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ANÁLISIS MEDIANTE SERIES DE POTENCIAS MODIFICADAS DE ECUACIONES DIFERENCIALES APLICADAS A LA CINÉTICA QUÍMICA

Analysis by modified power series of differential equations applied to chemical kinetics

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RESUMEN

Mediante ecuaciones diferenciales no lineales, se puede describir la cinética de reacciones químicas elementales homogéneas sucesivas que ocurren simultáneamente. Posteriormente, se presenta el modelo matemático que se deduce de la ley de acción de masas y se resuelve utilizando series de potencias modificadas para definir las funciones que rigen el fenómeno. Este artículo interpreta las oscilaciones resultantes de las ecuaciones diferenciales, denotando la interacción de las reacciones afectadas por sus estados anteriores. Las oscilaciones previas a la estabilización de la reacción pueden interpretarse como la velocidad de reacción, al hacerlo mediante series de potencias, se puede denotar que el comportamiento actual se ve afectado por el comportamiento anterior afectado por la monotonía de la función y el análisis de sus cambios en instantes anteriores. Este trabajo muestra una introducción a las ecuaciones diferenciales con retardo aplicadas a la observación de reacciones químicas, principalmente el aspecto del retardo en una reacción química que debe tenerse en cuenta en todos los casos de reacciones, para conocer cuáles son las consecuencias que se producen después de tener en cuenta los tiempos anteriores y sus respectivos casos de optimización.

Palabras claves: *ecuaciones diferenciales no lineales, química cinética, series de potencias modificadas.*

ABSTRACT

Using nonlinear differential equations, the kinetics of successive homogeneous elementary chemical reactions occurring simultaneously can be described. Subsequently, the mathematical model that is deduced from the law of mass action is presented and is solved using modified power series to define the functions that govern the phenomenon. This article interprets the oscillations resulting from differential equations, denoting the interaction of the reactions affected by their previous states. The oscillations before the stabilization of the reaction can be interpreted as the reaction rate. When doing so by power series, it can be denoted that the current behavior is affected by the previous behavior, affected by the monotony of the function, and the analysis of its changes in previous instants. This work shows an introduction to Differential Equations with delay applied to the observation of chemical reactions, mainly the aspect of delay in a chemical reaction that must be considered in all cases of reactions, to know the consequences that are carried out after taking into consideration previous times and their respective optimization cases.

Keywords: *nonlinear differential equations, kinetic chemistry, modified power series.*

I. INTRODUCTION

Many phenomena in nature are modeled by nonlinear systems, which are involved in fields such as physics, biology, chemistry, engineering, etc.(1) Chemical kinetics studies the speed of a chemical reaction, which is manifested in the change in concentration of the reactants or products with respect to time.(2)

In this article, we will pay attention to a nonlinear system that models different mechanisms, such as certain radioactive series, hydrolysis phenomena, and reactions involving potassium permanganate, oxalic sulfate, and manganous sulfate.(3)

The system represents reactions in series, since the product of the first reaction is the reagent of the consequent reaction. Through applied mathematical treatment and graphical analysis to express the model, it is intended to investigate the speed of the chemical phenomenon for its process control. The application of the modified power series method with arithmetic linear arrays is carried out, which allows us to deal with this type of complex nonlinear equations.(4,5)

In this research, we try to understand the oscillatory nature of the solutions of the models proposed for chemical reactions, thinking that these are due to the activation of energy and other factors that cause this behavior to exist until the reaction reaches equilibrium.

The analysis of differential equations in chemical systems has allowed for a better understanding of reaction processes, particularly in cases where delay plays a crucial role in the evolution of reactant and product concentrations. As noted in various sources.(6,7) The analytical solution of these equations using modified power series provides an efficient approximation to describe reaction dynamics in rigorous mathematical terms.

In the context of chemical reactions, modeling through non-standard differential equations allows for obtaining exact numerical solutions for delay equations, avoiding the cumulative errors that typically arise in conventional discretization methods.(2,8)

This methodology has been successfully applied to the description of chain reactions and systems with multiple intermediate species, as demonstrated by recent studies on advanced chemical kinetics.(9)

The oscillatory solutions observed in many chemical systems have been a subject of debate in the literature, particularly concerning their relationship with activation energy and cascade reaction mechanisms.(3,10) Based on the analysis of mathematical models involving differential equations, it has been determined that these behaviors emerge due to the competition between different reaction pathways, generating transient regimes with oscillations preceding the establishment of chemical equilibrium.(11)

The use of modified power series not only enables better prediction of these phenomena but also facilitates the formulation of optimization strategies in industrial processes where precise reaction rate control is essential.(12)

These techniques have been applied in chemical kinetics engineering, yielding promising results in terms of efficiency and operational cost reduction.(13)

Thus, the present study is framed within a well-established theoretical foundation for the mathematical modeling of complex chemical systems, supported by specialized literature and the development of innovative analytical tools for solving delay differential equations. The inclusion of these strategies in chemical sciences education and research will allow for a better understanding of kinetic phenomena and their impact on future industrial and experimental applications.

II. MATERIALS AND METHODS

In this sense, the photochemistry of thionitrites (RSNO) evidences a simultaneous chemical reaction where the photodissociation process via S-N bond cleavage yields RS· radicals,(14) which subsequently react to give a symmetric disulfide (RSSR) and nitrogen oxide.(15)

Figure 1 illustrates the general procedure of the reaction.

$$\begin{array}{ccccc} \text{R-SNO} & \longrightarrow & [2\ \text{R-S}\cdot] & \longrightarrow & \text{RS-SR} \\ (Y_1) & \longrightarrow & (Y_2) & \longrightarrow & (Y_3) \end{array}$$

Figure 1. *Photolysis of thionitrites.*

Considering the graphs observed and applied to Nitrosation, it is observed that in moments, stabilization is reached. It should be noted that chemically, the results observed in Figure 1 have a physical sense of the reaction when observed in the positive part of the *y*-axis. The reasons for the increase in the monotony of the function can be observed as an instant in which there is a majority of a reactant, and the existence of precipitation is observed in y_2.

III. RESULTS AND DISCUSSION

In this work, a nonlinear chemical system of ordinary differential equations of two consecutive chemical reactions whose mechanism is exemplified by certain radioactive series, hydrolysis, and reaction of potassium permanganate, oxalic sulfate, and manganous has been investigated.

By means of a power series, the formula has been solved Eq. (1. *a*), which, with initial conditions, has found its specific solution.

$$\frac{dy_1}{dt} = k_1 y_1 \qquad (1.\ a)$$

Through a mathematical artifice, an analytical solution for System:

$$\frac{dy_2}{dt} = y_2^2 - e^{-t} = 0 \qquad (1.\ b)$$

Where the system analysis is performed to understand the reaction, the mechanism is compared to the numerical solution obtained. And finally, to solve the formula (1. *c*). It has been cleared and (1. *c*) of the formula (2).

$$\frac{dy_3}{dt} = k_2 y_2^2 \qquad (1.\ c)$$

Considering that in the previous steps we found both y_1 and y_2:

$$y_1 + y_2 + y_3 = 0 \qquad (2)$$

From a mathematical standpoint, the well-posedness of the nonlinear system defined by equations (2.a)–(2.c), together with the conservation relation formula (2), can be established under standard regularity hypotheses on the reaction rate terms. In particular, the theoretical results developed in the doctoral thesis of Mayorga Arias guarantee the existence, uniqueness, and representability of solutions for nonlinear and delay-type differential systems via modified power series methods. This framework provides a rigorous mathematical foundation for the analytical procedure adopted in this work and supports the validity of the concentration profiles obtained.(16)

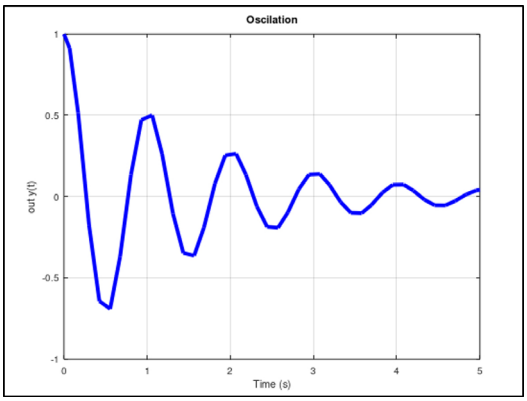

Figure 2. *Concentration profiles of reactants and products over time.*

Further analysis of the obtained data shows that the system exhibits oscillatory behavior in the concentration of reactants and products. This can be attributed to the presence of intermediate species that transiently accumulate before being fully converted into final products. Figure 2 presents a graphical representation of the concentration evolution over time, highlighting the oscillatory nature of the reaction kinetics. The numerical simulations confirm that small perturbations in the initial conditions can lead to significant variations in reaction times and final equilibrium states.(17)

The oscillatory behavior observed in Figure 2 is consistent with the qualitative properties derived from the analytical framework of delay and nonlinear differential equations. As established in the corresponding corollary of the theoretical results, solutions constructed via modified power series preserve the stability characteristics of the original system while allowing transient oscillations induced by nonlinear interaction terms. These oscillations are not numerical artifacts but arise naturally from the mathematical structure of the model, particularly from the coupling between intermediate species and the nonlinear reaction rates.(18,19)

The result will help in future research where it is required to know the concentration of the

reactant/product at any time *t*, (2.a), (2.b), and (2.c), which will have the following chemical system:

$$(Y_1) \longrightarrow (Y_2)$$
$$(Y_2) \longrightarrow (Y_3)$$

The modeling of a chain reaction not only helps us understand how and when the products of the reaction are generated, but it also allows us to modify this timing by understanding its behavior with certain catalysts and predicting the process's performance. (20) Being a chain reaction in the industrial application, the presence of the various products originating from the initial reagents is often needed in each of the different reactions. The graphs are useful for this type of situation because we can find the point at which the existence of the necessary products is observed at the same time without the need for the first product to be completely consumed, but to know the concentration graphs of the reactants and products with respect to time, the characteristic function of each reaction must be previously known, which is obtained by solving the differential equations explained in this paper.

IV. CONCLUSIONS

The oscillations shown are given thanks to the activation energies, reaching the activation energies to form the intermediates, and once formed, the next convexity is because it reaches another intermediary of better energy, to form the products, thus stabilizing the curve.(21)

Variations in temperature, pressure, and the active area of the catalyst, among others, can be factors that cause a delay in the chemical reaction. (22)

In radical reactions you need something to generate the radical; for example, in halogenation reactions two reactants are placed, and these two reactants can go a long time without reacting, but if they are affected by the delivery of energy, the reaction rate increases. This is because light causes the molecule to break and form radicals. This means that the bond is broken equally and each part of the molecule is left with an electron, generating new radicals.

Sometimes the reactants react with the walls of the vessels and change the monotony in the reaction. `

This mathematical model can be applied to various reactions to identify the factors of enthalpy and entropy, as well as to determine when these factors can begin to alter the behavior of concentration under the influence of a catalyst, as demonstrated in the application. (23)

We must then consider the concentration values that the model proposes to establish the influence of the activation energy of the chemical reaction, and to be able to explain the condensation plateau.(24)

Endothermic and exothermic processes must be considered, as well as the absorption or loss of energy until equilibrium is reached.(25)

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