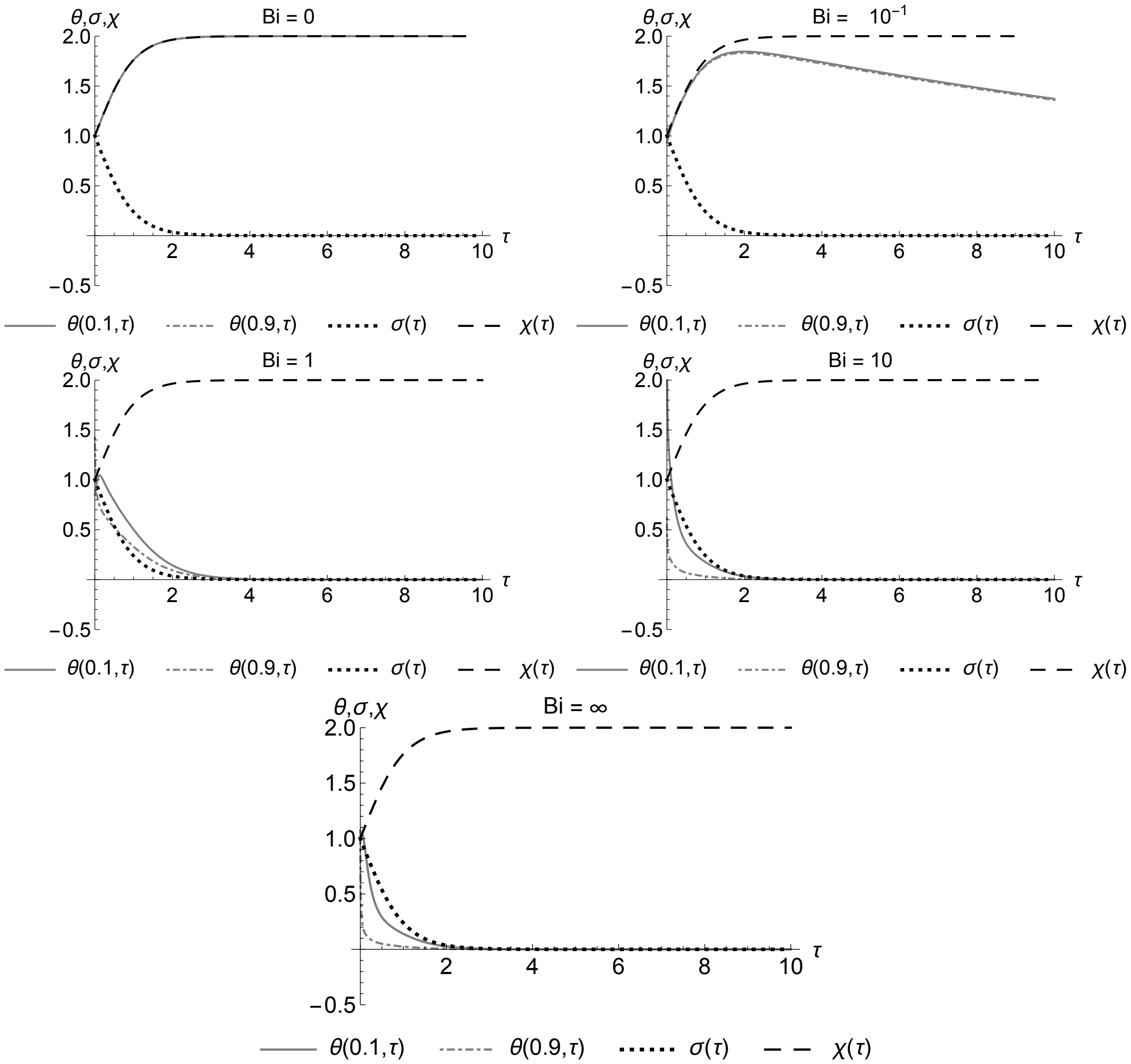

Figure 1. Temperature, biomass and substrate profiles with τ for different values of Bi.

4. CONCLUSIONS

The proposed study presented a simple mathematical formulation for an alcoholic fermentation process, which considers the concentration of single substrate, biomass and temperature as dependent variables. The model was then solved using the Generalized Integral Transform Technique, and computationally implemented using the Mathematica system. The convergence analysis showed that, in general, it is possible to obtain five converged digits with 60 terms in the truncated series, which shows the precision expected for the implemented technique. The convergence is slightly worse at near edge of the fermenter than is at the center for larger Biot numbers. When looking at the illustrative results for temperature and concentrations, it was seen that while the former depends on the Biot number, the concentrations don't. This was a result of a simplification made in this paper, which consider no dependency of the reaction velocity with temperature. As a continuation of this work, an improvement in the model and solution will include this dependency.

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