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Mathematical Modeling for 2-D Fluorescence Spectra Based Using Laplace Transform Method

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Abstract

In this article, Laplace transform and new perturbation methods are adopted to study the problem of the chemical kinetics problem. This article presents a new evaluation procedure of 2-D fluorescence spectra obtained during a yeast cultivation without performing a calibration measurement. The 2-D fluorescence spectra are used to predict the process variables biomass, glucose and ethanol. The new calibration procedure uses a mathematical model of these process variables, i.e., differential equations, to replace any calibration measurement. The mathematical model parameters are identified simultaneously during the calculation of the chemometric models. The approximate analytical solution of the concentration biomass, glucose and ethanol compared with numerical results.

Keywords : Mathematical model · Mass-action kinetics · Homotopy perturbation method· Laplace transform method · 2-D Fluorescence spectra.

1. Introduction

For on-line bioprocess monitoring many measurement devices have been developed, however, only few of them can really be applied to follow the actual state of the cells, i.e. intracellular conditions. Fluorescence make a noninvasive monitoring of intracellular compounds possible. Using a multi-wavelength excitation/emission spectrofluorometer, the fluorescence of fluorophors like NADH, amino acids (e.g. tyrosine and tryptophan) as well as vitamins (like pyridoxine and riboflavin) can be measured simultaneously in a so-called 2D-fluorescence spectrum (Stark ¨ et al., 2002). Therefore, the physiological state of the organisms under consideration can be detected by monitoring the culture fluorescence (Horvath et al., 1993). For quantification of 2D-spectra chemometric models are used, because theoretical models describing the culture fluorescence spectra by using exact fluorophor concentrations are much too complicated. One reason for this is, that the fluorescence spectra as well as quantum yield factors of amino acids can change significantly, if they are used as building blocks in different proteins. Furthermore, the fluorescence spectra depend on the inner filter and the cascade effect as well as on many bioprocess variables like, e.g. optical density, viscosity, ion concentration as well as the size and number of bubbles (Li and Humphrey, 1991). Therefore, to convert the spectra to meaningful information, chemometric modelling techniques, i.e. data driven techniques, must be applied.

One disadvantage of data driven modelling is the huge amount of calibration data necessary to calculate reliable models. For these calibration procedure a lot of off-line measurements of bioprocess variables are obligatory (Martens and Næs, 1989). However, if this time consuming task is performed well, after calibration these process variables can be predicted by the chemometric models out of the 2D-fluorescence spectra. In this contribution a new calibration methodology is presented, which do not require the time expensive collection and processing of samples for off-line measurement data. Instead a priori knowledge about the process is used such as a mathematical model, whose model parameter are determined during the calibration procedure, as well as the fact that the whole substrate has to be consumed at the end of the process run. The fluorescence data (1) discussed here are collected during the growth of Saccharomyces cerevisiae on a glucose medium.

$$\frac{dX(t)}{dt} = \mu_1 X(t) + \mu_1 X(t) = 0 \tag{2}$$

$$\frac{dS(t)}{dt} = -\mu_1 X(t) \frac{1}{Y_{XS}} \tag{3}$$

$$\frac{dE(t)}{dt} = \mu_1 X(t)\, Y_{ES} - \mu_2 X(t)\, Y_{XE} \tag{4}$$

*The initial condition becomes

$t = 0, \quad X = X_{in}, \quad S = S_{in}, \quad E = E_{in}$

If, the three reaction rates are moderately the numbers, are not greatly different in magnitude, then this is a straightforward problem.

Hussanan et al. 2014, Studied an influence of Newtonian heating on Casson fluid past an oscillatory vertical plate by Laplace transform. Kumar et al.2013, investigated a new approximate method, namely homotopy perturbation transform method (HPTM) which is a combination of homotopy perturbation method (HPM) and Laplace transform method (LTM) to provide an analytical approximate solution to time-fractional Cauchy-reaction diffusion equation. In this study, analytical approximation to the of the chemical kinetics problem using combination of new perturbation method and Laplace transform is presented.

2. Solving the concentrations in biomass, glucose and ethanol using new perturbation method and Laplace transform

Let us rewrite the Eqs. (2), (3) and (4) as:

$$X' = \mu_1 X + \mu_1 X = 0 \tag{5}$$

$$S' = -\mu_1 X \frac{1}{Y_{XS}} \tag{6}$$

$$E' = \mu_1 X Y_{ES} - \mu_2 X Y_{XE} \tag{7}$$

To illustrate new perturbation, we limit ourselves to consider the following system of nonlinear ordinary differential equations (NODEs) in the type of the solving Laplace transform method as follows:

Taking Laplace variables eqns. (5-7) and using new perturbation of initial substitute as follows:

$$L(X') - (\mu_1 + \mu_2) L(X) = 0 \tag{8}$$

$$L(S') + \frac{\mu_1}{Y_{XS}} L(S) = 0 \tag{9}$$

$$L(E') - \mu_1 Y_{ES} L(X) + \mu_2 Y_{XE} L(X) = 0 \tag{10}$$

We obtain the solution the eqns. (8), (9) and (10),

$$X(s) = \frac{X^*}{s - (\mu_1 + \mu_1)} \tag{11}$$

$$S(s) = \frac{S^*}{s} - \frac{\mu_1 X^*}{s Y_{XS} (s - (\mu_1 + \mu_2))} \tag{12}$$

$$E(s) = \frac{E^*}{s} + \frac{X^*}{s(s - (\mu_1 + \mu_2))} \left[\mu_1 Y_{ES} - \mu_2 Y_{XE} \right] \tag{13}$$

Finally, we take inverse Laplace transform for solutions (11), (12) and (13) we get

$$X(s) = X^* e^{(\mu_1 + \mu_1)t} \tag{14}$$

$$S(s) = S^* - \frac{\mu_1 X^*}{Y_{XS}} \left[\frac{e^{(\mu_1 + \mu_2)t} - 1}{\mu_1 + \mu_2} \right] \tag{15}$$

$$E(s) = E^* + \frac{X^* (\mu_1 Y_{ES} - \mu_2 Y_{XE})}{\mu_1 + \mu_2} \left[e^{(\mu_1 + \mu_2)t} - 1 \right] \tag{16}$$

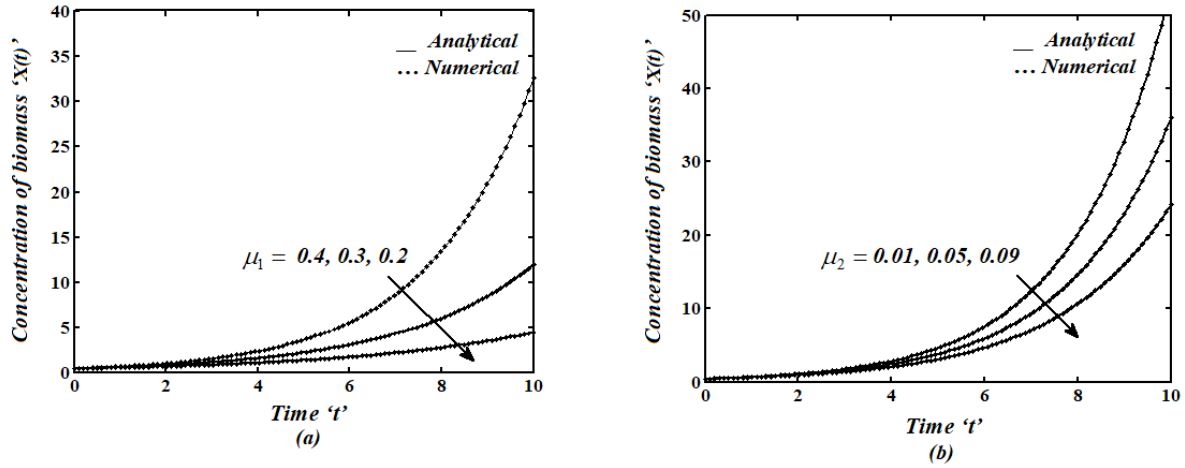

Figure 1. Comparison of analytical expression of the concentration profiles X(t) with simulation results for varies values of parameters, when $\mu_1 =$ = 0.4, $\mu_2 =$ 0.04 and X* =0.4.

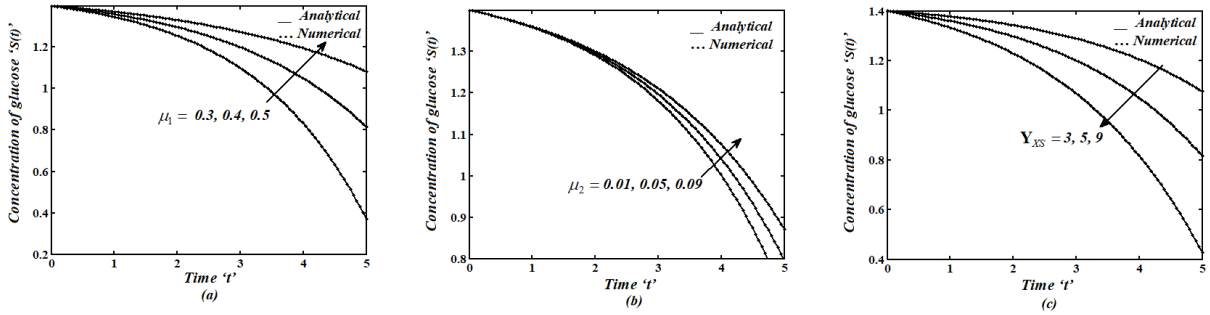

Figure 2. Comparison of analytical expression of the concentration profiles S(t) with simulation results for varies values of parameters, when $\mu_1 =$ = 0.4, $\mu_2 =$ 0.04, YXS=5, X* =0.4, and S* =1.4.

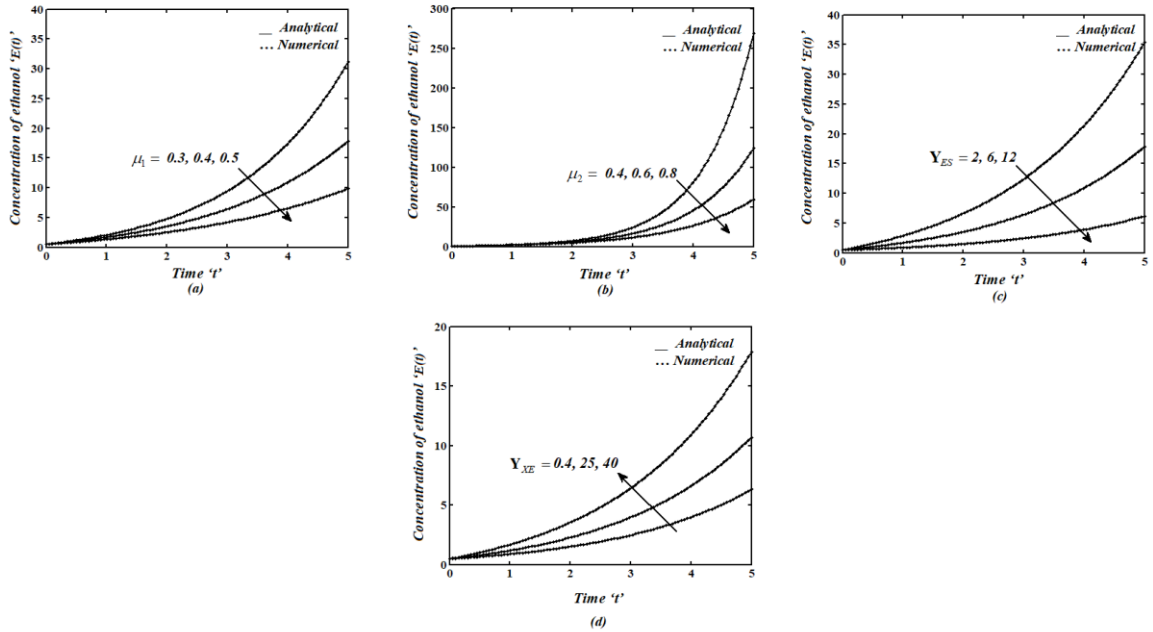

Figure 3. Comparison of analytical expression of the concentration profiles S(t) with simulation results for varies values of parameters, when $\mu_1 =$ 0.4, $\mu_2 =$ 0.04, YXS=5, YES = 6, YXE=0.5, X* =0.4, S* =1.4, and E* =0.48 .

3. Results and Discussion

In this study, this technique is used to solve the chemical kinetics problem. The governing equation which is a pair first order ordinary differential equations were solved analytically by using the new perturbation method (HPM) and Laplace transform. The approximate analytical solution of the concentration biomass, glucose and ethanol using the new perturbation method (HPM) and Laplace transform with those values obtained by the analytical method are given in Figs. 1–5.

The concentration profiles of biomass versus time are expressed in Figures 1(a) and 1(b). From these Figures, it is inferred that the value of the concentration of biomass decreases when the specific growth rate μ_2 increase. But the concentration of biomass increases when the specific growth rate constant μ_1 is increases. From Figure 2(a) – 2(c), it is inferred that the concentration of glucose is increases when yield coefficient glucose to biomass YXS is decreases. From Figure 2(c), it is observed the concentration of glucose increases when the specific growth rates μ_1 and μ_2 increases in Figures 3(a) and 3(b). From Figure 3(d), it is observed that an increase in the parameter yield coefficient ethanol to biomass YXE, the concentration of ethanol increases. From Figures 3(a) – 3(c), it is observed that the concentration of ethanol decreases when the parameters specific growth rates μ_1 , μ_2 and yield coefficient glucose to ethanol YES decreases.

4. Conclusion

In this paper, the new perturbation method and Laplace transform has been successfully applied to solve a system of ordinary differential equations which represent of one of a mathematical models of a chemical kinetics problem of the 2-D fluorescence spectra are used to predict the process variables biomass, glucose and ethanol. The new perturbation method and Laplace transform provides the solutions in the form of approximately with easily computed components. It is economical in terms of computer power/memory and does not involve tedious calculations without any restricted assumption and it is seeming that the new perturbation method and Laplace transform appears to be very accurate to employ with reliable results. The approximate analytical solution of the concentration biomass, glucose and ethanol compared with numerical results is presented.It has been achieved that from figures and table that the maximal error remainders decreased when the number of iterations are increased.

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