

Chemical reaction and diffusion dynamics

M.M.Stevanovic-Huffman and J. B.Savkovic-Stevanovic

Abstract- In this paper diffusion with chemical reaction was investigated. The concomitant advances in theory, measuring systems and computer simulation bring the new perspectives to the chemical reaction with diffusion studying. The chemical rate and diffusion rate parameters were considered. The obtained results shows effects the chemical reaction rate and diffusion rate. The obtained results demonstrate characterization of the dynamic and steady state conditions, transition between them and how it can be used to predict the stability of the system.

Keywords—: Chemical reaction rate, diffusion rate, reaction constants, diffusion coefficient, mutual effect.

I. INTRODUCTION

DIFFUSIONAL substance transfer rate has been investigated by many authors [1]-[4]. In the recent years, the subject of simultaneous diffusion and chemical reaction has received considerable attention from chemists and chemical engineers.

The dynamic, structure and function of the chemical reactions were studied in numerous literature. Synthetic analogous of naturally occurring esters find application in food industry, cosmetics, and pharmaceutical industry. There are many catalysts which catalyzed the synthesis of either aromatic and aliphatic esters[5]-[11]. Some kinetic models of the alkyl esters formation was derived and energy activation and frequency factor were determined [5],[6]. The specific chemical rate constant was determined and analysis of the product dynamic was performed in the previous paper. In addition to synthesis, these include “salvage” pathways for reesterification released by degradation of esters. The synthetic alkyl esters production with apple, pineapple and lemon aromas were examined in the paper [6]. Chemical rate theory was studied in the previous paper [14].

In cases where lack accurate information about a system or a system is complex to a point where a deterministic model is out of the question, resort is made to experimentation and statistics. In such cases, the system in question is treated as a black box or gray box, and its input-output relationships are studied through an experiment, which may be passive or active[13].

In this paper the chemical conversion taking into account reaction rate and diffusion rate was investigated. Because of the availability of modern computers the time is fast approaching when the scientist will be expected to be a conversant with the unsteady state solutions to systems as

was expected for the steady state solutions in the past.

II. SIMULTANEOUSLY CHEMICAL REACTION AND DIFFUSION OCCUR

Taking into account diffusion, microscopic description in of a chemical reaction, shown in Fig.1 can be described by equation (1)[13].

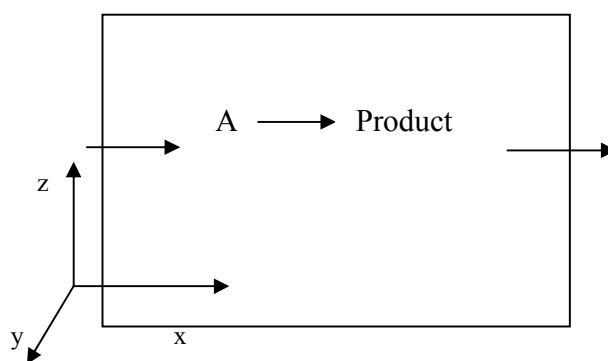


Fig.1 The chemical reaction scheme

$$\frac{\partial c_A}{\partial t} + v_x \frac{\partial c_A}{\partial x} + v_y \frac{\partial c_A}{\partial y} + v_z \frac{\partial c_A}{\partial z} + (-r_A) = D_{LA} \left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} \right) \quad (1)$$

$$\frac{\partial c_B}{\partial t} + v_x \frac{\partial c_B}{\partial x} + v_y \frac{\partial c_B}{\partial y} + v_z \frac{\partial c_B}{\partial z} + (-r_A) = D_{LB} \left(\frac{\partial^2 c_B}{\partial x^2} + \frac{\partial^2 c_B}{\partial y^2} + \frac{\partial^2 c_B}{\partial z^2} \right) \quad (2)$$

$$\frac{\partial c_C}{\partial t} + v_x \frac{\partial c_C}{\partial x} + v_y \frac{\partial c_C}{\partial y} + v_z \frac{\partial c_C}{\partial z} + (r_C) = D_{LC} \left(\frac{\partial^2 c_C}{\partial x^2} + \frac{\partial^2 c_C}{\partial y^2} + \frac{\partial^2 c_C}{\partial z^2} \right) \quad (3)$$

M. M. Stevanovic-Huffman, “Chemem”, Bartlett,
Memphis, TN38135, USA, email: serbhix@yahoo.com

J.B.Savkovic-Stevanovic, Faculty of Technology and Metallurgy,
Department of Chemical Engineering, 11000 Belgrade, Karnegijeva 4,
Serbia, e-mail: (savkovic@tmf.bg.ac.rs)

$$\frac{\partial c_D}{\partial t} + v_x \frac{\partial c_D}{\partial x} + v_y \frac{\partial c_D}{\partial y} + v_z \frac{\partial c_D}{\partial z} + (r_D) = D_{LD} \left(\frac{\partial^2 c_D}{\partial x^2} + \frac{\partial^2 c_D}{\partial y^2} + \frac{\partial^2 c_D}{\partial z^2} \right) \quad (4)$$

where c is the component concentration, x, y, z are space coordinates and t is time, v is geometrical velocity, (r) is reaction rate, and D is the diffusivity coefficient.

If mixing effects can be neglected equation (1) can be transformed:

$$\frac{\partial c_A}{\partial t} + v_x \frac{\partial c_A}{\partial x} + (-r_A) = D_{LA} \left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} \right) \quad (5)$$

If diffusion can be neglected in y and z direction equation (2) can be restarted in the form:

$$\frac{\partial c_A}{\partial t} + v_x \frac{\partial c_A}{\partial x} + (-r_A) = D_{LA} \left(\frac{\partial^2 c_A}{\partial x^2} \right) \quad (6)$$

The distribution $c_A(x, t)$ comes directly from the solution to the unsteady state diffusion in an infinite solid having a source at $x=0$, when $t=0$.

For the steady state condition and when velocity in the x direction can be neglected, equation (6) becomes:

$$D_{LA} \left(\frac{\partial^2 c_A}{\partial z^2} \right) = (-r_A) \quad (7)$$

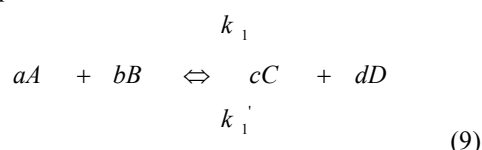
Now, this partial differential equation becomes, ordinary differential equation:

$$D_{LA} \left(\frac{d^2 c_A}{dx^2} \right) = (-r_A) \quad (8)$$

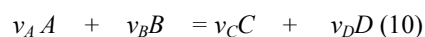
III. CHEMICAL REACTION RATE

The most fundamental description of a reaction system would be based on molecular considerations. The molecular description is distinguished by the fact that it treats an arbitrary system as if it were composed of individual entities, each obeys certain rules. Consequently the properties and state variables of the system are obtained by summing over all of the entities.

Let the considered reaction occurs in the liquid phase:



The reaction can be restarted in the following equivalent form:



where $v_A = -1$, $v_B = -b/a$, $v_C = c/a$, and $v_D = d/a$

Need to know something about the formulation of equations for the rate of chemical transformation from one species to another. This is subject of chemical kinetics. While it can not predict the rate of a chemical reaction, chemists can developed a number of valuable generalizations for formulating rate equations. It is necessary to understand these generalizations before proceeding with the design problem.

Chemical kinetics is the study of the rate and mechanism by which one chemical species is converted to another. The rate is the mass, in moles, of a product produced or reactant consumed per unit time. The mechanism is the sequence of individual chemical events whose overall results produce the observed reaction.

By mechanism is meant all the individual collisional or elementary processes involving molecules (atoms, radicals, and ions included) that take place simultaneously or consecutively in producing the observed overall rate. It is also understood that the mechanism of a reaction should give a detailed stereochemical picture of each step as it occurs. This implies a knowledge of so-called complex of transition state, not only in terms of the constituent molecules but also in terms of the geometry, such as interatomic distances and angles. In most instances the postulated mechanism is a theory devised to explain the end results observed by experiments. Like other theories, mechanisms are subject to change over the years as new data is uncovered or as new concepts regarding chemical interactions are developed.

It is not necessary to know the mechanism of a reaction in order to design. What is necessary is a satisfactory rate equation. A knowledge of the mechanism is of great value, however, in extending the rate data beyond the original experiments and in generalizing or systematizing the kinetics of reactions. Determining the mechanism of a reaction is a very difficult task and may require the work of many investigators over a period of many years. Reaction mechanisms are reliably known for only a few systems. However, postulated theories for mechanisms are available for a wide variety of reactions ranging from simple, gas-phase homogenous systems to complicated polymerization reactions involving initiation, propagation, and termination steps.

Successful procedures for predicting rates of reactions will not be developed until reaction mechanisms are better understood. It is important for those involved in reaction system design to be aware of developments in this area so that they may take advantage of new principles of chemical kinetics as they are developed.

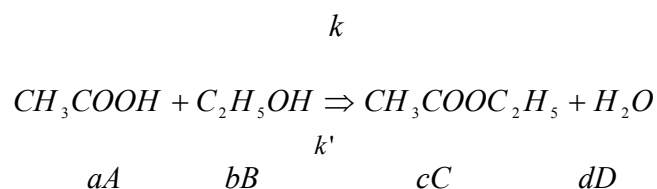
The rate of chemical reaction can vary from a value approaching infinity to essentially zero. In ionic reactions, such as those that occur on photographic film, or in high temperature combustion reactions, the rate is extremely fast. The rate of combination of hydrogen and oxygen in the

absence of a catalyst at room temperature is immeasurably slow. Most industrially important reactions occur at rates between these extremes, and it is in these cases that the designer must apply data on kinetics to determine finite sizes of reaction process. It is particularly important to know the rate changes with operating parameters, the most important of which are temperature, pressure, and composition of reaction mixture.

The science of kinetics is relatively young [15]. The first attempt to develop a theory explaining the manner in which molecules of a substance react was that of Arrhenius [16]. He postulated that the reactants had both inert and active molecules and that only active ones possessed sufficient energy to take part in the reaction. Since these early developments there have been a great many experimental studies of reaction rates for a wide variety of reactions, but few noteworthy advances in theory were made until the work of Eyring and Polanyi [17]. Using only such fundamental information as the configurations, dimensions, and interatomic forces of the reacting molecules, they postulated an activated-complex theory for predicting the rate of reaction. Lack of exact knowledge of the interatomic forces, and hence of energy-position relations, for any but the most simple molecules has prevented the activated-complex theory from being useful for predicting reaction rate data accurately enough for scientific work. While these theoretical developments have been of great value in the search for an understanding of how and why a chemical reaction takes place, the quantitative evaluation of the rate remains an experimental problem.

The large amount of experimental data on rates of chemical reaction have established reliable empirical forms for the mathematical expression of the effects of such variables as temperature and composition on the rate.

The early works in kinetics found that simple relations existed between rates of reaction and concentrations of reactants. For example, the rate of esterification was proportional to the first power of the concentration of ethanol and to the first power of the concentration of acetic acid. The rate is said to be first order with respect to each reactant. In general terms, suppose that the rate of the reaction



may be written

$$r_A = k c_A^{n_1} c_B^{n_2}$$

where $k = A_0 e^{-E/RT}$.

The dependency of k on temperature for an elementary process follows the Arrhenius equation. This provides a description of the rate in terms of the measurable variables, concentration and temperature. It is rigorously limited to an elementary process because the Arrhenius equation is too restricted. However, the exponential effect of temperature often accurately represents experimental rate data for an overall reaction, even though the activation energy is not clearly defined and may be a combination of energy values for several elementary steps.

The Arrhenius concept requires that molecules of reactants have an energy E above their normal, or average, energy, between initial, activated, and final states.

There is a possibility that some molecules will possess this excess because of the wide range over which the energy is distributed and the large number of molecules that make up the system.

In a view of the success of the Arrhenius equation, there have been many attempts to develop theoretical interpretations for the frequency factor A_0 and the activation energy E . The collision theory in which the frequency factor is treated as a collision rate, was inspired by the kinetic theory of gases. Subsequently the more sophisticated activated complex theory was developed to take advantage of the more detailed description of collisions made possible.

According to classical kinetic theory, some gaseous molecules will possess much larger amounts of translational energy than others because of variations in their molecular velocities. It is logical to suppose that collisions between these reactant molecules would provide the activation energy necessary for the reaction to occur. By assuming that the molecules behave as hard spheres, it is possible to develop simple expressions for the rate. This approach, originally advanced as the collision theory. The theory has a number of weaknesses and has been extended and supplemented by later developments. However, it offers a simple picture of the mechanism of reaction.

According to the collision theory, the number of molecules of product formed per unit time per unit volume is equal to the number of collisions multiplied by a factor, which takes into account the fact that only a fraction of the collisions involve molecules that possess the excess energy, activation energy, necessary for reaction.

The fraction of the molecules that possess the required excess energy for reaction should not depend on the number of collisions but on the magnitude of the energy itself. If Maxwellian is assumed the fraction of the total molecules having an energy at least equal to E can be shown to be $e^{-E/RT}$.

The collision theory has been found to give results in good agreement with experimental data for a number of bimolecular gas reactions. The theory has also been satisfactory for several reactions in solution involving simple ions. However, for many other reactions the predicted rates are much too large. Predicted frequency factors lie in the rather narrow range of 10^9 to 10^{11} , while measured values may be several orders of magnitude less. The deviation appears to

increase with the complexity of the reactant molecules. As a means of correcting for this disagreement it has been customary to introduce a probability, or steric factor. To retain the hard sphere concept must then explain why all the collisions supplying the necessary energy do not result in reaction.

Beginning at the last century activated complex theory was introduced [17]. This examination is based on the concept that molecules possess vibrational and rotational, as well as translational, energy levels.

The essential postulate is that an activated complex or transition state is formed from the reactant, and that this subsequently decomposes to the products. The activated complex is assumed to be in equilibrium with the reactants. Then the rate controlling step is the decomposition of the activated complex. The concept of an equilibrium activation step followed by slow decomposition is equivalent to assuming a time lag between activation and decomposition into the reaction products. It is the answer proposed by the theory to the question of why all collisions are not effective in producing a reaction.

Since equilibrium is assumed for the first step, the concentration of complex is that determined by the equilibrium constant. Then the rate of the overall reaction is equal to the product of the frequency of decomposition of the complex and its equilibrium concentration.

The collision theory does not offer a method for calculating the activation energy. The activated complex theory suggests that energy is enthalpy change for formation of the activated complex from the reactants.

In a reversible reaction, the reactions fail to complete conversion in the forward direction (specific reaction rate k) and the reaction proceeds in the reverse direction (specific reaction rate k'). Under the circumstances a situation occurs in which the rates of the forward and reverse reactions just balance each other, and a dynamic chemical equilibrium is established, which is defined by the equilibrium constant K . Therefore, in calculating reversible chemical reactions, the equilibrium constant should be derived from the law of mass action.

$$K = \frac{c_C^{v_C} c_D^{v_D}}{c_A^{v_A} c_B^{v_B}} = k / k' \quad (11)$$

where K is the equilibrium constant (at temperature constant characteristic of a given reversible reaction, c_A , c_B , c_C and c_D are the concentration of the reactants and products at the equilibrium, and k and k' are the rate constants for the forward and reverse reactions).

The molecularity describes the number of molecules participating in a reaction in accordance with its stoichiometric equation and must be an integer. There are reaction with a molecularity of one (monomolecular), two (bimolecular) and three (trimolecular).

The manner in which the rate of a chemical reaction is controlled by the concentration of each reactant is specified as a power exponent of that reactant's concentration, and this

is the reaction order with respect to that particular reactant. With several reactants, the overall reaction order is the sum of the power exponents of the reactants. Furthermore, the reaction order is proportional to the reactant's concentration in the case of a first order reaction, to the product of the concentration of two reactants for a second order reaction, to the product of the concentration of three reactants for the third order reaction, etc.

Rate of chemical reaction or reaction velocity, describes the change decrease or increase in the number of moles of the reactants due to a chemical interaction per unit time and unit volume. According to the law of mass action, the reaction rate is proportional to the current concentration of the reactants. For a second order reversible reaction, reaction rate is:

$$(r) = kc_Ac_B - k'c_Cc_D \quad (12)$$

where

$$\frac{dc_A}{dt} = \frac{dc_B}{dt} = (-kc_Ac_B + k'c_Cc_D) \quad (13)$$

$$\frac{dc_C}{dt} = \frac{dc_D}{dt} = (kc_Ac_B - k'c_Cc_D) \quad (14)$$

Change of the chemical reaction rate or reaction acceleration can be defined as:

$$\frac{d}{dt} \left(\frac{dc_A}{dt} \right) = \frac{d(-kc_Ac_B + k'c_Cc_D)}{dt} \quad (15)$$

Since a chemical reaction is accompanied by interaction of the reacting species at the molecular level, it is assumed that the reaction proceeds at the molecular level. These kinetic data are an essential block of an overall mathematical model.

In previous paper the ordinary differential equations solution by numerical method was provided. A computer program was written in BASIC programming language [14].

With elementary reactions, it is a simple matter to ascertain the mechanism and rate of reactions, because their stoichiometric equations uniquely define the respective mathematical models.

Kinetic data are usually determined from experimental measurements or they have taken from other authors.

For a closed system, kinetic data are derived by measuring time dependence of a chemical or physical observable variable which is a function of time.

These data can be written in forms:

Rate of change of concentration, c as a function of time t :

$$\frac{dc}{dt} = f(t) \quad (16)$$

Rate of change of concentration, c as a function of concentration:

$$\frac{dc}{dt} = f(c) \quad (17)$$

Concentration, c as a function of time, t .

$$c = f(t) \quad (18)$$

In principle rate versus concentration data are more useful because they may be directly used in equations of differential rates and this method is called differential.

Simulation on computers greatly speeds up the choice of constants for kinetic equations.

Thus, the first step in the chemical kinetic study for homogenous systems is to ascertain the manner in which the concentration of the reactant varies with time at the fixed temperature. The second step is to interpret the experimental relationships, $c=f(t)$, in order to find kinetic constants, namely the specific reaction rate and the reaction order, that is power exponents of the reactant concentrations. This can be done by two methods integral and differential.

Specific chemical rate constant can be determined by simulation using trial and error method observed curve $c=f(t)$. Comparison simulated and experimental curves it need to satisfied $c^{exp} - c^{cal} = min$.

IV. DIFFUSION RATE

The concept of diffusion may be viewed naively as the tendency for a group of particles initially concentrated near a point in space to spread out in time, gradually occupying an ever larger area around the initial point [14]. Herein the term particles refers not only to physical particles, but to any other identifiable units as well.

However, such a definition of diffusion is liable to invite confusion. For example, consider a number of particles released simultaneously from a point on a plane, each heading straight with its own speed and direction. Clearly, the particles will spread and occupy ever-increasing areas. However, such a process is not called diffusion.

Diffusion is a phenomenon by which the particle group as a whole spreads according to the irregular motion of each particle. Rephrasing, when the microscopic irregular motion of each particle gives rise to a regularity of motion of the total particle group, macroscopic regularity, the phenomenon of diffusion arises.

Problems involving diffusion can be handled from both the probabilistic considerations and the use of the known diffusion equations. Diffusion in a force field can be decomposed into random and nonrandom components. Random forces are related to the random motion of the individuals themselves and can be included in the diffusion process. In many cases they are parameterized by the diffusivity.

The Knudsen diffusion coefficient is expressed as [2]:

$$D = \frac{2r\bar{u}}{3} \quad (19)$$

where \bar{u} represents the average molecular velocity, and $2r$ is the molecular mean free path.

Einstein's definition of the diffusion coefficient has given by expression[3],[4]:

$$D = \frac{\bar{\lambda}^2}{2t} \quad (20)$$

where $\bar{\lambda}^2$ is the mean square distance a molecule travels in the x direction in a time t .

The point of departure for the theory of diffusion is the random walk. Let, consider the one-dimensional space illustrated in Fig.1. Each individual moves a short distance λ to the right or left in a short time t . This motion is taken to be completely random and probability of moving to either the right or left is $\frac{1}{2}$. After time t , a given population spreads, one half moving a distance λ to the right of the origin and one half moving the same distance to the left. It does not know which individual will belong to which half. Continuing, in the next time interval t , each individual moves a distance λ to the right or left, each alternative with a probability of $\frac{1}{2}$, independently of the previous motion. Thus $\frac{1}{4}$ of the population finds itself a distance 2λ to the right of the origin, $\frac{1}{4}$ is the same distance to the left, and $\frac{1}{2}$ returns to the origin. The population as a whole exhibits spreading. It should to know the form that the spatial distribution of population takes after time nt has passed.

V. MUTUAL EFFECTS CHEMICAL REACTION AND DIFFUSION ANALYSIS

In a mutual model structure pruning results candidate for a best match to the set of synthesis objectives. It can be viewed as a search through the space of candidate solutions to the problem. Production rules represent the knowledge consisting of phenomena objectives, coupling constraints user's requirements and performance expectations. The aim of pruning is to recommend plausible candidates for a solution to the problem with respect to the requirements and constraints.

To understand system phenomenon structure the following steps are required: specify of rules for selecting an entity for each specialization, for any entity with several aspects, specify rules for selecting a unique aspect, and for each aspect specify rules that ensure that the entities selected from specializations are configurable.

Transaction that take place the environment affect the system as its inputs, while the outputs that leave the system affect its environment. A transaction entering a model may pass through several steps before its transformation to an output. In addition to the input-system-output relationship, several complex relationships among these often exist.

In general, any two phenomena may be mutually exclusive, order dependent, order independent, or concurrent. Two are mutually exclusive phenomena when only one of them can be performed. Two phenomena are order dependent when one must be performed before the other phenomenon.

In recent years, the simultaneous diffusion and chemical reaction in porous catalysts has received considerable attention from chemists and chemical engineers. Diffusion and chemical reaction in a catalyst pore can be described by the above derived equations.

In a conventional fashion to problems of simultaneous diffusion and reaction quickly learns that the number of diffusion jumps required before a single reaction takes place is extremely large. This is because the reaction probability in the time interval of one collision is small in catalysts.

In order for the reaction to occur reactant molecules must migrate from the solution into the catalyst particle, and must react. The reaction product must then migrate back into the solution.

In film diffusion is much slower than the chemical reaction, it must obviously be rate controlling since, in this limiting case, all reactant molecules react as soon as they reach the reaction surface. If the chemical reaction is much slower than the diffusion processes sorption equilibrium of the reactants is established and upheld into the particle since diffusion is fast enough to make up for the disappearance of reactants by chemical reaction. The overall rate thus is controlled by the rate of the chemical reaction. If interparticle diffusion is much slower than the chemical reaction, the reaction molecules will react before they have time to penetrate into the interior. In this latter limiting case, the reaction occurs only in a thin layer at the particle surface and its rate is controlled by either film diffusion of chemical reaction at the surface.

If the simultaneous unsteady state process of diffusion and chemical reaction occur it can be described by the following equation:

$$\frac{\partial c_A}{\partial t} + (-r_A) = D_{LA} \left(\frac{\partial^2 c}{\partial x^2} \right) \quad (21)$$

for steady state is obtained:

$$(-r_A) = D_{LA} \left(\frac{d^2 c_A}{dx^2} \right)$$

or

$$D_{LA} \left(\frac{d^2 c_A}{dx^2} \right) + (-r_A) = 0 \quad (22)$$

This differential equation of the second order can be transformed into system equations of the first order as follows:

Introducing,

$$\xi = \frac{dc_A}{dt}$$

eq.(22) is transformed into system eqs.(23)

$$D_{LA} \left(\frac{d\xi}{dx} \right) + (-r_A) = 0 \quad (23)$$

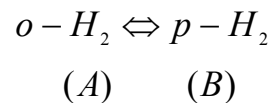
$$\xi = \frac{dc_A}{dx}$$

This system differential equations can be solved by known numerical methods [12].

VI. APPLICATION

Let consider, the ortho-para hydrogen conversion a reaction which maximum conversion is less than 100%. An understanding of the equilibrium conversion as a function of operating conditions is necessary before a satisfactory rate equilibrium can be formed.

The ortho-para hydrogen reaction is occurred at -196 °C and constant pressure in a flow reactor, with a nickel-on-Al₂O₃ catalyst as:



The rate data can be explained with an expression of the form:

$$r_A = k_r (y_{eq} - y)$$

show that this expression follows from the first order reversible rate equation.

General reaction rate is:

$$-\frac{dc_A}{dt} = kc_A - k'c_B$$

Assuming hydrogen is an ideal gas at reaction conditions and that P is the total pressure, it is obtained:

$$c_A = \frac{P}{RT} y_0$$

Since the system is binary one, then:

$$y_p = 1 - y_0, \text{ and}$$

$$c_A = \frac{P}{RT} (1 - y)_p,$$

and so,

$$c_{A,eq} = \frac{P}{RT}(1 - y_{eq})_p$$

$$-\frac{dc_A}{dt} = r \equiv k_r c_{A,eq} = \frac{k(K+1)}{K} \frac{P}{RT}(1 - y_{eq})_p$$

Solution of this equation for assumed initial conditions is shown in Fig.2. The computed concentration profile is shown for the first hour. Ratio of $(c_A / c_{A,eq})$ vs. time is shown in Fig. 4.

The concentration changing in x direction at the steady state conditions has shown in Fig.3.

Ratio of $(c_A / c_{A,eq})$ vs. time is shown in Fig. 4.

VII. CONCLUSION

In this paper the chemical rate reaction and diffusion rate for various dynamic and steady state conditions were examined. The analysis of the chemical reaction progress and diffusion progress characterization were developed. The obtained expressions show dynamic behavior of the component during the chemical reaction with reactants and products diffusion. Production requirements represent the knowledge consisting of reaction objectives, coupling constraints user's requirements and performance expectations.

The main contribution of this paper is advanced theory developing for the chemical reaction collisions and diffusion collisions.

Computer's simulation of the ortho -para hydrogen reaction was illustrated.

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B. Notation

- A-reactant 1
- A₀- acceleration factor, cm³ mol⁻¹ s⁻¹
- B-reactant 2
- C-product 1
- D-product 2
- D_L-diffusion coefficient
- c- concentration, cm³ mol⁻¹
- E-energy activation, J/mole
- k- specific rate constant in right side, cm³ mol⁻¹ s⁻¹
- k' - specific rate constant in left side, cm³ mol⁻¹ s⁻¹
- l- distance
- n- reaction order
- P-pressure
- (r_A)-reaction rate
- r - molecular mean free path
- R-universal gas constant
- t-time
- \bar{u} - represents the average molecular velocity
- x- radial distance
- y- o-H₂ composition

Greek symbols

- λ- distance a molecule travels

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A-reactant 1
B-reactant 2
C-product 1
D-product 2
L-liquid phase

Fig. 3 Concentration vs. distance

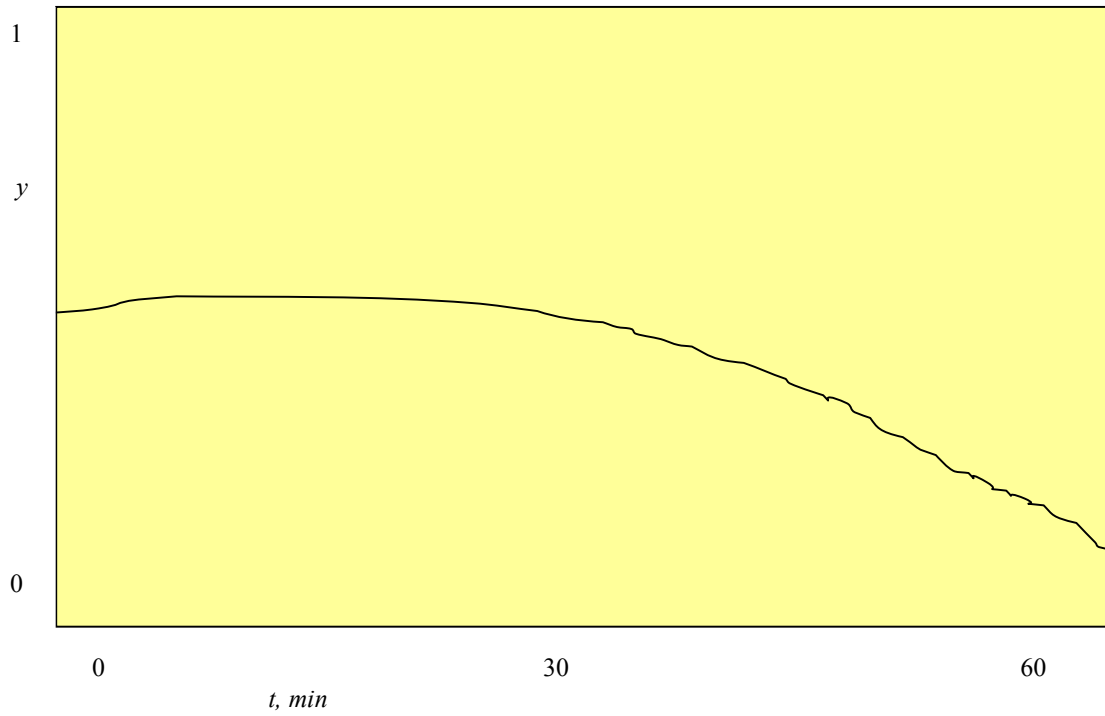
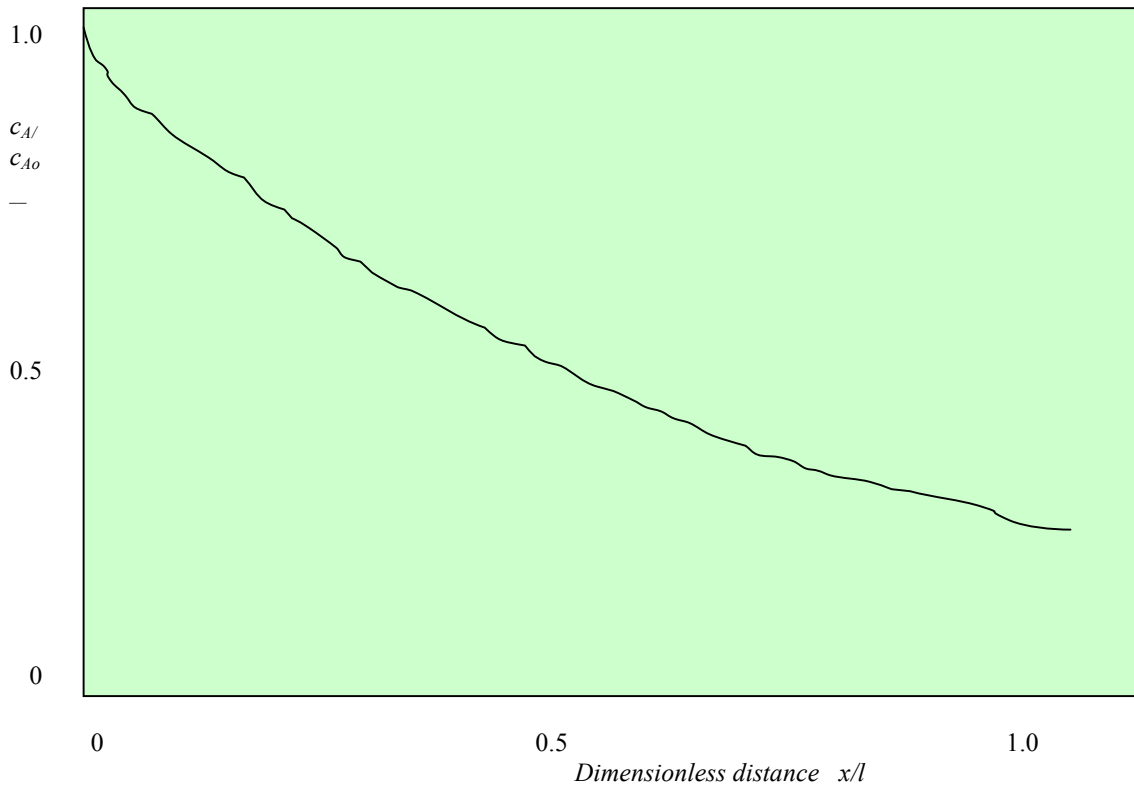


Fig.2 Dependence ortho- hydrogen concentration with time



papers in the Proceedings of International Conferences, in the above fields.

Other activities: Stevanovic-Huffman is a member of The American Chemical Society-Memphis.

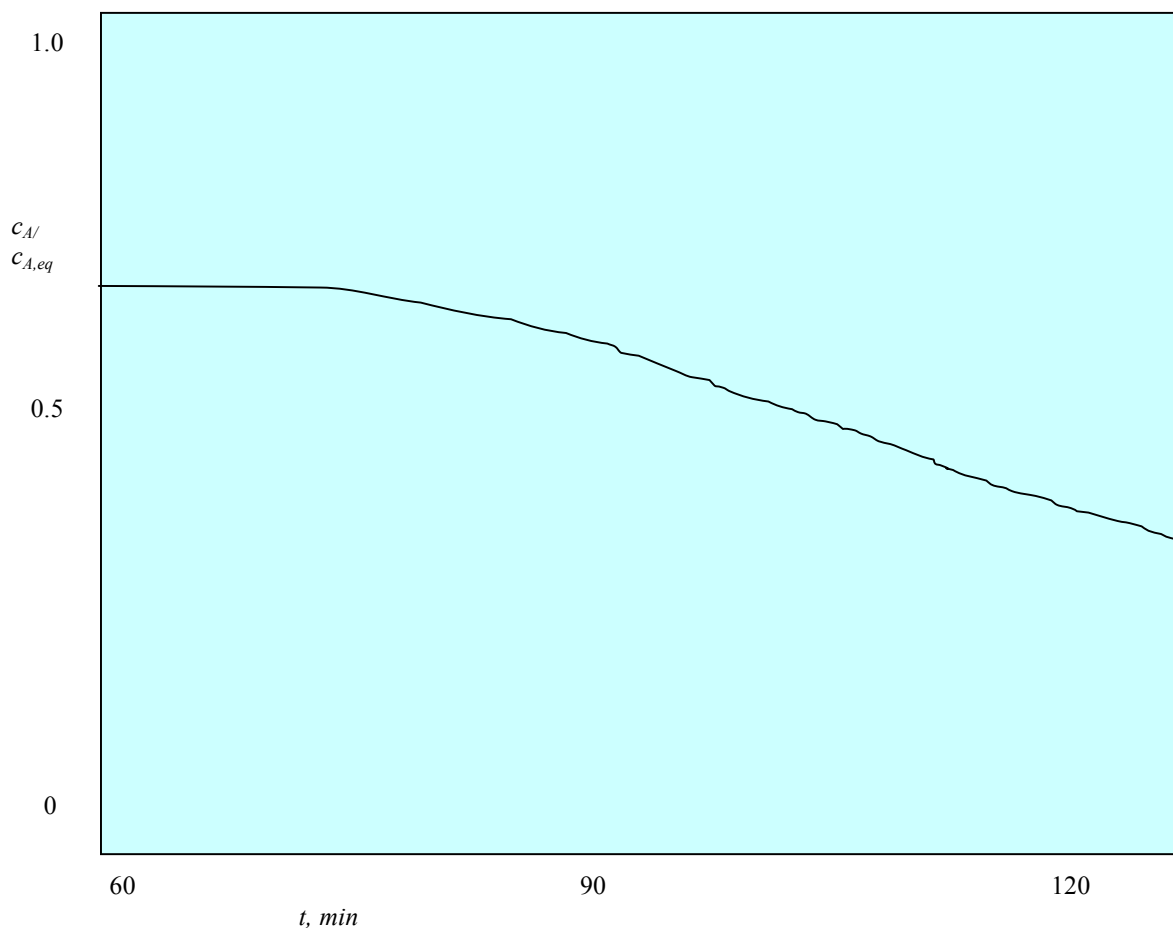


Fig.4 Ratio of the $(c_A / c_{A,eq})$ vs. time

Authors Biographical Data



Milena M. Stevanovic-Huffman graduated at the University of Memphis, U.S.A. **Education:** Her B.Sc. degree and M.Sc. degree at the University of Memphis, Department of Chemistry was achieved.

Research interest:: She's occupied with Chemical reaction dynamics, Oxidation-reduction systems, and Chemometric methods. She's published 3



Jelenka Savkovic-Stevanovic is full professor at the University of Belgrade, Faculty of Technology and Metallurgy, Serbia.

Education: B.Sc. and M.Sc. degree, University of Belgrade, Ph.D. University of Belgrade and Technical University of Berlin.

Research interest: She's occupied with Chemical Process Engineering, Pharmaceutical Engineering, and Ecological and Biomedical Engineering, especially, Modelling and Simulation Methods, Informatics, Artificial Intelligence, Bioinformatics and Toxicology. She published many papers, 10 professional books, patentee in the above fields.

Other activities: Prof. Savkovic-Stevanovic is an editor and chief of the *Computers & Ecological Engineering Journal*. Reviewer of many Journals and Projects. Consultant in companies and member of many professional organizations. She's cited in many monographs as 1000 Great minds of the World in 21st Century-ABI, U.S.A.. She's the first on the World's List of Scientists-IBC, U.K. from 2009 to 2012.

Many awards and honors: The best WSEAS articles, 2009, 2010: Savkovic-Stevanovic J., DNA polymeric chain, 2nd Inter. Conf. on Biomedical Electronics and Biomedical Informatics-BEBI09, pp.122-126, Moscow, August, 20-22, 2009; Savkovic-Stevanovic J., Learning and discovering in chemistry, 2nd International Conference on Mathematics and Computers in Biology and Chemistry, ID632-191, Iasi, Romania, 12-13 June, 2010, and *Transaction on Information*