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Ordinary Differential Equations with Applications in Chemical Reactions

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Abstract

Analytical chemical reactions are a very active interdisciplinary field, in which concepts, mathematical techniques and numbers are applied to a wide variety 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 useful 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 prove to have a wide range of applications in chemistry.

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

1. 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 recognized¹. 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. Statistical research (which does not study the article) can sometimes be used to construct and validate mathematical models².

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 equations³.

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)⁴,

Many of the fundamental laws of chemistry can be formulated in terms of differential equations. In chemistry, biology, medicine, bioengineering, differential equations are used to model the behavior of complex systems. The differential equations represented the fundamental discovery of Newton, who considered it necessary to keep secrets and to be published only in the form of an anagram "Data aequatione quotcunque fluentes quantitates involente fluctuacione invenire et vice-versa". In contemporary mathematical language, this means, "It is useful to solve differential equations"⁵. It is often desirable to describe the

behavior of a real-life system or phenomenon in mathematical terms, In solving differential equations (especially in the case of those with separable variables) we often have a solution that involves logarithms, A constant C will result from the indeterminate integration ⁶, In a mathematical model of a chemical reaction, variable time will often occur, Solving problems with the help of mathematical modeling can be done according to the following scheme ⁷,

2. Materials and methods

Differential equations belong to a wide class of equations in which the unknown is a function, They are called functional equations, Differential equations can be recognized because they contain derivatives of the unknown function, If the unknown function depends on a variable, the equation is called ordinary, The maximum order of the derivative that intervenes in the differential equation is called the *order of the equation* ⁸ The general form of a first order equation can be defined as:

$$f(t, x(t), \frac{dx}{dt}) = 0 \tag{1}$$

where, $f : D \rightarrow R, D \subset R^3$ is an unknown function, and is the solution of the differential equation, In this article we will deal with the *normal form* of a differential equation:

$$\frac{dx}{dt} = f(t, x(t)) \tag{2}$$

where: $f : D \rightarrow R, D \subset R^2$

It is called a solution of equation (2), a function $x = x(t) : D \rightarrow R$, where is a range of real numbers that satisfies the conditions ⁹ :

$$\{(t, x(t)) \in D, t \in I\} \tag{3}$$

3. Results & Discussion

The notion of solving a differential equation is equivalent to the notion of integrating this equation into the indicated domain of definition, From a geometric point of view, a solution represents an integral curve in the plane (xOt), If the solutions of some differential equations can be given with the help of formulas in which integrals of some known functions intervene, we will say that the equation is solvable by squaring ⁹,

We will consider the *chemical reaction*: $aA + bB \rightarrow cC$, where A, B are the reactants, is the product, and a, b, c they are called stoichiometric coefficients ¹⁰, The reaction rate is defined as follows:

$$r = -\frac{1}{a} \frac{d(A)}{dt} = -\frac{1}{b} \frac{d(B)}{dt} = -\frac{1}{c} \frac{d(C)}{dt} \tag{4}$$

where $(A), (B), (C)$ are the concentrations of the three substances,

We consider an irreversible reaction process in

which reactants A and B produce compound C : $A+B \xrightarrow{k} C$, where, k is the reaction constant, Whether $x = [A], y = [B], z = [C]$ concentrations of reactants A, B and C ¹¹,

Then the *differential equation* that models this process is:

$$\frac{dz}{dt} = kxy \tag{5}$$

For a *biochemical reaction* of the form: $A+B \xrightarrow{k} C+D$, the differential equation that models this reaction is:

$$-\frac{dx}{dt} = \alpha x(t)y(t) \tag{6}$$

where $x(t), y(t)$ represents the number of gram molecules present in A and respectively B , is a constant that depends on the type of reaction ¹²,

If we consider the *reaction irreversible*: $A \xrightarrow{k} B$ then we get:

$$\frac{dx}{dt} = \frac{dy}{dt} = -\kappa x \tag{7}$$

where x is the amount of substance (mol / liter) in A , y is the amount of substance (mol / liter) in B , and κ is the reaction rate constant, Any metabolic processes can be described by such reactions, For a *biochemical reaction* of the form: $2A+B \xrightarrow{k} C$, the differential equation that models this reaction is ¹³,

$$\frac{1}{2} \frac{dx}{dt} = -\frac{dy}{dt} = \kappa x^2 y \tag{8}$$

If we consider the *reaction* : $\begin{cases} A \xrightarrow{\kappa_1} B \\ B \xrightarrow{\kappa_2} A \end{cases}$ then we get:

$$\begin{cases} \frac{dx}{dt} = -\kappa_1 x + \kappa_2 y \\ \frac{dy}{dt} = \kappa_1 x + \kappa_2 y \end{cases} \tag{9}$$

where x is the amount of substance (mol / liter) in A , y is the amount of substance (mol / liter) in B , and κ_1, κ_2 are the reaction rate constants ¹⁴,

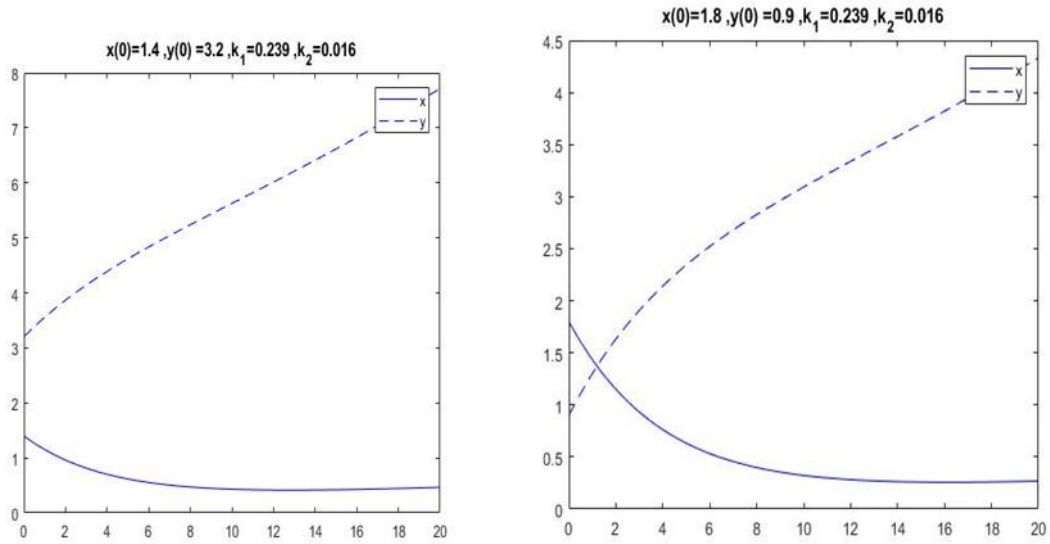


Fig. 1: Numerical simulation of the solution of the differential equation (9) for: $x(0) < y(0)$ and $x(0) > y(0)$

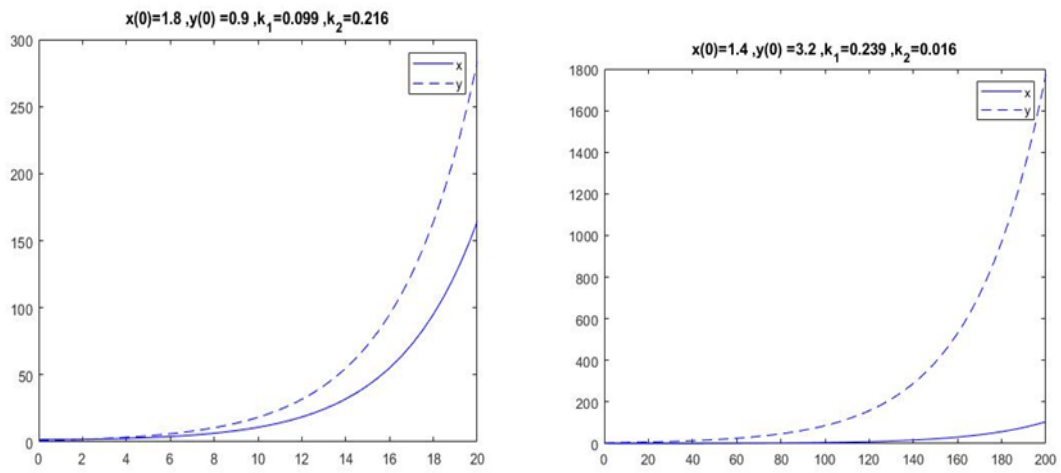


Fig. 2: Numerical simulations of the solution of the differential equation (9) for: $k_1 < k_2$ and $k_1 > k_2$

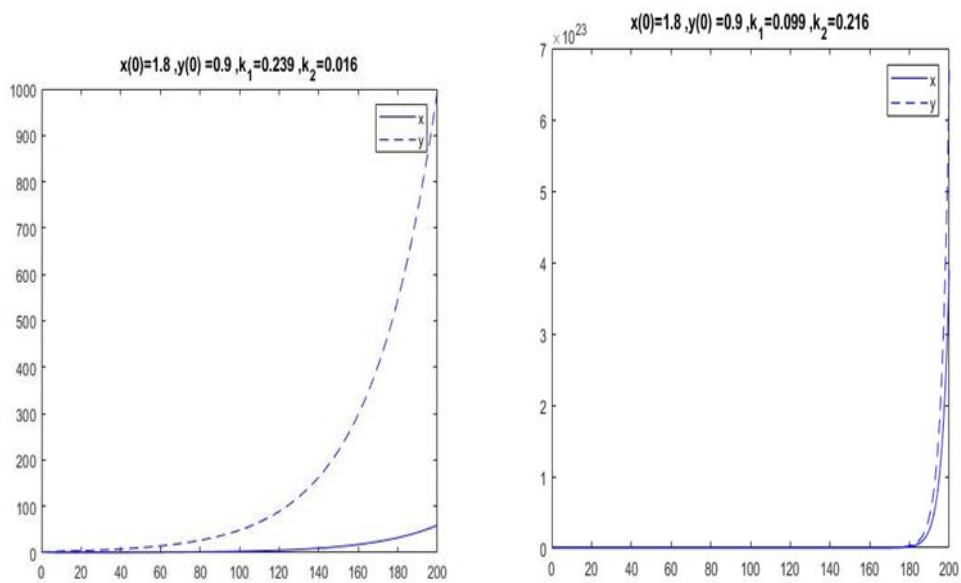


Fig. 3: Numerical simulation of the solution of the differential equation (9) for: $t_{\max} = 200$

For the reaction: $H_2 + O_2 \xrightarrow{\alpha} 2HO$, we will find the differential equation :

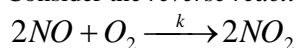
$$\frac{d(HO)}{dt} = 2\alpha(H_2)(O_2) \tag{10}$$

where α represents the reaction rate constant,

The main oxides of nitrogen are nitrogen monoxide (NO) and nitrogen dioxide (NO₂), and together they are called NO noxious substances, In terms of health effects, NO is considered harmless, at least at the concentrations that usually exist in the street, NO₂, on the other hand, can have the worst effects, Only a small fraction of the gases emitted

$$\left\{ \begin{aligned} x' &= -\alpha x^2(t) \rightarrow \frac{1}{x^2(t)} dx = -\alpha dt \rightarrow \int \frac{1}{x^2} dx = -\alpha \int dt \rightarrow \frac{1}{x} = -\alpha t + C \rightarrow x(t) = \frac{1}{\alpha t + C} \\ \int \frac{1}{x^2} dx &= -\frac{1}{x} + C_1 \end{aligned} \right.$$

Consider the reverse reaction:



We will note through x the initial amount of propane (NO_2), through y_0 the initial amount of (NO)

$$\left\{ \begin{aligned} \frac{dx}{dt} &= k(y_0 - x)^2(z_0 - \frac{x}{2}) \rightarrow \frac{dx}{(y_0 - x)^2(2z_0 - x)} = \frac{k}{2} dt \rightarrow \int \frac{dx}{(y_0 - x)^2(2z_0 - x)} = \frac{k}{2} \int dt \\ \int \frac{dx}{(y_0 - x)^2(2z_0 - x)} &= \int (\frac{A}{y_0 - x} + \frac{B}{(y_0 - x)^2} + \frac{C}{2z_0 - x}) dx = -A \ln|y_0 - x| + \frac{B}{y_0 - x} - C \ln|2z_0 - x| + C_1 \\ A &= -\frac{1}{(2z_0 - y_0)^2}, B = \frac{1}{2z_0 - y_0}, C = \frac{1}{(2z_0 - y_0)^2} \\ \frac{1}{(2z_0 - y_0)^2} \ln|2z_0 - x| &+ \frac{1}{(y_0 - x)(2z_0 - y_0)} = \frac{k}{2} t + C_2 \end{aligned} \right.$$

Tert-butyl chloride (C_4H_9Cl) is a colorless organic compound in liquid form at room temperature, It is slightly soluble in water, The compound is flammable and volatile, and its main use is in nucleophilic substitution reactions, to produce different substances, ranging from alcohols to

$$\left\{ \begin{aligned} x' &= -\delta x(t) \rightarrow \frac{1}{x(t)} dx = -\delta dt \rightarrow \int \frac{1}{x} dx = -\delta \int dt \rightarrow \ln|x| = -\delta t + C \\ \int \frac{1}{x} dx &= \ln|x| + C_1, \delta = 0,1223 / \text{sec} \\ x(0) = x_0 &\rightarrow C = x_0 \rightarrow x(t) = x_0 e^{-\delta t} \end{aligned} \right.$$

(13)

by the engines is NO_2 , the main quantity being NO, Present NO_2 in ambient air is mainly due to subsequent oxidation of NO¹⁵, We will consider the breakdown of nitrogen dioxide: $2NO_2 \rightarrow 2NO + O_2$

Because this reaction requires two molecules of NO_2 , the rate at which the reaction takes place is proportional to the square of the concentration of NO_2 where $x(t)$ is the concentration of nitrogen dioxide at time t ,

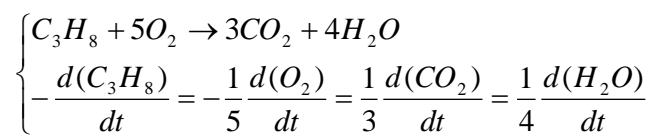
(11)

and through z_0 the amount of oxygen, The differential equation that models this phenomenon is form¹⁶,

(12)

salts, During a certain chemical reaction, the concentration $x(t)$ de C_4H_9Cl obeys the equation¹⁷,

A grate gas works using the chemical reaction:



(14)

We will mark by the initial amount of propane (C_3H_8), through b the amount of oxygen and through x the

amount of grill gas, The differential equation that models this phenomenon is form:

$$\begin{cases}
 \frac{dx}{dt} = \alpha(a-x)(b-x)^5 \rightarrow \frac{dx}{(a-x)(b-x)^5} = \alpha dt \rightarrow \int \frac{dx}{(a-x)(b-x)^5} = \alpha \int dt = \alpha t + C_6 \\
 \int \frac{dx}{(a-x)(b-x)^5} = \int \left(\frac{A}{a-x} + \frac{B}{(b-x)} + \frac{C}{(b-x)^2} + \frac{D}{(b-x)^3} + \frac{E}{(b-x)^4} + \frac{F}{(b-x)^5} \right) dx \\
 \int \frac{1}{a-x} dx = -\ln|a-x| + C_1, \int \frac{1}{(b-x)^2} dx = \frac{1}{b-x} + C_2, \int \frac{1}{(b-x)^3} dx = \frac{1}{2} \frac{1}{(b-x)^2} + C_3 \\
 \int \frac{1}{(b-x)^4} dx = \frac{1}{3} \frac{1}{(b-x)^3} + C_4, \int \frac{1}{(b-x)^5} dx = \frac{1}{4} \frac{1}{(b-x)^4} + C_5 \\
 A \ln|a-x| + B \ln|b-x| - \frac{C}{b-x} - \frac{D}{2(b-x)^2} - \frac{E}{3(b-x)^3} - \frac{F}{4(b-x)^4} = -\alpha t - C_6
 \end{cases}
 \tag{15}$$

Constants A, B, C, D, E, F is determined by the method of indeterminate coefficients,

Hydrobromic acid is a strong inorganic acid, The salts of hydrobromic acid are called bromides, The chemical formula of hydrobromic acid is HBr , Under normal conditions of temperature and pressure, hydrobromic acid is a colorless gas that smokes in the air, being very greedy for water¹⁸,

$$\begin{cases}
 H_2 + Br_2 \rightarrow 2HBr \\
 \frac{d(HBr)}{dt} = \alpha H_2 Br_2^{\frac{1}{2}}
 \end{cases}
 \tag{16}$$

We will note through a the initial amount of hydrogen (H_2) through b cantity of Br_2 and through x the amount of grill gas, The differential equation that models this phenomenon is form:

$$\begin{cases}
 \frac{dx}{dt} = \alpha(a-x)\sqrt{b-x} \rightarrow \frac{dx}{(a-x)\sqrt{b-x}} = \alpha dt \rightarrow \int \frac{dx}{(a-x)\sqrt{b-x}} = \alpha \int dt \\
 -\frac{2}{\sqrt{a-b}} \operatorname{arctg} \sqrt{\frac{b-x}{a-b}} = \alpha t + C \rightarrow \operatorname{arctg} \sqrt{\frac{b-x}{a-b}} = -\frac{\alpha(a-b)}{2} + C_2 \\
 \sqrt{\frac{b-x}{a-b}} = \operatorname{tg} \left(C_2 - \frac{\alpha a - \alpha b}{2} \right) \rightarrow x(t) = b - (a-b) \operatorname{tg}^2 \left(C_2 - \frac{\alpha a - \alpha b}{2} \right) \\
 \int \frac{dx}{(a-x)\sqrt{b-x}} = \begin{cases} \sqrt{b-x} = t \rightarrow b-x = t^2 \rightarrow x = b - t^2 \rightarrow dx = -2tdt \\ -2 \int \frac{dt}{(a-b+t^2)} = -\frac{2}{\sqrt{a-b}} \operatorname{arctg} \sqrt{\frac{b-x}{a-b}} + C_1 \end{cases}
 \end{cases}
 \tag{17}$$

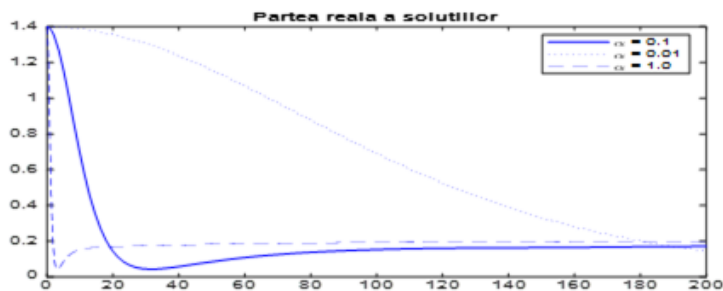


Fig. 4: The real part of the solution of differential equations (17) for different values of the parameter α

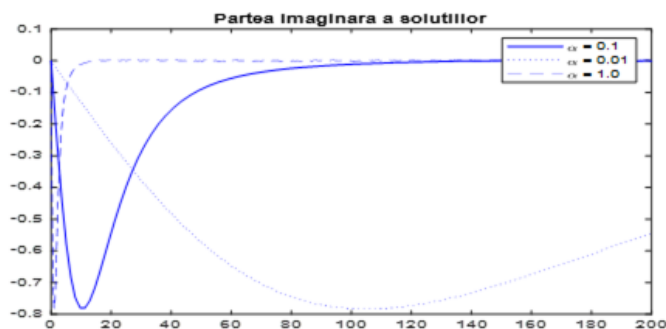
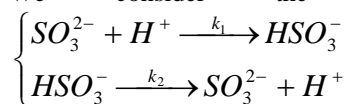


Fig. 5: The imaginary part of the solution of differential equations (17) for different values of the parameter α

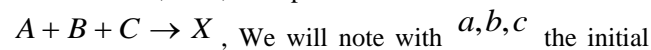
We consider the reaction reversible:



We will note through x the initial amount of hydrogen (

$$\begin{cases} \frac{dz}{dt} = k_1(x_0 - z)y - k_2(z_0 + z) \rightarrow \frac{dz}{k_1(x_0 - z)y - k_2(z_0 + z)} = dt \\ z(t) = [e^{(-k_1y - k_2)(t+C)} - (k_1x_0y - k_2z_0)] \frac{1}{(-k_1y - k_2)} \\ \int \frac{dz}{z(-k_1y - k_2) + (k_1x_0y - k_2z_0)} = \int dt \rightarrow \frac{1}{-k_1y - k_2} \ln|z(-k_1y - k_2) + (k_1x_0y - k_2z_0)| = t + C \end{cases} \tag{18}$$

Let be an irreversible reaction process in which the reactants A, B, C produce the substance X :



We will note with a, b, c the initial

$$\begin{cases} \frac{dx}{dt} = k(a-x)(b-x)(c-x) \rightarrow \frac{dx}{(a-x)(b-x)(c-x)} = kdt \rightarrow \int \frac{dx}{(a-x)(b-x)(c-x)} = k \int dt \\ \int \frac{dx}{(a-x)(b-x)(c-x)} = \int \left(\frac{A}{a-x} + \frac{B}{b-x} + \frac{C}{c-x} \right) dx = -A \ln|a-x| - B \ln|b-x| - C \ln|c-x| + C_1 \\ |(a-x)|^A |(b-x)|^B |(c-x)|^C = -kt + C_2 \\ \begin{cases} A+B+C=0 \\ A(-b-c) + B(-a-c) + C(-a-b) = 0 \rightarrow A = \frac{1}{(a-b)(a-c)}, B = \frac{1}{(b-a)(b-c)}, C = \frac{1}{(a-c)(b-c)} \\ A+B+C=1 \end{cases} \\ |(a-x)|^{\frac{1}{(a-b)(a-c)}} |(b-x)|^{\frac{1}{(b-a)(b-c)}} |(c-x)|^{\frac{1}{(a-c)(b-c)}} = -kt + C_2 \\ x(0) = 0 \rightarrow C_2 = a^{\frac{1}{(a-b)(a-c)}} b^{\frac{1}{(b-a)(b-c)}} c^{\frac{1}{(a-c)(b-c)}} \end{cases} \tag{19}$$

SO_3^{2-}) through y cantity of H^+ and through z cantity of (HSO_3^-) , The differential equation that models this phenomenon is form ¹⁹,

concentrations of the three substances, The mathematical model is of the form ²⁰,

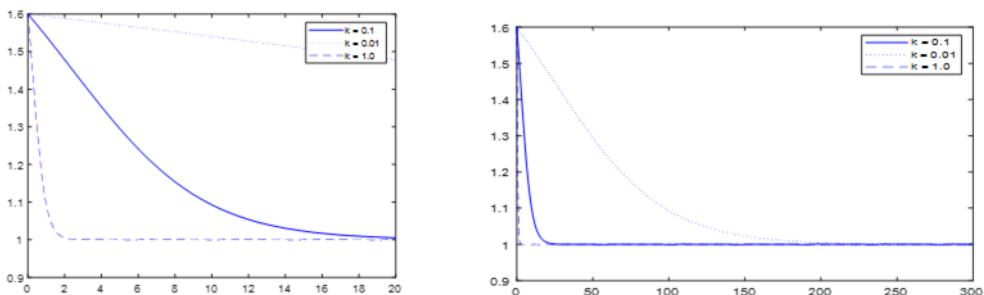


Figure 6, Numerical simulation of the solution of the differential equation (19) for: $t_{max} = 20$ and $t_{max} = 200$

If we consider the general reaction: $mA + nB \rightarrow A_m B_n$ we get:

$$\frac{da}{dt} = -ka^m b^n \tag{20}$$

Where the initial concentration b_0 of the substance B far exceeds the initial concentration of the substance A , then the concentration of the substance B will be relatively constant during the reaction, and the reaction will be an order reaction m ²¹,

$$\frac{dx}{dt} = -k_1 x^m \rightarrow \frac{dx}{x^m} = -k_1 dt \rightarrow \int \frac{dx}{x^m} = -k_1 \int dt \rightarrow \frac{1}{1-m} x^{1-m} = -k_1 t + C \rightarrow x(t) = \sqrt[1-m]{(1-m)(-k_1 t + C)} \tag{21}$$

Radium is a radioactive chemical element that has the symbol Ra and atomic number 88, Its appearance is almost pure white, but it is light, it oxidizes on exposure to air, Radium is an alkaline earth metal found in uranium ores, It is extremely radioactive, its most stable isotope, Ra^{226} , it

has a half-life of 1602 years and disintegrates ²², Whether $x(t)$ cantity of Ra^{226} (grams) left at the moment t , then:

$$\begin{cases} x' = -0,0004332x(t) \rightarrow \frac{1}{x(t)} dx = -0,0004332dt \rightarrow \int \frac{1}{x} dx = -0,0004332 \int dt \\ \int \frac{1}{x} dx = \ln|x| + C_1 \\ x(0) = x_0 \rightarrow C = x_0 \rightarrow x(t) = x_0 e^{-0,0004332t} \end{cases} \quad (22)$$

To place these discoveries in time, paleontologists use several fossil dating techniques, The best known of these is radiocarbon dating, using *carbon-14*, an unstable carbon isotope formed by cosmic ray collisions with nitrogen atoms in the upper atmosphere, An accurate measurement of the carbon-14 ratio can then be transformed into an estimate of the death time ²³, *Carbon-14* is suitable for this type of estimation because the decay rate is very slow, Then, the rate of decay of the

radioactive material is directly proportional to the amount of radioactive material, Suppose there is a certain amount of radioactive material defined by the variable x , where $x(t)$ is the amount of radioactive material at time t, The probability that each atom will disintegrate in a short period of time (Δt) it is independent of what other molecules do :

$$\begin{cases} x' = ax(t) \rightarrow \frac{1}{x(t)} dx = a dt \rightarrow \int \frac{1}{x} dx = a \int dt \rightarrow x(t) = C_1 e^{at} \rightarrow x(t) = x_0 e^{a(t-t_0)} \\ \int \frac{1}{x} dx = \ln|x| + C \\ x(t_0) = x_0 \rightarrow C_1 = x_0 e^{-at_0} \end{cases} \quad (23)$$

where $x(t)$ is the amount of radioactive material at a time, We are interested in *finding the half-life* for this isotope (the time interval in which half of the organic material disintegrates),

$$\begin{cases} x(t) = \frac{x_0}{2} \rightarrow \frac{x_0}{2} = x_0 e^{-at} \rightarrow e^{at} = 2 \end{cases} \quad (24)$$

For Carbon-14, the half-life is $t = 5715$ years, For $t = 5715$ years, we get: $a = -0,0001213$,

*Plutonium*²¹⁰ is an isotope of plutonium, The number of atoms of *plutonium*²¹⁰ stay after t days, with an initial value of radioactive atoms x_0 , is given by:

Plutonium is the chemical element in the actinide series with atomic number 94 in the periodic table of elements,

$$\begin{cases} t = \frac{\ln 2}{a} = \frac{0.693}{4,95 * 10^{-3}} = 140 \text{days} \end{cases} \quad (25)$$

In 1986, a reactor at the *Chernobyl* nuclear power plant exploded and spread radioactive materials over Europe, This disaster is considered to be the worst accident in the history of nuclear energy, It was estimated that half the amount of cesium (Cs^{137}) and iodine (I^{131}) and 5% of

the remaining radioactive elements present in the reactor were released into the atmosphere ²⁴, The two radioactive elements were iodine-131 (I^{131}) whose half-life is 8 days and cesium-137 (Cs^{137}) whose half-life is 30 years,

- For I^{131} we will get:
$$\begin{cases} t = \frac{\ln 2}{a} = \frac{0.693}{8} = 0,0866 \\ x_I(t) = x_0 e^{-0,0866t} \end{cases} \quad (26)$$

- For Cs^{137} we will get:
$$\begin{cases} t = \frac{\ln 2}{a} = \frac{0.693}{30} = 0,023 \\ x_{Cs}(t) = x_0 e^{-0,023t} \end{cases} \quad (27)$$

Uranium is a chemical element, a metal, from the actinide series of the periodic table of elements, *Uranium*²³⁷ is an

isotope of uranium ²⁵, The number of atoms of *Uranium*²³⁷ left after t days, with an initial value of radioactive

atoms x_0 , is given by:

$$\begin{cases} t = \frac{\ln 2}{a} = \frac{0.693}{6,8} = 0,1022 \\ x_{U^{237}}(t) = x_0 e^{6,8t} \end{cases} \quad (28)$$

4, Conclusions

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,

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