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Approximate Analytical Solution of Coincidences in Chemical Kinetics : Laplace Transform Method

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Abstract : In this article, Laplace transform method are adopted to study the problem of the chemical kinetics problem analytically. The basis of the mathematical model used to describe and simulate the analyzed process is a system of ordinary differential equations. As a result, is obtained a single algebraic equation in terms of the complex variable *s*. In order to study the dynamics of the system these equations should be reverted to the time domain by performing an inverse Laplace transform. New properties of intersections and coincidences of transient concentration curves were discovered and are presented analytically using the classical consecutive mechanism A$\rightarrow$ $B \rightarrow C$ as an example. The analytical solutions obtained allow a full description of the response curves for only one kinetic parameters.

Keywords : Kinetic dependence; coincidence; intersection; consecutive mechanism $A \rightarrow B \rightarrow C$; golden ratio; time of intersection; Laplace transform method.

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1. Introduction

Among the innumerable processes which take place in chemistry and chemical engineering, there are some whose features have as yet been woefully neglected. The goal of the present paper is to distinguish and describe one family of such features, i.e., intersection and coincidences of dependencies which exhibit an unexpected elegance, both physical-chemical and mathematical. Most of the results will be obtained analytically, computer calculations will be used only to solve certain transcendental equations and be mentioned as such [1].

The Laplace transform has been studied by many authors over the years due to the wide array of applications of the Laplace transform technique to different areas of science. There have now been many publications, for example the book written by Widder (1941) [2] about the Laplace transform and inversion formulas, the book written by Jaeger in 1961 [3] describes applied the Laplace transform with engineering applications. A nice review of this transform applied to Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs) is given in Poularikas [4]. There are also articles describing the use of the Laplace transform in chemical engineering, e.g. articles written by Kolev and Linden [5], Ahmed and Batin [6], Ahmed and Kalita [7], Membrez and others [7]. Kolev and Linden [5] used Laplace transform for the solution of partial equations describing the transient masstransfer in laminar flow systems and heat-transfer in single and multi-stream flow systems. The papers [6] and [7] describe the use of the Laplace transform for analysis the transient convection-radiation magnetohydrodynamic viscous flow in a porous medium and study hydromagnetic flow in chemical reactors. Membrez and others [8] used the Laplace transform technique of find the kinetic parameters for the adsorption of a protein on porous beads. A bibliography of a great many papers are available on the WEB.Recently, many analytical methods such as theVariational Iteration method [9], Adomain decomposition

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method [10], Taylor series method [11], Homotopy analysis method [12] and Homotopy perturbation method [13] are compared to these methods.

The MHD free convection of water at 4°C through a fluid flow bounded by a moving boundary layer was portrayed mathematically [14]. An analytical approximation to the solution of the problem of forced convection over a horizontal flat plate using a combination of the Homotopy perturbation method and Laplace transform is presented [15]. In this study, the analytical approximation of the chemical kinetics problem using a combination of the Laplace transform is presented. In this paper, application of Laplace transform technique for analysis of the problem of the chemical kinetics is presented. The actual investigation has three main aims. The determination of the Laplace transform makes easier solution finding and the analysis of the answer of the analytic system.

2. Mathematical Formulation: Consecutive reactions

Consecutive reactions are one of the best-known basic mechanisms in chemical kinetics. The simplest example of such sequential reactions is $A \rightarrow B \rightarrow C$. Many important chemical processes are described via this scheme of reactions. The simplest kinetic model is presented as follows:

$$\frac{dC_A}{dt} = -k_1\ C_A \tag{1}$$

$$\frac{dC_B}{dt} = k_1\ C_A - k_2\ C_B \tag{2}$$

$$\frac{dC_C}{dt} = k_2\ C_B \tag{3}$$

where C_A, C_B, C_C are the concentrations of the substances A, B, C respectively, and k_1 and k_2 ([1/s]) are the rate constants of the first and second reaction, respectively. Otherwise, when $k_1 = k_2$ the system has a different type of solution due to

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the coincidence of both exponential decays. By direct solution or using the Laplace transform method it is seen that

$$C_A(t) = C_{A,0}\ \exp(-k_1\ t) \tag{4}$$

$$C_B(t) = (C_{A,0}\ k_1\ t + C_{B,0})\ \exp(-k_1\ t) \tag{5}$$

$$C_C(t) = C_{A,0}\,(1-(1+k_1\,t)\exp(-k_1\ t)) + C_{B,0}(1-\exp(-k_1\ t)) \tag{6}$$

From here on we assume also $C_{A,0}$ = 0 and $C_{B,0}$ = 0. Such formulas can be found e.g. in (Eremin, 1976) [16] and (Bairamov, 2003) [17] p. 49, who presented this solution for $C_A(t)$, $C_B(t)$ and $C_C(t)$.

3. Result and discussion

The analysis that we presented significantly improves our ability to distinguish mechanisms; previously, we considered that observing a maximum of C_B is a sufficient indication to distinguish the consecutive mechanism $A \rightarrow B \rightarrow C$ from the parallel $A \rightarrow B$, $A \rightarrow C$. Now we are able based on our six possible scenarios, either to falsify the hypothesis of the $A \rightarrow B \rightarrow C$ consecutive mechanism or to justify it and infer some conditions on the ratio ρ of the rate constants.

Figure 1, represents the concentrations of substances $C_A(t)$, $C_B(t)$ and $C_C(t)$ using analytical solution for fixed values for $C_{A,0} = 1$ and $C_{B,0} = 1$. The rate constants of the reaction k_1 is fixed for all concentration of substances. As the systems considered grow more complex, the number of intersection and maximum points and of their orderings will grow rapidly: polynomially for the former, combinatorically for the latter. This increasing complexity can to some extent be matched by automatic methods, whether numerical and symbolic depending on what the theoretical setting will allow. Ultimately, we expect that

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unifying properties will emerge; indeed, we generally believe that the analysis of intersections and coincidences presents a source of vast information for new families of patterns for distinguishing mechanisms and parameter domains, and might even find applications outside the domain of chemical kinetics.

Figures 2 and 3, illustrates the effect of rate constants of the reaction k_1 on concentration profiles $C_A(t)$ and $C_B(t)$. It represents the concentration profile is decreasing with increasing values of reaction k_1 solution for fixed values for $C_{A,0}=1$ and $C_{B,0}=1$. Figure 4, shows the effect of first reaction k_1 on the concentration of the profile $C_C(t)$. From this figure, we observed that the concentration increases as the increasing value of a parameter k_1 for fixed values of $C_{A,0}=1$ and $C_{B,0}=1$.

We will analyse such models both for close systems and for open systems with mass exchange. An interesting opportunity of these are provided by thermos-desorption and thermos-gravimetric problems: in both cases, there is a sequence of linear processes and the kinetic model reflects this sequence and the change of other factor(s) as well. In the first case, the change of temperature in time; in the second, the loss of weight over time. The problem of intersection can be presented for exit flow dependencies for diffusion-reaction models (related to the Temporal Analysis of Products, TAP, data), etc. Special attention will be paid to the analysis of multi-step radioactive decay, where the coefficients are known very accurately.

4. Conclusions

This method is a powerful mathematical tool for solving any system of linear and nonlinear differential equations. Nonlinear differential equations have been done by the homotopy perturbation method, and the effect of several physical parameters attempting to control the velocity and temperature profiles is shown graphically and briefly discussed. As the

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magnetic parameter rises, we can see that the velocity profile reduces in the flow region. Thus, we conclude that we can control the velocity field by introducing a magnetic field, but the reversed phenomenon is noted by increasing the permeability parameter value. Therefore, this technique is a powerful mathematical tool to solve any scheme of linear and nonlinear differential equations.

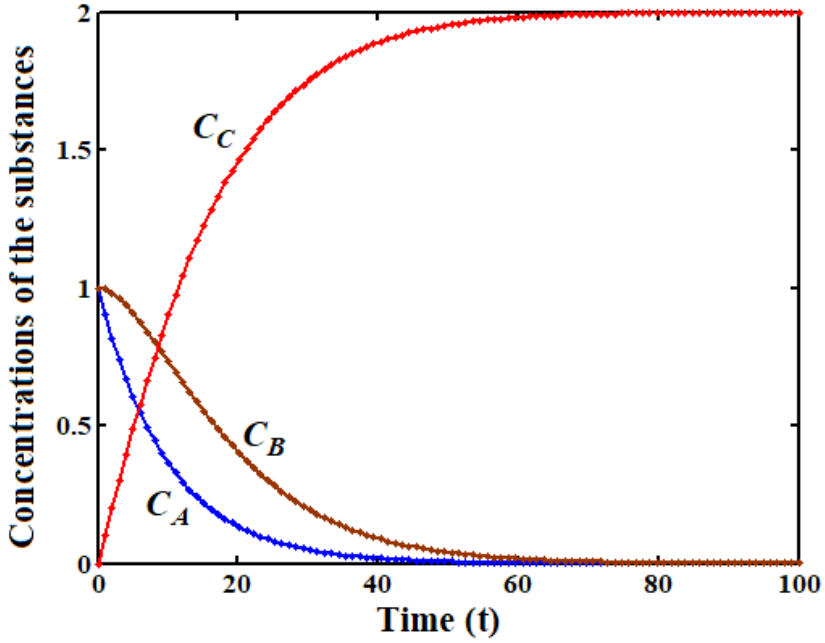

Fig.1. The concentrations of substances $C_A(t)$, $C_B(t)$ and $C_C(t)$ using analytical solution for fixed values for $C_{A,0}=1$ and $C_{B,0}=1$.

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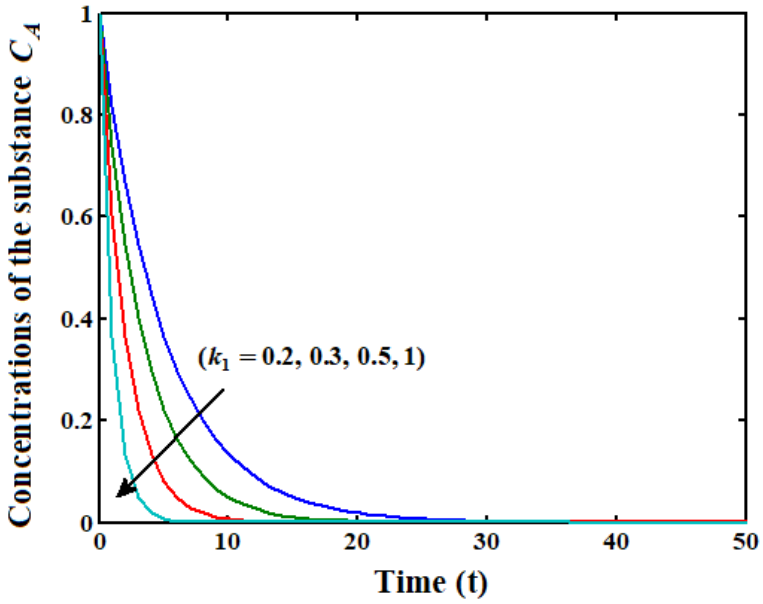

Fig.2. The concentrations of substance $C_A(t)$ using analytical solution for fixed values for $C_{A,0} = 1$ and $C_{B,0} = 1$.

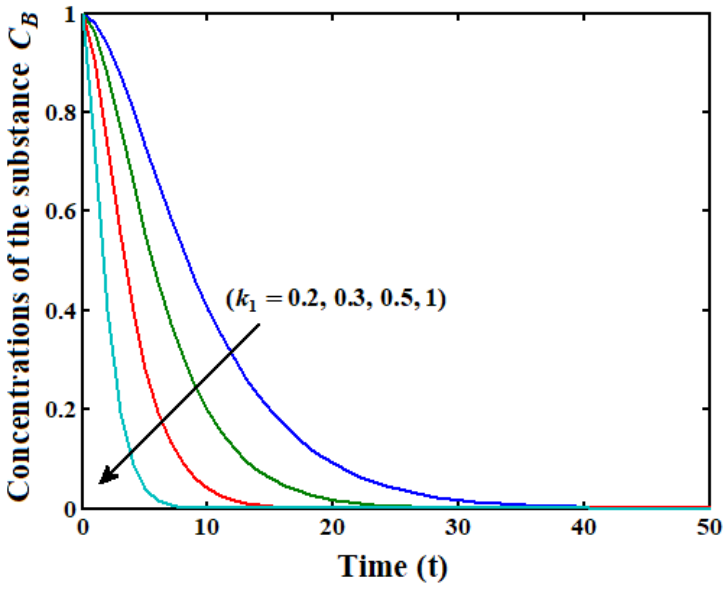

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Fig.3. The concentrations of substances $C_B(t)$ using analytical solution for fixed values for $C_{A,0}=1$ and $C_{B,0}=1$.

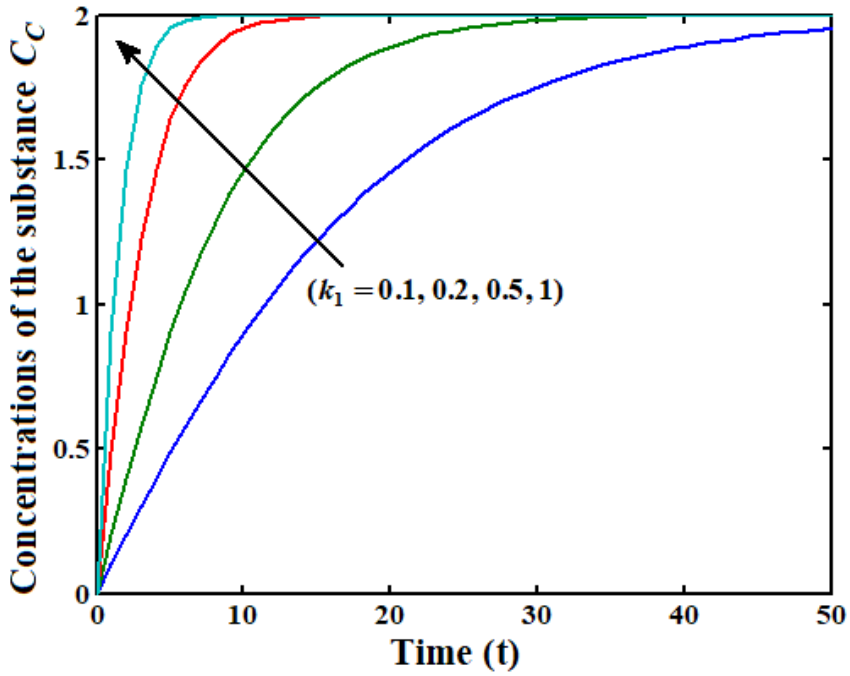

Fig.4. The concentrations of substances $C_C(t)$ using analytical solution for fixed values for $C_{A,0}=1$ and $C_{B,0}=1$.

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