CHAPTER - I

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1.1 INTRODUCTION

1.1.1. Mathematical modeling

The term model has a different meaning in model theory, a branch of mathematical logic. Models describe our beliefs about how the world functions. In mathematical modeling, we translate those beliefs into the language of mathematics. The process of beginning with a situation and gaining understanding about that situation is generally referred to as “modeling”. If the understanding comes about through the use of mathematics, the process is called mathematical modeling. Mathematical modeling is the link between mathematics and the rest of the world.

Mathematical modeling is the process of constructing mathematical objects whose behaviors or properties correspond in some way to a particular real-world system. A mathematical object could be a system of equations, a stochastic process, a geometric or algebraic structure, an algorithm, or even just a set of numbers. The term real-world system could refer to a physical system, a financial system, a social system, an ecological system etc.

Mathematical modeling is the art of translating problems from an application area into tractable mathematical formulations whose theoretical and numerical analysis provides insight, answers, and guidance useful for the originating application. Mathematical modeling

* is indispensable in many application

* is successful in many further applications
A mathematical model is a description of a system using mathematical concepts and language. The process of developing a mathematical model is termed mathematical modeling. Mathematical models are used particularly in the natural sciences (such as physics, biology, earth science, meteorology) and engineering disciplines (computer science, artificial intelligence) but also in the social sciences (such as economics, psychology, sociology and political science), physicists, engineers, statisticians, operations research analysts and economists.

Mathematical modeling is mostly used in the following areas with reference to biology such as protein folding, humane genome project, population dynamics, morphogenesis, evolutionary pedigrees, spreading of infectious diseases (AIDS) and animal and plant breeding (genetic variability). Particularly in chemistry, it is used in reaction dynamics, molecular modeling and electronic structure calculations. In physics, it is used in elementary particle tracking, quantum field theory predictions (baryon spectrum) and laser dynamics. In artificial intelligence also the following branches make use of mathematical modeling such as computer vision, image interpretation, robotics, speech recognition, optical character recognition and reasoning under uncertainty. In computer science, it is used in image processing, realistic computer graphics. In chemical engineering, it is used in chemical equilibrium and planning of production units.
Advantages of mathematical modeling

- Mathematics is a very precise language. This helps us to formulate ideas and identify underlying assumptions.
- Mathematics is a concise language, with well-defined rules for manipulations.
- All the results that mathematicians have proved over hundreds of years are at our disposal.
- Computers can be used to perform numerical calculations.

In this thesis some of the mathematical models in physical sciences are discussed.

1.1.2. Initial and boundary value problem

The general solution of differential equations gives information about the structure of the complete solution space for the problem. However, in practice, one is often interested only in particular solutions that satisfy some conditions related to the area of application. These conditions are usually of two types. They are called such as initial value problems and boundary value problems.

Boundary value problems are similar to initial value problems. A boundary value problem has conditions specified at the boundaries of the independent variable in the equation whereas an initial value problem has all of the conditions specified at the same value of the independent variable.

The symbolic solution of both initial value problems and boundary value problems requires knowledge of the general solution for the problem. The final step, in which the particular solution is obtained using the initial or boundary values, involves mostly algebraic operations, and is similar for initial value problems and boundary value problems.
Initial value problems and boundary value problems for linear differential equations are solved rather easily, since the final algebraic step involves the solution of linear equations. In non-linear differential equations, the solution could have several branches, or the arbitrary constants from the general solution could occur in different arguments of transcendental functions. As a result, it is not always possible to complete the final algebraic steps for non-linear problems. In this thesis some of the initial boundary value problems has been solved using various analytical techniques.

1.2 NON-LINEAR PROBLEMS IN PHYSICAL SCIENCE

1.2.1. Modeling of packed-bed immobilized enzyme reactor

Any realistic analysis of the packed-bed enzymatic reactor should include some fundamental aspects of the process such as liquid-phase and the solid-phase mass transfer, intrinsic kinetic parameters, and reactor hydrodynamics. Packed-beds are commonly employed for solid-fluid contacting in heterogeneous catalysis for several reasons: (i) it facilitates the contact and subsequent separation between reactant and catalyst; (ii) it allows reuse of the enzyme without the need for a prior separation; (iii) a continuous mode of operation can be used easily.

Lilly et al. [12] proposed a method to characterize packed-bed immobilized enzyme (IME) reactors, in which the exit concentration of substrate consumed is linearly plotted against fraction of substrate and the apparent Michaelis constant. On the other hand, Peter et al. [13] found that such a plot, made by using experimental data in the packed-bed immobilized β-galactosidase reactor, was deviated from linearity. Although several attempts [14,15] were made to theoretically interpret the experimental results, no decisive conclusion
has been derived because the models introduced were not sufficient. Shiraishi
previously derived expressions for the apparent kinetic parameters of IME reactions [16].
Shiraishi studied the design equation for a packed-bed immobilized enzyme reactor is
expressed in terms of apparent kinetic parameters and the relationship between the exit
concentration of substrate consumed and the logarithm of the exit unconverted fraction of
substrate [17]. In packed-bed immobilized enzyme reactor, the governing non-linear reaction
/ diffusion equation is expressed in the following non–dimensional form [17]:

\[ \frac{d^2U}{dX^2} + \frac{G-1}{X} \frac{dU}{dX} = \frac{\gamma_E U}{1 + \alpha U} \]  

(1.1)

with the boundary conditions:

\[ X = 0, \frac{dU}{dX} = 0 \]  

(1.2)

\[ X = 1, \frac{dU}{dX} = m(1-U) \]  

(1.3)

The effectiveness factor is given by

\[ Ef = \frac{(1 + \alpha)}{\gamma_E} \left[ \frac{dU}{dX} \right]_{X=1} \]  

(1.4)

Where \( U \) represent the dimensionless concentration and \( X \) is distance. \( \alpha \) and \( \gamma_E \) are
dimensionless parameters. To the best of author’s knowledge, no general analytical results of
substrate concentration and effectiveness factor for all values of dimensionless parameters \( \alpha \)
and \( \gamma_E \) have been published. In this thesis, an approximate analytical expressions for the
steady-state concentrations and effectiveness factor for all values of parameters \( \alpha \) and \( \gamma_E \)
are obtained by using the Homotopy perturbation method.
1.2.2. Modeling of immobilized glucoamylase kinetics by flow calorimetry

Wide applications of glucoamylase in starch industry, motivate the research aimed in the improvement of the enzyme properties by methods of enzyme screening, molecular biology and enzyme engineering. The potential improvement of industrial process by glucoamylase immobilization still intrigues researchers. This research can be facilitated by developing suitable method for the investigation of kinetic properties of immobilized glucoamylase. Immobilized glucoamylase kinetics by flow calorimetry is expressed in the following dimensionless form [18]:

\[
\frac{d^2 u}{dX^2} + \frac{2}{X} \frac{du}{dX} - \frac{ku}{1 + \alpha u + \beta u^2} = 0
\]  

(1.5)

With the boundary conditions:

\[
\frac{du}{dX} = 0 \text{ at } X = 0
\]  

(1.6)

\[u = 1 \text{ at } X = 1\]  

(1.7)

The dimensionless effective factor (\(\eta\)) is given by

\[
\eta = \frac{R^2 \varepsilon V}{3(1 - \varepsilon)C_{sb}} = \left(\frac{du}{dX}\right)_{X=1}
\]  

(1.8)

Where \(u\) represent dimensionless concentration, \(X\) is dimensionless distance, \(k, \alpha\) and \(\beta\) are dimensionless parameters. Vladimir Stefuca et.al [18] simplified this task by reducing the experiment to the initial rate measurement in combination with the FC avoiding the requirement of a more complicated chemical analysis. For the purpose of the methodology development, the enzyme was immobilized in controlled-pore glass (CPG) particles and a
well defined substrate – maltodextrin (MDX) - was used. However, to the best of author’s knowledge, the steady state analytical expression of immobilized glucoamylase and effectiveness factor have not been derived. In this thesis, we have obtained the analytical expression of immobilized glucoamylase and effectiveness factor for all values of parameters for steady state condition using the modified Adomian decomposition method.

1.2.3. Modeling of chemical absorption of carbon dioxide and phenyl glycidyl ether solution

The chemical fixation of carbon dioxide has received much attention in view of environmental problems. An attractive strategy to deal with this situation is converting carbon dioxide into valuable substances. The overall reaction between CO$_2$ and phenyl glycidyl ether (PGE) to form the 5 – membered cyclic carbonate is as follows [19]:

$$\text{R} + \text{CO}_2 \rightarrow \text{R} - \text{O} - \text{C}_6\text{H}_5$$

where R is a functional group of –CH$_2$-O-C$_6$H$_5$. The overall reaction of equation (1.9) consists of two consecutive steps: 1) a reversible reaction between PGE (B) and THA-CP-MS41 (QX) to form an intermediate complex (C$_1$); 2) an reversible reaction between C$_1$ and CO$_2$ (A) to form QX and five-membered cyclic carbonate (C):

$$B + QX \rightleftharpoons C_1$$

$$A + C_1 \rightarrow C + QX$$

Mass transfer with chemical reaction using absorption of carbon dioxide into phenyl glycidyl ether solution is expressed in the following dimensionless form as [19]:
\[
\frac{d^2 a}{dx^2} = \frac{\alpha_1 ab}{1 + \beta_1 a + \beta_2 b} \tag{1.12}
\]

\[
\frac{d^2 b}{dx^2} = \frac{\alpha_2 ab}{1 + \beta_1 a + \beta_2 b} \tag{1.13}
\]

With the boundary conditions:

\[
a = 1, \quad \frac{db}{dx} = 0 \quad \text{at} \quad x = 0
\tag{1.14}
\]

\[
a = k, \quad b = 1 \quad \text{at} \quad x = 0
\tag{1.15}
\]

The flux of carbon dioxide is given by

\[
\beta = \left( \frac{da}{dx} \right)_{x=0}
\tag{1.16}
\]

Where \(a\) is the concentration of CO\(_2\), \(b\) is the concentration of PGE, \(\alpha_1, \alpha_2, \beta_1, \beta_2\) are normalized parameters and \(x\) is the dimensionless distance. Park et al. [19] investigated the chemical absorption of carbon dioxide and phenyl glycidyl ether solution containing the catalyst THA-CP-MS41 in a heterogeneous system. To our knowledge no analytical solutions of this model have been reported. In this thesis, we present the simple approximate analytical expression for the steady-state concentrations of CO\(_2\), PGE and flux using the Adomian decomposition method.

1.2.4. Mathematical modeling of a biofilm

Biofilms occur when microorganisms (bacteria, algae, unicellular organisms) adhere to the interfaces between gas and liquid phases (e.g., the water surface), liquid and solid phases (e.g., the stony bottom), or two liquid phases (e.g., an oil drop in water) [20].
Of greatest importance are vander Waals forces, electrostatic attraction, or hydrogen bonds. Their activity can have an adverse effect, e.g., if biofilms damage materials (biocorrosion) [21], or it can also be beneficial, e.g., in water purification in nature and technology [22].

Steady state problem of substrate consumption by a biofilm is expressed in the following form [26]:

\[
D_f \frac{d^2 S_f}{dz^2} = q \frac{S_f}{K + S_f} X_f
\]  

(1.17)

The boundary conditions are

\[
z = 0, \quad \frac{dS_f}{dz} = 0 \quad (1.18)
\]

\[
z = L_f, \quad S_f = S_i \quad (1.19)
\]

Where \( S_f \) is the substrate concentration in the biofilm, \( K \) is the Michaelis-Menten constant, \( z \) is the co-ordinate, \( L_f \) is the biofilm thickness, \( D_f \) is the diffusion coefficient within the biofilm, \( q \) is the substrate consumption rate constant and \( S_i \) is the substrate concentration outside the biofilm. Dueck et al., [23-25] described the mathematical modeling of evaluation of biofilm with allowance for its erosion. Recently, Minkov et al., [26] obtained the analytical expression for the substrate flux into the biofilm as the function of volumetric flow rate of the substrate solution. To my knowledge no rigorous analytical solution of concentration of substrate and flux into the biofilm for a square law of microbial death rate with steady-state conditions has been reported. In this thesis, we present an approximate analytical expressions for the steady-state concentration of substrate and flux into the biofilm using the Adomian decomposition method for all values of biofilm thickness and substrate concentration outside the biofilm.
1.3 OBJECTIVES AND SCOPE OF THE PRESENT INVESTIGATION

The objectives of the present investigation are as follows:

* To derive the analytical expression of concentration of substrate and effectiveness factor in a packed-bed immobilized enzyme reactor using Homotopy perturbation method.

* To find the approximate analytical expression of substrate concentration and effectiveness factor of immobilized glucoamylase kinetics by flow calorimetry using modified Adomian decomposition method. The model is based on non stationary diffusion equation containing a non-linear term related to kinetics of the enzymatic reaction.

* To evaluate approximate analytical expression of carbon dioxide and phenyl glycidyl ether solution for all values of parameters by solving system of non linear diffusion equations.

* To present the mathematical modeling of biofilm by solving single non-linear ordinary differential equation using Adomian decomposition method. Analytical results compare with the available numerical results.

1.4 ORGANIZATION OF THE RESEARCH WORK

This thesis presents theoretical results on the development of mathematical expressions to study the physical science problems. Particular emphasis is put on solving the system of non-linear differential equations in initial boundary value problems at physical science. The overall objective of the work is to produce analytical, or approximate expressions and numerical solutions which predict the assessment of the substrate
concentrations in packed-bed immobilized enzyme reactor, immobilized glucoamylase kinetics by flow calorimetry, carbon dioxide and phenyl glycidyl ether solution, and biofilm.

In Chapter 1, a short introduction to mathematical modeling and initial boundary value problem was presented.

In Chapter 2, a simple and closed approximate analytical expression of the steady-state concentrations and effectiveness factor in a packed-bed immobilized enzyme reactor for all values of the reaction diffusion parameters using Homotopy perturbation method was presented. This model is based on system of reaction-diffusion equations containing a non-linear term related to Michaelis-Menten kinetics of the enzymatic reaction. The result of this work is simple approximate calculations of concentration and effectiveness factor for all values of dimensionless parameters $\alpha$ and $\gamma_E$.

In Chapter 3, a non-linear reaction differential process in immobilized glucoamylase kinetics by flow calorimetry is discussed. This model is based on steady-state diffusion reaction equation containing a non-linear term in reaction rate. An approximate analytical expression of substrate concentration and effectiveness factor for all possible values of the kinetic parameters are derived using the modified Adomian decomposition method. The obtained results are compared with numerical simulation and are found to be in good agreement.

In Chapter 4, mathematical analysis corresponding to the diffusion and reaction kinetics in chemical reaction between carbon dioxide and phenyl glycidyl ether solution is presented. The approximate analytical expressions for the steady state concentration of carbon dioxide, phenyl glycidyl ether and flux are obtained for all values of parameters using Adomian decomposition method. The obtained results are compared with numerical simulation and are found to be in good agreement.
In Chapter 5, a mathematical model by a biofilm is discussed. The second order non-linear differential equation is solved both analytically and numerically. The approximate analytical expressions for the steady state substrate concentrations for all values of biochemical parameters were obtained using Adomian decomposition method. Furthermore, an analytical expression corresponding to the steady state flux response is also presented. The obtained results are compared with numerical simulation and are found satisfactory agreement with the existing result.

In Chapter 6, we discuss about overall conclusion and future enhancements of the thesis.