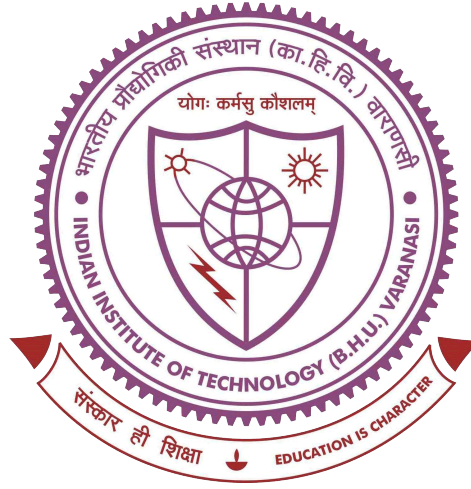


NUMERICAL STUDY OF SOME FRACTIONAL ORDER
REACTION-DIFFUSION PROBLEMS



Thesis submitted in partial fulfillment for the

Award of Degree

DOCTOR OF PHILOSOPHY

By

Manpal Singh

DEPARTMENT OF MATHEMATICAL SCIENCES

INDIAN INSTITUTE OF TECHNOLOGY

(BANARAS HINDU UNIVERSITY)

VARANASI -221005

Roll No: 18121022

June 2024

CERTIFICATE

It is certified that the work contained in this thesis titled “*Numerical study of some fractional order reaction-diffusion problems*” by *Manpal Singh* has been carried out under our joint supervision and co-supervision, and this work has not been submitted elsewhere for a degree.

It is further certified that the student has fulfilled all the requirements of Comprehensive Examination, Candidacy and SOTA for the award of Ph.D. degree.


03/06/24
Dr. Rajeev

(Supervisor)

Associate Professor
Department of Mathematical Sciences
Indian Institute of Technology
(Banaras Hindu University)
Varanasi-221005



Prof. Subir Das

(Co-Supervisor)

Professor
Department of Mathematical Sciences
Indian Institute of Technology
(Banaras Hindu University)
Varanasi-221005

DECLARATION BY THE CANDIDATE

I, *Manpal Singh*, certify that the work embodied in this thesis is my own bonafide work and carried out by me under the supervision of *Dr. Rajeev* and co-supervision of *Prof. Subir Das* from *July, 2018* to *June, 2024* at the *Department of Mathematical Sciences, Indian Institute of Technology (Banaras Hindu University), Varanasi*. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, *etc.*, reported in journals, books, magazines, reports dissertations, thesis, *etc.*, or available at websites and have not included them in this thesis and have not cited as my own work.


Date: 03/06/2024


Place: Varanasi


(Manpal Singh)

CERTIFICATE BY THE SUPERVISORS

It is certified that the above statement made by the student is correct to the best of our knowledge.


(Dr. Rajeev)
(Supervisor)
Associate Professor
Department of Mathematical Sciences
Indian Institute of Technology(BHU)
Varanasi-221005


(Prof. Subir Das)
(Co-Supervisor)
Professor
Department of Mathematical Sciences
Indian Institute of Technology(BHU)
Varanasi-221005


03.06.2024

Head of the Department
Department of Mathematical Sciences
Indian Institute of Technology(BHU)
Varanasi-221005

COPYRIGHT TRANSFER CERTIFICATE

Title of the Thesis: *Numerical study of some fractional order reaction-diffusion problems.*

Name of the Student: *Manpal Singh*

Copyright Transfer

The undersigned hereby assigns to the Indian Institute of Technology (Banaras Hindu University), Varanasi all rights under copyright that may exist in and for the above thesis submitted for the award of the Ph.D. degree.

Date: 03/06/24

Place: Varanasi

MSingh
03/06/24
(Manpal Singh)

Note: However, the author may reproduce or authorize others to reproduce material extracted verbatim from the thesis or derivative of the thesis for author's personal use provided that the source and the Institute copyright notice are indicated.

ACKNOWLEDGEMENTS

This thesis is not the outcome of the efforts of entirely one individual. Many people have contributed to its development. At this amenity of successful integrating of my work, I bow my head on the feet of lord almighty for the numerous blessing. He has bestowed upon me blessings throughout my PhD journey. There is hardly any task which is more pleasant than acknowledgment. My gratitude to all those who have helped in so many ways in preparing this work.

First of all, I would like to express my sincere thanks to my respected supervisor and co-supervisor, **Dr. Rajeev** and **Prof. Subir Das**, respectively for their excellent guidance, continuous encouragement, patience and advice during the whole span of Ph.D. I have been very lucky to have such supervisors who cared so much about my work, have shaped my understanding on the subject that has given me confidence to work independently. I also learnt from them which is much more than one could have expected from the supervisor.

I express my cordial thanks to **Prof. S.K. Pandey, Head**, and **Dr. Anuradha Banerjee, Convener, DPGC, of the Department of Mathematical Sciences IIT(BHU)** and RPEC members, including Dr. B. Biswas and Dr. V.K. Singh, for their valuable suggestions and encouragement. I am thankful to all the Department of Mathematical Sciences faculty members. I will also take a moment to express my appreciation and thank all the non-faculty members for their support

I am very grateful to have supportive seniors and lab-mates Dr. Rakesh Kumar, Dr. Anuwedita Singh, Dr. Abhishek Kumar, Dr. Umesh Kumar, Dr. Ankit Kumar, during my Ph.D. Journey. I would also like to thanks to sincere juniors of my lab

Mr. Sunny Singh, Ms. Anshika, Mr. Shivshankar Chauhan, Ms. Sapna Baluni, Mr. Shivshankar Das, Mr. Shubham Tiwari, Ms. Anjuman, Ms. Lipi Jain, Ms. Rashmi Sharma, Ms. Jaya Joshi, Ms. Arpita Charan and all the research scholars of the department for their moral supports.

I have very special thanks to my seniors *Dr. Kushal Dhar Dwivedi, Dr. Sachin Kumar, Dr. Prashant Pandey, and my colleagues Mr. Promod Sharma and Dr. Yashveer Kumar* and all the research scholars of the department for their moral supports.

I am also grateful to my Institute, IIT(BHU), for providing necessary resources throughout my research. I express my thanks to all non teaching staff members of the department for their supports.

I express my sincere and cordial gratitude to my parents, my sibling ***Mohit Kumar*** and ***Sangita***, my grandparent ***Mr.Prem Singh*** and ***Mrs.Vimla Devi***, my maternal uncle ***Dr.Santos Kumar Ravi, Mr.Yashvendra Singh and Mr.Rahul Kumar*** who always stood with me throughout my academic journey and provide moral as well as financial support. It was their love, care and patience which encouraged me to move on. Special love to my sweet maternal cousin ***Lakshya, Golu, Aadi & Parv.***

My acknowledgment will be incomplete if I do not mention **Pt. Madan Mohan Malaviya** with whose blessings and support I could be able to achieve my goal successfully.

Manpal Singh

PREFACE

The study of reaction-diffusion problems has long been a cornerstone of mathematical modeling in fields ranging from biology and chemistry to physics and engineering. These models describe how substances or populations interact and spread over time and space, capturing the essence of processes like chemical reactions, biological pattern formation, and ecological dynamics. However, classical reaction-diffusion models often assume integer-order derivatives, which may not fully capture the complexities of real-world systems where memory effects, anomalous diffusion, or spatial heterogeneities play significant roles.

In recent years, fractional calculus has emerged as a powerful tool for extending classical models to include non-integer or fractional derivatives. This generalization provides a more flexible framework for modeling processes that exhibit non-locality and history dependence, which are frequently observed in natural systems. Despite its growing importance, the study of fractional-order reaction-diffusion problems remains a challenging and rapidly evolving area of research. The primary objective of this thesis is to find the numerical solution of some fractional-order reaction-diffusion problems by developing efficient and accurate methods. Special attention is given to the spectral and operational matrix methods that can handle the unique demands of fractional order models.

This thesis has six chapters; Chapter 1 serves as an introduction to the thesis, covering topics such as the diffusion process and the reaction-advection-diffusion equation. It also includes a historical background of fractional calculus theory and its related definitions. Basic concepts of fractional order reaction-advection-diffusion equations and a literature review on the topic are discussed in this chapter. Additionally, the methods used in the thesis rely heavily on Lucas and Vieta-Fibonacci polynomials,

so a brief introduction to these polynomials, along with some of their important properties, is provided in this chapter.

In chapter 2, the author has developed a numerical method to solve the two-dimensional nonlinear and multi-term time-fractional diffusion equations with the help of Lucas's operational matrix. In the proposed method, solutions to the problems are expressed in terms of Lucas polynomial as basis function. The concerned method provides a highly accurate numerical solution. The accuracy of the approximate solution of the problem can be increased by expanding the polynomial terms. The accuracy and efficiency of the concerned method have been authenticated through error analyses with some existing problems whose solutions are already known.

In chapter 3, a new scheme has been developed for the numerical solution of the fractional order reaction advection-diffusion equation. To approximate the problem, the authors used Vieta-Fibonacci polynomials as basis functions and derived the operational matrices with the said polynomials for integer and fractional order Caputo differential operators for the first time. Lastly, the method is used to solve an unsolved reaction-advection diffusion model and observe the effect on solute concentration due to changes in various parameters of the model.

In Chapter 4, an innovative approach for the numerical solution of a three-component time-fractional order Brusselator reaction-diffusion system using the Vieta-Fibonacci wavelet and collocation method has been developed. The proposed method involves the derivation of operational matrices for both integer and fractional order derivatives. The existence, uniqueness of the solution, and Ulam-Hyers stability of the model are rigorously discussed. The numerical experiments showcase the method's superior performance in terms of accuracy and computational efficiency. The application of the Vieta-Fibonacci wavelet method to the three-component fractional

order Brusselator reaction-diffusion system marks a significant advancement in the field of computational mathematics.

In chapter 5, we consider a nonlinear reaction-diffusion equation with a Caputo-Fabrizio derivative, and its solution is obtained by the finite difference collocation method. First, we approximate the Caputo-Fabrizio derivative with the aid of shifted Legendre polynomials. To deal with the time derivative, a finite difference scheme is applied, and to deal with the spatial Caputo-Fabrizio derivative, the shifted Legendre spectral collocation method is used. To signify the efficiency and validity of the developed scheme, a few numerical examples are solved, and the absolute error between exact and numerical results is presented in tabular form.

In Chapter 6, overall work has been concluded, and also the future works have been presented.

Contents

List of Figures	xi
List of Tables	xiii
Preface	xv
1 Introduction	1
1.1 Diffusion process	1
1.2 Reaction-advection-diffusion equation	2
1.3 Fractional calculus	5
1.4 Special functions	9
1.4.1 Euler's Gamma function	9
1.4.2 Mittag-Leffler function	9
1.4.3 Wright function	10
1.4.4 Error function and complementary error function	11
1.5 Fractional order reaction-advection-diffusion equation	11
1.6 Basic definitions of fractional calculus	12
1.6.1 Riemann-Liouville fractional integral	13
1.6.2 Riemann-Liouville fractional derivative	13
1.6.3 Caputo derivative	14
1.7 Mathematical preliminaries	15
1.7.1 Lucas polynomials	15
1.7.2 Vieta-Fibonacci polynomials	16
1.7.3 Shifted Vieta-Fibonacci polynomials	17
1.7.4 Kronecker product	18
1.8 Challenges and motivation	19
2 Numerical solution of two-dimensional nonlinear fractional order reaction-advection-diffusion equation by using collocation method	21
2.1 Introduction	21

2.1.1	Approximation of function	24
2.2	OM of derivative in terms of Lucas polynomials	24
2.3	Numerical method to solve two-dimensional fractional order diffusion model	26
2.4	Numerical examples	29
2.5	Solution of the problem	36
2.6	Conclusion	38
3	Novel operational matrix method for the numerical solution of non-linear reaction-advection-diffusion equation of fractional order	39
3.1	Introduction	39
3.1.1	Function approximation	43
3.2	Formation of shifted Vieta-Fibonacci operational matrix	44
3.3	Application of the proposed method	47
3.4	Convergence analysis	49
3.5	Numerical applications	52
3.6	Solution of the problem	55
3.7	Conclusion	58
4	An innovative Vieta-Fibonacci wavelet collocation method for the numerical solution of three-component Brusselator reaction diffusion system of fractional order	61
4.1	Introduction	61
4.2	Vieta-Fibonacci wavelets	65
4.2.1	Vieta-Fibonacci wavelets	66
4.3	Derivation of VF wavelet OM	67
4.3.1	OM of integer order derivative	68
4.3.2	OM of fractional order derivative	69
4.4	Existence, uniqueness, and stability results	72
4.4.1	Existence and uniqueness	73
4.4.2	Ulam-Hyers stability	83
4.5	Implementation of the approach	87
4.6	Error bound analysis	90
4.7	Numerical results	94
4.8	Conclusion	102
5	Numerical solution of nonlinear reaction-advection-diffusion equation in sense of Caputo-Fabrizio derivative with finite difference and collocation method	103
5.1	Introduction	103
5.2	Preliminary definitions	105
5.2.1	C-F derivative and integral	105

5.2.2	Shifted Legendre polynomials	106
5.3	C-F approximation	107
5.4	Numerical technique	109
5.5	Error analysis	112
5.6	Numerical results and discussion	116
5.7	Conclusion	126
6	Conclusion and future work	127
6.1	Future work	128
	Bibliography	131

List of Figures

2.1	Plots of solute profile vs. x and y for non-conservative system with sink term ($k = -1$) for various values of α	37
2.2	Plots of solute profile vs. x and y for conservative and non-conservative systems for $\alpha=1$ at $t=0.5$	37
3.1	Behaviour of exact and numerical solutions for $n = 8$ at $\alpha = 0.5$ for Example 3.1.	53
3.2	Behaviour of exact and numerical solutions for $n = 3$ at $\alpha = 0.7$ for Example 3.2	55
3.3	Variations of $u(x, 0.5)$ vs. x for various values of α for $\lambda_1 = 0.5$, $\lambda_2 = 1$ at $t = 0.5$	56
3.4	Variations of $u(x, 0.5)$ vs. x for various values of α for $\lambda_1 = 0.5$, $\lambda_2 = 0$ at $t = 0.5$	56
3.5	Variations of $u(x, 0.5)$ vs. x for various values of α for $\lambda_1 = 0.5$, $\lambda_2 = -1$ at $t = 0.5$	57
3.6	Variations of $u(x, 0.5)$ vs. x for various values of λ_2 for $\alpha = 1$, $\lambda_1 = 0.5$ at $t = 0.5$	57
3.7	Variations of $u(x, 0.5)$ vs. x for various values of λ_1 for $\alpha = 1$ and $\lambda_2 = 1$ at $t = 0.5$	58
4.1	Behaviour of exact solutions and their corresponding Error graph at $t = 0.5$ for Example 4.1 at $\hat{m} = 9$	96
4.2	Graph for the variation in concentrations for different values of α at $t = 0.1$ for Example 4.1 at $\hat{m} = 8$	97
4.3	Behaviour of exact solutions and their corresponding Error graphs at $t = 0.5$ for Example 4.2 at $\hat{m} = 12$	99
4.4	Graph for the variation in concentrations for different values of α at $t = 0.1$ for Example 4.2 at $\hat{m} = 8$	100
4.5	Variations in errors for different values of \hat{m} at $t = 0.5$ and $\alpha = 0.70$ for Example 4.3.	101
5.1	Plot of $u(x, t)$ versus x for Example 5.1 in case of Exact and Numerical solution.	117
5.2	Plot of $u(x, t)$ versus x for Example 5.2 in case of Exact and Numerical solution.	119

5.3	Plot of $u(x, t)$ versus x for Example 3 in case of Exact and Numerical solution.	120
5.4	Plot of $u(x, t)$ versus x for Example 4 in case of Exact and Numerical solution.	122
5.5	Plot between $u(x, 0.5)$ versus x for Example 5.5 at $\beta = 1.5$ for various values of α	124
5.6	Plot between $u(x, 0.5)$ versus x for Example 5.5 at $\beta = 1.9$ for various values of α	124
5.7	Plot between $u(x, 0.5)$ versus x for Example 5.5 at $\alpha = 0.5$ for various values of β	125
5.8	Plot between $u(x, 0.5)$ versus x for Example 5.5 at $\alpha = 0.9$ for various values of β	125

List of Tables

2.1	The absolute errors for $n = 8$ and $n = 10$ with $\alpha = 0.4$ at $t = 0.5$ for Example 2.1	31
2.2	The absolute errors for $n = 8$ and $n = 10$ with $\alpha = 0.8$ at $t = 0.5$ for Example 2.1	31
2.3	The absolute errors for $n = 8$ and $n = 10$ at $t = 0.5$ for Example 2.2 .	32
2.4	The absolute errors for $n = 8$ and $n = 10$ at $t = 0.5$ for Example 2.3 .	33
2.5	The absolute errors for $n = 8$ and $n = 10$ at $t = 0.5$ for Example 2.4 .	34
2.6	The absolute errors for $n = 8$ and $n = 10$ at $t = 0.5$ for Example 2.5 .	35
3.1	The maximum absolute errors at $t = 1$ for different values of α for Example 3.1	53
3.2	The maximum absolute errors at $t = 0.5$ for $n = 6$ for Example 3.2 . .	54
4.1	Tabular presentation of absolute errors for different values of α at $t = 0.5$ and $\hat{m} = 12$ for Example 4.1	95
4.2	Tabular presentation of absolute errors for different values of \hat{m} at $\alpha = 0.73$ and $t = 0.5$ for Example 4.2	98
4.3	Comparison of exact and numerical solution at $\alpha = 0.70$ and $t = 0.4$ for Example 4.3	101
5.1	variations of absolute errors at $x = 0.5$ and for different values of h for Example 5.1	118
5.2	variations of absolute errors at $x = 0.5$ and for different values of h for Example 5.2	119
5.3	variations of absolute errors at $x = 0.5$ and for different values of h for Example 5.3	121
5.4	Comparison of absolute errors at $h = \frac{1}{512}$ and for different values of x for Example 5.4	122