2020 3rd International Seminar on Research of Information Technology and Intelligent Systems, ISRITI 2020
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Some Numerical and Analytical Solutions to an Enzyme-Substrate Reaction-Diffusion Problem (Conference Paper)

Mungkasi, S.

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Sanata Dharma University, Faculty of Science and Technology, Department of Mathematics, Yogyakarta, Indonesia

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Abstract

We consider an enzyme-substrate reaction-diffusion problem . Unsteady and steady state models are recalled. For the unsteady state case, the model is in the form of a second order partial differential equation. We solve the unsteady state model using the explicit numerical finite difference method, which is forward difference in time and centered difference in space. For the general steady state case, the model is in the form of a second order ordinary differential equation. We solve the general steady state model using the explicit first order Euler's numerical method. For the particular steady state case of the unsaturated catalytic kinetics, we derive the exact analytical solution using the characteristic method of ordinary differential equations. For the particular steady state case of the saturated catalytic kinetics, we derive the exact analytical solution using the direct-integration method. The obtained exact analytical solutions are identical with the existing exact analytical solutions derived using the variational iteration method. With the aid of computer, the enzyme-substrate reaction-diffusion problem can be solved and simulated successfully for both unsteady and steady state cases. © 2020 IEEE.

Author keywords

enzyme-substrate system | finite difference method | reaction-diffusion problem | saturated steady state | unsaturated steady state

Indexed keywords

Engineering controlled terms: Diffusion in liquids | Enzymes | Finite difference method | Intelligent systems | Iterative methods | Ordinary differential equations

Engineering uncontrolled terms: Characteristic method | Direct integration method | Exact analytical solutions | Reaction diffusion problems | Second-order ordinary differential equations | Second-order partial differential equation | Steady-state modeling | Variational iteration method

Engineering main heading: Numerical methods

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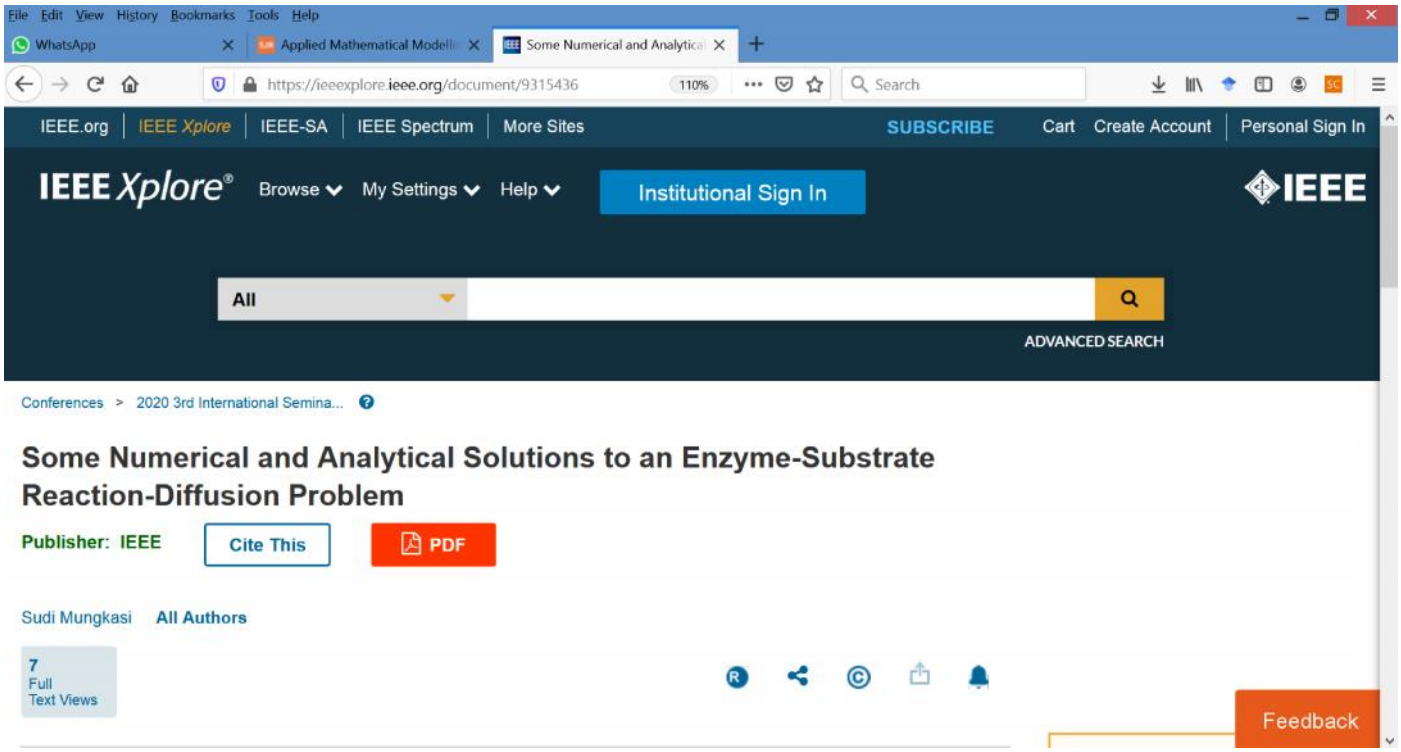

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Sudi Mungkasi All Authors

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Conference Location: Yogyakarta, Indonesia, Indonesia

I. Introduction

Chemical reaction problems may incorporate diffusion. This process is then called a reaction-diffusion problem. The reaction-diffusion process has been modelled into a mathematical equation. The derivation involves the so called Michaelis-Menten kinetics. The Michaelis-Menten kinetics itself has been widely recognised in chemistry for reaction problems [1]–[7].

Authors

Figures

References

Keywords

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Ignasius Boli Suban; Andi W. R. Emanuel
Publication Year: 2020 , Page(s): 100 - 105

Abstract (355 Kb)

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Husein Mubarok; Agus Ardiansyah
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Publication Year: 2020 , Page(s): 650 - 654

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Network Attack Detection System Using Filter-based Feature Selection and SVM
Ventje Jeremias Lewi Engel; Firhat Hidayat; Richard Dwiputra
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Abstract (497 Kb)

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Modification of Wireless Reverse Charging Scheme with Bundling Optimization Issues
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Abstract (327 Kb)

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Abstract (487 Kb)

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Comparison of the Latest DTM with DEM Pleiades in Monitoring the Dynamic Peatland

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Abstract (2038 Kb)

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Abstract (772 Kb)

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Detection of Sensor Node-less Area Using A Genetic Algorithm for Wireless Sensor Network
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Abstract (461 Kb)

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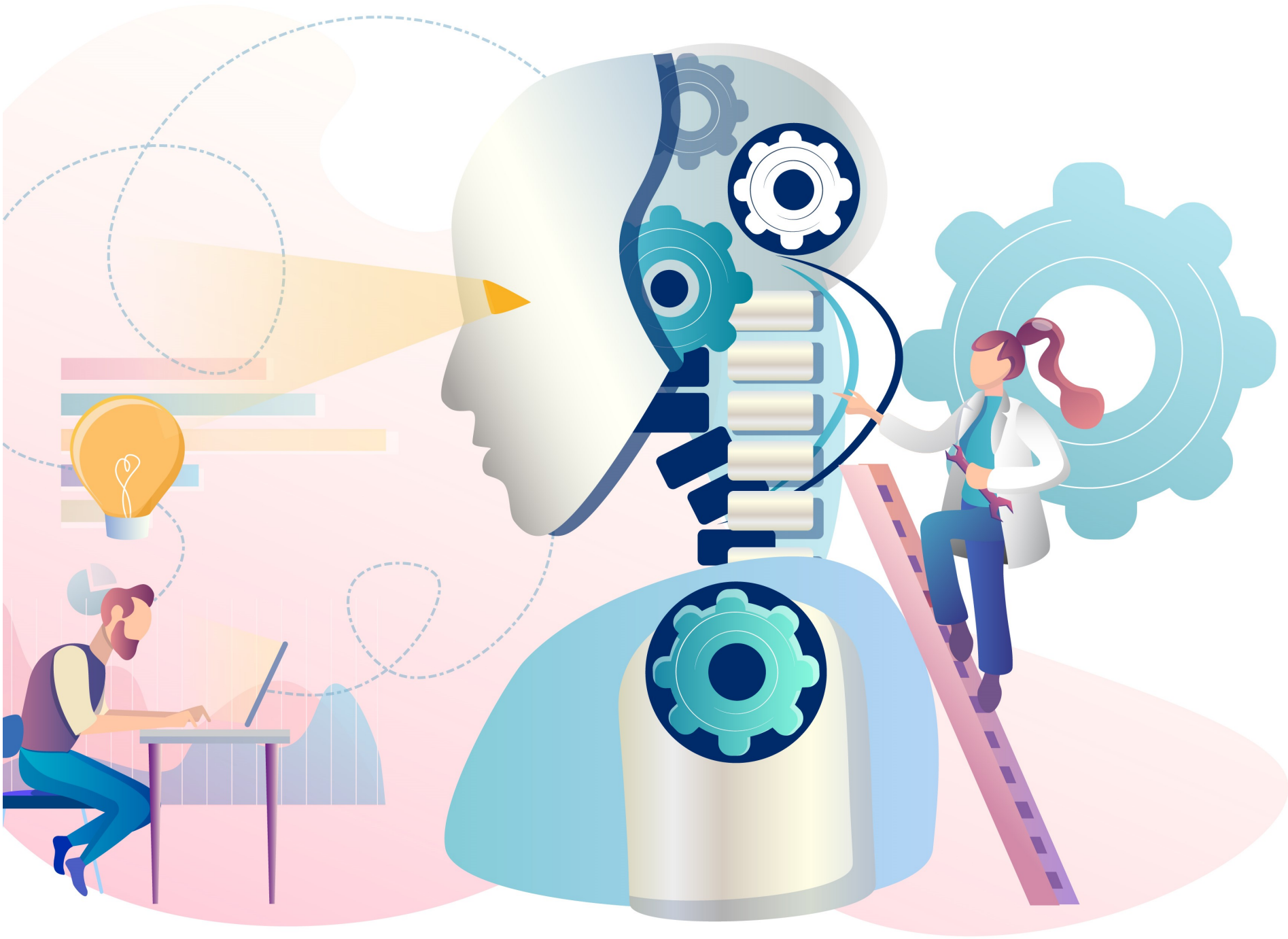

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We inform you that the **STMIK AKAKOM Yogyakarta** will organize **The 3rd International Seminar on Research of Information Technology and Intelligent Systems 2020 (ISRITI 2020)** (http://isriti.akakom.ac.id/). This seminar will take place from **10 December 2020** in **Grand Inna Malioboro Hotel, Yogyakarta**, **Indonesia**. This seminar will be connection to the most influential ideas and systems in the field of information technology and intelligent systems. Join us at 3rd ISRITI 2020 and contribute to the research-led exploration and discussion of the current, development, and emerging state of the information technology and intelligent systems.

The purpose of this seminar is to provide a platform for academics, practitioners, researchers, and governments to identify and explore the issues, opportunities, and solutions that promote information technology and intelligent system convergences, developments and find new business, technology, and societal value from the information technology and intelligent systems.

Call for Papers

We invite submissions in all areas of information technology and intelligent systems research. In particular, we encourage submissions related to the seminar theme :***Artificial Intelligence for Social Interactions***. We, in the name of the committe, hope you enjoy this seminar and have a great day in Yogyakarta.

All accepted papers must be presented orally (offline) or online in the Conference in order to be published in the proceeding, unless their paper will not be published in the proceeding.

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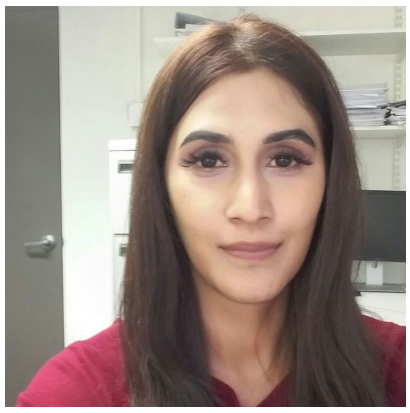

Dr. Zoohan Gani

Victoria University, Sydney
Australia

Assoc.Prof.Dr. Ahmad Hoirul Basori

King Abdulaziz University, Rabigh, Makkah
Saudi Arabia

Submission

Submission Type: **Full Paper**

Important Dates

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Paper Submission: ~~**31 July 2020**~~
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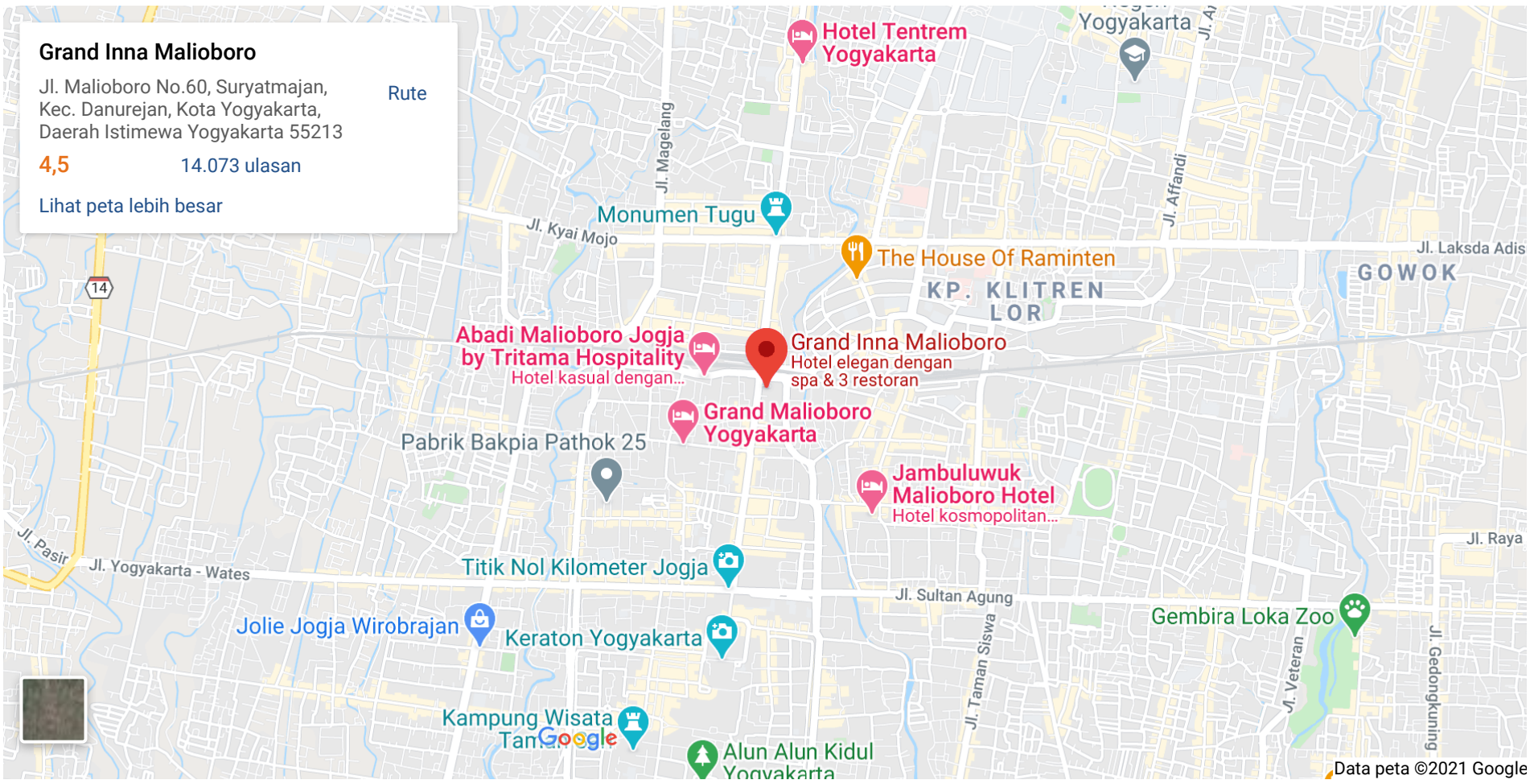

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#3rd ISRITI 2020

Yogyakarta - Indonesia
10 December 2020

ARTIFICIAL INTELLIGENCE for SOCIAL INTERACTIONS

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WELCOME SPEECH FROM THE CHAIRMAN OF STMIK AKAKOM YOGYAKARTA

The honourable
Keynote Speakers (Dr. Zoohan Gani from Victoria University and Assc. Prof. Ahmad Hoirul Basory from King Abdul Azis University)
Chairman of Widya Bakti Foundation and his staffs,
Representatives from IEEE Indonesia Chapter and Central IEEE,
Team of Indonesia Researcher and Scientist Institute,
Researchers and conference attendees,
Ladies and Gentlemen,

Assalamu'alaikum Wr. Wb.
May peace and health be upon us all.

First of all, let us express our utmost gratitude to God Almighty (SWT) for His blessings and grace so that even though in this coronavirus pandemic atmosphere, we can all still participate in the third iSriti international conference. On this occasion, let me express my sincere appreciation to the Keynote Speakers: Dr. Zoohan Gani from Victoria University, Sydney Australia, and Assoc. Prof. Dr. Ahmad Hoirul Basory from King Abdul Azis University, Rabig, Makkah, Saudi Arabia for their willingness to share their brilliant ideas and insights to be presented at this conference.

Dear ladies and gentlemen
On this occasion, as the head of STMIK AKAKOM Yogyakarta, I am saddened to state that the third iSriti conference had to be held online, considering that the coronavirus pandemic has not ended. Even though a pandemic currently hits us, the researchers' enthusiasm is apparent in the number of research articles submitted. We received up to 262 articles from 17 countries. Around 135 articles were accepted to be readily presented online in a conference forum with the theme: Artificial Intelligence for Social Interactions.
As the organizers of iSriti, we are very proud and grateful for the researchers' participation who have been willing to submit their research results to be published in this conference forum. We would also like to thank IEEE and IRSI, who have trusted and supported this conference from the very beginning. We still hope to build networks and information exchange between academics, practitioners, researchers, and the government to identify and explore issues, opportunities, and solutions to face challenges in the current era of technological disruption.

Finally, on this occasion, I would like to express my utmost gratitude to:
1) The distinguished keynote speakers who have been willing to share their valuable knowledge in this conference;
2) The third iSriti researchers who have presented and will present their research results;
3) Reviewers who have carefully reviewed the articles of the researchers;
4) Moderators who are more than willing to lead the plenary session;
5) IEEE for trusting us to hold this international conference;
6) IRSI, which has supported the third iSriti activities until now;
7) The committee that has been working hard to prepare this international conference according to plan;

Last but not least, as the organizer, I would like to sincerely apologize for any shortcomings or inconveniences during this event.

Thank you very much for your kind attention, and *Wassalamu'alaium Wr. Wb.*
Yogyakarta, 10 December 2020

The Chairman of STMIK AKAKOM Yogyakarta

Totok Suprawoto, M.M., M.T.

WELCOME SPEECH FROM THE GENERAL CHAIR OF THE 3rd ISRITI 2020

Dear colleagues and friends.

On behalf of the organizing committee, I am delighted to welcome all participants to the 3rd International Seminar on Research of Information Technology and Intelligent Systems (ISRITI 2020). This conference is the third international conference held by STMIK Akakom Yogyakarta, Indonesia and the first to be held by STMIK Akakom in virtual form on December 10th, 2020.

In this conference, the committee decided to choose the following theme: "Artificial Intelligence for Social Interactions". This highlight was chosen because various advances in the field of AI have recently raised concerns that AI will replace various things that are the human domain. For us, AI can be used to better understand social interactions and to build machines that work more collaboratively and effectively with humans. Therefore, by highlighting that theme in ISRITI 2020, we hope we can raise awareness towards AI for social interactions.

The aim of the conference is to provide an interactive international forum for sharing and exchanging information on the latest research in the area of information technology, computer sciences, informatics, and related fields. Nearly 135 academicians, researchers, practitioners, and presenters from 17 countries (Indonesia, Malaysia, India, USA, Brazil, Australia, South Korea, Hungary, Morocco, Vietnam, Iraq, China, Thailand, Turkey, Ireland, Romania, Russia, and Saudi Arabia) gathered in this event. In total, there are 262 active papers submitted to this conference. Each paper has been reviewed with tight criteria from our invited reviewers. Based on the review result, 135 papers have been accepted, which lead to an acceptance rate of 51.5%. This conference will not be successful without extensive effort from many parties. First, I would like to thank all keynote speakers for allocating their valuable time to share their knowledge with us. I would also like to express my sincere gratitude to all participants who participate in this conference. Special acknowledgement should go to the Technical Program Committee Chairs, Members, and Reviewers for their thorough and timely reviewing of the papers. We would also like to thank our sponsors: IEEE Indonesia Section and Research and Society Service Institution at STMIK Akakom. Last but not least, recognition should also go to the Local Organizing Committee members who have put enormous effort and support for this conference. At last, we hope that you have an enjoyable and inspiring moment during our conference. Thank you for your participation in ISRITI 2020.

Yogyakarta, 10 December 2020
General Chair of the 3rd ISRITI 2020

Dr. Bambang Purnomosidi D. P.

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PREFACE

A language and reasoning can be said as some of the characteristics of human abilities. On the other hand, the ability of human thinking can be modeled as computation. The development of cognitive science that combines scientific development with technology began to appear in the 1960s. In those years, human behavior did not adequately explain cognitive processes. Although, there has been much debate by behaviorist experts regarding the cognitive science approach. However, with a variety of approaches, there is something quite encouraging that computer models of cognition can be used as an alternative approach to these various models. Furthermore, computers can be used to test hypotheses where computation itself is the subject of the mind. So that there are various kinds of models developed in the field of cognitive science with different fields of science, including anthropology, artificial intelligence (AI), philosophy, linguistics, neuroscience, and psychology. Even though there are different scientific fields, it turns out that they can work together in explaining various kinds of cognitive science models. AI is a part of the field of computer science that can describe intelligent computer systems. This system can show characteristics related to intelligence in human behavior, such as reasoning, understanding language, learning, solving problems, and so on. This intelligent system has a long-term goal of equaling or surpassing human intelligence. The approach used in simulating this system uses mathematical approaches, discursive reasoning, language, and so on. New developments related to the paradigm in this field emerged in the mid-80s, bringing together developments in the fields of philosophy, AI, and cognitive science.

Human intelligence is illustrated as a result of a program running on the human brain. In connectionist's view, information processing on computer devices is a fundamental difference from the brain. In the context-sensitive cognition model, human intelligence depends on the physical properties of the neurons. So that artificial intelligence requires brain-like computer skills, better known as neurocomputers. The purpose of this terminology is to design hardware compatible with neuro-computing. In this case, the model that is later known massively is an artificial neural network in which this model is trained, not programmed. Much information is extracted deeper than a representation that is presented in various forms that can be understood by humans. In the past, artificial emotions were somewhat neglected in AI and cognitive science. However, currently, emotional intelligence is one of the things that is raised with relevant information indicators in solving a case or problem. Emotion has an important domain in motivating and directing behavior. So that discussions in cognitive science and AI become one of the raw materials in representing information, then use it in social interactions. This representation is a language capable of thinking about problem-solving and social processes. This explains the systematics or methods used are very important in understanding cognition and communication in the context of social interaction. This pattern has appeared in the childhood phase in the learning process until later understanding their identity and interacting with others in the form of communication. The basis for this transformation is then essential in solving many cases in the world of science and technology.

Editor of 2020 3rd ISRITI

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Some Numerical and Analytical Solutions to an Enzyme-Substrate Reaction-Diffusion Problem

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***Abstract*—We consider an enzyme-substrate reaction-diffusion problem. Unsteady and steady state models are recalled. For the unsteady state case, the model is in the form of a second order partial differential equation. We solve the unsteady state model using the explicit numerical finite difference method, which is forward difference in time and centered difference in space. For the general steady state case, the model is in the form of a second order ordinary differential equation. We solve the general steady state model using the explicit first order Euler's numerical method. For the particular steady state case of the unsaturated catalytic kinetics, we derive the exact analytical solution using the characteristic method of ordinary differential equations. For the particular steady state case of the saturated catalytic kinetics, we derive the exact analytical solution using the direct-integration method. The obtained exact analytical solutions are identical with the existing exact analytical solutions derived using the variational iteration method. With the aid of computer, the enzyme-substrate reaction-diffusion problem can be solved and simulated successfully for both unsteady and steady state cases.**

***Index Terms*—enzyme-substrate system, finite difference method, reaction-diffusion problem, saturated steady state, unsaturated steady state**

I. Introduction

Chemical reaction problems may incorporate diffusion. This process is then called a reaction-diffusion problem. The reaction-diffusion process has been modelled into a mathematical equation. The derivation involves the so called Michaelis–Menten kinetics. The Michaelis–Menten kinetics itself has been widely recognised in chemistry for reaction problems [1, 2, 3, 4, 5, 6, 7].

A number of authors provide some studies of reaction-diffusion in chemical reaction problems. Lyons et al. [8, 9] derived a dimensionless model of the problem, where the system was a boundary value problem. The model of Lyons et al. [8, 9] was then studied by Rahamathunissa and Rajendran [10], where the system was changed to an initial value problem. Furthermore, Mahalakshmi and Hariharan [11] provide an approximation method for solving the initial value problem that was considered by Rahamathunissa and Rajendran [10]. The unsaturated and saturated steady state solutions to the initial value problem have been obtained by Rahamathunissa and Rajendran [10] using a variational iteration method. The variational iteration method was due to He [12, 13, 14] and it has been successfully used to solve various problems [15, 16, 17, 18, 19, 20, 21, 22, 23, 24] including the mathematical chemistry areas [25, 26, 27, 28, 29, 30].

In this paper, we provide an alternative method to solve unsaturated and saturated steady state problems. We implement the characteristic and direct-integration methods for ordinary differential equations in solving the unsaturated and saturated steady state problems. We also provide the unstability property of the equilibrium solution. In addition, finite difference methods for solving the unsteady and steady state problems are provided. Finite difference method has been shown to be powerful for solving various problems [31, 32, 33, 34, 35], which also include mathematical chemistry areas [36, 37, 38, 39, 40, 41, 42, 43, 44, 45].

This paper is simply organised as follows: we recall the mathematical models and provide their analytical properties; then, numerical finite difference methods are presented; afterwards, numerical results and discussion are provided; and finally, some concluding remarks are written.

II. Mathematical Models and Their Properties

Enzyme-substrate reaction-diffusion models have been derived by Lyons et al. [8]. In this section, we recall the models of unsteady and steady state cases.

A. Unsteady state model

We consider the following unsteady state dimensionless model

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\gamma u(x,t)}{1+\alpha u(x,t)} \tag{1}$$

with initial condition

$$u(x,0) = 0, \tag{2}$$

and boundary conditions

$$\frac{\partial u(0,t)}{\partial x} = 0, \qquad u(1,t) = 1. \tag{3}$$

Here the space domain is $0 \leq x \leq 1$, the time domain is $t \geq 0$, and $u(x,t)$ represents the concentration of substrate at any position x at any time t. In addition, parameters α and γ are positive constants relating to the reaction process (see [8, 9, 10, 11] for details).

B. Steady state model

For the steady state condition, time t does not influence the dynamics of the system. Therefore, the steady state model is the following ordinary differential equation

$$\frac{d^2 u(x)}{dx^2} - \frac{\gamma u(x)}{1+\alpha u(x)} = 0. \tag{4}$$

Let us consider the function

$$f(u) = -\frac{\gamma u}{1+\alpha u}. \tag{5}$$

This function f is zero if and only if $u = 0$. This $u = 0$ is the equilibrium solution. As

$$f'(u) = -\frac{\gamma}{(1+\alpha u)^2}, \tag{6}$$

we obtain $f'(0) = -\gamma$, which is a negative value. Here $f'(u) = df(u)/du$. Based on the theory of linear stability of equilibrium points [46], we infer that the equilibrium solution $u = 0$ is unstable. It means that any perturbation of the solution to the equilibrium solution $u = 0$ moves away (gets larger in amplitude) from this equilibrium.

1) Unsaturated catalytic kinetics: The unsaturated catalytic kinetics is achieved when $\alpha u << 1$. In this case, equation (4) can be reduced to

$$\frac{d^2u(x)}{dx^2} - \gamma u(x,t) = 0. \tag{7}$$

Here, we shall provide our contribution in providing the exact solution to equation (7) with boundary conditions

$$u'(0) = 0, \qquad u(1) = 1. \tag{8}$$

We derive the exact solution using the characteristic method of ordinary differential equation, as follows. Let us denote that λ is the characteristic variable. Then, the characteristic equation for equation (7) is

$$\lambda^2 - \gamma = 0. \tag{9}$$

The caracteristic roots of equation (9) is $\lambda_1 = \sqrt{\gamma}$ and $\lambda_2 = -\sqrt{\gamma}$. The general solution to equation (7) is

$$u(x) = c_1 \exp(\sqrt{\gamma}\, x) + c_2 \exp(-\sqrt{\gamma}\, x), \tag{10}$$

where c_1 and c_2 are constants. Incorporating boundary conditions (8) to general solution (10), we obtain that

$$c_1 = c_2 = \frac{1}{\exp(\sqrt{\gamma}) + \exp(-\sqrt{\gamma})}. \tag{11}$$

Therefore, the exact solution to equation (7) with boundary conditions (8) is

$$u(x) = \frac{\exp(\sqrt{\gamma}\, x) + \exp(-\sqrt{\gamma}\, x)}{\exp(\sqrt{\gamma}) + \exp(-\sqrt{\gamma})}. \tag{12}$$

We note that Rahamathunissa and Rajendran [10] used variational iteration method to obtain the exact solution to equation (7) with initial conditions

$$u(0) = a, \qquad u'(0) = 0, \tag{13}$$

where $u'(x) = du(x)/dx$. The exact solution to equation (7) with initial conditions (13) is [10]

$$u(x) = a \cosh(\sqrt{\gamma}\, x). \tag{14}$$

Here, we shall also provide an alternative derivation of the exact solution to equation (7) with initial conditions (13) using the characteristic method of ordinary differential equation, as follows. Knowing the general solution to equation (7) is given by equation (10), we incorporate initial conditions (13) to it. Then, we obtain

$$c_1 = c_2 = \frac{a}{2}. \tag{15}$$

Therefore, the exact solution to equation (7) with initial conditions (13) is

$$u(x) = \frac{a}{2}\left(\exp(\sqrt{\gamma}\, x) + \exp(-\sqrt{\gamma}\, x)\right). \tag{16}$$

Function (16) is identical with function (14).

2) Saturated catalytic kinetics: The saturated catalytic kinetics is achieved when $\alpha u >> 1$. In this case, equation (4) can be reduced to

$$\frac{d^2u(x)}{dx^2} - \frac{\gamma}{\alpha} = 0. \tag{17}$$

Here, we shall provide our contribution in providing the exact solution to equation (17) with boundary conditions (8). Integrating (17) twice with respect to x, we obtain that the general solution to equation (17) is

$$u(x) = \frac{\gamma}{2\alpha}x^2 + c_1 x + c_2, \tag{18}$$

where c_1 and c_2 are constants. Incorporating boundary conditions (8) with equation (17), we obtain

$$c_1 = 0, \qquad c_2 = 1 - \frac{\gamma}{2\alpha}. \tag{19}$$

Therefore, the exact solution to equation (17) with boundary conditions (8) is

$$u(x) = \frac{\gamma}{2\alpha}x^2 + 1 - \frac{\gamma}{2\alpha}. \tag{20}$$

Rahamathunissa and Rajendran [10] used variational iteration method to obtain the exact solution to equation (17) with initial conditions (13), and obtained that it is

$$u(x) = a + \frac{\gamma}{2\alpha}x^2. \tag{21}$$

Here, we provide an alternative derivation of exact solution (21), as follows. Recall that if we integrate (17) twice with respect to x, we obtain (18) where c_1 and c_2 are constants. Incorporating initial conditions (13) with equation (18), we obtain

$$c_1 = 0, \qquad c_2 = a. \tag{22}$$

Then, the exact solution to equation (17) with initial conditions (13) is

$$u(x) = \frac{\gamma}{2\alpha}x^2 + a, \tag{23}$$

which is identical with function (21).

III. Numerical Methods

Suppose that we are given a closed domain, where $x \in [0, 1]$ and $t \in [0, t_f]$, in which $t_f > 0$ is the final time. We take discrete points $\{x_0 = 0, x_1, x_2, ..., x_M = 1\}$ of space and $\{t^0 = 0, t^1, t^2, ..., t^N = t_f\}$ of time. Here $\Delta x = x_m - x_{m-1}$ for $m = 1, 2, 3, ..., M$, and $x_m = m\,\Delta x$ for $m = 0, 1, 2, ..., M$; in addition, $\Delta t = t^n - t^{n-1}$ for $n = 1, 2, 3 ..., N$, and $t^n = n\,\Delta t$ for $n = 0, 1, 2, ..., N$. We denote $u_m^n \approx u(x_m, t^n)$.

A. Finite difference method for the unsteady state model

A semi-discrete finite difference scheme for solving the unsteady state model (1) is

$$\frac{du_m}{dt} = \frac{u_{m+1} - 2u_m + u_{m-1}}{\Delta x^2} - \frac{\gamma u_m}{1 + \alpha u_m}. \tag{24}$$

Using the Euler method, the semi-discrete scheme (24) can be discretised further with respect to time t, so we obtain the fully-discrete finite difference scheme

$$u_m^{n+1} = u_m^n + \frac{\Delta t}{\Delta x^2}\left(u_{m+1}^n - 2u_m^n + u_{m-1}^n\right) - \frac{\gamma u_m^n \Delta t}{1 + \alpha u_m^n}. \tag{25}$$

Numerical treatment for the boundary conditions are as follows. The boundary condition at $x = 1$ is fixed to be

$u_M = 1$. For the boundary condition at $x = 0$, we introduce an artificial point $x = -\Delta x$, where the value at this artificial point is $u_{-1} = u_1$; this is in order that we enforce $du/dt = 0$, as required by the problem, at the second order accuracy.

B. Runge–Kutta methods for the steady state model

The steady state model (4) can be written equivalently into a system of two first order ordinary differential equations

$$\frac{du}{dx} = v, \tag{26}$$

$$\frac{dv}{dx} = \frac{\gamma u}{1 + \alpha u}. \tag{27}$$

The simplest Runge–Kutta type method for solving system (26)-(27) is the Euler's method given by

$$u_{m+1} = u_m + \Delta x\, v_m, \tag{28}$$

$$v_{m+1} = v_m + \Delta x\, \frac{\gamma u_m}{1 + \alpha u_m}. \tag{29}$$

The Euler method (28)-(29) is a first order accurate method.

There are many other Runge–Kutta type methods for solving system (26)-(27) with higher order accuracy, such as the second order Heun's method, third order Runge–Kutta method, fourth order Runge–Kutta method, and fifth order Dormand–Prince method. The later is a famous one due to Dormand and Prince [47] which is implemented in the MATLAB software as the ode45 algorithm [48, 49].

It is important to note that Runge–Kutta type methods are applicable for initial value problems. Because our problem is not an initial value one, but it is a boundary value problem, a Runge–Kutta method should be combined with another numerical method for solving the boundary value problem. For example, if we use a shooting method for boundary value problems, then we need to combine an ordinary differential equation solver (such as a Runge–Kutta method) with a root-finding method. However, this strategy may not be efficient. It is more convenient for us to run the finite difference method for the unsteady state case for a sufficient time; when the solution does not change with respect to time, then we have reached the steady state solution.

IV. Numerical Results and Discussion

In this section we report our numerical experiments and discussion about them. Both the unsteady and steady state cases are considered.

A. Unsteady state experiments

For the unsteady state experiments, we take $\gamma = 1$, $\alpha = 0.1$, $\Delta x = 0.1$, and $\Delta t = 0.01\Delta x$. Results for $t = 0.1$, $t = 0.3$, and $t = 9.0$ are plotted in Figure 1. We obtain that for $t = 0.1$ and $t = 0.3$, the system is unsteady. However, for large time, such as $t = 9.0$, the system has reached the steady state condition. The steady state condition is observed using the finite difference method in which the solution does not change with respect to time.

When the solution is unsteady, as time evolves, the solution graph moves from below going up until it reaches the steady state condition. This is realistic physically and matches mathematically with the fact that the equilibrium solution $u = 0$ is unstable. This means that if there exists a perturbation of the solution around $u = 0$, the perturbation moves away from the equilibrium solution $u = 0$.

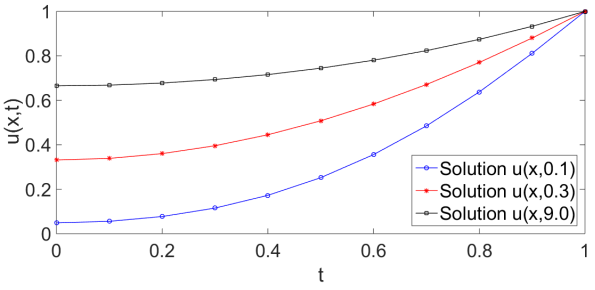

Fig. 1. Numerical results of the unsteady state solutions at time $t = 0.1$ and $t = 0.3$ together with the steady state solution at $t = 9.0$.

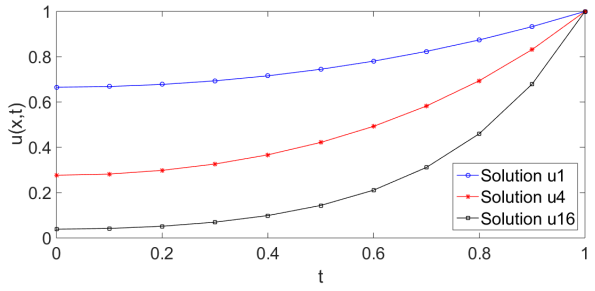

Fig. 2. Numerical results of the steady state solutions. Those for $\gamma = 1$ are denoted by u1, those for $\gamma = 4$ are denoted by u4, and those for $\gamma = 16$ are denoted by u16.

B. Steady state experiments

For the steady state experiments, we take $\alpha = 0.1$. Results for $\gamma = 1$, $\gamma = 4$, and $\gamma = 16$ are plotted in Figure 2. Here we use the finite difference method for the unsteady state case for a sufficient time; when the solution does not change with respect to time, then we have reached the steady state solution. We use the stopping criterion that the average of absolute difference between two consecutive iterative solutions is less than 10^{-15}.

We obtain that for steady state solutions, the larger the value of γ leads to the lower the concentration of the substrate in the system. This is realistic, because large value of γ corresponds to highly reactive system. That is, the substrate has a fast reaction in the system when γ is large.

V. Conclusion

We have solved the reaction-diffusion model using the characteristic and direct-integration methods analytically and finite difference method numerically. The exact solution to the unsaturated steady state case is derived based on the characteristic method for ordinary differential equations. The exact solution to the saturated steady state case is derived based on the direct-integration method. The finite difference method solves both the unsteady and steady state cases. Our results are applicable for electroactive polymer films. This research is limited to one-dimensional problems. Future research direction could model and solve problems in two and/or three dimensions.

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