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Numerical Approch of First Order Differential Equations Arising in The Modeling of Chemical Reactions

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ABSTRACT

Analytical chemical reactions are a very vigorous interdisciplinary field, in which concepts mathematical techniques and numbers are applied to a large diversity of phenomena in medicine and bioengineering. The theory of ordinary differential equations is a fundamental field of mathematics with many applications in chemistry, biology, medicine and bioengineering. Many chemical reactions can be described quantitatively by ordinary differential equations. In this article we have presented some applications of ordinary differential equations in analytical chemistry. An extremely functional principle used in modeling chemical reactions has proven to be the principle of mass conservation. All the models presented are solved analytically, using different integration techniques specific to ordinary differential equations. By proper interpretation, the models presented to have a broad range of applications in chemistry.

Keywords: Models , Mathematical models, Chemical reactions, Ordinary differential equations

I. INTRODUCTION

Although the development of chemistry has been essentially influenced by the development of mathematics, in recent decades the importance of completing the descriptive study of some chemical phenomena or mechanisms with aspects related to the processing and interpretation of the obtained data is recognized , The most advanced form of the use of mathematics in chemistry is mathematical chemistry, It aims at the mathematical modeling of chemical processes and the study of models using methods specific to mathematics, The possibility of the abstract is the essential advantage of mathematical modeling in the case of chemical reactions, A mathematical model is a device that helps the chemist predict or explain the behavior of a chemical reaction, chemical experiment, or event, A mathematical model is a simplification of a complex real-world problem in the form of mathematical equations , To write a mathematical model, the following steps are followed: • The problem is identified; • The working hypotheses, the variables, as well as the relations between the variables and the model are formulated; • Resolves the model; • Check the model (testing with real data) , Many of the fundamental laws of chemistry can be formulated in terms of differential equations, In contemporary mathematical language, this means, "It is useful to solve differential equations".

In chemical reaction engineering, simulations are useful for investigating and optimizing a particular reaction process or system. Modeling chemical reactions helps engineers virtually understand the chemistry, optimal size and design of the system, and how it interacts with other physics that may come into play. This is the first of a series of blog posts on chemical reaction engineering, and here we will have a look at the initial stages of modeling the application: the chemical reaction kinetics.

Creating models of chemical reactions is super important to help students understand how things change and how atoms balance. In this activity, students will create a grid that illustrates four chemical reactions. They should be sure to include the reactants, products, and the equation in their finished product. To extend this activity, ask students to add a cell that explains what type of reaction it is (exothermic vs endothermic) and what happens during the process.

The models represented by differential equations presented in this article offer some significant advantages compared to other models proposed in chemistry, namely: they can model evolutionary processes, allow a compartmental analysis of the modeled process, allow determining the stability of equilibrium configurations, allow sensitivity analysis ¸ in relation to the reaction parameters, From a mathematical point of view, the theory of differential equations is well developed both qualitatively and numerically, As a disadvantage, they cannot model phenomena with a high degree of heterogeneity, These models can be used successfully in developing inverse methods for determining one or more reaction parameters involved in the model, The accuracy of the predictions of these models is strongly influenced by the internal kinetics, by the spatial-temporal scale of evaluation of the reaction parameters, by the control of the error of solving the mathematical model, An extremely useful principle used in modeling chemical reactions has proven to be the principle of mass conservation,

Many processes and phenomena in chemistry, and generally in sciences, can be described by first-order differential equations. These equations are the most important and most repeatedly used to illustrate natural laws. Even though the math is the same in all cases, the student may not always easily understand the similarities because the relevant equations appear in different topics and contain different quantities and units. This text was written to present a unified view on various examples; all of them can be mathematically described by first-order differential equations. The following example is discussed like modeling chemical reactions.

Example

During a chemical reaction, substance A is converted into substance B at a rate that is proportional to the square of the amount of A. When 60 grams of A are present, and after 1 hour only 10 grams of A remain unconverted. How much of A is present after 2 hours?

Solution:

Let *y* be the unconverted amount of substance A at any time *t*.
From the given assumption about the conversion rate, we can write the differential equation as follows.

$$\frac{dy}{dt} = ky^2 \qquad (1)$$

Where $\frac{dy}{dt}$ is Rate of change of y

k is proportional constant

using separable method, integrating (1), we get

$\int \frac{dy}{y^2} = \int kdt + C$, C be a integrating constant

Therefore $y(t) = \frac{-1}{kt+C}$ (2)

When t = 0 , y= 60

Equation (2) implies that C = $\frac{-1}{60}$

When t = 1 , y = 10

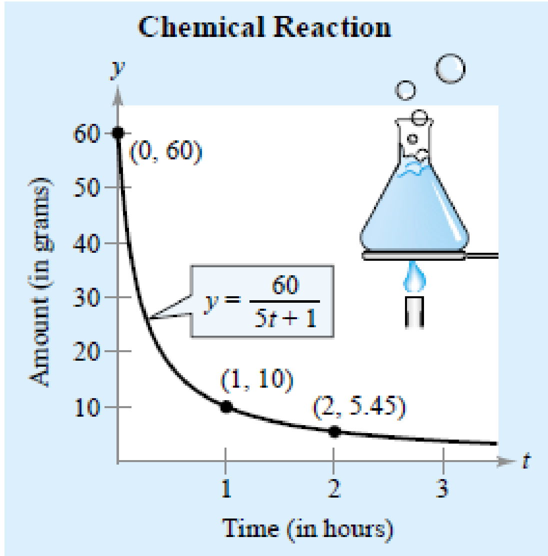
Equation (2) implies that k= $\frac{-1}{12}$

Now equation (1) implies that $y(t) = \frac{-1}{\frac{-t}{12}-\frac{1}{60}}$

Using the model, we can can determine that the unconverted amount of substance A after 2 hours

when t = 2 hours

$$y(t) = 5.45 \text{ grams (approximately)}$$



In above Figure we note that the chemical conversion is occurring rapidly during the first hour. Then, as more and more of substance A is converted, the conversion rate slows down.

The next example describes growth model called a Gompertz growth model. This model assumes that the rate of change of *y* is proportional to *y* and the natural log of $\frac{L}{y}$ where *L* is the population limit.

II. MODELING POPULATION GROWTH

A population of 20 wolves has been introduced into a national park. The forest service estimates that the maximum population the park can sustain is 200 wolves. After 3 years, the population is estimated to be 40 wolves. If the population follows a Gompertz growth model, how many wolves will there be 10 years after their introduction?
Solution: Let *y* be the number of wolves at any time *t*.
From the given assumption about the rate of growth of the population, we can write the differential equation as follows.

$$\frac{dy}{dt} = ky\ ln\frac{200}{y} \qquad (3)$$

Where $\frac{dy}{dt}$ is Rate of change of y
k is proportional constant
Using variable separable method, Integrating (3) we get

$$y(t) = 200e^{-Ce^{-kt}} \qquad (4)$$

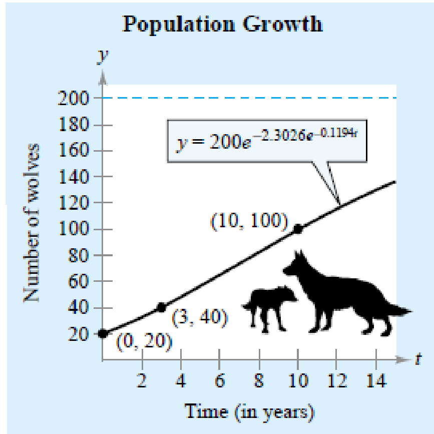
When t = 0 , y = 20
Equation (4) implies that C = $-ln\left(\frac{1}{10}\right) = ln(10) \approx 2.3026$
When t = 3 , y = 40
Equation (4) implies that k ≈ 0.1194
Therefore equation (4) implies that

$$y(t) = 200e^{-2.3026e^{-0.1194t}} \qquad (5)$$

Using this model ,we can estimate the wolf population after 10 years

$$y(t) = 200e^{-2.3026e^{-0.1194X10}}$$

$$\approx 100 \ wolves$$



From the above figure, we note that after 10 years the population has reached about half of the estimated maximum population

CONCLUSION

In this paper, we discussed the importance of first order differential equations in many areas such as physics, chemistry and engineering. It should be mentioned that there are many other processes in science, which are based on first-order differential equations like modeling chemical reactions.

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