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Chapter 2

Mathematical Modeling and Simulation of Nonlinear Process in Enzyme Kinetics

Lakshmanan Rajendran, Mohan Chitra Devi, Carlos Fernandez and Qiuming Peng

Additional information is available at the end of the chapter

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Abstract

A deep and analytical understanding of the enzyme kinetics has attracted a great attention of scientists from biology, medicine, chemistry, and pharmacy. Mathematical models of enzyme kinetics offer several advances for this deep and analytical understanding due to their in compensable potential in predicting kinetic processes and anticipating appropriate interventions when required. This chapter concerns mathematical modeling analysis and simulation of enzyme kinetics. Experimental data and available knowledge on enzyme mechanics are used in constituting a mathematical model. The models are either in the form of linear or nonlinear ordinary differential equations or partial differential equations. These equations are composed of kinetic parameters such as kinetic rate constants, initial rates, and concentrations of enzymes. The nonlinear nature of enzymatic reactions and a large number of parameters have caused major issues with regard to efficient simulation of those reactions. In this work, an enzymatic system that includes Michaelis-Menten and Ping Pong kinetics is modeled in the form of differential equations. These equations are solved numerically in which the system parameters are estimated. The numerical results are compared with the results from an existing work in literature.

Keywords: mathematical modeling, enzyme kinetics, chemical kinetics, nonlinear reaction-diffusion equation, amperometric, cyclic voltammetry, chronoamperometric

1. Introduction

Enzyme kinetics is a challenging research field nowadays incorporating modern applied mathematics into biotechnology, engineering science, and pharmacy. Moreover, in medical studies, scientists work on human metabolism to improve the capabilities of some metabolites or enzymes in metabolic pathways. In industrial applications, kinetics methods are also widely used to
develop certain methods for improving functionality of some molecules in a cell. Many problems in theoretical and experimental biology/chemistry involve the solution of the steady-state reaction diffusion equation with nonlinear chemical kinetics. Such problems also arise in the formulation of substrate and product material balances for enzymes immobilized within particles [1, 2], in the description of substrate transport into microbial cells [3–5], in membrane transport, in the transfer of oxygen to respiring tissue [6, 7], and in the analysis of any artificial kidney system [8].

To impose the functionality of some molecules in a cell, a mathematical model of such metabolic systems must be constructed and simulated. Most of the dynamical systems can be approximated by various types of differential and integral equations involving finite number of variables and parameters. Thus, the future behavior of the system can be predicted if model kinetics parameters and initial states of the variables are available. In particular, ordinary and partial differential equations (ODEs and PDEs) are popular in modeling of the metabolic pathways or enzyme kinetics.

Releasing enzyme-substrate reactions under single-molecule kinetics was reported by Shlomi et al. [9]. An integral equation method with Michaelis-Menten kinetics to solve nonlinear diffusion problems in spherical coordinates was stated by Tosaka and Miyale [10]. Maalmi et al. [11] reported numerical and semianalytical solutions of nonlinear equations, which covered diffusivity, size, bulk concentration of reactant, binding constant of Michaelis-Menten kinetics, and site reactivity values. Merchant [12] stated the M-M decay reaction terms and the Gray-Scott scheme along with the semianalytical method to nonlinear reaction-diffusion systems. Indira and Rajendran [13] described a homotopy perturbation method to obtain substrate and product concentrations within the enzymatic layers. Removal of substrate from Michaelis-Menten kinetics governed the extravascular partition in which the analytical solution for the steady-state condition was investigated by Bucolo and Tripathi [14]. Dang Do and Greenfield [15] utilized the finite integral transform method to elucidate the problem based on the nonlinear reaction diffusion coupled with the chemical kinetics of a general shape solid. Chapwanya et al. [16] conveyed an epidemiological model with the Michaelis-Menten contact rate formulation to investigate variations in the enzyme kinetics with a simple susceptible infected recovered (SIR) model. Napper [17] proposed the Michaelis-Menten kinetics model to investigate the oxygen transport to heart tissue. Regalbuto et al. [18] presented an analytical methodology for obtaining solutions based on the maximum principle to nonlinear reaction-diffusion boundary value problems.

Rajendran and Saravanakumar [19] discussed mediated bioelectrocatalysis in order to build bioreactors, bio fuel cells, and biosensors.

Due to the difficulties in solving nonlinear differential equations in enzyme kinetics, some recent advanced analytical and numerical simulation techniques are used to solve the problems in chemical kinetics. Thus, in this review, all analytical and numerical works in enzyme kinetics are summarized.

2. Reaction diffusion systems

Reaction diffusion system is a mathematical model based on how the concentration of substances/products is disseminated over space changes under the influence of diffusion and a local
3. Nonlinear phenomena

The modern theory of the nonlinear reaction diffusion process is an important field in today’s science. The nonlinear system and coherent structures represent an interdisciplinary area with many nonlinear applications in various fields. Those applications can be divided into six disciplines: chemistry (autocatalytic chemical and enzyme reactions), physics (nonlinear optics and electric circuits, plasmas and states of solid, condensed atomic gases, hydrodynamics, galaxy dynamics and cosmology, fluid dynamics, and celestial mechanics), general relativity, biology (biofuel cell, bioreactor and biosensor, atmosphere and oceans, and animal dispersal), random media, and modern telecommunications. A great variety of phenomena in physics, chemistry, or biology can be described by nonlinear ODE/PDEs and particularly by reaction-diffusion equations. For these reasons, the theory of the analytical solutions of the reaction-diffusion equations is considered.

In reaction diffusion systems, nonlinear phenomena play a crucial role in applied mathematics and chemistry. Exact (closed-form) solution of nonlinear reaction diffusion equations plays an important role in the proper understanding of qualitative features of many phenomena and processes in various areas of natural science. The main result obtained from reaction and diffusion systems is that nonlinear phenomena include diversity of stationary and spatio-temporary dissipative patterns, oscillations, different types of waves, excitability, biostability, etc. But it is difficult for us to obtain the exact solution for these problems. The investigation of exact solution of nonlinear equation is interesting and important. In general, this results in the need to solve linear and nonlinear reaction diffusion equations with complex boundary conditions. The enzyme kinetics in biochemical systems have usually been modeled by differential equations, which are based only on reaction without spatial dependence of the various concentrations. The dimensionless nonlinear reaction diffusion equations are described below:

\[
\frac{\partial S}{\partial \tau} = \nabla^2 S - f(R, \tau, S, P) \tag{1}
\]

\[
\frac{\partial P}{\partial \tau} = \nabla^2 P + g(R, \tau, S, P) \tag{2}
\]
where $S$ and $P$ represent the dimensionless concentrations of substrate and product, $\tau$ represents the dimensionless time, and $R$ is the dimensionless radial co-ordinate of the particle. The first term on the right-hand side of the above equation accounts for active species (substrate or product) diffusion, whereas the second term $f(R, \tau, S, P)$ and $g(R, \tau, S, P)$ represents the homogeneous reaction term (nonlinear term), generally polynomial in the concentrations and time.

4. Common geometries and nonlinear reaction

Most commonly used electrodes/microelectrodes consist of a conducting metal/glassy carbon or semiconducting surface embedded in an insulating wall. When the conducting surface is a rectangle or disc of a few millimeters, this is known as a “planar” electrode. Diffusion to this surface is effectively planar (the effects of the edges are negligible), hence the nonlinear one-dimensional reaction diffusion equation is given by:

$$\frac{\partial[C]}{\partial \tau} = D \frac{\partial^2[C]}{\partial x^2} + f([C])$$  (3)

Two other electrode geometries where diffusion occurs in only one spatial dimension are the hemispherical and hemicylindrical electrodes. The nonlinear two-dimensional (hemispherical or spherical) reaction diffusion equation is:

$$\frac{\partial[C]}{\partial \tau} = D \left( \frac{\partial^2[C]}{\partial x^2} + \frac{2 \partial[C]}{r \partial r} \right) + f([C])$$  (4)

and for the latter is:

$$\frac{\partial[C]}{\partial \tau} = D \left( \frac{\partial^2[C]}{\partial x^2} + \frac{1 \partial[C]}{r \partial r} \right) + f([C])$$  (5)

The hemisphere can be achieved experimentally via a small drop of mercury positioned over a smaller conducting disc. A soft polymer, rubber, or other similar materials are usually employed to fabricate a hemicylinder. The electrodes are usually employed in theoretical studies due to the low dimensionality of the mass-transport equation. Additional terms such as diffusion and nonlinear reaction allow the equation to be solved analytically. Furthermore, the electrodes are not accurately or easily fabricated for practical geometries.

The corresponding nonlinear reaction-diffusion issues in enzyme kinetics are focused on the mathematical resolution. Table 1 shows the response of particular electrodes with special emphasis on earlier theoretical works in the field.

Example 1: Michaelis-Menten kinetics and microcylinder electrodes

The model is written for an enzyme reaction to generate an electro-active product (e.g., hydrogen peroxide from an oxidase enzyme) that reacts at an immobilization matrix, which
<table>
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<td>A. Meena et al.</td>
<td>Journal of Electroanalytical Chemistry 641(2010)35–44</td>
<td>Amperometric</td>
<td>$S + E_1 S_1 [E_1 S_1] E_2 \rightarrow P + E_2$</td>
<td>Homotopy perturbation method (HPM)</td>
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<tr>
<td>Author</td>
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<td>G. Rahamathunissa et al.</td>
<td>Journal of Mathematical Chemistry 9(2011)457–474</td>
<td>Chronoamperometric</td>
<td>$R + Z^k \rightarrow O + \text{Products}$</td>
<td>VIM</td>
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<td>S. Logambal, L. Rajendran</td>
<td>Journal of Membrane Sciences 373(2011)20–28</td>
<td>Amperometric</td>
<td>$E_{OX} + S + \frac{k_{cat}}{C_0} E \rightarrow E_{red} + P$</td>
<td>Homotopy perturbation method (HPM)</td>
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<td>S. Anitha et al.</td>
<td>Electrochimica Acta 56(2011)3345–3352</td>
<td>Amperometric</td>
<td>$E_{OX} + S + \frac{k_{cat}}{C_0} E \rightarrow E_{red} + P + E_2 A \rightarrow B$</td>
<td>Homotopy perturbation method (HPM)</td>
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<td>K. Indra, L. Rajendran</td>
<td>Electrochimica Acta 56(2011)6411–6419</td>
<td>Chronoamperometric</td>
<td>$S_1 + O_2 + P_2 + H_2O V_1$, $P_2 + 2e^- + 2H^+ \rightarrow S_2 E_1 + P$, $S_2 + \frac{1}{2} O_2 \rightarrow P_2 + H_2O V_2$</td>
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<td>S. Thiagarajan et al.</td>
<td>Journal of Mathematical Chemistry DOI: 10.1007/s10919-011-9854-z</td>
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<td>$S + M_{red} \rightarrow S M_{red} + P + M_{red}$</td>
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<td>M. Uma Maheswari, L. Rajendran</td>
<td>Journal of Mathematical Chemistry DOI: 10.1007/s10919-011-9853-0</td>
<td>Chronoamperometric</td>
<td>$E + S \rightarrow k_{cat} E \rightarrow E + P$</td>
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<td>P. Rijiravanich et al.</td>
<td>Electroanalytical Chemistry 589(2006)249</td>
<td>Amperometric</td>
<td>$O_2 + 2\text{catechol} \rightarrow 2$ o–quinone + $2H_2O$, o–quinone + $2H^+ + 2e^-$ \rightarrow $\text{catechol}$</td>
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<td>A. Eswari, L. Rajendran</td>
<td>Journal of Electroanalytical Chemistry 660(2011)200–208</td>
<td>Amperometric</td>
<td>$O_2 + 2\text{catechol} \rightarrow 2$ o–quinone + $2H_2O$, o–quinone + $2H^+ + 2e^-$ \rightarrow $\text{catechol}$</td>
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<td>G. Varatharajan, L. Rajendran</td>
<td>Applied Mathematics 2(2011)1140–1147</td>
<td>Amperometric</td>
<td>$S + E + \frac{k_{cat}}{k_{red}} \text{C}<em>{Q\text{red}} \rightarrow P + E$, $E</em>{red} \rightarrow E$</td>
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<td>K. Venugopal et al.</td>
<td>Journal of Biomedical Science and Engineering 4(2011)31–641</td>
<td>Chronoamperometric</td>
<td>$O_2 + 2\text{catechol} \rightarrow 2$ o–quinone + $2H_2O$, o–quinone + $2H^+ + 2e^-$ \rightarrow $\text{catechol}$</td>
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<td>K. Indra, L. Rajendran</td>
<td>Journal of Mathematical Chemistry DOI: 10.1007/s10919-011-9968-3</td>
<td>Chronoamperometric</td>
<td>$A \rightarrow B + C$, $B \pm e^- \rightarrow \text{products}$</td>
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<td>Journal of Mathematical Chemistry DOI: 10.1007/s10910-011-9973-6</td>
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<td>Author</td>
<td>Reference</td>
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<tr>
<td>S. Sevukaperumal et al.</td>
<td>Applied Mathematics 3(2012)373–381</td>
<td>Chronoamperometric</td>
<td>$\text{Glucose} + O_2 \rightarrow \text{gluconic acid} + H_2O_2$</td>
<td>Homotopy analysis method (HPM)</td>
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<td></td>
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<td>$\text{H}_2\text{O}_2 \rightarrow H_2\text{O}_2 + \frac{1}{2} \text{O}_2$</td>
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<td>V. Ašerisa et al.</td>
<td>Journal of Electroanalytical Chemistry 685(2012)63–71</td>
<td>Amperometric parallel substrates conversion</td>
<td>$S_i \rightarrow \frac{1}{2}p_1$</td>
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<td>V. Flexer et al.</td>
<td>Bioelectrochemistry 74(2008)201–209</td>
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<td>$S + E_{OX} \rightarrow S_i E \rightarrow p + E_{red}$</td>
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<td>R. Baronas et al.</td>
<td>Chemometrics and Intelligent Laboratory Systems 126(2013)108–116</td>
<td>Amperometric</td>
<td>$E + S_i h_i \rightarrow E S_{i E} \rightarrow E + P_i, i = 1, \ldots, k$</td>
<td>Numerical simulation</td>
</tr>
<tr>
<td>R. Baronas et al.</td>
<td>Sensors 12(2012)9146–9160</td>
<td>Amperometric</td>
<td>$E_{OX} + S_i h_i \rightarrow E_{red} + P_i E_{OX} + n_i e^{-}$</td>
<td>difference technique</td>
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<td></td>
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<td></td>
<td>Analytical, HPM&amp;HAM, VIM,ADM, etc.</td>
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</table>

Table 1. Contributions to the theoretical modeling of enzymatic electrodes.
is metallically conducting sites/particles. The reaction within the film under the Michaelis-Menten kinetics may be written as follows:

\[ S + E \xrightarrow{k_1} [E_1S] \xrightarrow{k_{cat}} P + E_2 \]  

(6)

The consumption rate of \( S \) is given by \( k_{cat}c_Sc_E/\frac{1}{K_M} \), where \( c_i \) denotes the concentration of species \( i \). The rate is equivalent to \( (k_{cat}/K_M)c_sc_E \), where \( K_M = (k_{-1}+k_{cat})/k_1 \). The consumption rate of \( S \) in the film is compensated by diffusion. If the solution is stirred uniformly, so that \( S \) is constantly supplied to the film, the mass balance for \( S \) can be written in cylindrical coordinates:

\[ \frac{D_S}{r} \frac{d}{dr} \left( r \frac{dc_S}{dr} \right) - k_{cat}c_Ec_S/\frac{1}{c_S + K_M} = 0 \]  

(7)

where \( c_S \) is the concentration profile of substrate, \( c_E \) is the concentration profile of enzyme, \( D_S \) is its diffusion coefficient, and \( K_M \) is the Michaelis constant. The rate of consumption will be \( v(r) = k c_H \), where \( k \) is the rate constant for the hydrogen peroxide reaction and \( c_H \) is the peroxide concentration. Then, the equation of continuum for hydrogen peroxide is generally expressed in the steady-state by

\[ \frac{D_H}{r} \frac{d}{dr} \left( r \frac{dc_H}{dr} \right) + k_{cat}c_Ec_S/\frac{1}{c_S + K_M} - v(r) = 0 \]  

(8)

At the electrode surface (\( r_0 \)) and at the film surface (\( r_1 \)), the boundary conditions are [29]:

\[ r = r_0 : \frac{dc_S}{dr} = 0, \quad c_H = 0 \]
\[ r = r_1 : c_S = c_S^*, \quad c_H = 0 \]  

(9)

where \( c_S^* \) is the bulk concentration of \( S \) scaled by the partition coefficient of the film. The current is provided by the consumption rate at each site. Thus, the total current at an electrode of length \( L \) is expressed by [29]

\[ I/nF = 2\pi L \int_{r_0}^{r_1} rv \, dr \]  

(10)

The analytical results of the problem are discussed by Eswari and Rajendran [30].

**Example 2: enzyme catalysis reaction**

The reactions without spatial dependence on various concentrations have modeled the enzyme kinetics in biochemical systems. Nonlinear systems of ordinary differential equations are solely based on that. Michaelis and Menten were pioneers in explaining the enzyme reaction model. In addition, they also reported the free enzyme binding to the reactant, which
produced an enzyme-reactant complex. Eq. (11) illustrates the Michaelis-Menten kinetics, in which the enzyme-substrate complex is formed after the enzyme is combined with the substrate.

\[
E + S \xrightarrow{k_1} ES \xrightarrow{k_2} E + P
\]  

(11)

As can be seen from Eq. (11), the product \( P \) is released by the binding of substrate \( S \) with enzyme \( E \). The product released is not reversible; however, the substrate binding is reversible. The reactants’ concentrations in Eq. (11) are represented by the following letters:

\[
s = [S], \ e = [E], \ c = [SE], \ p = [P]
\]  

(12)

The law of mass action leads to the system of following nonlinear reaction equations [31],

\[
\frac{ds}{dt} = -k_{1e}s + k_{-1}c
\]  

(13a)

\[
\frac{de}{dt} = -k_{1e}s + (k_{-1} + k_2)c
\]  

(13b)

\[
\frac{dc}{dt} = k_{1e}s - (k_{-1} + k_2)c
\]  

(13c)

\[
\frac{dp}{dt} = k_2c
\]  

(13d)

where \( k_1 \) is the forward rate of ES complex formation and \( k_{-1} \) is the backward rate constant.

The above problem is discussed theoretically by Meena et al. [32].

Example 3: Michaelis-Menten mechanism for co-substrate and substrate

Figure 1 illustrates Michaelis-Menten reaction kinetics scheme for co-substrate and substrate. Limoges et al. [33] reported for a redox enzymatic homogenous system along with one-dimensional mass transport equation a concise discussion and derivation.

When the enzyme is being solubilized, the electrochemical signal that is produced during the reaction is governed by the following set of nonlinear partial differential equations.

\[
\frac{\partial Q}{\partial t} = D_P \frac{\partial^2 Q}{\partial x^2} - \frac{C_E^0}{k_{1Q} + \frac{1}{k_{1Q}'} + \frac{1}{k_{1Q}''} + \frac{1}{k_{1Q}'''} + \frac{1}{k_{1Q}''''}}
\]  

(14)

\[
\frac{\partial S}{\partial t} = D_S \frac{\partial^2 S}{\partial x^2} - \frac{C_E^0}{k_{1S} + \frac{1}{k_{1S}'} + \frac{1}{k_{1S}''} + \frac{1}{k_{1S}'''} + \frac{1}{k_{1S}''''}}
\]  

(15)

where \( D_P, D_S \) are the diffusion coefficients of co-substrate and substrate, respectively; \( Q, S \) are the concentrations of co-substrate and substrate, respectively; \( x \) is the distance from the
electrode surface; $C^0$ is the bulk concentration of substrate; $C^T$ is the total concentration of enzyme; $k_1$, $k_2$, and $k_3$ are the reaction rate constants; and $t$ is the time. The initial and boundary conditions for Eqs. (14) and (15) are given by:

$$t = 0, x \geq 0, \text{ and } x = \infty, [S] = C^0_S$$

(16)

$$x = 0, t \geq 0 : [Q] = \frac{C^0_P}{1 + \exp \left( \frac{E - E^\circ_{P/Q}}{RT} \right)}, \ \frac{\partial [S]}{\partial x} = 0$$

(17)

$$x = \infty, \frac{\partial [Q]}{\partial x} = 0$$

(18)

The analytical expressions corresponding to the concentration of co-substrate for steady and nonsteady state conditions have been obtained by solving the above nonlinear equation using a new approach to homotopy perturbation method (HPM). Analytical expressions of the plateau current are also presented for steady and nonsteady state conditions:

$$i = FS D_P \left( \frac{\partial [Q]}{\partial x} \right)_{x=0}$$

(19)

where $E$ is the electrode potential, $E^\circ_{P/Q}$ is the standard potential of the P/Q couple, $F$ is the Faraday constant, and $S$ is the surface area of the electrode. The above problem is discussed theoretically by Rasi et al. [34].

5. Analytical solutions

To study many of the physical phenomena, the exact solutions of nonlinear partial or ordinary differential equations play an important role. In order to understand the mechanism of complicated dynamical processes and physical phenomena modeled by nonlinear differential equations, the existence of approximate analytical and exact solutions is very important. In
addition, nonlinear differential equations can also assist to investigate the stability of these solutions as well as checking the simulation analysis. Nonlinear partial differential equations govern a significant variety of phenomena including physical, chemical, and biological. The development of techniques aimed at exact solutions of nonlinear differential equations with nonsteady and steady state [35] has been one of the most exciting advances of nonlinear science and theoretical physics/chemistry. An important role in nonlinear science is played by exact solutions of differential equations. Furthermore, this can be especially observed in nonlinear physical chemistry science. This can be attributed to the provision of physical information as well as more insight into the physical aspects of the problem, which could lead to further applications. Over the past few decades, different methods have been reported to solve analytical solutions such as Tanh-sech [36], extended tanh [37], Jacobi elliptic function expansion [39], hyperbolic function [38], F-expansion [40], and the First integral [41]. To solve different types of nonlinear systems of PDEs, the sine-cosine method [42] has been employed. A variety of powerful analytical methods such as homotopy perturbation method [43–45], homotopy analysis method [46, 47], Adomian decomposition method [48, 49], wavelet transform method [50], etc. are applied to solve the nonlinear problems (e.g., Eqs. (8) and (13)–(15)) in chemical kinetics [51].

6. Numerical solutions

Many differential equations cannot be solved analytically. For practical purpose, however, such as in physical engineering sciences, a numerical approximation to the solution is often sufficient. The numerical method is mainly to solve complex problem physically or geometrically. It is also used to validate the experimental results. Some of the nonlinear equations in chemical kinetics were solved using numerical methods [52–56].

7. Summary

Most mathematical models of enzyme kinetics are based on reaction diffusion equations or rate equations containing nonlinear terms related to the kinetics of the enzyme reaction. Powerful and accurate analytical (HPM, HAM, ADM, etc.) and numerical mathematical methods have been employed for their resolution under steady and nonsteady state conditions. The theoretical results provide very useful insight into the effects on the performance of the thickness and structure of the enzymatic film, the loading of the different species, the diffusivity of the mediator, etc. Also, the theoretical modeling and simulation of these systems enable us to characterize the enzymatic reactions (i.e., rate constant, turnover rate, and Michaelis-Menten constants).

In spite of the above-mentioned benefits, there are only limited theoretical studies addressing kinetics of enzyme reaction and most of them include a number of simplifying assumptions mainly related to the mass and charge transport inside and outside the biocatalyst film, the enzymatic kinetic scheme, and the electrode morphology. Experimental validation of proposed
models is even more seldom. Therefore, more effort in the future research is needed in this direction in order to develop more detailed models and accurate simulations that can assist the rational development and optimization of enzyme electrodes.

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