PREFACE

The thesis is divided into six chapters, in which Chapter 1 is an introduction and covers groundwater contamination, fractional calculus, reaction-advection-diffusion equations, and fractional-order equations. This chapter has also covered the fundamentals of reaction-advection-diffusions, definitions, and a review of the relevant literature. This chapter covers the mathematical models for using the shifting Legendre collocation, and finite difference methods to solve solute transport issues.

In chapter 2, a one-dimensional variable-order nonlinear partial integro-differential equation viz., reaction-advection-diffusion equation with initial and boundary conditions are solved using Legendre wavelet approximation and operational matrices. The solution of solute concentration is calculated numerically and also presented graphically. Using the shifted Legendre collocation points, the model is reduced to a system of algebraic equations, which are solved using Newton-Cotes method. The error is then calculated by comparing the numerical solution obtained from the system of algebraic equations and the known exact solution of an existing problem to validate the efficiency of the proposed numerical scheme. The main point of the chapter is to show that the diffusivity of solute concentration is directly proportional to the order of non-linearity for different particular cases in less computational time by using the reliable and efficient Legendre wavelet approximation and operational matrices method.

In Chapter 3, the fractional order nonlinear reaction-advection-diffusion equation describing contaminant transport in groundwater has been solved using shifted Legendre collocation method. The shifted Legendre polynomial is used to approximate the function. After that the operational matrix for fractional order derivative in Caputo sense is applied on it. The shifted Legendre collocation points are employed to obtain a system of nonlinear algebraic equations which have been solved using Newton method. The shifted Legendre collocation method is validated by comparing the numerical results with those obtained using exact solutions through error analyses and the results are shown in graphical as well as tabular forms which clearly exhibits that the method is effective and reliable. The salient feature of the chapter is the explanation of the damping of the solution profile as the system approaches to fractional order from standard order.

In Chapter 4, the spatio-temporal fractional-order nonlinear reaction-advection-diffusion equation is solved using the neural network method (NNM). Shifted Legendre orthogonal polynomials with variable coefficients are used in the network's construction. The characteristics of a fractional-order derivative are used to determine the loss function of a neural network. The permissible learning rate range is discussed in detail, assuming that the Lipschitz hypothesis is accurate for the nonlinearity in reaction term. The effects of reaction term and also the degree of nonlinearity in reaction and advection terms on the solution profile are visualized through graphical presentations for specific test cases.

Chapter 5 is concerned with the numerical solution of a two-dimensional nonlinear fractional-order partial differential equation (FPDE) with Riesz space fractional derivative (RSFD) using a fast compact implicit integration factor (FcIIF) with non-uniform time meshes. Here two types of FPDE-RSFD are considered, the first one is a two-dimensional nonlinear Riesz space-fractional reaction-diffusion equation (RSFRDE) and the second one is a two-dimensional nonlinear Riesz space-fractional reaction-advection-diffusion equation (RSFRADE). The validation and effectiveness of the numerical method is given by considering some existing models.

The thesis is concluded in Chapter 6, and future work is presented.