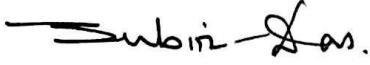


CERTIFICATE

It is certified that the work contained in this thesis titled "*Numerical study of fractional diffusion equations and its applications*" by *Sachin Kumar* has been carried out under my supervision and that 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.



Prof. Subir Das
(Supervisor)
Professor
Department of Mathematical Sciences
Indian Institute of Technology
(Banaras Hindu University)
Varanasi-221005

पर्यवेक्षक/Supervisor
गणितीय विज्ञान विभाग
Department of Mathematical Sciences
भारतीय प्रौद्योगिकी संस्थान
Indian Institute of Technology
(काशी हिन्दू विश्वविद्यालय)
(Banaras Hindu University)
वाराणसी/Varanasi-221005

DECLARATION BY THE CANDIDATE

I, *Sachin Kumar*, certify that the work embodied in this thesis is my own bonafide work and carried out by me under the supervision of *Prof. Subir Das* from *July, 2017* to *July, 2021* 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, theses, *etc.*, or available at websites and have not included them in this thesis and have not cited as my own work.

Date: *October 6, 2021*

Place: Varanasi

Sachin Kumar
(Sachin Kumar)

CERTIFICATE BY THE SUPERVISOR

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

Subir Das

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

पर्यवेक्षक/Supervisor
गणितीय विज्ञान विभाग
Department of Mathematical Sciences
भारतीय प्रौद्योगिकी संस्थान
Indian Institute of Technology
(काशी हिन्दू विश्वविद्यालय)
(Banaras Hindu University)
वाराणसी/Varanasi-221005

T. Som
6/10/21

(Prof. T. Som)
Professor and Head
Department of Mathematical Sciences
Indian Institute of Technology
(Banaras Hindu University)
Varanasi-221005

विभागाध्यक्ष/HEAD
गणितीय विज्ञान विभाग
Department of Mathematical Sciences
भारतीय प्रौद्योगिकी संस्थान
Indian Institute of Technology
(काशी हिन्दू विश्वविद्यालय)
(Banaras Hindu University)
वाराणसी/Varanasi-221005

COPYRIGHT TRANSFER CERTIFICATE

Title of the Thesis: *Numerical study of fractional diffusion equations and its applications.*

Name of the Student: *Sachin Kumar*

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: *October 6, 2021*

Place: Varanasi

Sachin Kumar

(Sachin Kumar)

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

The work presented in this thesis would not have been possible without my close association with many people. I take this opportunity to extend my sincere gratitude and appreciation to all those who made this Ph.D thesis possible. I would like to express my sincere gratitude to the Indian Institute of Technology (B.H.U) for letting me fulfill my dream of being a student here. I would like to extend my sincere gratitude to my research guide *Dr. Subir Das, Professor*, for introducing me to this exciting field of applied mathematics and for his dedicated help, advice, inspiration, encouragement and continuous support, throughout my Ph.D. His enthusiasm, integral view on research and his mission for providing high-quality work, has made a deep impression on me. I could not have imagined having a better advisor and mentor for my Ph.D. study.

My sincere thanks also goes to *Prof. T Som*, Head, and *Prof. Santwana Mukhopdhyaya*, Associate Dean, and the RPEC Members *Dr. Rajeev* and *Prof. S.K. Singh, Department of Computer Science* for their support throughout my research work. I acknowledge my deep sense of gratitude to all the Faculty Members of the Department of Mathematical Sciences for their valuable suggestions, appreciation, and encouragement.

My special thanks to fellow lab mates, *Dr. Vijay Kumar Yadav, Dr. Anup Singh, Rakesh Kumar, Anuwedita Singh, Kushal Dhar Dwivedi, Prashant Pandey* and *Umesh Kumar* for always standing by my side and sharing a great relationship as compassionate friends. I will always cherish the warmth shown by them.

I feel a deep sense of gratitude for my father, Mr. *Vinod Raghav*, mother, *Mrs. Babita Devi*, who formed part of my vision and taught me good things that really matter in life. Their infallible love and support has always been my strength.

A special thanks to my younger brother *Govind*, sisters *Khushi* and *Deepika*, for their love and affection. I have no words to express my gratitude to my family.

Above all I thank to Lord Shiva, the Highest and Almighty one, for letting me through this journey of life. You are the one who has done a great and tremendous job for this thesis. Thank you Lord, for your endless blessing that has showered upon me.

Sachin Kumar

Contents

List of Figures	ix
List of Tables	xi
Preface	xii
1 Introduction	1
1.1 Fractional Calculus	1
1.1.1 Classical fractional derivative	2
1.1.2 Fractional operator with non-singular kernel	5
1.1.3 Variable order fractional derivative and integration [4]	5
1.2 Diffusion Phenomena	7
1.2.1 Derivation of diffusion equation [6]	7
1.3 Application of diffusion equation	13
1.3.1 Medical Science [7]	13
1.3.2 Geological Science [8]	14
1.3.3 Chemical Science [9]	14
1.3.4 Physical Science [10]	14
1.3.5 Ground water contamination problem [11]	15
1.3.6 Economics [12]	15
1.4 Numerical methods	15
2 Operational matrix method for solving nonlinear space-time fractional order reaction-diffusion equation based on Genocchi polynomial	18
2.1 Introduction	18
2.2 Preliminaries	23
2.2.1 Genocchi polynomial and its properties [13, 14]	24
2.3 Approximation of a arbitrary function	26
2.4 Genocchi operational matrix of fractional derivative [15]	26
2.4.1 Lemma	26

2.5	Error bound and stability analysis	28
2.6	Solution of the problem	30
2.7	Results and discussion	32
2.8	Conclusion	39
3	Numerical solution of two dimensional reaction-diffusion equation using operational matrix method based on Genocchi polynomial	41
3.1	Introduction	41
3.2	Preliminaries	42
3.2.1	Kronecker product of two matrix	42
3.2.2	Approximation of an arbitrary function	43
3.2.3	Genocchi operational matrix of fractional derivative	43
3.3	Error bound and stability analysis	44
3.4	Solution of the problem	46
3.5	Results and discussion	49
3.6	Conclusion	55
4	Gegenbauer wavelet operational matrix method for solving variable order non-linear reaction-diffusion and Galilei invariant advection-diffusion equations	57
4.1	Introduction	57
4.2	Preliminaries	60
4.2.1	Variable-order derivatives of Type 1(V1) and Type 2(V2)	60
4.2.2	Gegenbauer polynomial and Gegenbauer wavelet	61
4.3	Function Approximation	63
4.4	Error bound and stability analysis	64
4.5	Operational matrix of derivative	68
4.5.1	Gegenbauer wavelet operational matrix of variable-order fractional derivative	69
4.6	Proposed model	72
4.7	Description of proposed method	73
4.8	Results and discussion	75
4.9	Conclusion	85
5	Analysis of tumor cells in the absence and presence of chemotherapeutic treatment: The case of Caputo-Fabrizio time fractional derivative	86
5.1	Introduction	86
5.2	Derivation of C-F fractional differential operational matrix	90
5.2.1	Approximate expression of C-F derivative of simple polynomial function	90
5.2.2	Chebyshev polynomials [16]	91

5.3	Description of model representing the chemotherapy effect on behavior of tumor cells	96
5.4	Solution of the problem	99
5.5	Numerical simulation and results	101
5.5.1	Variation of tumor cells when chemotherapy drug is not injected	103
5.5.2	Behavior of tumor cells after applying chemotherapeutic treatment	104
5.5.3	Discussion of the nature of model in fractional order system and future scope	105
5.6	Conclusion	107
6	Conclusion and scope of future work	109
	 Bibliography	 112

List of Figures

1.1	Minion	9
2.1	Plots of $u(x, t)$ vs. x and t for $M = 3$ in case of approximate solution.	34
2.2	Plots of $u(x, t)$ vs. x and t for $M = 3$ in case of exact solution.	34
2.3	Plots of $u(x, t)$ vs. x for various α at $t=1$ when $\lambda = -1, \beta = 1$	36
2.4	Plots of $u(x, t)$ vs. x for various β at $t=1$ when $\lambda = -1, \alpha = 1$	36
2.5	Plots of $u(x, t)$ vs. x for different values of λ at $t=1$ when $\alpha = 1, \beta = 1, \psi(x, t) = 0$	38
2.6	Plots of $u(x, t)$ vs. x for different values of λ at $t=1$ when $\alpha = 1, \beta = 1, \psi(x, t) = x - xt^2$	39
3.1	Plots of $u(x, y, t)$ vs. x and y for $M = 4$ in case of numerical and exact solution for $t = 0.5$	51
3.2	Plots of $u(x, y, t)$ vs. x and y for $M = 4$ in case of numerical and exact solution for $t = 0.5$	52
3.3	Plots of $u(x, y, t)$ vs. x and y for various α at $t=0.5$ when $\kappa_3 = 1, \beta = \gamma = 2$	53
3.4	Plots of $u(x, y, t)$ vs. x and y for various β at $t=0.5$ when $\kappa_3 = 1, \alpha = 1, \gamma = 2$	54
3.5	Plots of $u(x, y, t)$ vs. x and y for various γ at $t=0.5$ when $\kappa_3 = 1, \beta = 2, \alpha = 1$	54
3.6	Plots of $u(x, y, t)$ vs. x and y for various β at $t=0.5$ when $\beta = 2, \alpha = 1, \gamma = 2$	55
4.1	Plots of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ in case of numerical and exact solution for $t = 0.5$	77
4.2	Plots of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ in case of numerical and exact solution for $t = 0.5$	78
4.3	Plots of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ in case of numerical and exact solution for $t = 0.5$	80
4.4	Plots of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ in case of numerical and exact solution for $t = 0.5$	81
4.5	Behavior of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ at $t = 0.5$	81
4.6	Behaviour of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ at $x = 0.5$	82

4.7	Behaviour of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ at $x = 0.5$	82
4.8	Plots of $u(x, t)$ for $\hat{m} = 4$ and $\lambda = 2$ in case of numerical and exact solution for $t = 0.5$	84
5.1	Growth of tumor cells at different time periods in absence of chemotherapeutic (a) for integer order system ($\alpha = 1, \beta = 1, \gamma = 1, \zeta = 1$) (b) for C-F fractional order system ($\alpha = 0.9, \beta = 0.9, \gamma = 0.9, \zeta = 0.9$).	104
5.2	Graphical representation of tumor cells in presence of chemotherapeutic drug with different time intervals.	105
5.3	Plots of normal cells $N(x, t)$ for different values of α	106
5.4	Plots of tumor cells $T(x, t)$ at different values of β	106
5.5	Plots of Immune cells $I(x, t)$ for different values of γ	107
5.6	Plots of concentration of chemotherapeutic drug $U(x, t)$ for different values ζ	107
5.7	Dynamics of tumor cells at time $t = 0.5$ with different immune levels.	108

List of Tables

1.1	Different type of fractional diffusion	12
2.1	variations of L_∞ and L_2 for different time for first case taking $M = 3$.	33
2.2	variations of L_∞ and L_2 for different time for second case taking $M = 3$.	35
2.3	variations of L_∞ and L_2 for different time for second case taking $M = 4$.	35
2.4	Comparison of absolute errors for proposed method and the method given in [17].	37
3.1	variations of absolute error for different time and space for first case taking $M = 4$	50
3.2	variations of absolute error for different time and space for first case taking $M = 4$	52
4.1	Variations of absolute error for different x at $t = 0.5$, $\lambda = 2$ and various \hat{m}	76
4.2	Comparison of absolute error for method given in [18] and the proposed method for different x at $t = 1$	76
4.3	Variations of absolute error for different x at $t = 0.5$, $\lambda = 2$ and various \hat{m}	78
4.4	Comparison of absolute error for method given in [19] and proposed method	78
4.5	Variations of absolute error for different x at $t = 0.5$, $\lambda = 2$ and various \hat{m}	79
4.6	comparison of L_∞ error for method given in [20] and proposed method	79
4.7	Variations of absolute error for different x at $t = 0.5$, $\lambda = 2$ and various \hat{m}	80
4.8	Variations of absolute error for different x at $t = 0.5$, $\lambda = 2$ and various \hat{m}	83
4.9	Variations of absolute error for different x at $t = 0.5$, $\lambda = 2$ and various \hat{m}	85
5.1	Description and approximate numerical values of parameters used in model (5.38 – 5.41).	98
5.2	Variations of absolute error for the unknown functions at fixed spatial point $x = 1$ for $m = 8$	103

PREFACE

In this thesis, the numerical study of fractional diffusion equation has been done which has applications in porous media and tumor analyses. Chapter 1 contains the introduction part of the thesis. In this chapter, firstly the history of fractional calculus with evolution has been discussed. The definition of different types of fractional order derivatives like Caputo, Riemann-Liouville, and Atangana-Baleanu derivatives with constant and variable order is given which will be used through the article. In the last, the background, derivation of the fractional diffusion equation and its applications in different fields with a list of numerical methods dealing with it are incorporated in this chapter.

Chapter 2 contains the analysis of the one-dimensional reaction-diffusion equation. The Genocchi operational matrix of differentiation with collocation method has been used in solving the model. The validation of the method is shown by solving the particular cases of the reaction-diffusion model. For accuracy of the method, the error table has been incorporated and results are compared with the existing numerical results from previous literature. In the end, the application of this model in the groundwater contamination problem has been presented.

The two-dimensional version of the previous reaction-diffusion model along with Neumann boundary conditions has been studied in Chapter 3. The Genocchi operational matrix with collocation method has been used for solving this model. The validation and accuracy of the method are depicted through error tables and also from the plots between the exact and numerical solution.

In chapter 4, two models have been considered, out of which one is variable order non-linear reaction-diffusion model and another one variable order advection-diffusion

model. Here, the operational matrix of the ultraspherical wavelet is used in finding the numerical solutions of aforementioned models. The validation of the method is shown by solving the numerical examples for the particular cases of both models. The effect of reaction term on solution profile is depicted through figures.

In chapter 5, the applications of diffusion equation are shown in the tumor analysis with the absence and presence of chemotherapeutic treatment. A model of four coupled diffusion equations is considered with exponential kernel non-singular fractional order derivative for the analysis of the behavior of tumor cells, normal cells, and immune cells. The spectral method based on the Chebyshev polynomials is used for the investigation of the model. The results for tumor cells' behavior in presence of chemotherapeutic treatment and the dynamic behavior of all types of cells concerning different fractional order are shown with the help of figures. In the end, the response of the immune system against tumor cells has been depicted.