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Karbala International Journal of Modern Science xx (2017) 1–13
http://www.journals.elsevier.com/karbala-international-journal-of-modern-science/

Homotopy perturbation method for kinetic analysis of thermal inactivation of jack bean urease

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Received 3 July 2017; revised 1 October 2017; accepted 12 October 2017

Abstract

In this work, theoretical modeling and determination of molar concentration of the native and denatured jack bean urease (EC 3.5.1.5) are presented. A three-reaction kinetic model of thermal inactivation of urease is analyzed using homotopy perturbation method. The obtained analytical solutions are used to study the kinetics of thermal inactivation of the enzyme as applied in biotechnology. From the results, it is established that the molar concentration of native enzyme decreases as the time increases while the molar concentration of the denatured enzyme increases as the time increases. The time taken to reach the maximum value of the molar concentration of native enzyme is the same as the time taken to reach the minimum value of the molar concentration of the denature enzyme. The molar concentration of the denatured enzyme reaches the steady state value when reaction time is less than or equal to 5s. Also, the molar concentration of the denatured enzyme becomes zero when rate constant of dissociation reaction of the native form of the enzyme into a denatured form, is less than or equal to 0.01 s^{-1}. The analytical solutions are verified with numerical solutions using Runge–Kutta with shooting method and good agreements are established between the solutions. The information given in this theoretical investigation will assist in the kinetic analysis of the experimental results over handling rate constants and molar concentrations.

Keywords: Kinetics; Thermal activation; Jack bean urease; Enzyme; Homotopy perturbation method

1. Introduction

Functionally, urease (urea amidohydrolase E.C.3.5.1.5) is a part of the superfamily of amidohydrolases and phosphotriesterases. It is a highly efficient catalyst for the hydrolysis of urea into carbon dioxide and ammonia. It catalyzes at a rate approximately 10^{14} times faster than the rate of the non-catalyzed reaction [1–12]. The hydrolysis of urea is catalyzed by urease to produce ammonia and carbamate and the carbamate produced is subsequently degraded by spontaneous hydrolysis to produce another ammonia and carbonic acid. Urease activity tends to increase the pH of its environment as it produces ammonia.

Jack bean urease, which is the most widely used plant urease, is a nickel containing oligomeric enzyme exhibiting a high degree of specificity to urea [2]. The importance and the various applications of the urease as

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Peer review under responsibility of University of Kerbala.

https://doi.org/10.1016/j.kijoms.2017.10.003

a good catalyst for hydrolysis of urea have attracted several research interests [2–21] especially in biotechnology and biomedical engineering studies. Also, the thermostability of jack bean urease has often been a subject of investigation [22–25]. However, there are few studies where the temporal loss of enzyme activity and the kinetic analysis of heat induced decay of enzyme activity were presented. Moreover, none of these studies involved consistent evaluation of kinetics of the urease inactivation. Most of the past studies described the complex mechanisms of thermal deactivation of enzymes as a "one step – two states" process where the native (active) form is transformed in the denaturated (inactive) form by a first order unimolecular irreversible reaction [24]. This unifying simplification is of interest for people focusing attention to phenomenological rather than mechanistic description of the kinetics of heat induced enzyme deactivation. However, the multitemperature evaluation revealed that an adequate kinetic model had to incorporate at least three reaction steps [24]. While the three-step mechanism model of inactivation of the enzyme has been developed by Illeova et al. [24], there is no provision of analytical solutions (except by Ananthi et al., [26]) for the predictions of model concentrations of the native enzyme, denature enzyme and temperature for thermal inactivation of urease. Ananthi et al., [26] applied homotopy analysis method to develop approximate analytical solutions for the analysis of kinetic and thermal inactivation of the enzyme. Although, the homotopy analysis method (HAM) is a reliable and efficient semi-analytical technique, but it suffers from a number of limiting assumptions such as the requirements that the solution ought to conform to the so-called rule of solution expression and the rule of coefficient ergodicity. Also, the use of HAM in the analysis of linear and nonlinear equations requires the determination of auxiliary parameter which will increase the computational cost and time. Also, the lack of rigorous theories or proper guidance for choosing initial approximation, auxiliary linear operators, auxiliary functions, and auxiliary parameters limit the applications of HAM. Moreover, such method requires high skill in mathematical analysis and the solution comes with large number of terms. In practice, analytical solutions with large number of terms and conditional statements for the solutions are not convenient for use by designers and engineers [26]. The determination of Adomian polynomials as carried out in Adomian decomposition method (ADM), the need for small perturbation parameter as required in traditional PMs, the rigor of the derivations of differential transformations or recursive relation as carried out in differential transformation method (DTM), the lack of rigorous theories or proper guidance for choosing initial approximation, auxiliary linear operators, auxiliary functions, auxiliary parameters, and the requirements of conformity of the solution to the rule of coefficient ergodicity as done in HAM, the search Langrange multiplier as carried out in variational iteration method (VIM), and the challenges associated with proper construction of the approximating functions for arbitrary domains or geometry of interest as in Galerkin weighted residual method (GWRM), least square method (LSM) and collocation method (CM) are some of the difficulties that are not experienced in HPM. Furthermore, in the class of the newly developed approximate analytical methods, homotopy perturbation method is considered to relatively simple with fewer requirements for mathematical rigor or skill. HPM solves differential equations, difference equation, differential-difference equations, fractional differential equation, pantograph equation and integro-differential equation. It solves nonlinear integral and differential equations without linearization, discretization, closure, restrictive assumptions, perturbation, approximations, round-off error and discretization that could result in massive numerical computations. It does not require small parameter in the algebraic or differential equation as done in the other traditional perturbation methods (Regular and singular perturbation). It provides excellent approximations to the solution of non-linear equation with high accuracy. Also, most of the above methods are limited to small domains. Applying the methods to large or infinite domain problems are often carried out with the applications of before-treatment techniques such as domain transformation techniques, domain truncation techniques and conversion of the boundary value problems to initial value problems or with the use of after-treatment techniques such as Pade-approximant, basis function, cosine after-treatment techniques, sine-after-treatment techniques and domain decomposition techniques. Indisputably, such additional computations through the before- and after-treatment techniques increase the computational cost and time. Furthermore, the search for a particular value that will satisfy second the boundary condition in DTM, HAM, ADM, and VIM necessitated the use of software and such could result in additional computational cost in the generation of solution to the problem. This drawback in the other approximation analytical methods is not experienced in HPM. HPM is a powerful method that gives acceptable analytical and accurate results with

Please cite this article in press as: M.G. Sobamowo, O.A. Adeleye, Homotopy perturbation method for kinetic analysis of thermal inactivation of jack bean urease, Karbala International Journal of Modern Science (2017), https://doi.org/10.1016/j.kijoms.2017.10.003