COMPLEX BOUNDARY VALUE PROBLEMS OF NONLINEAR DIFFERENTIAL EQUATIONS

SYNOPSIS SUBMITTED TO MADURAI KAMARAJ UNIVERSITY IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE OF

DOCTOR OF PHILOSOPHY

IN

MATHEMATICS

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JUNE - 2019

INTRODUCTION

1. Mathematical Modeling

Mathematical modeling is the art of building mathematical objects, such as equations, shapes, or games, which share certain desired properties with observed phenomena. Also, the mathematical model is a mathematical framework based on a piece of the real world. It could be of varying levels of descriptive detail like sketches of a flower in an artist's the real world, but nevertheless they are extremely useful, and mathematics also lets us carefully study those assumptions and minimize their impact. The modeling process may or may not result to solving the problem entirely, but it will shed light to the situation under investigation [1].

Also, mathematical modeling is a principled activity that has both principles behind it and methods that can be successfully applied. The principles are over-arching or meta-principles phrased as questions about the intentions and purposes of mathematical modeling. These meta-principles are almost philosophical in nature [2]. The methodological modeling principles are also captured in the following list of questions: what are we looking for?, what do we want to know?, what do we know?, what can we assume?, how should we look at this model?, what will our model predict?, are the predictions valid?, are the predictions good?. The figure below shows key steps in modeling process.

From the modeling process, the problem situation has to be understood by the problem solver, this means that situation model has to be constructed. Then the situation has to be simplified and structured leading to a real model of the situation. Mathematization transforms the real model into a mathematical

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model which consists here of certain equations. Working mathematically (calculating, solving the equations, etc.) yields mathematical results, which are interpreted in the real world as real results.
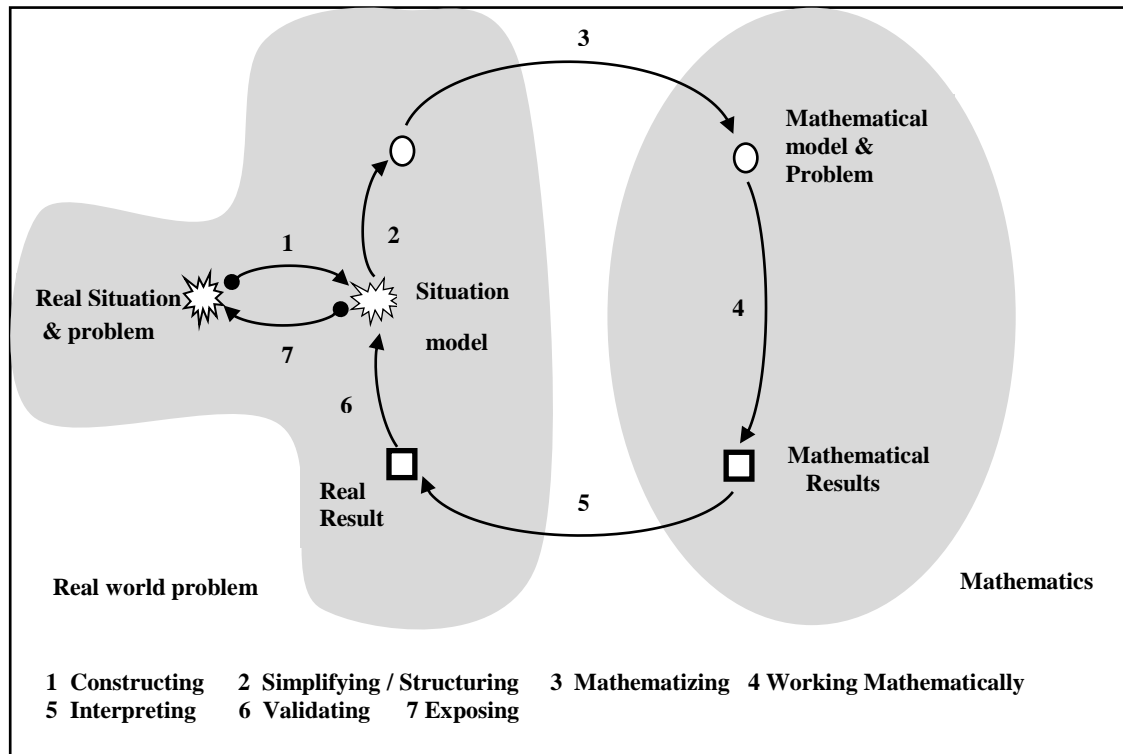

Fig. 1: Schematic diagram of the mathematical modeling cycle.

In this chapter, mathematical modeling of the SCR reaction network, mathematical modeling of multi-step enzyme systems immobilized on porous electrodes, mathematical modeling of a solid catalyzed reactive HiGee stripping, mathematical modeling of diffusion and reaction within the E-matrix of sandwich type amperometric biosensor and mathematical modeling of amperometric enzyme electrodes and mathematical modelling of the ethanol and acetaldehyde in a fixed bed laboratory reactor are discussed.

2. Nonlinear Phenomena

Nonlinear phenomena are phenomena, which, in contrast to a linear system, cannot be explained by a mathematical relationship of proportionality (that is, a linear relationship between two variables). For example, the spread of an infectious disease is most often exponential, rather than linear, with time. Also, many plausible dynamical models of complex biological systems, ranging from representations of the mode of action of enzymes, via the regulation of the vertebrate immune system, to species interactions at the population level, exhibit highly nonlinear patterns of behavior [3 - 5]. In mathematical point of view, we cannot obtain the exact solution for non-linear systems. But it's difficult to solve, nonlinear systems are commonly approximated by linear equations.

Also, Nonlinear phenomena frequently appear in many areas of the natural sciences such as physics [6-8], chemistry [9-11], biology [11-13], general relativity [14], random media [15-17], modern telecommunication[18,19], and so on. It can be narrated by the nonlinear differential system (ODE/PDEs) and specifically by reaction - diffusion equations.

3. Complex Boundary Value Problems

Complex boundary value problems of nonlinear differential equations have merged as an interesting and fascinating branch of applied mathematics and pure mathematics with a wide range of applications in industry, economics, biology, physics, chemistry, social, and pure and applied sciences. A boundary value problem in one dimension is an ordinary differential equation together with conditions involving values of the solution and/or its derivatives at two or more points. The number of conditions imposed is equal to the order of the differential

equation. Usually, boundary value problems of any physical relevance have these characteristics: (1) The conditions are imposed at two different points; (2) the solution is of interest only between those two points; and (3) the independent variable is a space variable, which we shall represent as x [20].

In a mathematical modelling system of nonlinear initial and boundary value problems appear in many areas such as physics, chemistry, biology, engineering, and so on. Also, a solution of initial and boundary value problem is a solution to the differential equation which also satisfies the boundary conditions. Problems involving non-linear differential equations are extremely, diverse, and methods of solution or analysis are problem dependent. In this thesis, some of the initial and boundary value problems in chemical sciences are solved using the Homotopy perturbation method, Modified Adomian decomposition method, Akbari - Ganji's Method and He's Variational Iteration Method.

4. Reaction Diffusion Systems

Reaction - diffusion systems are mathematical models which describe the behaviour of a large range of chemical systems where diffusion of material competes with the production of that material by some form of chemical reaction. Also, it arises in many branches of physics, chemistry, biology, ecology etc. Reviews of the theory and applications of reaction-diffusion systems can be found in books and numerous articles (see, for example [21 - 23]). These arise in a large variety of application areas, such as flow in porous media [24], heat conduction plasma [25], combustion problems [26], liquid evaporation [27], and of more recent interest, image processing [28].

Exact solution of nonlinear reaction diffusion equations plays an important role in proper understanding of qualitative features of many phenomena and reaction diffusion systems is that nonlinear phenomena include diversity of stationary and spatio-temporal dissipative patterns, oscillations, different types of waves, excitability, bistability 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 the reaction without spatial dependence of the various concentrations. The dimensionless nonlinear reaction diffusion equations are

$$\frac{\partial S}{\partial \tau} = \nabla^2 S - f(R, \tau, S, P)$$
$$\frac{\partial P}{\partial \tau} = \nabla^2 P - g(R, \tau, S, P)$$

(1)

Where S and P represent the dimensionless concentrations of substrate and product, τ represents the dimensionless time and R is the dimensionless radial coordinate of the particle. The first term on the right hand side of the above equation accounts for active species (substrate and product) diffusion, whereas the second term $f(R, \tau, S, P)$ and $g(R, \tau, S, P)$ represent the homogeneous reaction term (nonlinear term), generally polynomial in the concentrations and time.

5. Using Asymptotic Methods to solve the Strongly Nonlinear Differential Equations
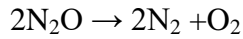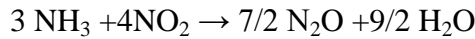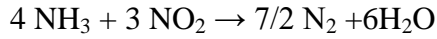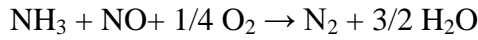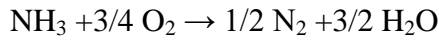
In recent years much of the attention is devoted to finding the analytical solution for the case of strongly nonlinear differential equations using some asymptotic techniques. Analytical solution provides a clear view into how variables and interactions between the variables affect the result. It is more efficient than numerical solution. Solving system of nonlinear differential equations helps the researcher to understand a physical problem better, and may help in improving the future procedures and designs used to solve their problems. Several asymptotic methods like Pade approximation method (PAM)[29], Variational iteration method (VIM)[30], Homotopy analysis method (HAM)[31], Homotopy perturbation method (HPM) [32], Modified Adomian decomposition method (MADM) [33], Akbari-Ganji's Method (AGM) [34], and He's Varaitional Iteration method [35] and so on are available to find analytical solutions of strongly nonlinear differential equations in any branches of physics, chemistry, biology, ecology etc.

6. Mathematical Modeling of Chemical Science

The Mathematical modeling framework for biochemical systems based on ordinary differential equations (ODE) or partial differential equations (PDE), in which biochemical processes are represented. In this thesis, nonlinear differential equations of the SCR reaction network, multi-step enzyme systems, catalyzed reactive HiGee stripping amperometric biosensor and electroactive polymer film are considered for a theoretical analysis.

6.1 Reaction Equations for the Global Kinetic Model in SCR Reaction Network

The mathematical model studied in the present work concerns the reaction - diffusion equations for different enzymatic reaction mechanisms. The model develops the reaction-diffusion equation in the global kinetic model and the steady-state equations to determine the concentration profiles of NH_3, NO, NO_2 and N_2O to assess the design and performance of such reactors [36]. In the SCR reaction network, there are seven reactions estimate in the global kinetic model and parameter estimation as follows:

$NH_3 + 3/4 \ O_2 \rightarrow 1/2 \ N_2 + 3/2 \ H_2O$

$NO + 1/2 \ O_2 \rightleftarrows NO_2$

$NH_3 + NO + 1/4 \ O_2 \rightarrow N_2 + 3/2 \ H_2O$

$2 \ NH_3 + NO + NO_2 \rightarrow 2N_2 + 3 \ H_2O$ \hfill (2)

$4 \ NH_3 + 3 \ NO_2 \rightarrow 7/2 \ N_2 + 6H_2O$

$3 \ NH_3 + 4NO_2 \rightarrow 7/2 \ N_2O + 9/2 \ H_2O$

$2N_2O \rightarrow 2N_2 + O_2$

For the above reaction schemes, the kinetic equations for NH_3, NO, NO_2 and N_2O are as follows:

$$r_1 = \frac{k_1 \, C_{NH_3} \, C_{O_2}}{1 + K_{NH_3} \, C_{NH_3}} \; ; r_2 = k_2 \left(C_{NO} \, C_{O_2}^{0.5} - C_{NO_2} / K_{NO}^{eq.} \right); r_3 = \frac{k_3 \, C_{NH_3} \, C_{NO} \, C_{NO_2}}{1 + K_{NH_3} \, C_{NH_3}} \; ;$$

$$r_4 = \frac{k_4 \, C_{NH_3} \, C_{NO} \, C_{NO_2}}{1 + K_{NH_3} \, C_{NH_3}} \; ; \; r_5 = \frac{k_5 \, C_{NH_3} \, C_{NO_2}}{1 + K_{NH_3} \, C_{NH_3}} \; ; r_6 = \frac{k_6 \, C_{NH_3} \, C_{O_2}}{1 + K_{NH_3} \, C_{NH_3}} \; ; r_7 = k_7 \, C_{N_2O} \, C_{NO_2} \quad (3)$$

The nonlinear differential equation that reaction rate for each component in the medium is evaluated as:

$$\frac{dC_{NH_3}}{d[W/Q]} = -\left(r_1 + r_3 + 2\,r_4 + 4\,r_5 + 3\,r_6\right) \tag{4}$$

$$\frac{dC_{NO}}{d[W/Q]} = -\left(r_2 + r_3 + r_4\right) \tag{5}$$

$$\frac{dC_{NO_2}}{d[W/Q]} = r_2 - r_4 + 3\,r_5 - 4\,r_6 \tag{6}$$

$$\frac{dC_{N_2O}}{d[W/Q]} = \frac{7}{2}\,r_6 - 2\,r_7 \tag{7}$$

where C_i is the concentration of i species calculated in the kinetic model ($i = NH_3$, NO, NO_2 and N_2O), k_i is the kinetic rate constants of reaction i ($i = 1$ to 7), K_{NH_3} and $K^{eq.}_{NO}$ are the equilibrium constant of NH_3 and NO respectively, r_j is the rate of reaction j ($j = 1$ to 7), and W/Q is the space time.

The corresponding an initial condition for the Eqns. (4) - (7) is followed:

at $[W/Q] = 0$; $C_{NH_3} = a_1, C_{NO} = a_2, C_{NO_2} = a_3$ and $C_{N_2O} = a_4$ \tag{8}

In this thesis the Homotopy perturbation method is employed to solve the above system of nonlinear diffusion equations for the steady-state condition, in particular, this problem has faster convergence when the above said method is applied.

6.2 Reaction - Diffusion Equations Within the E-Matrix of Sandwich Type Amperometric Biosensor

Amperometric biosensors measure the changes in current at the working electrode that resulted from the biochemical and electrochemical reaction. In amperometric biosensors, the potential is held constant and the current is measured [37, 38]. Of the various types of available enzymatic biosensors, the sandwich type amperometric biosensors have been widely used due to sensitivity and rapid responsiveness. In order to model the response of enzymatic nanobiosensors more complicated mathematical approaches have to be employed [39]. The reaction that occurs within the enzymatic membrane is as follows [39]:

$$E_r + S \underset{k_{-1}}{\overset{k_1}{\leftrightarrow}} E_r S \xrightarrow{k_2} E_o + R \tag{9}$$

$$E_o + M \underset{k_{-3}}{\overset{k_3}{\leftrightarrow}} E_o M \xrightarrow{k_4} E_r + P \tag{10}$$

where E_r and E_o are the reduced and oxidized forms of the enzyme, while $E_r S$ and $E_o M$ are the intermediate complexes of the enzyme with substrate and mediator, respectively. The reaction at the electrode surface is

$$P \xrightarrow{-2e^-} M \tag{11}$$

where 'P' and 'M' is the oxidized and reduced form of the mediator.

From Eqns.(9) and (10) the following expression for the reaction rate can be obtained

$$v = \frac{v_{max}}{1 + K_S / C_S + K_M / C_M} \tag{12}$$

where $K_S = k_4(k_{-1} + k_2)[(k_2 + k_4)k_1]^{-1}$, $K_M = k_2(k_{-3} + k_4)[(k_2 + k_4)k_3]^{-1}$,

$$v_{max} = C_E k_{cat} = C_E k_2 k_4 [(k_2 + k_4)]^{-1},$$

where K_S and K_M are usually called the Michaelis-Menten constants for S and M respectively. The reaction on the enzymatic matrix for the steady-state condition can be described by the set of nonlinear reaction / diffusion equations as follows:

$$D_S \frac{d^2 C_S}{dx^2} = D_M \frac{d^2 C_M}{dx^2} = -D_P \frac{d^2 C_P}{dx^2} = -D_R \frac{d^2 C_R}{dx^2} = v \qquad (13)$$

where D_S, D_M, D_P and D_R are the diffusion coefficients for the species within the membrane respectively. Here x denotes distance, C_S, C_M, C_P and C_R are the concentrations of S, M, P and R respectively. The boundary conditions for the above system of nonlinear equation are as follows:

$$\frac{dC_S}{dx} = 0; \frac{dC_M}{dx} = 0; C_P = 0; \frac{dC_R}{dx} = 0 \qquad \text{at} \qquad x = 0 \qquad (14)$$

$$C_S = C_S^*; C_M = C_M^*; C_P = C_R = 0 \qquad \text{at} \qquad x = l \qquad (15)$$

where l denotes the thickness of the E-matrix. C_S^* and C_M^* are the concentrations in the external solution. In this thesis, the modified Adomian decomposition method is employed to solve the above system of coupled nonlinear diffusion equations for the steady - state condition, as it has rapid convergence for this kind of rate equations.

7. Objectives and scopes of the present investigation

The objectives of the present investigation are as follows:

➢ To derive the approximate analytical expressions corresponding to the concentration of NH_3, NO, NO_2 and N_2O in the global kinetic model of the SCR network model using the Homotopy perturbation method.

- To obtain the analytical expressions to the concentration of the substrate and mediator multi – step enzyme electrodes using the Homotopy perturbation method.

- To discuss the mathematical model for solid catalyzed reactive HiGee stripping model.

- To derive the closed – form of analytical expressions of the concentrations of substrate, mediator and product in the E-matrix of sandwich type amperometric biosensor using the Modified Adomian decomposition method (MADM).

- To evaluate the approximate analytical solution of the concentration of substrate in electroactive polymer film using the Akbari - Ganji's Method (AGM).

- To derive the analytical expersions for the concentrations of the ethanol and acetaldehyde in a fixed bed laboratory reactor by using the He's variational iteration method.

8. Organization of the Research Work

- This thesis presents the approximate analytical expression on the development of a mathematical model to study the kinetics of reaction diffusion processes in boundary value problems. In particular, it is put on solving the nonlinear differential equations with boundary condition on reaction and diffusion process. The overall objective of this thesis is to provide analytical expressions for the concentrations, the validity of the present solution, estimation of kinetic parameter etc. A variety of analytical and numerical methods are employed to obtain the analytical expressions under steady - state conditions.

- ➤ **Chapter one** presents a brief introduction to mathematical modeling, the relevant systems of equations describing reaction diffusion process, nonlinear phenomena, various asymptotic techniques and biochemical systems.

- ➤ **Chapter two** analyzes the mathematical model of the SCR reaction network model. The approximate analytical expressions corresponding to the concentration of NH_3, NO, NO_2 and N_2O have been obtained using the Homotopy perturbation method (HPM).

- ➤ **Chapter three** presents the diffusion-kinetic model of the steady-state concentration and current density for immobilization of all enzymes. Furthermore, it is possible to calculate the approximate amounts of the concentrations and current corresponding to a nonlinear Michaelis – Menten kinetic scheme.

- ➤ **Chapter four** discusses the mathematical model for the solid catalyzed reactive HiGee stripping under the three phases of reaction viz. Catalyzed phase, Liquid phase and Gas phase. This model is based on the nonlinear reaction diffusion equations. The developed second order governing differential equations represents catalyzed phase is solved analytically and numerically using modified Adomain decomposition method and Finite element method using a MATLAB program respectively. Also, we have derived the analytical solutions for liquid and gas phases using Homotopy perturbation method. In addition, we have presented the analytical expression for the effectiveness factor for all the concentration under the diffusional restrictions.

- ➤ **Chapter five** discusses the E-matrix of sandwich type amperometric biosensor for steady-state condition of the diffusion and reaction. The model is based on the diffusion equation involving non-linear terms related to enzyme kinetics. A closed-form of analytical expressions of concentrations corresponding to the

biosensor current for the steady-state condition is derived. Concentrations of substrate, mediator and product are expressed in terms of single dimensionless parameters. Adomian decomposition method (ADM) is employed to solve the system of non-linear reaction diffusion equations. The analytical results are compared with the experimental and numerical results. The analytical current curve fits very well with the experimental current curves.

➢ **Chapter six** analyzes the mathematical modeling of the electroactive polymer film. This mathematical model describes substrate is considered to form a complex with the immobilized catalyst which subsequently decomposes to form a product. We will apply the AGM for an analytical approximation of substrate in the electroactive polymer film. The AGM yields a rapidly convergent, easily computable and readily verifiable sequence of analytic approximations that are convenient for parametric simulations.

➢ **Chapter seven** investigated the effects of nonlinear behaviour of the dimensionless concentrations of the ethanol and acetaldehyde in a fixed bed laboratory reactor. The main aim of this study is based on solving the nonlinear differential equation of concentration of the ethanol and acetaldehyde by using the He's variational iteration method. The analytical solution have been compared with numerical result in order to achieve conclusions based on not only for accuracy and efficiency of the solutions, but also the simplicity of the taken procedures which would have remarkable effects on the time devoted for solving process.

➢ **Chapter eight** is the overall conclusion and future enhancements of the thesis.

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PROPOSED CONTENTS OF THE THESIS

CHAPTER I: **INTRODUCTION**

CHAPTER II: **ANALYTICAL SOLUTION FOR THE MATHEMATICAL MODELING OF THE SCR REACTION NETWORK USING HPM**

CHAPTER III: **ANALYTICAL EXPRESSIONS OF THE SUBSTRATE AND MEDIATOR OF MULTI-STEP ENZYME ELECTRODES**

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CHAPTER V: **AKBARI - GANJI'S METHOD (AGM) FOR SOLVING NONLINEAR REACTION DIFFUSION EQUATION IN THE ELECTROACTIVE POLYMER FILM**

CHAPTER VI: **A THEORETICAL STUDY ON THE DIFFUSION AND REACTION PROCESS THAT OCCURS WITHIN THE E-MATRIX OF A SANDWICH-TYPE AMPEROMETRIC BIOSENSOR**

CHAPTER VII: **VARIATION ITERATION METHOD FOR SOLVING ETHANOL AND ACETALDEHYDE CONCENTRATIONS IN A FIXED BED LABORATORY REACTOR**

CHAPTER VIII: **CONCLUSION AND FUTURE ENHANCEMENT**

LIST OF PUBLICATIONS BASED ON THE THESIS

- **M. Veeramuni** and K.M. Dharmalingam, Analysis through an analytical solution for the SCR reaction network using HPM, **International Journal of Computational Engineering Research**, 08(2018), 50 – 56. **(UGC Approved Journal)**

- K.M. Dharmalingam, **M. Veeramuni** and T. Praveen, Analytical expressions of the substrate and mediator of multi-step enzyme electrodes, **Journal of Mathematical Chemistry**, 57(2019), 986 - 1000. **(Springer)**

- **M. Veeramuni**, K.M. Dharmalingam, and T. Praveen, Analysis Through an Analytical Solution of the Mathematical Model for Solid Catalyzed Reactive HiGee Stripping, **Chemistry Africa**, (2019). **(Springer - In press)**

- K.M. Dharmalingam, **M. Veeramuni**, Akbari-Ganji's Method (AGM) for solving nonlinear reaction diffusion equation in electroactive polymer film, **Journal of Electroanalytical chemistry,** 844 (2019), 1 - 5. **(Elsevier)**

- **M. Veeramuni**, K.M. Dharmalingam, and T. Praveen, A theoretical study on the diffusion and reaction process that occurs within the E-matrix of a sandwich - type amperometric biosensor, **Electrochemistry Communication**. **(Communicated - Elsevier)**

- K.M. Dharmalingam, **M. Veeramuni**, Variation Iteration Method for solving ethanol and acetaldehyde concentrations in a fixed bed laboratory reactor, **Proceeding in 5th International Conference on Emerging Trends in Multidisciplinary Research, Organised by Arunai International Research Foundation & National University of Singapore, Singapore.**

LIST OF CONFERENCES / SEMINARS / WORKSHOPS PRESENTED AND PARTICIPATED

- Presented a paper at the National conference on "ADVANCES IN MATHEMATICS AND ITS APPLICATION TO SCIENCE AND ENGINEERING" organized by Department of Mathematics, University College of Engineering Pattukkottai, Rajamadam, Thanjavur, 22nd January 2016.

- Participated in National conference on "RECENT ADVANCEMENTS IN PURE AND APPLIED MATHEMATICS" organized by Department of Mathematics, N.M.S. Sarmathai Vasan College for Women, Madurai, 5th January 2017.

- Participated in the Science Academies' Lecture Workshop on "MATHEMATICAL MODELLING" organized by Department of Mathematics, The Madura College, Madurai, 10th & 11th February 2017.

- Presented a paper in the "INTERNATIONAL CONFERENCE ON MATHEMATICAL MODELING AND COMPUTATIONAL METHODS IN SCIENCE AND ENGINEERING (ICMMCMSE - 2017)" organized by Ramanujan Centre for Higher Mathematics and Department of Mathematics, Alagappa University, Karaikudi, 20th – 22nd February 2017.

- Presented a paper in the "INTERNATIONAL CONFERENCE ON MATHEMATICAL METHODS, MODELING AND SIMULATION IN CHEMICAL SCIENCE" organized by Department of Mathematics, Department of Chemical Enginnering, SSN CE Society for the Advancement of Chemical Sciences and Education, Kalpakkam, SSN College of Enginnering, Chennai, 06th - 10th December 2018.