



Application of Weighted Residual and Orthogonal Finite Element Computational Techniques to Nonlinear Boundary Value Problems

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Application of weighted residual and Orthogonal Finite Element Computational Techniques to Nonlinear Boundary Value Problems

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Science Graduate program at Addis Ababa University in Partial
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**Supervised by
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Collage of Natural and Computational Science

Computational Science Graduate program

This is to certify that this thesis entitled as “*Application of weighted residual and Orthogonal Finite Element Computational Techniques to Nonlinear Boundary Value Problems*”, submitted in partial fulfillment of the requirements for the degree of Master of Science in Computational Science to the Collage of Natural and Computational Science Graduate program Addis Ababa University, done by **Getenet Tamiru** is an authentic work carried out by him under our guidance. The theme embedded in this thesis has not been submitted earlier for the award of any degree or diploma in any other university to the best of our knowledge.

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As thesis research advisor, I hereby certify that I have read and evaluated this thesis prepared under my guidance by GETENET TAMIRU entitled “**Application of weighted residual and Orthogonal Finite Element Methods Computational Techniques to Nonlinear Boundary Value Problems**” The work is original in nature and is suitable for the award of Master’s Degree in Computational Science.

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Date

Declaration

I, Getenet Tamiru, declare that this work entitled “**Application of Weighted Residual and Orthogonal Finite Element Methods Computational Techniques to Nonlinear Boundary Value Problems**”, is the outcome of my own effort and study and that all sources of materials used for the study have been duly acknowledged. I have produced it independently except for the guidance and suggestion of my research supervisor and examiner. This study has not been submitted for any degree in this University or any other University. It is offered for the partial fulfillment of the degree of Master of Science in Computational Science.

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Abstract

The main focus of this thesis is to examine the applications of weighted residual and orthogonal collocation finite element computational techniques to nonlinear boundary value problems. The application of WRM and OCFE method for solving nonlinear boundary value problems are examined. A detailed comparison with their procedures is made. The orthogonal collocation finite element method is compared to the Subdomain, Galerkin, and Collocation weighted residual methods and the advantage are illustrated. The sensitivity of the orthogonal collocation method to different parameters is studied. Orthogonal collocation on finite elements is used to solve nonlinear BVPs and its superiority over the weighted residual method is shown. To this end, application of Subdomain Weighted Residual method, Galerkin Weighted Residual method, Collocation Weighted Residual and the orthogonal collocation on finite elements is also used to solve nonlinear boundary value problems, namely the steady state exothermic chemical reaction in a slab of combustible material, the catalytic reactions in a flat particle, the thermal explosion in a vessel, Troesch boundary value problem for temperature distribution, reaction-diffusion equation and temperature distribution in straight fins with temperature dependent thermal conductivity to their respect mixed boundary conditions for different parameters. We also analyzed computational cost by measuring elapsed and CPU time for the applications of WRM and OCFEM. The results agree remarkably with those from the literature.

Key words: *BVPs, Weighted Residual, Subdomain WRM, Galerkin WRM, Collocation WRM, Orthogonal Collocation Finite Element method*

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Notations

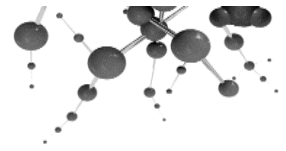
$\phi(x)$	Nonlinear BVP solution
N	Order of polynomial
N_e	Number of elements
$w(x)$	Weight function
R	Residual
λ	Frank-kameneskii parameter
ε	Activation energy parameter
δ	Heat loss parameter
m	Numerical exponent
x	Domain of interest
x_k	Interpolation nodes
l_k	Lagrange polynomial function
M	dimensionless thermo-geometric fin parameter
n	convective heat transfer power
Q	dimensionless heat transfer
γ	dimensionless internal heat generation parameter
ω	thermal conductivity parameter or non-linear parameter

List of Acronyms

DE	Differential Equation
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
BVP	Boundary Value Problem
WR	Weighted Residual
WRM	Weighted Residual Method
FEM	Finite Element Method
SD	Subdomain
GRK	Galerkin
COL	Collocation
OCFE	Orthogonal Collocation Finite Element
FDM	Finite Difference Method
SDWM	Subdomain Weighted Residual Method
GRKWM	Galerkin Weighted Residual Method
COLWM	Collocation Weighted Residual Method
OCFEM	Orthogonal Collocation Finite Element Method
HAM	Homotopy Analysis Method
DTM	Differential Transformation Method
HPM	Homotopy Perturbation Method
LMM	Leibnitz-Maclaurin Method

Chapter 1

INTRODUCTION



1.1 Background

Numerical methods are applicable in real life and also numerical methods have key role in any profession [1] [2] and are represented into mathematical models. Numerical methods tend to emphasize the implementation of algorithms. The aim of numerical methods is therefore to provide systematic methods for solving problems in a numerical form. Numerical methods are becoming more and more important in engineering applications [3], simply because of the difficulties encountered in finding exact analytical solutions but also, because of the ease with which numerical techniques can be used in conjunction with modern high-speed digital computers. A differential equation is any equation which contains derivatives, either ordinary derivatives or partial derivatives.

An *ordinary differential equation* is one in which an ordinary derivative of a dependent variable ϕ with respect to an independent variable x is related in a prescribed manner to x , ϕ and lower derivatives [1] [4]. The most general form of an explicit *ordinary differential equation* of n^{th} order is given by:

$$\frac{d^n \phi}{dx^n} = f \left(x, \phi, \frac{d\phi}{dx}, \frac{d^2\phi}{dx^2}, \dots, \frac{d^{n-1}\phi}{dx^{n-1}} \right) \quad (1.1 \text{ eq. } 1)$$

A *partial differential equation* is an equation involving partial derivatives of an unknown function of two or more independent variables [2]. For two independent variables, such equations can be expressed in the following general form (provided that it is linear):

$$A \frac{\partial^2 \phi}{\partial x^2} + B \frac{\partial^2 \phi}{\partial x \partial y} + C \frac{\partial^2 \phi}{\partial y^2} + D = 0 \quad (1.1 \text{ eq. } 2)$$

Where A , B , and C are functions of x and y and D is a function of x , y , ϕ , $\partial\phi/\partial x$, and $\partial\phi/\partial y$.

In differential equations approximate solutions can satisfy only part of the conditions of the problem. The differential equation may be satisfied only at a few positions, rather than at each

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point. The approximate solution is expanded in a set of known functions with arbitrary parameters.

Approximation is anything that is similar, but not exactly equal, to something else. A calculation can be approximated by rounding the values within it before performing the operations. Sometimes it is difficult to solve an equation exactly. When the governing equation which is formed to represent the complex behavior and problems do not have solution, develop one consistent, stable and convergent approximate solution is preferable. Handling of large system of equation, complicated geometries etc. are some of the advantages and the capability of numerical methods. However, an approximate solution may be accurate enough for solving the considered equation. This study explains the methods or techniques for finding approximate solution to differential equations:

The first one is the method of weighted residuals, depending on the problem of the governing differential equation there are two types of approximate methods, namely variational methods and weighted residual methods. Finding the extremum or stationary values of a functional with respect to the variables of the problem is called *variational principle*. The functional include all the intrinsic features of the problem, such as the governing equations and boundary conditions. The variational methods of approximation are Ritz, Galerkin, least-squares or Collocation method.

In weighted residual method, assumed approximate solution is substituted into the governing differential equation. Since the approximate solution does not satisfy the equation, a residual is obtained. The residual is multiplied by a weighting function and the integral of the product is required to be zero. The number of weighting functions is equal to the number of unknown coefficients in the approximate solution. There are several choices for the weighting functions, and some of the more popular choices have been assigned names. Engineers were using MWR to find approximate solutions [5]. This study has implemented on ODE problems with boundary conditions and solutions. This study explains about Galerkin, Collocation, Subdomain weighted residual methods.

The second tools for finding approximate solution is Orthogonal Collocation Finite Element Method, using collocation points chosen as the roots of orthogonal polynomials and chose the trial functions as the Jacobi polynomials thence, picked the collocation points as the

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corresponding zeros of these polynomials [6] [7] . This study has implemented on problems with mixed boundary conditions and smooth solutions.

1.2 Statement of the Problem

Researchers and scholars forwarded their own ideas on the areas of weighted residuals methods (Galerkin, collocation, Sub domain, Ritz, Least square method of moment) and orthogonal collocation finite element method. Some of them have tried to describe the details analysis of these methods. Some authors depicted the applications of these methods, rather than doing detail analysis. In this section some related works are reviewed.

Weighted residual methods (WRM) can be used in solving the nonlinear problems of differential equations and provide simple and highly accurate solutions of BVPs [8]. Prof. Bruce listed in the table about the histories of approximate methods on his research in [9]. A detailed analysis was done by Bruce A. Finlayson in [5] , [9] about weighted residual for different methods. The types of weighted residual methods and their steps was done in [10].

Salih reported in [11] gives brief of how these methods are working and also Ali reported in [10] about the Methods of weighted residuals and their steps, Finlayson in [5] tells us application of weighted residuals in fluid mechanics and heat transfer, also Akalu and his colleagues in [12] tell the numerical solutions for the linear BVP using Galerkin weighted residual method and result comparison with the exact solution, for the Galerkin¹ weighted residual method Lars-Erik Lindgren in [8] gave us a brief explanation, Obuka and his colleagues reported in [13] for periodic boundary value problem for the Galerkin method. Erik Lindgren and Bruce in [8] [5] gave an idea about collocation method, we also learnt from Bruce Finlayson the subdomain method investigated around 1923 E.C [9].

The other method for the solution of boundary value problem is orthogonal collocation finite element. Bruce A. Finlayson reported in [14] about the method and the steps, he also used it to solve problems in chemical reaction engineering as he stated in [7]. Margaret in [15] studied comparative analysis for orthogonal collocation method and give us an idea for the application

¹ **Boris Grigorievich Galerkin** was Born on 4th of March 1871 at Polotsk, Belarus and died 12 June 1945 at Moscow, USSR. He was a Soviet mathematician and engineer best known for his method of approximate integration.

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of linear second order differential equation. The Lagrange interpolation polynomial was explained and defined in [16]. Like the above researchers and authors, Rajiv Jain in [17] gave idea of how to apply orthogonal collocation on elements with each element having interior collocation points to get the solution of second order differential equations using OCFEM.

This research fills the gaps mentioned above. Thus, the main purpose of this study is application of weighted residual and Orthogonal Finite Element Computational Techniques to Nonlinear Boundary Value Problems. In this, we study the application of Galerkin weighted residual method, collocation weighted residual method, sub domain weighted residual method and orthogonal collocation finite element method to nonlinear boundary value problems, which are the steady state exothermic chemical reaction in a slab of combustible material, the catalytic reactions in a flat particle, the thermal explosion in a vessel, Troesch boundary value problem for temperature distribution, reaction-diffusion equation and temperature distribution in straight fins with temperature dependent thermal conductivity, which have mixed boundary conditions and dirichlet boundary condition.

1.3 Objective

1.3.1 General Objective

The main objective of this study is application of weighted residual and orthogonal finite element computational techniques to nonlinear boundary value problems. Based on our general objective we specifically set our objective as followed:

1.3.2 Specific Objectives

- ✍ To find numerical solution of nonlinear BVPs
- ✍ To find numerical solution of nonlinear BVPs using Galerkin weighted residual method;
- ✍ To find numerical solution of nonlinear BVPs using Collocation weighted residual method;
- ✍ To find numerical solution of nonlinear BVPs using Sub domain weighted residual method;
- ✍ To find numerical solution of nonlinear BVPs using orthogonal collocation finite element method;
- ✍ To show the applications of weighted residual methods to nonlinear BVPs;
- ✍ To show the applications of orthogonal collocation finite element method to nonlinear BVPs;

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 Application of weighted residual and Orthogonal Finite Element Computational Techniques to
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1.4 Methodology

Mainly, nonlinear boundary value problems were considered to describe a density of a dimensionless concentration or density of concentration a temperature. We find out numerical solutions of the models BVP by using the weighted residual method and orthogonal collocation method.

Our point of view here is to examine and show different computational techniques to weighted residual and orthogonal finite element methods. At the same time, we aim to develop numerical solution to nonlinear boundary value problems. All the simulations would be done using MATLAB R2019b version 9.7.0 [18] [19].

1.5 Thesis Outline

This thesis is organized as follows

In chapter 2, the numerical solutions of nonlinear boundary value problems using weighted Residuals and orthogonal collocation finite element method are discussed. Galerkin, Collocation and Subdomain methods of weighted residuals are discussed, techniques and algorithms are given for weighted residual and orthogonal finite element methods and experimented boundary value problems are described.

In this chapter 3, application of weighted residual methods to nonlinear boundary value problems that have mixed and Dirichlet boundary conditions are applied to examine the accuracy of the methodology and validate the solution with the analytical solution. Computational analysis and interpretations are presented.

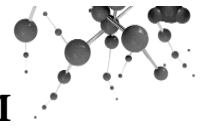
In Chapter 4, application of Orthogonal Collocation Finite element to nonlinear BVP is discussed. Numerical experiment is given for different number of elements. And computational comparisons interpretations among its elements are explained.

In Chapter 5, give the concluding remarks and future work of the weighted residual and orthogonal collocation finite element method.

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Chapter 2

NONLINEAR BOUNDARY VALUE PROBLEM



2.1 Boundary Value Problems

A Boundary Value Problems (BVP) is a differential equation along with a set of additional restrictions on the boundaries, called the boundary conditions. A solution to the boundary value problem is also a solution to the differential equation which satisfies the boundary conditions. BVPs arise in several branches of science. For instance, in physical differential equation for a few problems involving the wave equation, like the determination of normal modes, are often stated as boundary value problems. To be useful in applications, a boundary value problem should be well-posed this implies that given the input to the problem there exists a unique solution, which depends continuously on the input. For a boundary value problem, information about a solution to the differential equation(s) is also generally specified at over one point. A simple and common form for two-point boundary value problem involve a second order differential equation is:

$$\phi'' = f(x, \phi, \phi'), a \leq x \leq b \quad (2.1 \text{ eq. 1})$$

together with the boundary conditions

$$\phi(a) = \gamma \text{ and } \phi(b) = \beta \quad (2.1 \text{ eq. 2})$$

where α and β are known constants and the known endpoints a and b may be finite or infinite.

Now, let us consider boundary value problems in which the conditions are specified at more than one point. The main distinction between initial values problems and boundary value problems is that in the former case we are able to start an acceptable solution at its beginning (initial values) and just march it along by numerical integration to its end (final values); while within the present case, the boundary conditions at the starting point do not determine a unique solution to start with and a “random” choice among the solutions that satisfy these (incomplete) starting boundary conditions is almost certain not to satisfy the boundary conditions at the other specified points.

A more mathematical way to describe the difference between an initial value problem and a two-points boundary value problem is that (IVP) has all of the conditions specified at the same value of the independent variable in the equation and that value is at the lower boundary of the domain, thus the term "initial value". Whereas, a two-point boundary value problem has conditions specified at the extremes of the independent variable [20] [1].

In a boundary value problem, we are trying to satisfy a steady state solution everywhere in the domain that agrees with our prescribed boundary conditions. For a flux conservative problem, the problem becomes finding the set of fluxes at all the nodes such that for every node, what comes in goes out. In general, boundary value problems will reduce, when discretized, to a large and sparse set of linear (and sometimes nonlinear) equations. The following sections will first develop some physical intuition into the types and sources of boundary value problems, then show how to discretize them and finally present a potpourri of solution techniques.

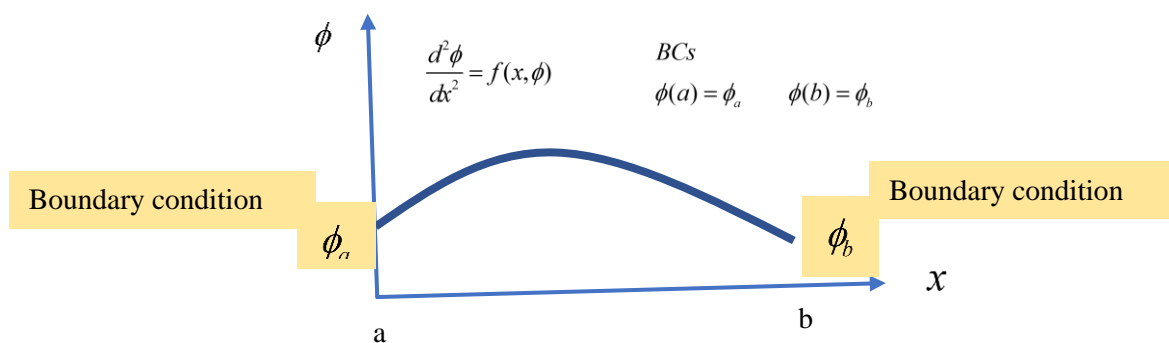


Figure 1: graphical scheme of BVP

2.1.1 Boundary Conditions

Boundary conditions exist in the form of mathematical equations, exert a set of additional constraints to the problem on specified boundaries. Boundary conditions can be applied to both ordinary and partial differential equations.

In this study, for the experimented nonlinear BVPs, the following types of boundary conditions are considered

1. Dirichlet Boundary Condition

when the boundary prescribes a value to the dependent variable(s) then the boundary is Dirichlet boundary condition.

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$$\begin{aligned}\phi(a) &= A \\ \phi(b) &= B\end{aligned}\tag{2.1 eq. 3}$$

2. Neumann Boundary Condition

In the Neumann boundary condition, the derivative of the dependent variable is known in all parts of the boundary.

$$\begin{aligned}\frac{d\phi}{dx}(a) &= C \\ \frac{d\phi}{dx}(b) &= D\end{aligned}\tag{2.1 eq. 4}$$

Note: Dirichlet and Neumann are predominant. In present study, the Dirichlet and Neumann boundary conditions have been proposed for the governing differential equations.

3. Mixed Boundary Condition

Mixed boundary condition refers when Dirichlet boundary conditions are prescribed in some parts of the boundary while Neumann boundary conditions given in the others.

$$\begin{aligned}\frac{d\phi}{dx}(a) &= C \\ \phi(b) &= B\end{aligned}\tag{2.1 eq. 5}$$

2.1.2 Solutions of boundary value problems

2.1.2.1 Analytic solutions of BVP

For many problems in engineering and physics, the techniques lead us to linear and nonlinear boundary. There are challenges in the formulation of solution in equations of mathematical physics for the mathematical modeling of problems of chemical reactions, heat- and mass-transfer, unsteady thermal streams. [21] A solution to a boundary value problem is a solution to the differential equation which also satisfies the boundary conditions [22]. BVPs arise in applied mathematics, engineering and several branches of physics. However, for nonlinear boundary value problems, it is usually difficult to obtain closed-form solutions for BVPs. In some cases, in solutions of equations of mathematics, the analytical or the approximate analytical methods can compete with the numerical methods Ali Belhocine [23] presented an analytic solution for bvps. Most of the time, only numerical approximate solutions will be expected. Semi

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analytic/approximate analytic solutions like: Perturbation method [24], Traditional non-perturbation methods and Adomian's decomposition method [25] have been developed for solving boundary value problems.

2.1.2.2 Numerical Method of solving BVP

Numerical methods have been developed for obtaining approximate solutions to boundary value problems. Some of them are summarized here:

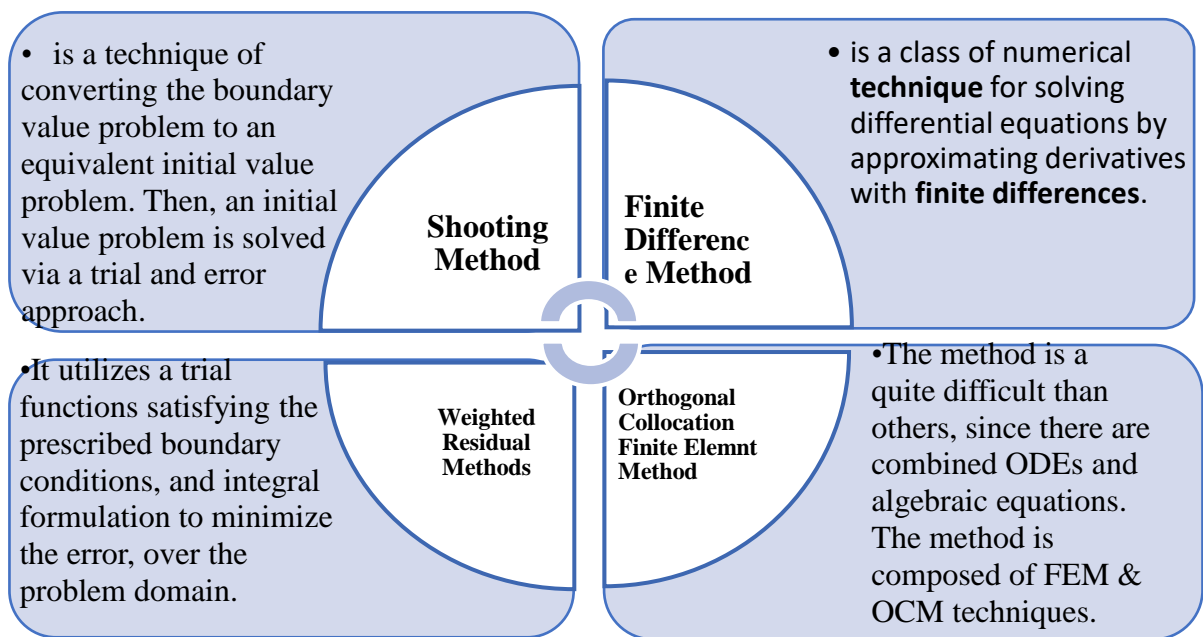


Figure 2: Numerical methods of solving BVP

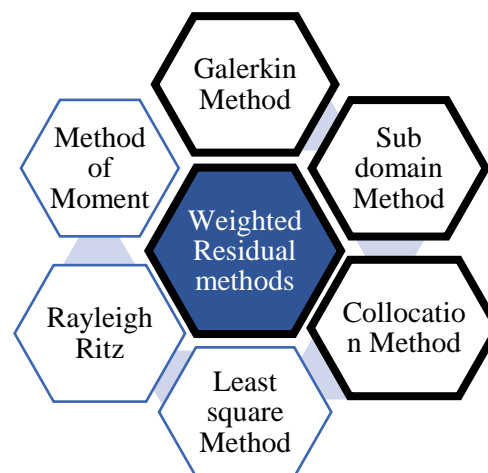


Figure 3: Weighted residual methods of solving BVP

Application of weighted residual and Orthogonal Finite Element Computational Techniques to
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2.1.2.2.1 Shooting method

M.R. Osborne reported that we can find numerical solution by using shooting method in [26]. Shooting method is a technique of converting the boundary value problem to an equivalent initial value problem. Then, an initial value problem is solved via a trial and error approach, by analogy to the procedure of shooting the object at a stationary target.

The shooting technique for the nonlinear second-order BVP is similar to the linear technique, except that the solution to a nonlinear problem cannot be expressed as a linear combination to two initial value problems.

2.1.2.2.2 Finite difference

We can also find the numerical solution of BVP by using finite difference method. The most common alternatives to the shooting method are finite-difference approaches. The finite difference method is used to solve ordinary differential equations that have conditions imposed on the boundary or simply problems are called boundary-value problems.

$$\phi'(x) = \frac{\phi(x+h) - \phi(x-h)}{2h} + O(h) \quad (2.1 \text{ eq. 6})$$

$$\phi''(x) = \frac{\phi(x+h) - 2\phi(x) + \phi(x-h)}{h^2} + O(h^2) \quad (2.1 \text{ eq. 7})$$

where h is the step size

2.2 Weighted Residual Method

2.2.1 Motivation

One of the approximate techniques for solving boundary value problems is Method of Weighted Residuals (MWR). It utilizes a trial functions satisfying the prescribed boundary conditions, and integral formulation to minimize the error, over the problem domain. Weighted residual methods (WRM) can be used in solving the nonlinear problems of differential equations and provide simple and highly accurate solutions of BVPs [10]. Prof. Bruce described in the table about the histories of approximate methods on his research in [9].

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Application of weighted residual and Orthogonal Finite Element Computational Techniques to
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As any other numerical method, the objective is to obtain of algebraic equations, that, when solved, produce a result with an acceptable accuracy. If we are seeking the values of a_i that would reduce the residue $R(x)$ all over the domain, we may integrate the residue over the domain and evaluate it!

2.2.2 General Concept

The general concept is described for a one-dimensional case. But the concept can easily be extended to two-dimensional and three-dimensional cases.

Given a differential equation of the general form,

$$D[\phi(x), x] = 0 \quad a < x < b \quad (2.2 \text{ eq. } 1)$$

Subject to boundary conditions

$$\phi(a) = \phi(b) = \gamma \quad (2.2 \text{ eq. } 2)$$

The method of weighted residuals seeks an approximate solution in the form:

$$\phi^*(x) = \sum_{i=1}^n c_i N_i(x) \quad (2.2 \text{ eq. } 3)$$

Where ϕ^* is the approximate solution expressed as the product of c_i unknown (i.e. constant parameters to be determined), and $N_i(x)$ are trial functions.

When the assumed solution of (2.2 eq. 3) is substituted into the differential equation of (2.2 eq. 1), a residual error $R(x)$ (residual) will result, which is given by

$$R(x) = D[\phi^*(x), x] \neq 0 \quad (2.2 \text{ eq. } 4)$$

The method of weighted residuals (MWR) requires that the unknown parameters c_i be evaluated such that,

$$\int_a^b w_i(x) R(x) dx = 0 \quad i = 1, n \quad (2.2 \text{ eq. } 5)$$

Where $w_i(x)$ represents n arbitrary weighting functions.

Note: On integration, (2.2 eq. 5) results in n algebraic equations, which can be solved for the n^{th} values of c_i . (2.2 eq. 5), expresses that the sum (integral) of the weighted residual error over the domain of the problem is zero.

The solution is exact at the end points (the boundary conditions must be satisfied) but, in general, at any interior point the residual error is nonzero.

Note: Several variations of the MWR exist and the techniques vary primarily on how the weighting factors are selected. The most common techniques are collocation, subdomain, Rayleigh-Ritz, least squares and the Galerkin's method.

We will discuss the Galerkin's, Collocation, Subdomain methods as they are quite simple to use and adaptable to the finite element method.

2.2.3 Experimented BVPs Trial Solution

Getting the trial/approximate solution $\phi(x)$

To formulate trial solution the following are pre-required

- Order of the governing equation (n)
- Degree of polynomial ($p = n+1$)
- Number of parameters to be determined ($c_i = p+1$)

Thus, all examined BVPs on section 2.6 are 2nd order but they have different boundary conditions due to that our trial/ approximate function formulation would not be the same. Based on their boundary conditions, let us group them, then follow the procedures and formulate the trial solution.

We formulate the trial solution: a quadratic trial solution shown in was adopted in this work.

$$\phi = c_1 + c_2x + c_3x^2 \quad (2.2 \text{ eq. } 6)$$

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2.2.4 General Algorithm to Weighted Residual Method

Algorithm 1: General algorithm for weighted residual

- 1) Assume that the functional form of the approximate solution $\phi(x)$ is given by

$$\phi^*(x) = \sum_{i=1}^n c_i N_i(x)$$

Choose the functional form of the trial function $\phi_i(x)$. Make sure that linearly independent and satisfy the boundary conditions.

- 2) Substitute the approximate solution $\phi(x)$ into the ODE. Then, define the residual as

$$R(x)$$

- 3) Choose the weighting functions

$$w_i(x), \quad i = 1, 2, \dots$$

- 4) Find the weighted residuals $w_i(x)R(x)$;

This section discusses the three weighted residual method, namely Galerkin's method, Sub Domain and Collocation Method as follow below:

2.2.5 Galerkin² Method

Galerkin's weighted residual method, the weighting functions are chosen to be identical to the trial functions, i.e.

$$w_i(x) = N_i(x) \quad i = 1, n$$

Therefore, the unknown parameters are determined by integrating them over the range of integration, and setting the integrals of the weighted residuals equal to zero to give equations for the evaluation of the coefficients c_i of the trial function $N_i(x)$.

² Boris Grigorievich Galerkin (1871–1945) Russian Mathematician. Galerkin's method was published in Russian in 1915 [9].

$$\int_a^b w_i(x)R(x)dx = 0 \quad i = 1, n$$

Again, the above integration results in n algebraic equations for evaluation of the n unknown parameters.

The Algorithm or the steps for the Galerkin weighted residual method as Ali Ümit in [10] listed are the following:

2.2.5.1 Algorithm to the Galerkin's method

We use the steps in above general algorithm for weighted residual methods and then after step 4 we apply the following steps.

Algorithm 2: Algorithm for Galerkin weighted residual

5) Set the integrals of the weighted residuals equal to zero;

$$\int_a^b w_i(x)R(x)dx = 0$$

6) Integrate, and solve the system of weighted residual integral equations for the coefficients c_i , $i = 1, 2, \dots, n$. Apply this method for the solution.

2.2.6 Sub Domain Method

This method doesn't use weighting factors explicitly, so it is not, strictly speaking, a member of the Weighted Residuals family. However, it can be considered a modification of the collocation method. The idea is to force the weighted residual to zero not just at fixed points in the domain, but over various subsections of the domain. To accomplish this, the weight functions are set to unity, and the integral over the entire domain is broken into a number of subdomains sufficient to evaluate all unknown parameters in many cases an equal division of the total domain is likely the best choice.

2.2.6.1 Algorithm to the Sub domain method

We use the steps in above general algorithm for weighted residual methods and then after step 4 we apply the following steps.

Algorithm 3: Algorithm for Sub domain weighted residual

- 5) we choose another middle limit (let us call it c) between the upper & lower
 6) Set the integrals of the weighted residuals equal to zero;

$$\int_a^c R(x)dx = 0$$

$$\int_c^b R(x)dx = 0$$

Integrate, and solve the system of weighted residual integral equations for the coefficients c_i , $i = 1, 2, \dots, n$. Apply this method for the solution.

2.2.7 Collocation Method

In the collocation method, we select at least the same number of collocation points as the unknown parameters and determine the parameters ϕ_j such that the residual is zero at the selected points. Or the idea of the collocation method is to demand that R vanishes at $N+1$ selected points x_0, \dots, x_N

$$R(x_i; c_0, \dots, c_N) = 0, \quad i \in \mathcal{I}_s \quad (2.2 \text{ eq. } 7)$$

Assume a solution, then force the residue to be zero at the collocation points

2.2.7.1 Algorithm to the Collocation's Method

We use the steps in above general algorithm for weighted residual methods and then after step 3 we apply the following steps.

Algorithm 4: Algorithm for Collocation weighted residual

3. Set $R(x, c_i) = 0$, and solve the system of residual equations for the coefficients c_i . Apply this method for the solution of the equation.

2.3 Orthogonal Collocation Finite Element Method

For problems whose solution has steep gradients, the orthogonal collocation method on finite elements is a useful method, and therefore the method can be applied to time dependent problems, too. The method is quite difficult than others, since there are combined ordinary differential equations and algebraic equations. Researchers and authors have developed and extended the Orthogonal Collocation method on finite elements. The OCFE method is generalization of OCM method [14]. The method of OCFE gives better results than orthogonal collocation method. Converging rate of OCFE method is much better than OCM method. The method of orthogonal collocation on finite elements (OCFE) is composed of two technique, these are finite element method (FEM) and orthogonal collocation method (OCM).

2.3.1 Method of Solutions

Let us assume that a second order nonlinear differential equation in the dependent variable ϕ and independent variable x is defined on the domain $[a, b]$, with two known boundary conditions. This domain $[a, b]$ is divided into smaller sub-domains or elements N_e , then the orthogonal collocation method is applied within each element. The solution is hence a function of the number of elements N_e and will sometimes be denoted by ϕ_{Ne} for equally spaced elements and ϕ_{Ne} for unequally spaced elements in order to avoid confusion [27]

In this study, the principle of orthogonal collocation is studied in conjunction with finite elements, i.e., orthogonal collocation on finite elements (OCFE). The domain of interest is called global domain. To apply collocation, the global domain is divided into small subdomains called elements. After applying collocation, the resulting system of equations is compiled to get the required solution.

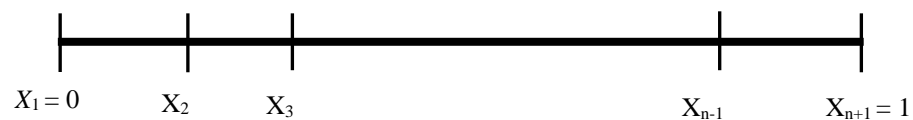


Figure 4: Application of finite element on the global domain

The domain of interest $0 \leq x \leq 1$ is divided into subdomains $0 = x_1 < x_2 < \dots < x_{ne+1} = 1$ called elements with $h_k = x_{k+1} - x_k$. The global variable x varies in the k^{th} element, where $k = 1, 2, \dots, N_e$.

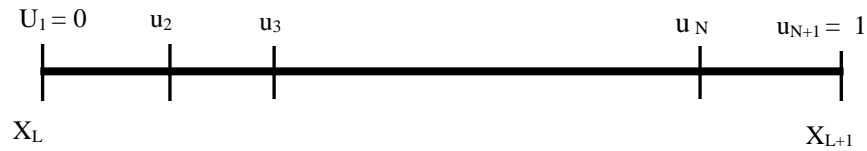


Figure 5: Application of orthogonal collocation on the local domain

A new variable $v = \frac{(x - x_k)}{h_k}$ is introduced in such a way that as x varies from x_k to x_{k+1} , v varies from 0 to 1. Then orthogonal collocation method is applied on the new variable v .

2.3.2 Element Distribution

One of the challenging tasks here is identifying how to distribute elements within given domain $[a, b]$. We will choose Finlayson [14] as he proposed that better results can be obtained in the case of unequal element spacing than the equal element spacing. However, Investigators like Carey and Finlayson [28], Paterson and Creswell [29], have given several formulas for placing elements.

2.3.3 Algorithm

The following algorithm is constructed from [14] [15] [7]

Algorithm 5: Algorithm for Orthogonal Collocation Finite Element

1. Consider an orthogonal function $\phi(u)$ which satisfies the linear or nonlinear differential equation $\phi(u)$ with two known boundary conditions and is defined on the domain $[a, b]$.
2. This domain $[a, b]$ $0 \leq x \leq 1$ is divided into subdomains $0 = x_1 < x_2 < \dots < x_{ne+1} = 1$ called elements with $h_k = x_{k+1} - x_k$.
3. A new variable u is introduced

$$v = \frac{(x - x_k)}{h_k} \quad (2.3 \text{ eq. 1})$$

4. The orthogonal collocation method is applied within each element.
5. We let $\phi^i(u)$ as a trial solution at the i^{th} element.

$$\phi^i(v) = \sum_{k=1}^{N+1} c_k^i l_k(v) \quad (2.3 \text{ eq. 2})$$

6. Substituting the approximate solution in from step 5 into the differential equation gives the residual in the i^{th} element
7. We compute the Lagrange polynomial of degree k in the variable u .

$$l_k(v) = \prod_{\substack{j=1 \\ j \neq k}}^{N+1} \frac{v - v_j}{v_k - v_j} \quad (2.3 \text{ eq. 3})$$

Here $v_j, j=1,2,\dots,N+1$ are the interpolation points with $v_1 = a, v_{N+1} = b$ and $v_j = 2,3,\dots,N$ are the root then we evaluate u from step 3 (2.3 eq. 1) and recover the approximate solution from step 5 (2.3 eq. 2)

8. The continuity of the functions and the continuity of the derivatives should be adjusted up to the last element. We have a system of equations which we choose to arrange in the order.
9. Then finally this gives a matrix vector form $Ac = b$ which is depicted in the system of equations.

2.4 Accuracy and Convergence

In numerical computations very often, it becomes essential to find the functional approximation of a set of discrete data points and this approximation is done by minimizing some norm of the error.

The most important reason for estimating error is to gain some confidence in the numerical solution. There is some cost associated with estimating error and adapting the step size/method, but generally this is a bargain because the IVP is solved more efficiently. Three kinds of norms

are commonly used for the functional approximation, viz. L1, L2 and L-infinity. This project describes the three kinds of norms for both discrete data set and continuous functions.

2.4.1 Absolute Error

Absolute error is the value that shows how far away the approximate is as a numerical value.

$\phi_{numerical}$ is the approximate of ϕ_{exact} .

$$Absolute\ Error = |\phi_{exact}(i) - \phi_{numerical}(i)| \quad (2.3\ eq.\ 4)$$

Where:

ϕ_{exact} = the exact value of the given equation

$\phi_{numerical}$ = The numerical value of the method

2.4.2 Relative Error

It gives a value that shows how far away the approximate is as a decimal.

$$Relative\ Error = \frac{\phi_{exact}(i) - \phi_{numerical}(i)}{\phi_{exact}(i)} \quad (2.3\ eq.\ 5)$$

Where:

ϕ_{exact} = the exact value of the given equation and $\phi_{exact}(i) \neq 0$

$\phi_{numerical}$ = The numerical value of the method

2.4.3 Norm

2.4.3.1 L2 Norm

L2 norm is a standard method to compute the length of a vector in **Euclidean** space, L2 norm of x is defined as the square root of the sum of the squares of the values in each dimension. we symbolize its norm by $\|A\|$.

$$\|A\|_2 = \sqrt{\sum_{j=1}^n (\phi_{exact} - \phi_{numerical})^2} \quad (2.3\ eq.\ 6)$$

Where:

ϕ_{exact} = the exact value of the given equation

$\phi_{numerical}$ = The numerical value of the method

2.4.3.2 L - Infinity Norm

This is the easiest to find. The largest absolute value of components of a vector.

$$\|A\|_{\infty} = \text{Max} |\phi_{exact} - \phi_{numerical}| \quad (2.3 \text{ eq. } 7)$$

Where:

ϕ_{exact} = the exact value of the given equation

$\phi_{numerical}$ = The numerical value of the method

2.4.3.3 Root Mean Square (RMS) Norm

RMS error is Acronym for root mean square error. A measure of the difference between locations that are known and locations that have been interpolated or digitized. RMS error is derived by squaring the differences between known and unknown points, adding those together, dividing that by the number of test points, and then taking the square root of that result. The regression line predicts the average y value associated with a given x value. Note that is also necessary to get a measure of the spread of the y values around that average. To do this, we use the root-mean-square error (r.m.s. error). To construct the r.m.s. error, first need to determine the residuals. Residuals are the difference between the actual values and the predicted values.

$$RMS = \sqrt{\frac{\sum_{j=1}^n (\phi_{exact} - \phi_{numerical})^2}{n}} \quad (2.3 \text{ eq. } 8)$$

where ϕ_{exact} is the observed value for the j^{th} observation and

$\phi_{numerical}$ is the predicted value.

They can be positive or negative as the predicted value under or over estimates the actual value. Squaring the residuals, averaging the squares, and taking the square root gives us the RMS error. Then use the RMS. error as a measure of the spread of the ϕ values about the predicted ϕ value.

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We choose the list of BVP problems and equations below to solve using, Sub domain, Galerkin and collocation weighted residual methods.

2.5 Computational Cost

Computational cost is used to measure the execution time per time step during computation. To estimate the time that it takes for your computation to execute on real-time hardware, estimate the simulation execution-time budget for your real-time target machine.

2.5.1 Elapsed Time

Macmillan dictionary defined Elapsed time in [30], “The amount of time that has passed since a particular process started, especially compared with the amount of time that was calculated for it in a plan”. As the same meaning as the dictionary, for computational analysis, elapsed time means the total amount of time in seconds that a certain function/instruction takes for execution. MathWorks briefly described about elapsed time in [31] `toc` reads the elapsed time since the stopwatch timer started by the call to the `tic` function. `t = toc` returns the **elapsed time** in `t`. `time` measures the amount of **time MATLAB** takes to complete one or more operations, and displays the **time** in seconds. This example measures how the **time** required to solve a nonlinear BVPs using Weighted residual orthogonal collocation finite element methods.

2.5.2 CPU Time

CPU time returns the total CPU time (in seconds) used by MATLAB® application from the time it was started. This number can overflow the internal representation and wrap around.

2.6 Preliminaries of the Experimented Boundary Value Problems

For the application of weighted residual method and orthogonal collocation finite element method, here we have selected six boundary value problems for different types of boundary conditions.

2.6.1 Exothermic Chemical Reaction in a Slab of Combustible Material

2.6.1.1 Motivation

Frank-Kamenetskii’s disapproval of Semenov’s logic theorized that the difference between the temperatures at the center of the solid and its surface is the cause of the explosion [32].

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The study of thermal decomposition of reactive material in a slab is vital in understanding the heat transfer of engineering processes. It is notable that thermal decomposition of various materials is reliant on size, shape and surface or natural temperature just as the physical properties of the material and condition. As such, for some random calculation, there is a basic size and surface temperature above which the heat generation inside the strong surpasses the heat scattering to the environment [33].

In several industrial applications theoretical study of transient heating in a slab of combustible material due to exothermic chemical reaction plays an important part. These include: heavy oil recovery, cellulosic material storage, biomass, solids combustion, waste incineration, carbon gasification, etc. Without sufficient knowledge of a reacting system, exothermic chemical processes can dramatically increase leading to a runaway reaction, potential explosion, economic losses and toxic gas emissions, such as carbon [34].

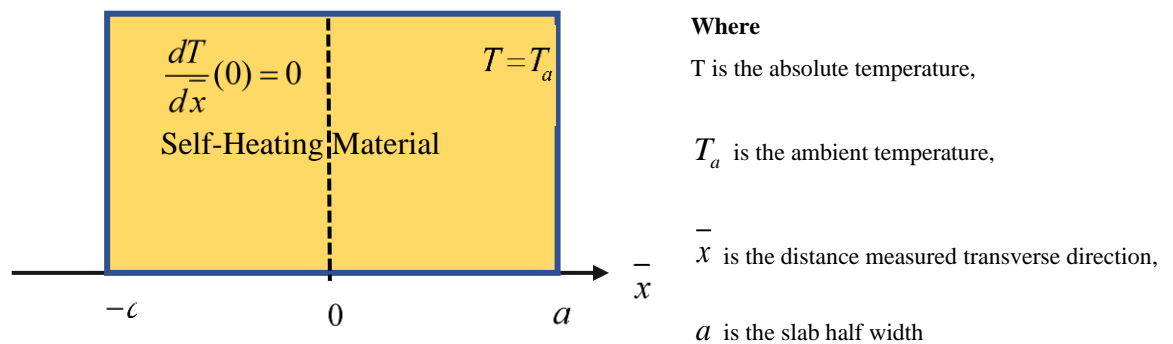


Figure 6: Geometry of the Problem

2.6.1.2 Problem Definition

Due to exothermic chemical reaction, the study of transient heating in a slab of combustible material plays a significant role in many industrial applications. For example: storage of cellulosic materials, heavy oil recovery, the pyrolysis of biomass and coal, the combustion of solids, waste incineration, coal gasification, etc. Estomih S Massawe, Wilson Mahera Charles, and Oluwole D Makinde in [35] studied this problem by using Perturbation technique together with a special type of Hermite-Padé series summation and improvement method. However, in this study, we investigate a numerical solution for this problem using weighted residual and orthogonal collocation method.

Governing Differential equation [35]

$$\frac{d^2\phi}{dx^2} + \lambda \left[(1 + \varepsilon\phi)^m e^{\left(\frac{\phi}{1+\varepsilon\phi}\right)} - \delta\phi \right] = 0 \quad (2.4 \text{ eq. 1})$$

(2.4 eq. 2)

$$\frac{d\phi}{dx} = 0, \quad \phi(1) = 0$$

where

λ is the Frank – Kameneskii parameter,

ε the activation energy parameter,

δ the heat loss parameter,

m is the numerical exponent.

The parameters in (2.4 eq. 1) for the thermal decomposition of the reacting combustible material which are of great importance with respect to applications in the area of industrial safety and handling techniques of explosives. we used the following parameter values for $\lambda, \delta, \varepsilon, m$.

Table 1: exothermic explosion problem parameter definition

Row #	Varying parameters					Constant/Fixed parameters
	Parameter name	1st Parameter	2 nd Parameter	3 rd Parameter	4 th Parameter	
1	λ	0.1	0.2	0.3	0.4	$\delta = 0.1, \varepsilon = 0.1, m = 0.5$
2	δ	0	0.1	0.2	--	$\lambda = 0.1, \varepsilon = 0.1, m = 0.5$
3	m	-2	0	0.5	--	$\lambda = 0.1, \varepsilon = 0.5, \delta = 0.1$

The analytical solution for the exothermic explosion problem is given by in [35] using iterative

$$\begin{aligned} \theta(x) = & \frac{\lambda}{2}(x^2-1) - \frac{\lambda^2}{24}(x^2-1)(x^2-5)(-1-m\varepsilon+\delta) + \frac{\lambda^3}{720}(x^2-1)(-2\delta x^4 + 8m\varepsilon x^4 + 4x^4 \\ & - 2m\varepsilon x^4\delta - 3m\varepsilon^2 x^4 - 6\varepsilon x^4 + \delta^2 x^4 + 4m^2\varepsilon^2 x^4 - 14\delta^2 x^2 - 52m\varepsilon x^2 + 28\delta x^2 + 12m\varepsilon^2 x^4 \\ & - 26x^2 + 24\varepsilon x^2 - 26m^2\varepsilon^2 x^2 + 28m\varepsilon x^2\delta - 66\varepsilon + 61\delta^2 + 94 + 188m\varepsilon + 94m^2\varepsilon^2 - 122m\varepsilon\delta \\ & - 122\delta - 33m\varepsilon^2) \end{aligned} \quad (2.4 \text{ eq. 3})$$

2.6.1.3 Weighted and Approximate Function

The given boundary conditions for both are the same $\frac{d\phi}{dx} = 0$, $\phi(1) = 0$. Thus, (2.2 eq. 6) could satisfies the boundary conditions in (2.4 eq. 2), this yields

$$c_2 = 0 \quad (2.4 \text{ eq. 4})$$

$$c_1 = -c_3 \quad (2.4 \text{ eq. 5})$$

Thus, the functional form of the approximate solution $\phi(x)$ that satisfies the boundary conditions could be written as

$$\phi(x) = c_3(-1 + x^2) \quad (2.4 \text{ eq. 6})$$

And the weight function is

$$N(x) = -1 + x^2 \quad (2.4 \text{ eq. 7})$$

The derivative of the approximating function or trial function is used

First order

$$\frac{d\phi}{dx} = 2c_3x \quad (2.4 \text{ eq. 8})$$

Second order

$$\frac{d^2\phi}{dx^2} = 2c_3 \quad (2.4 \text{ eq. 9})$$

After substituting the first derivative from (2.4 eq. 8), second derivative from (2.4 eq. 9) and the approximate function from (2.4 eq. 6) into equation (2.4 eq. 1), the residual would be

$$R = 2c_3 + \lambda \left[(1 + \varepsilon(-c_3 + c_3x^2))^m e^{\left(\frac{-c_3 + c_3x^2}{1 + \varepsilon(-c_3 + c_3x^2)}\right)} - \delta(-c_3 + c_3x^2) \right] \quad (2.4 \text{ eq. 10})$$

After this we follow the procedures as per the algorithms for weighted residuals in the above section for each method.

2.6.2 Catalytic Reactions in a Flat Particle

2.6.2.1 Motivation

Researchers studied about simultaneous mass and heat transfer inside a porous catalyst particle have been widely studied. Many chemical and biochemical reactions take place within porous catalyst particles. This example arises in a study of heat and mass transfer for a catalytic reaction within a porous catalyst flat particle [32]. The differential equation is the direct result of a material and energy balance. Let us consider a flat geometry for the particle and that conductive heat transfer is negligible compared to convective heat transfer yields the differential equation.

2.6.2.2 Problem Definition

Governing Differential equation [36]

$$\frac{d^2\phi}{dx^2} = \lambda\phi \exp\left[\frac{\gamma\beta(1-\phi)}{1+\beta(1-\phi)}\right] \quad (2.4 \text{ eq. 11})$$

$$\frac{d\phi}{dx} = 0, \quad \phi(1) = 1 \quad (2.4 \text{ eq. 12})$$

where

ϕ is Dimensionless *concentration*,

λ is Dimensionless *parameter*,

β is Dimensionless *parameter*,

γ is Dimensionless *parameter*,

we used the following parameter values for λ, γ, β .

Table 2: catalytic reaction problem parameter definition

Row #	Varying parameters					Constant/Fixed parameters
	Parameter name	1st Parameter	2 nd Parameter	3 rd Parameter	4 th Parameter	
1	λ	0.01	0.5	2	5	$\gamma = 1, \beta = 0.2$
2	β	0.001	0.01	0.03	0.05	$\gamma = 5, \lambda = 1$

The analytical Solution for the catalytic reaction problem is given by in [36].

$$\phi(x) = \left(1 + \frac{\lambda\beta\gamma(\cosh(2k) - 3)}{6k^2(1+\beta)^2 \cosh^2(k)} \right) \left(\frac{\cosh(kx)}{k} \right) + \left(\frac{\gamma\lambda\beta(3 - \cosh(2kx))}{6(1+\beta)^2 \cosh^2(k)} \right) \quad (2.4 \text{ eq. 13})$$

where

$$k = \sqrt{\lambda + \frac{\lambda\beta\gamma}{(1+\beta)}}$$

2.6.2.3 Weighted and Approximate function

The given boundary conditions for both are the same $\frac{d\phi}{dx} = 0$, $\phi(1) = 1$. Thus, we formulate the trial solution: a quadratic trial solution shown in was adopted in this work.

$$\phi = c_1 + c_2x + c_3x^2 \quad (2.4 \text{ eq. 14})$$

(2.2 eq. 6) could satisfies the boundary conditions in (2.4 eq. 2), this yields

$$c_2 = 0 \quad (2.4 \text{ eq. 15})$$

$$c_1 = 1 - c_3 \quad (2.4 \text{ eq. 16})$$

Thus, the functional form of the approximate solution $\phi(x)$ that satisfies the boundary conditions could be written as

$$\phi(x) = 1 - (1 + x^2)c_3 \quad (2.4 \text{ eq. 17})$$

And the weight function is

$$N(x) = 1 + x^2 \quad (2.4 \text{ eq. 18})$$

The derivative of the approximating function or trial function is used

First order

$$\frac{d\phi}{dx} = 2c_3x \quad (2.4 \text{ eq. 19})$$

Second order

$$\frac{d^2\phi}{dx} = 2c_3 \quad (2.4 \text{ eq. 20})$$

After we substitute the corresponding terms first derivative from (2.4 eq. 19), second derivative from (2.4 eq. 20) and the approximate function from (2.4 eq. 17) into equation(2.4 eq. 11) , the residual would be

$$R = 2c_3 - \lambda(1 - c_3 + c_3x^2)e^{\left[\frac{\gamma\beta(1-(1-c_3+c_3x^2))}{1+\beta(1-(1-c_3+c_3x^2))}\right]} \quad (2.4 \text{ eq. 21})$$

After this we follow the procedures as per the algorithms for weighted residuals in the above section for each method.

2.6.3 Thermal Explosion Problem

2.6.3.1 Motivation

Researchers like D.A Kamenetskii [37] and Ya.B.Zeldovich [38] had done a lot of research work in the field of thermal explosion theory. A solution of thermal equation exists if λ is small enough meaning that chemical heat production can be entirely balanced by conduction. However, for increasing λ the solution suddenly does not exist anymore. This phenomenon is referred to as *a thermal explosion*.

2.6.3.2 Problem Definition

Wang, Xijian And Zeng, Tonghua in [39] investigated this problem model by using central difference and newton iteration method. In this study, we find numerical solutions using weighted residual methods and OCFE method.

Governing Differential equation [39]

$$\frac{d^2\phi}{dx^2} + \lambda e^{(\phi)} = 0 \quad (2.4 \text{ eq. 22})$$

$$\frac{d\phi}{dx} = 0, \quad \phi(1) = 0 \quad (2.4 \text{ eq. 23})$$

where

λ is Dimensionless *parameter*

The analytical Solution for the exothermic explosion problem is given by in [39].

$$\phi(x) = \ln\left(\frac{2\phi^2}{\lambda}\right) - 2\ln(\cosh(\phi x))$$

where the parameter ϕ satisfies the relation (2.4 eq. 24)

$$\cosh \phi = \sqrt{\frac{2}{\lambda\phi}}$$

2.6.3.3 Weighted and Approximate Function

The given boundary conditions for both are the same $\frac{d\phi}{dx} = 0$, $\phi(1) = 0$. Thus, (2.2 eq. 6) could satisfies the boundary conditions in (2.4 eq. 2), this yields

$$c_2 = 0 \quad (2.4 \text{ eq. 25})$$

$$c_1 = -c_3 \quad (2.4 \text{ eq. 26})$$

Thus, the functional form of the approximate solution $\phi(x)$ that satisfies the boundary conditions could be written as

$$\phi(x) = c_3(-1+x^2) \quad (2.4 \text{ eq. 27})$$

And the weight function is

$$N(x) = -1+x^2 \quad (2.4 \text{ eq. 28})$$

The derivative of the approximating function or trial function is used

First order

$$\frac{d\phi}{dx} = 2c_3x \quad (2.4 \text{ eq. 29})$$

Second order

$$\frac{d^2\phi}{dx^2} = 2c_3 \quad (2.4 \text{ eq. 30})$$

We get the residual after we substitute the corresponding terms first derivative from (2.4 eq. 29), second derivative from (2.4 eq. 30) and the approximate function from (2.4 eq. 27) into equation (2.4 eq. 22).

$$R = 2c_3 + \lambda e^{(-c_3+c_3x^2)} \quad (2.4 \text{ eq. 31})$$

.....

After this we follow the procedures as per the algorithms for weighted residuals in the above section for each method.

2.6.4 Temperature Distribution in Straight Fins with Temperature Dependent Thermal Conductivity

2.6.4.1 Motivation

Heat transfer is the process of thermal energy exchange due to a temperature difference in a medium or between media. as P.S. Ghoshdastidar [40] reported on his book in industry and nature, the applications of heat transfer are diversified. such as, formation of rain and snow are for the natural phenomena wherein heat transfer plays assertive role. and also heat transfer important in industry for medical applications, like Bioheat transfer, Materials processing, etc [41]. M.G. Sobamowo in [42] solved longitudinal fin with temperature-dependent properties and internal heat generation using Galerkin's weighted residual method. Pinar Mert Cuce, Erdem Cuce and Cemalettin Aygun in [43] used Homotopy perturbation method for to solve temperature distribution problems. On the other hand, Promise Mebine and Nataliya Olali [44] applied the SDC technique which is a token of power series solution called Leibnitz-Maclaurin Method (LMM) for the problem of fin efficiency for convective straight fin with temperature-dependent thermal conductivity. A.A. Joneidi, D.D. Ganji, M. Babaelahi in [45] together solved the same problem by using DTM (Differential Transformation Method) . we also examined and reported fin in our previous research in [46] using for a Temperature-Dependent Thermal Conductivity Fin with Internal Heat Generation .

In this work, therefore, we apply the weighted residual methods for the problem of fin efficiency for convective straight fin with temperature-dependent thermal conductivity.

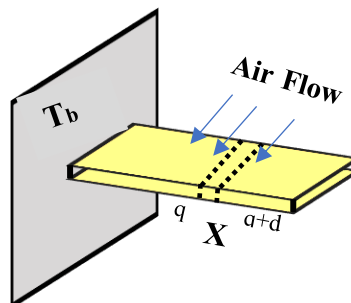


Figure 7: Schematic of straight fin geometry with the internal heat generation

2.6.4.2 Problem Definition

The differential equation is [44]:

$$\frac{d^2\phi}{dx^2} + \beta\phi \frac{d^2\phi}{dx^2} + \beta\left(\frac{d\phi}{dx}\right)^2 - \psi^2\phi = 0 \quad (2.4 \text{ eq. 32})$$

$$\begin{aligned} \frac{d\phi}{dx} &= 0, \text{ when } x=0 \\ \phi(1) &= 1, \text{ when } x=1 \end{aligned} \quad (2.4 \text{ eq. 33})$$

where

ϕ is the dimensionless temperature,

x is the non-dimensional coordinate,

β is the non-dimensional parameter describing thermal conductivity, and

ψ is the thermogeometric fin parameter.

The semi analytical Solution for the Fin problem is given by [47]

$$\begin{aligned} \phi(x) &= \alpha + \frac{x^2}{2!} \left(\frac{\alpha\psi^2}{(1+\alpha\lambda)} \right) + \frac{x^4}{4!} \left(\frac{\alpha\psi^4}{(1+\alpha\lambda)^2} - \frac{3\alpha^2\psi^4\lambda}{(1+\alpha\lambda)^3} \right) \\ &+ \frac{x^6}{6!} \left(\frac{\alpha\psi^6}{(1+\alpha\lambda)^3} - \frac{18\alpha^2\psi^6\lambda}{(1+\alpha\lambda)^4} + \frac{45\alpha^3\psi^6\lambda^2}{(1+\alpha\lambda)^5} \right) \\ &+ \frac{x^8}{8!} \left(\frac{\alpha\psi^8}{(1+\alpha\lambda)^4} - \frac{66\alpha^2\psi^8\lambda}{(1+\alpha\lambda)^5} + \frac{669\alpha^3\psi^8\lambda^2}{(1+\alpha\lambda)^6} - \frac{1440\alpha^4\psi^8\lambda^3}{(1+\alpha\lambda)^7} \right) \end{aligned} \quad (2.4 \text{ eq. 34})$$

where $\alpha = \phi(0)$

2.6.4.3 Weighted and Approximate Function

The given boundary conditions for both are the same $\frac{d\phi}{dx} = 0$, $\phi(1) = 1$. Thus, we formulate the

trial solution: a quadratic trial solution shown in was adopted in this work.

$$\phi = c_1 + c_2x + c_3x^2 \quad (2.4 \text{ eq. 35})$$

(2.2 eq. 6) could satisfies the boundary conditions in (2.4 eq. 2), this yields

$$c_2 = 0 \quad (2.4 \text{ eq. 36})$$

$$c_1 = 1 - c_3 \quad (2.4 \text{ eq. 37})$$

Thus, the functional form of the approximate solution $\phi(x)$ that satisfies the boundary conditions could be written as

$$\phi(x) = 1 - (1 + x^2)c_3 \quad (2.4 \text{ eq. } 38)$$

And the weight function is

$$N(x) = 1 + x^2 \quad (2.4 \text{ eq. } 39)$$

The derivative of the approximating function or trial function is used

First order

$$\frac{d\phi}{dx} = 2c_3x \quad (2.4 \text{ eq. } 40)$$

Second order

$$\frac{d^2\phi}{dx^2} = 2c_3 \quad (2.4 \text{ eq. } 41)$$

Residual function is

$$R = 2c_3 + \beta(1 - c_3 + c_3x^2)2c_3 + \beta(2c_3x)^2 - \psi^2(1 - c_3 + c_3x^2) \quad (2.4 \text{ eq. } 42)$$

After this we follow the procedures as per the algorithms for weighted residuals in the above section for each method.

2.6.5 Troesch Boundary Value Problem for Temperature Distribution

2.6.5.1 Motivation

The Troesch's problem is a nonlinear boundary-value problem. And it had been first described and solved Troesch's problem comes from a system of nonlinear ordinary differential equations which occur in an investigation of the confinement of a plasma column by applying radiation pressure and via the gas porous electrodes theory [48] [49].

As [47] experimented HPM, it is a modern technique for iteratively constructing analytic solutions to nonlinear equations. By using Homotopy Perturbation Method we can get the semi exact solution and also we can use the HPM method as semi analytic solution for Troesch problem [50]. Thus, the semi analytical solution for the Troesch problem is given by in [47].

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2.6.5.2 Problem Definition

The differential equation is:

Governing Differential equation [47]

$$\frac{d^2\phi}{dx^2} = \lambda \sinh(\lambda\phi) \quad (2.4 \text{ eq. 43})$$

$$\phi(0) = 0$$

$$\phi(1) = 1 \quad (2.4 \text{ eq. 44})$$

where λ is Dimensionless parameter,

The semi analytical Solution for the Troesch problem is given by [47].

$$\begin{aligned} \phi(x) = & x + \frac{1}{120} \lambda^4 x^5 + \frac{1}{6} \lambda^2 x^3 + \left(-\frac{1}{120} \lambda^4 - \frac{1}{6} \lambda^2 \right) x + \frac{1}{17280} \lambda^8 x^9 \\ & + \frac{11}{5040} \lambda^6 x^6 + \frac{1}{120} \lambda^4 x^5 - \frac{1}{4800} \lambda^8 x^5 - \frac{1}{240} \lambda^6 x^5 - \frac{1}{720} \lambda^3 x^6 \\ & - \frac{1}{36} \lambda^4 x^3 + \left(\frac{13}{86400} \lambda^8 + \frac{17}{5040} \lambda^6 + \frac{7}{360} \lambda^4 \right) x \end{aligned} \quad (2.4 \text{ eq. 45})$$

2.6.5.3 Weighted and Approximate Function

The given boundary conditions for both are the same $\phi(0) = 0$, $\phi(1) = 1$. Thus,

we formulate the trial solution: a quadratic trial solution shown in was adopted in this work.

$$\phi = c_1 + c_2 x + c_3 x^2 \quad (2.4 \text{ eq. 46})$$

(2.2 eq. 6) could satisfies the boundary conditions in (2.4 eq. 2), this yields

$$c_1 = 0 \quad (2.4 \text{ eq. 47})$$

$$c_2 = 1 - c_3 \quad (2.4 \text{ eq. 48})$$

Thus, the functional form of the approximate solution $\phi(x)$ that satisfies the boundary conditions could be written as

$$\phi(x) = x - (x + x^2)c_3 \quad (2.4 \text{ eq. 49})$$

And the weight function is

$$N(x) = x + x^2 \quad (2.4 \text{ eq. } 50)$$

The derivative of the approximating function or trial function is used

First order

$$\frac{d\phi}{dx} = 1 - c_3 + 2c_3x \quad (2.4 \text{ eq. } 51)$$

Second order

$$\frac{d^2\phi}{dx^2} = 2c_3 \quad (2.4 \text{ eq. } 52)$$

As per (2.4 eq. 49) , (2.4 eq. 52) the residual function is

$$R = 2c_3 - \lambda \sinh(\lambda(x - c_3x + c_3x^2)) \quad (2.4 \text{ eq. } 53)$$

After this we follow the procedures as per the algorithms for weighted residuals in the above section for each method.

2.6.6 Reaction Diffusion Equation

2.6.6.1 Motivation

Reaction-diffusion equation have been applied in many areas of specialization for example, in developmental biology Alan Turing reported in [51], neuroscience in [52] a detailed analysis was done on Action Potential Propagation by Hodgkin-Huxley, James Sneyd reported about Calcium dynamics in [53] [54].

The analytical solution for the reaction-diffusion equation is taken from Vembu Ananthaswamy, Lakshmanan Rajendran report in [36].

2.6.6.2 Problem Definition

The differential equation is: [55]

$$\frac{d^2\phi}{dx^2} + \lambda e^{\left(\frac{\phi}{(1+\alpha\phi)}\right)} = 0 \quad (2.4 \text{ eq. } 54)$$

$$\phi(0) = 0, \quad \phi(1) = 0 \quad (2.4 \text{ eq. } 55)$$

where

λ is Dimensionless *parameter*,

The analytical Solution for the reaction diffusion equation problem is given by [36].

$$\begin{aligned} \phi(x) = & \left(\frac{\alpha(b^2 + 3)}{2} - 1 \right) + \left(1 - \frac{\alpha(2b^2 + 4)}{3} + \alpha b \sqrt{\lambda} x \right) \cos(\sqrt{\lambda} x) \\ & + \frac{\alpha(b^2 - 1) \cos(2\sqrt{\lambda} x)}{6} - \left(\frac{\alpha b \sin(2\sqrt{\lambda} x)}{3} \right) \\ & + \sin(\sqrt{\lambda} x) \left\{ (b - \alpha \sqrt{\lambda} x) + \left(\frac{\alpha}{\sin(\sqrt{\lambda})} \right) \left[\sqrt{\lambda} \sin(\sqrt{\lambda}) \right. \right. \\ & \left. \left. + \frac{b \sin(2\sqrt{\lambda})}{3} \frac{(b^2 + 3)}{2} - \frac{(b^2 - 1) \cos(2\sqrt{\lambda})}{6} + \left(\frac{2b^2 + 4}{3} - b \sqrt{\lambda} \right) \cos(\sqrt{\lambda}) \right] \right\} \end{aligned} \quad (2.4 \text{ eq. } 56)$$

2.6.6.3 Weighted and Approximate Function

The given boundary conditions for both are the same $\phi(0) = 0$, $\phi(1) = 0$. Thus,

we formulate the trial solution: a quadratic trial solution shown in was adopted in this work.

$$\phi = c_1 + c_2 x + c_3 x^2 \quad (2.4 \text{ eq. } 57)$$

(2.2 eq. 6) could satisfies the boundary conditions in (2.4 eq. 2), this yields

$$c_1 = 0 \quad (2.4 \text{ eq. } 58)$$

$$c_2 = -c_3 \quad (2.4 \text{ eq. } 59)$$

Thus, the functional form of the approximate solution $\phi(x)$ that satisfies the boundary conditions could be written as

$$\phi(x) = (-x + x^2)c_3 \quad (2.4 \text{ eq. } 60)$$

And the weight function is

$$N(x) = -x + x^2 \quad (2.4 \text{ eq. } 61)$$

The derivative of the approximating function or trial function is used

First order

$$\frac{d\phi}{dx} = -c_3 + 2c_3 x \quad (2.4 \text{ eq. } 62)$$

Second order

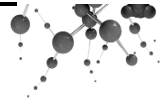
$$\frac{d^2\phi}{dx} = 2c_3 \quad (2.4 \text{ eq. } 63)$$

Residual function

$$\mathbf{R} = 2\mathbf{c}_3 + \lambda e^{\left(\frac{-c_3x+c_3x^2}{(1+\alpha(-c_3x+c_3x^2))}\right)} \quad (2.4 \text{ eq. } 64)$$

After this we follow the procedures as per the algorithms for weighted residuals in the above section for each method.

Chapter 3



APPLICATION OF WEIGHTED RESIDUALS FOR SOLVING NONLINEAR BVPs

We choose the list of BVP problems and equations namely, for the steady state exothermic chemical reaction in a slab of combustible material, thermal explosion in a vessel, catalytic reactions in a flat particle, temperature distribution in straight fins with temperature dependent thermal conductivity, reaction-diffusion equation, Troesch boundary value problem for temperature distribution using, SD, GRK and COL weighted residual methods.

3.1 Subdomain Method

We have seen the methods and algorithms for SDWRM on section 2.2.6 based on that in this section, we validate the SDWRM for the experimented BVPs on section 2.6.

3.1.1 Numerical Experiments

3.1.1.1 Exothermic Chemical Reaction in a Slab of Combustible Material

In this section, we validate exothermic thermal explosion problem (2.4 eq. 1) with the boundary conditions in (2.4 eq. 2). The exact solution of the equation is taken from (2.4 eq. 3). By using its algorithm and physically realistic values of various embedded parameters that we defined in the above Table 1: exothermic explosion problem parameter definition, for the numerical experiment. Based on Algorithm 3 on Chapter 2, and section 2.6.1.3, we seen the trial/approximate solution for the general application of weighted residual method. The Subdomain's formulation of the Exothermic thermal explosion (2.4 eq. 1) equation is as per Algorithm 3 let us choose another middle limit ($c = 0.5$) between the upper ($b = 1$) and lower ($a = 0$) and we integrate them separately. Integrating the residual function (2.4 eq. 10) using the middle limit $c = 0.5$ and lower limit $a = 0$, we have;

$$\int_0^{0.5} R dx \quad (3.1 \text{ eq. } 1)$$

And again, integrate the residual function (2.4 eq. 10) using the middle limit $b = 1$ and lower limit $c = 0.5$, we have;

.....

$$\int_{0.5}^1 R dx \tag{3.1 eq. 2}$$

We finally get the integration of the residue using the upper limit $b = 1$ and lower limit $a = 0$

$$\int_0^1 \left[2c_3 + \lambda \left[(1 + \varepsilon(-c_3 + c_3x^2))^m e^{\left(\frac{-c_3 + c_3x^2}{1 + \varepsilon(-c_3 + c_3x^2)}\right)} - \delta(-c_3 + c_3x^2) \right] \right] dx \tag{3.1 eq. 3}$$

then we compute and solve the above equation (3.1 eq. 3), based on the above Algorithm 3 on Chapter 2, page 15, we developed a user defined computer program for solving exothermic explosion problem for Subdomain method by us by using MATLAB version R2019b v9.7.0, for the numerical experiment, we defined parameters in the above Table 1, row 1.

Figures (7)-(11) illustrate the effects of various thermophysical parameters on the steady state temperature profiles. The temperature is maximum along the centerline and minimum at the surface. for the experimentation parameters we define on Table 1, row 1.

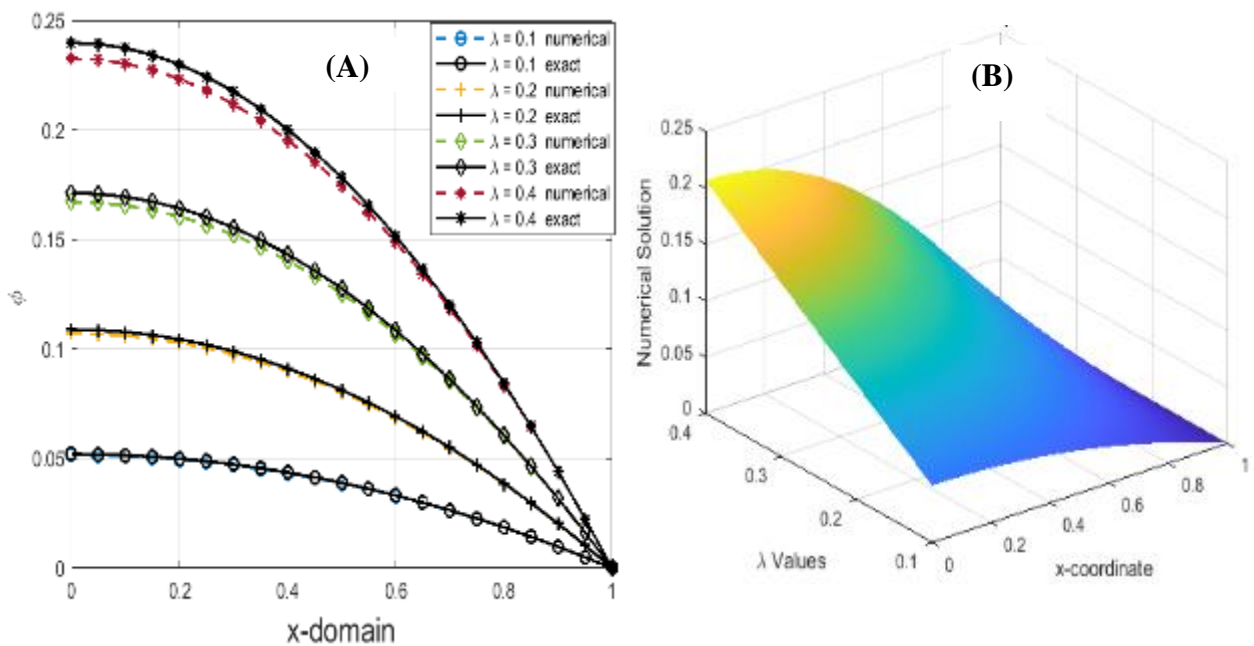


Figure 8: solution for exothermic thermal explosion problem using subdomain WRM

when $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

For both numerical and analytic solutions Figure 8 (A) show that the slab temperature increases with an increase in the parameter values of λ . As the Frank-Kamenetskii parameter (λ) increases,

.....

and the other remaining parameters (i.e activation energy(\mathcal{E}), heat loss (δ), numerical exponent (m)) remains fixed, then the slab internal heat generation due to exothermic reaction increases, this invariably leads to an elevation in the slab temperature. And Figure 8 (B) shows the 3D plot for the influence of the parameter (λ) values on the dependent variable (ϕ) along the x coordinate.

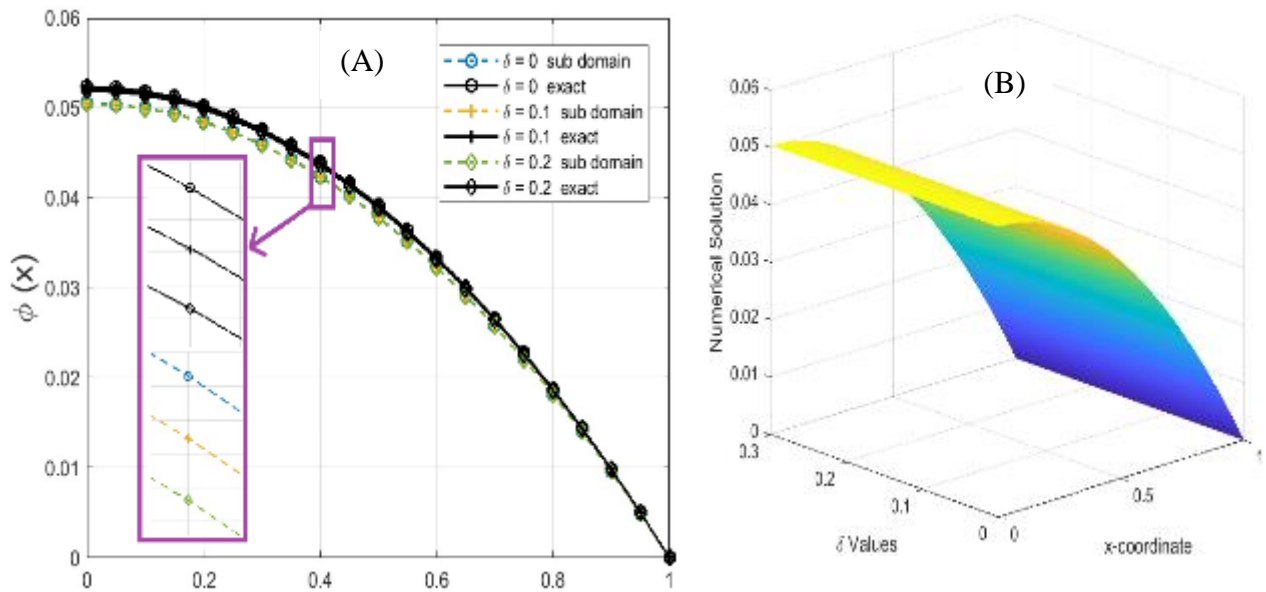


Figure 9: effect of heat loss on slab temperature profiles using subdomain WRM

when $\lambda = 0.1$, $m = 0.5$, $\mathcal{E} = 0.1$

For the parameter definition on row 2, In Figure 9 (A) we observe that the slab temperature decreases with an increase in the heat loss parameter values of (δ). The decrease in the slab temperature with increasing (δ) can be attributed to the cooling action of heat loss on the slab. But the other remaining parameters (i.e the activation energy(\mathcal{E}), Frank Kamenskii (λ), numerical exponent(m)) remains fixed. Figure 9 (B) shows the influence of (δ) values on solutions (ϕ) along x coordinate using 3D graph.

For row 3 of parameter definition on Table 1, Figure 10 (A) show that the slab temperature is highest during bimolecular reaction $m = 0.5$ and lowest for sensitized reaction $m = -2$, hence confirming the earlier results in the literature. The slab temperature increases with an increase in the numerical exponent parameter values of (m).

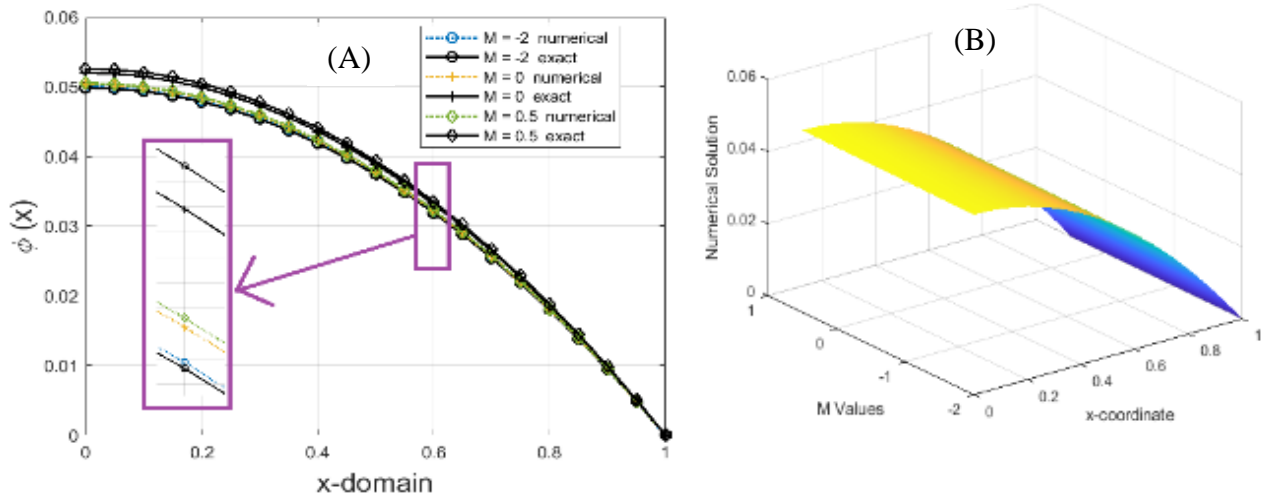


Figure 10: Subdomain and Analytic Solution for solving Exothermic Explosion problem when $\lambda = 0.1$, $\varepsilon = 0.5$, $\delta = 0.1$

Figure 10 (B) tell us the effect of their changes of these three components (x , m and ϕ) by using 3D plot. It is clear that the obtained results in our method are in very good agreement with the exact solution, which proves the reliability of the method.

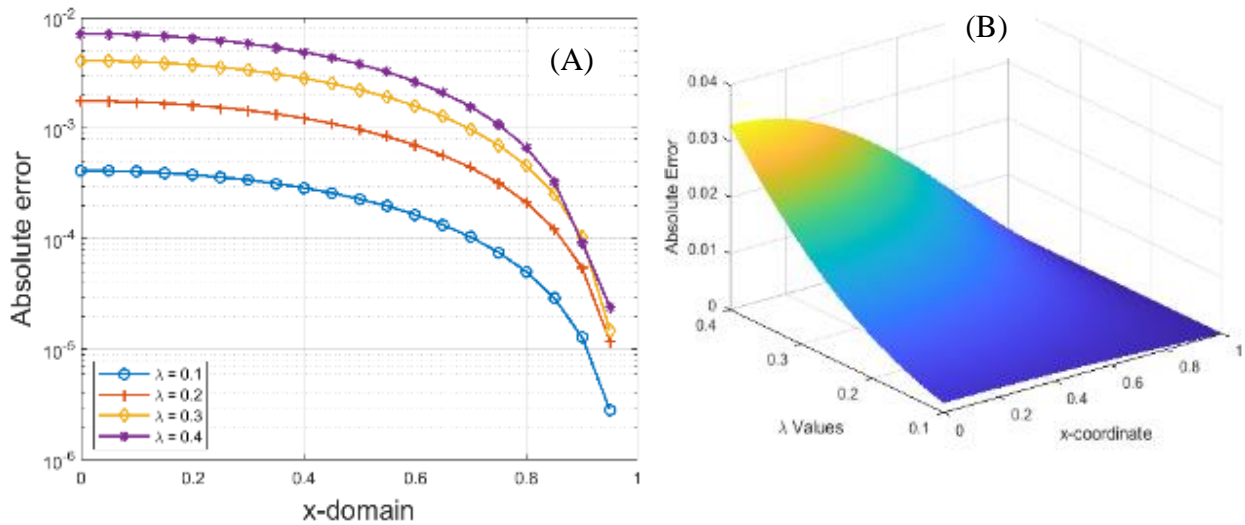


Figure 11: Absolute Error for solving Exothermic Explosion problem when $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Absolute error is the prominent techniques to check the accuracy of numerical method. Thus, as we discussed the types and formulations of errors on Chapter 2, section 2.4, here absolute

error is carried out for the subdomain weighted residual method of exothermic thermal explosion problem.

From Figures (10)-(12), we observe that the *absolute errors* are decreasing from left boundary to the right for all lambda values. Figure 11 (A) shows the absolute error as lambda vary and m, ϵ, δ keeps fixed and the error is decreasing (e.g for $\lambda = 0.1$ when $x = 0.05$ abs error = 0.001685 and when $x = 0.95$, abs error=0.000127). Figure 11 (B) show us the 3D view of the error plot as λ and x are going increasing.

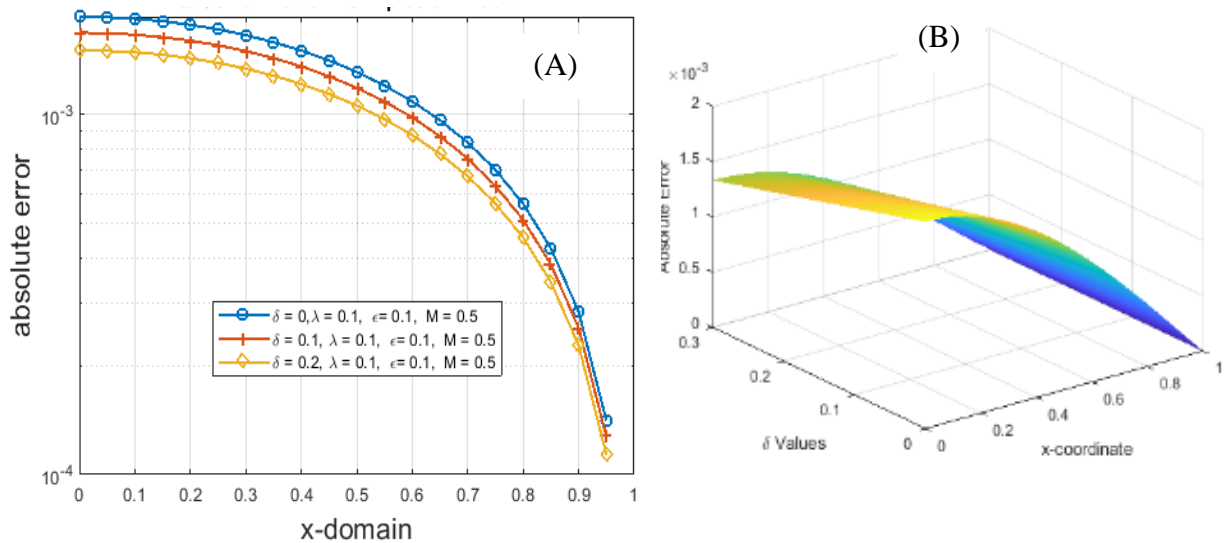


Figure 12: Absolute Error for solving Exothermic Explosion problem

when $\lambda = 0.1$, $m = 0.5$, $\epsilon = 0.1$

Figure 12 (A) shows that absolute error drastically decreases to the boundary this is also reflected when the heat loss parameter values of (δ) is increase and λ, m, ϵ keeps fixed the absolute error is decreasing (e.g for $\delta = 0$ when $x=0.05$ abs error = 0.001866 and when $x = 0.95$, abs error = 0.000141) this confirms that our numerical solution is accurate. Figure 12 (B) show that the 3D view of the error plot as δ and x are going increasing.

We observe from Figure 13 (A) absolute error is decrease from left to the right boundary and we get the similar observation as reaction type index increase on temperature profiles (e.g for $m = -2$ when $x = 0.05$ absolute error = 0.000140 and when $x = 0.90$, absolute error = 0.000001).

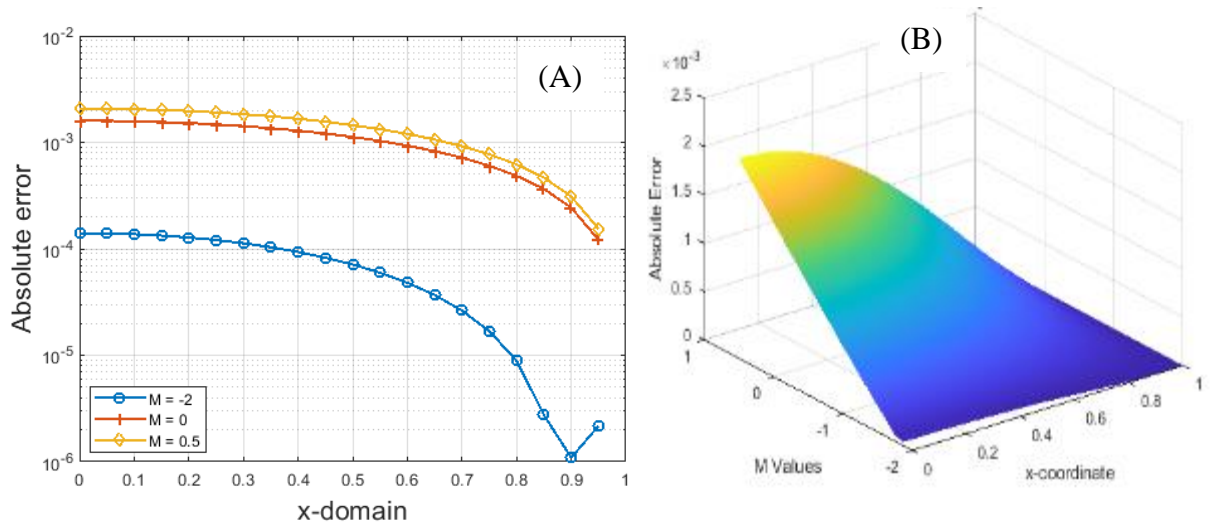


Figure 13: Absolute error for solving exothermic explosion problem

when $\lambda = 0.1, \varepsilon = 0.5, \delta = 0.1$

Figure 13 (B) tells us the effects of the changes of m and x on the absolute error using 3D diagram. Thus, the above absolute error results show us our subdomain method is very close to the exact solution.

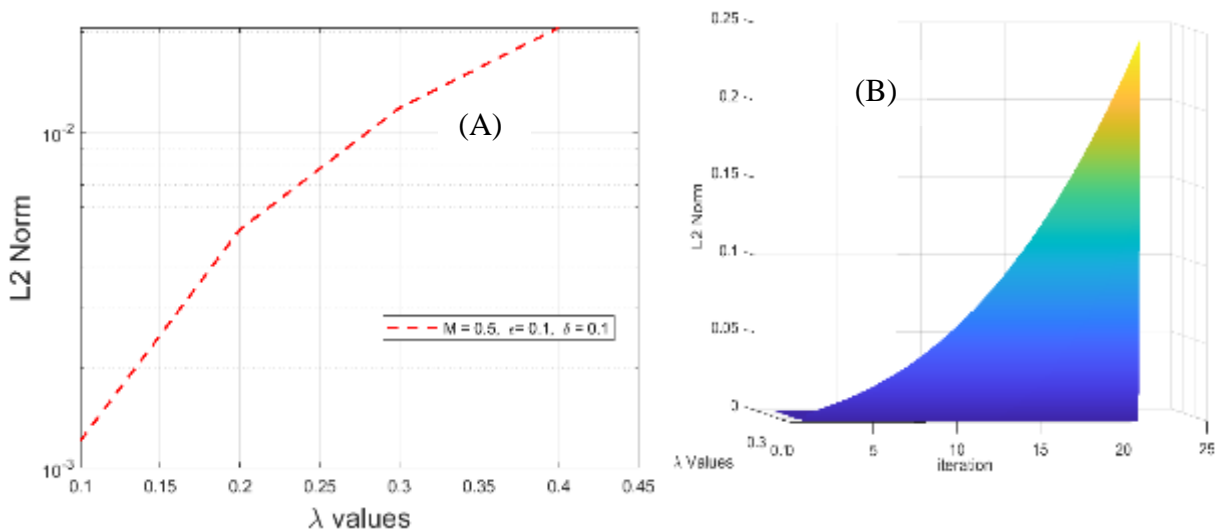


Figure 14: L_2 norm for exothermic thermal explosion problem

when λ vary and $m = 0.5, \varepsilon = 0.1, \delta = 0.1$

Like the absolute error, the other technique to check the accuracy of numerical method is using L_2 norm. As we described the types and formulations of norms on Chapter 2 section 2.4 , here

L2 norm is carried out for the subdomain weighted residual method of exothermic thermal explosion problem. Figures (14) - (16), show us the accuracy of our numerical method.

Figure 14 (A) tells us the L2 norm increases with an increase in the parameter values of λ . (e.g at $\lambda = 0.1$ $L_2 = 0.005457728$ and at $\lambda = 0.3$ $L_2 = 0.056145304$). We observe from Figure 14 (B) the effect of the L2 norm with an increase λ values and the iteration by using 3D graph(e.g. we observe there is the lowest L2 norm at 1st iteration & $\lambda = 0.1$, and there is the highest L2 norm at 21st iteration & $\lambda = 0.4$).

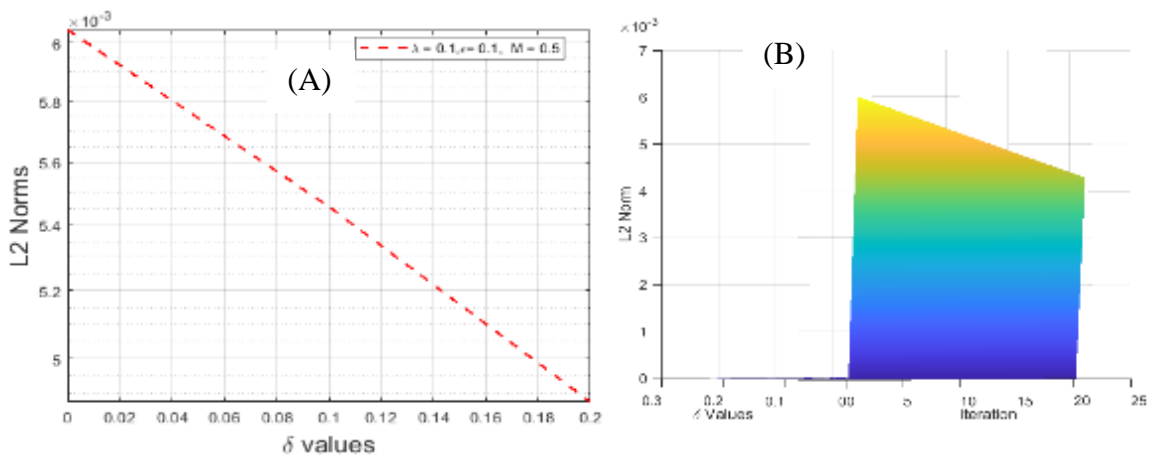


Figure 15: L2 norm when $\lambda = 0.1, m = 0.5, \epsilon = 0.1$

Figure 15(A) show us L2 norm is decreasing even heat loss parameter values of (δ) is increasing (e.g at $\delta = 0.0$ $L_2 = 0.006044074$ and at $\delta = 0.2$ $L_2 = 0.004876619$).

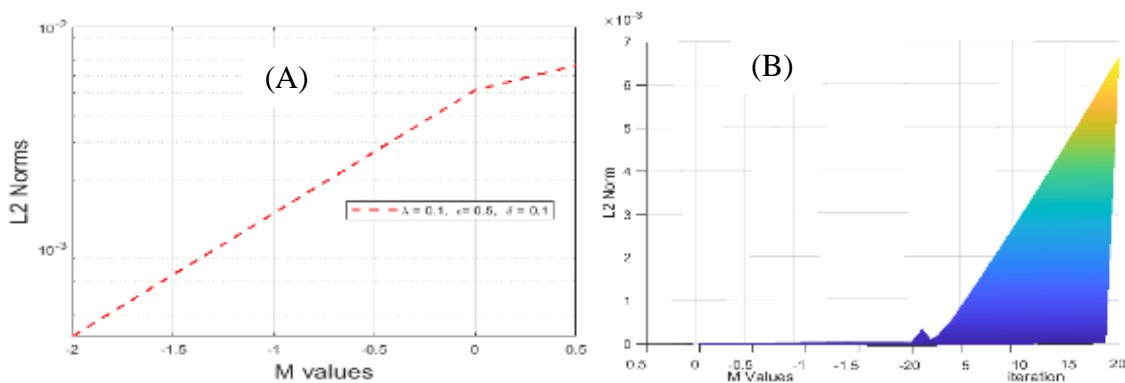


Figure 16: L2 Norm when $\lambda = 0.1, \delta = 0.1, \epsilon = 0.5$

We observed from Figure 16 that the increment of L2 norm due to an increase values of m .

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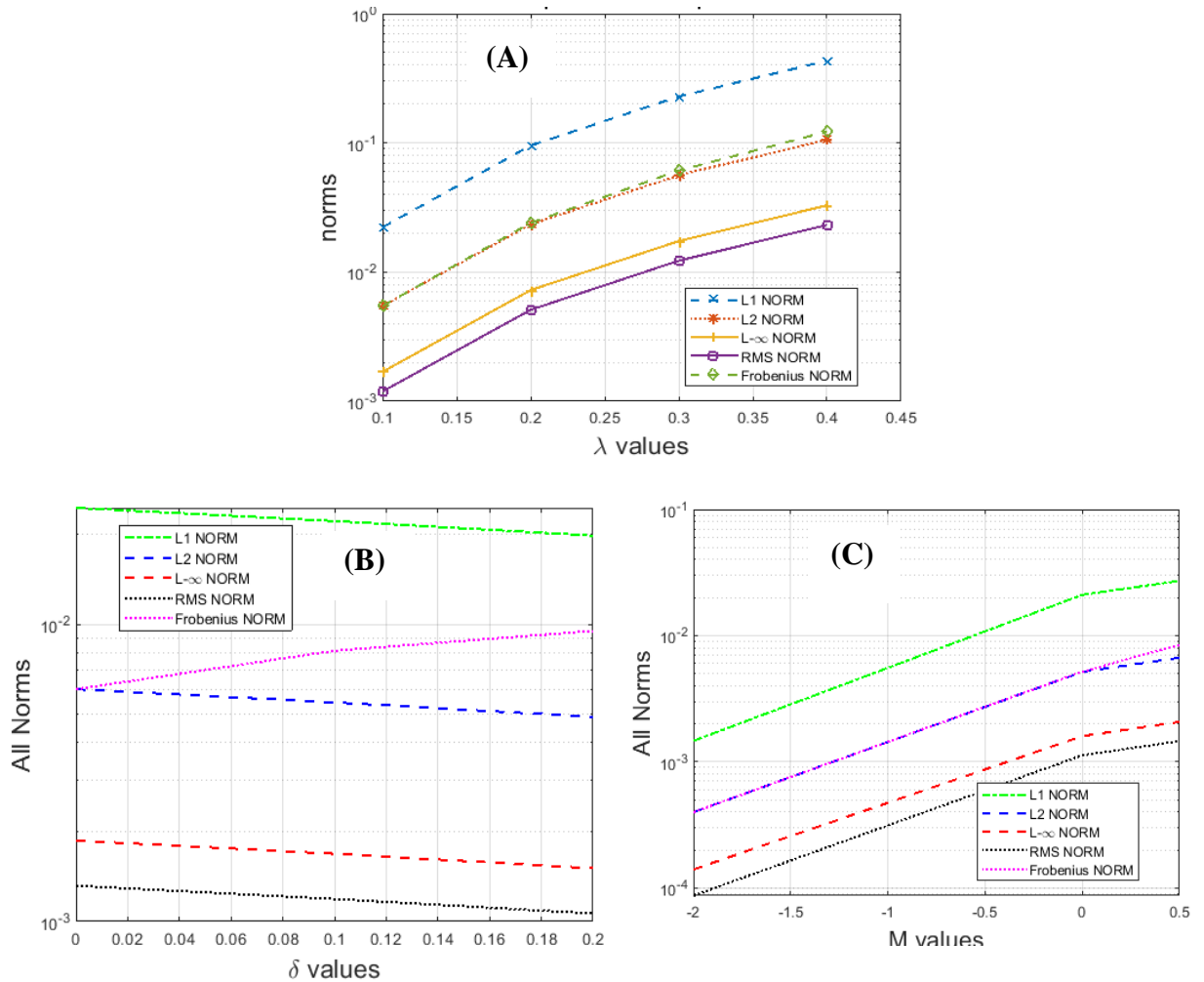


Figure 17: other norms computation for the exothermic explosion problem

when (A) $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$; (B) $\lambda = 0.1$, $m = 0.5$, $\varepsilon = 0.1$; (C) $\lambda = 0.1$, $\delta = 0.1$, $\varepsilon = 0.5$

Figure 17 (A) - (C) illustrate the plots of L_2 -norm, L-infinity norm, root mean square (RMS), L_1 -norm and frobenius norm of the numerical solution of (2.4 eq. 1) for the parameter values of $\lambda, m, \varepsilon, \delta$. Here we observe that at the beginning of the simulations, L_2 and Frobenius seems like the same plots, indeed due to their characteristics they are the same at the beginning but they are not the same after their second vary parameter respectively since frobenius norm is a matrix norm. In addition, L_1 , L_2 and Frobenius norms are larger than infinity norm and RMS, the infinity norm is also larger than root mean square (RMS).

Figure 17 (A) shows plots of norms due to the influence of Frank-Kamenetskii parameter (λ). All norms are increasing as Frank-Kamenetskii parameter (λ) values are increase but the other

remaining parameters (i.e activation energy(ε), heat loss(δ), numerical exponent(m)) keeps as fixed parameters. We observe from Figure 17 (B) as heat loss (δ) increase, all norm values are decreasing but the other remaining parameters (i.e Frank-Kamenetskii parameter (λ), activation energy (ε), numerical exponent(m)) keeps as fixed. Figure 17 (C) depicts plots of norms for the parameter values of $\lambda = 0.1$, $\delta = 0.1$, $\varepsilon = 0.5$ for different values of numerical exponent(m). When m increases all norm, values show fast increasing up ($m=0$), after this point norms are increasing but not fast. This validates the numerical formulation.

3.1.1.2 Catalytic Reaction Problem

We validate here the Subdomain weighted residual method for the cases of catalytic reaction problem (2.4 eq. 11) with the boundary conditions in (2.4 eq. 12). The exact solution of the equation is taken from (2.4 eq. 13). By using its algorithm and physically realistic values of various embedded parameters that we defined in the above Table 2, for the numerical experiment.

Based on Algorithm 3 on Chapter 2 of section 2.6.2.3, we seen the trial/approximate solution for the general application of weighted residual method. The Subdomain's formulation of the catalytic reaction problem (2.4 eq. 11) equation as Algorithm 3, let us choose another middle limit ($c = 0.5$) between the upper ($b = 1$) and lower ($a = 0$) and we integrate them separately. Integrating the residual function (2.4 eq. 21) using the middle limit $c = 0.5$ and lower limit $a = 0$, we have;

$$\int_0^{0.5} R dx \quad (3.1 \text{ eq. } 4)$$

And again, integrate the residual using the middle limit $b = 1$ and middle limit $c = 0.5$, we have;

$$\int_{0.5}^1 R dx \quad (3.1 \text{ eq. } 5)$$

The integration of the residue using the upper limit $b = 1$ and lower limit $a = 0$ is

$$\int_0^1 \left[2c_3 - \lambda(1 - c_3 + c_3 x^2) e^{\left[\frac{\gamma\beta(1-(1-c_3+c_3x^2))}{1+\beta(1-(1-c_3+c_3x^2))} \right]} \right] dx \quad (3.1 \text{ eq. } 6)$$

We compute and solve the above equation (3.1 eq. 6) using computational techniques based on Algorithm 3, for the numerical experiment, we defined parameters on Table 2, row 1 of section 2.6.2.2. We developed a user defined computer program code for solving catalytic reaction problem for Subdomain method by using MATLAB version R2019b v9.7.0. Based on the algorithm and computer result, we validated the Subdomain weighted residual method. Accordingly,

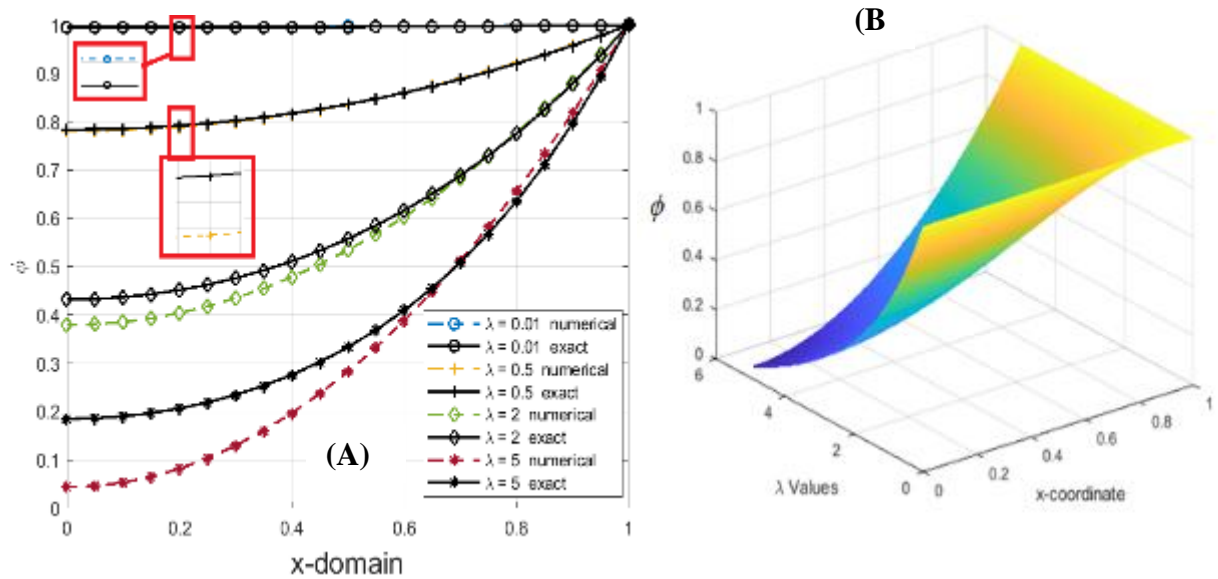


Figure 18: Solution for solving Catalytic problem

$$\text{when } \gamma = 1, \beta = 0.2$$

Figure 18 (A) shows the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless distance down the reactor x obtained from Equations (2.4 eq. 11) Table 2, row 1. From these figures it is clear that the concentration (ϕ) decreases for the fixed values of β and γ for the different values of λ . Figure 18 (B) shows the 3D plot for the influence of the parameter (λ) values with the independent variable on the dependent variable (ϕ) or solution.

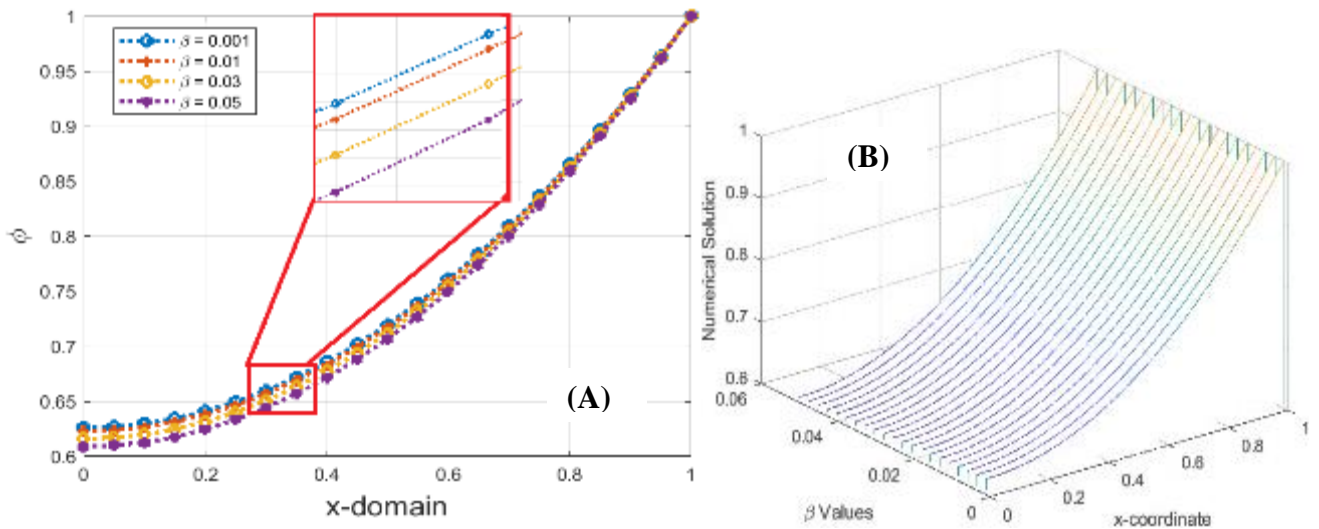


Figure 19: solution for solving catalytic problem using subdomain WRM when $\lambda = 1, \gamma = 5$

Figure 19 (A) tells us the influence of β on the dimensionless concentration (ϕ) versus the dimensionless distance down the reactor x obtained from equations (2.4 eq. 11), Table 2, row 2. From these figures it is clear that the concentration (ϕ) decreases for the fixed values of λ and γ for the different values of β . Figure 19(B) shows the 3D plot for the influence of the parameter (β) values with the independent variable on the dependent variable (ϕ) or solution.

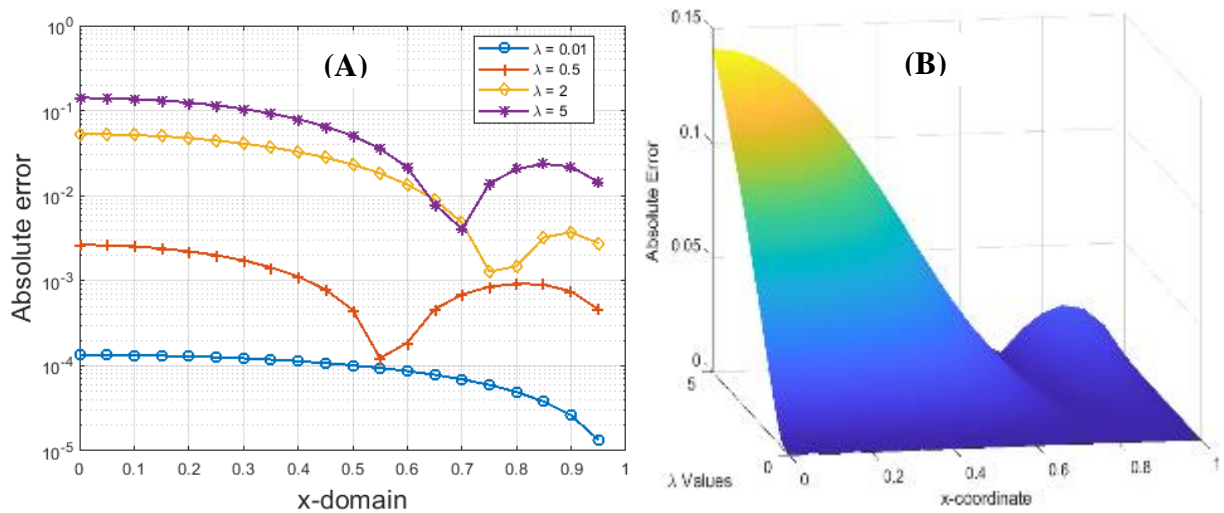


Figure 20: Absolute error for solving catalytic reaction problem when $\gamma = 1, \beta = 0.2$

Figure 20(A) and Figure 21(B) showed that the accuracy of our numerical method using computation of absolute error. These the sub domain method is very close to the analytic solution for parameter values mentioned on Table 2,row 1 when λ vary and $\gamma=1, \beta=0.2$.

Figure 20(B) show us three-dimensional view of the absolute errors.

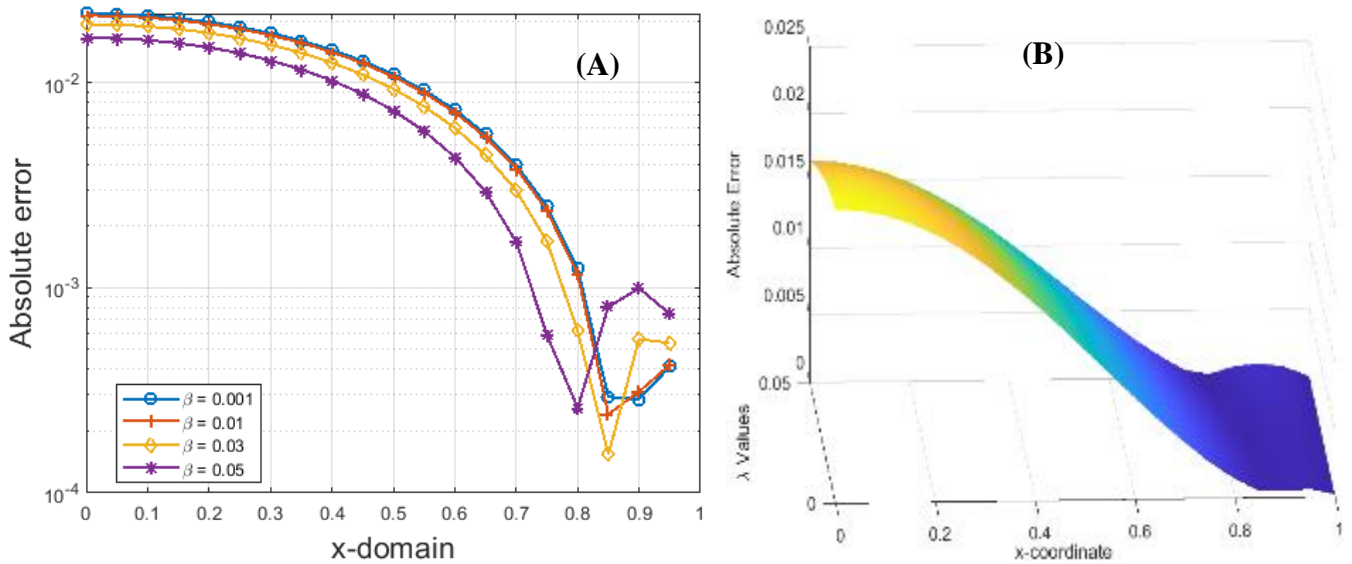


Figure 21: Absolute Error for solving Catalytic reaction problem when $\lambda = 1, \gamma = 5$

Figure 21 (A) and Figure 21(B) tells us the accuracy of our numerical method using computation of absolute error. These the sub domain method is very close to the analytic solution for parameter values mentioned on Table 2 and row 2 when β vary and $\lambda = 1, \gamma = 5$.

Figure 21 (B) show us three-dimensional view of the absolute errors.

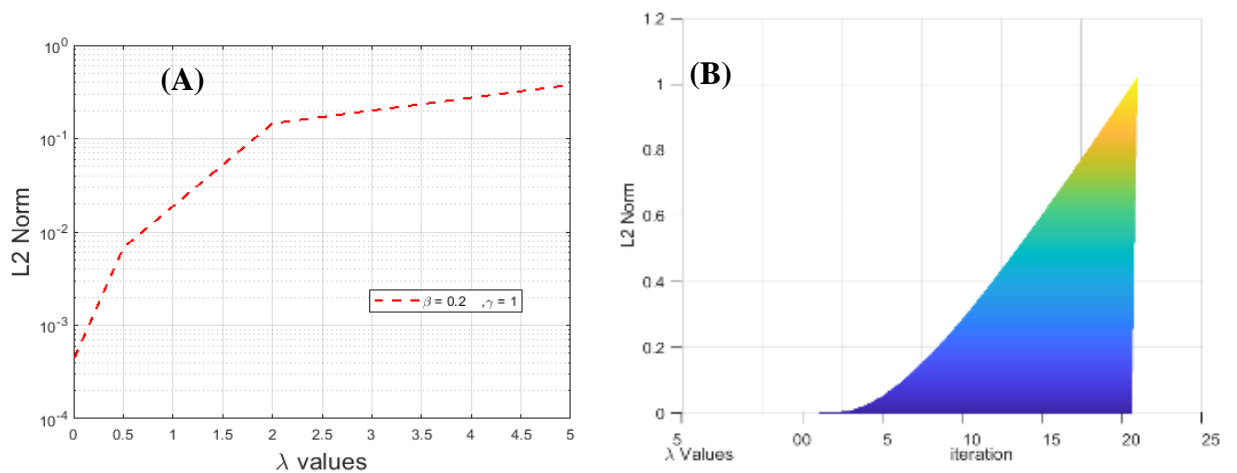


Figure 22: L2 Norm when $\gamma = 1, \beta = 0.2$

We observe from Figure 22(A) L2 norm is increasing for the fixed values of β and γ for the different values of λ . Figure 22 (B) & Figure 23 (B) show us 3D view of parameters and iterations versus L2 norm. Figure 23 showed L2 norm decreasing for the fixed values of λ and γ for the different values of β .

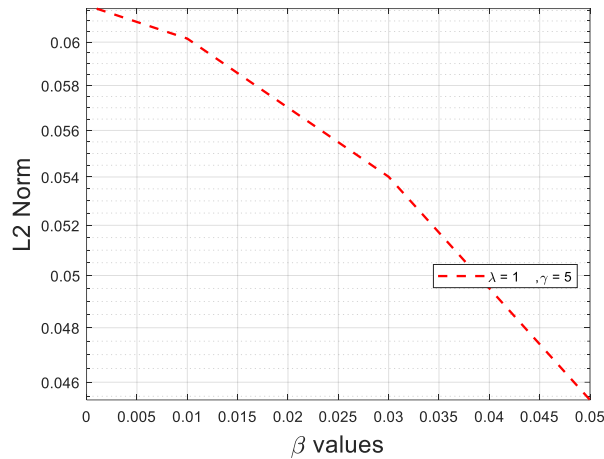


Figure 23: L2 Norm when $\gamma = 5, \lambda = 1$

Figure 24 illustrate the plots of L_2 - norm, $L-\infty$ norm, root mean square (RMS), L_1 -norm and frobenius norm of the numerical solution of (2.4 eq. 11) for the parameter values under Table 2.

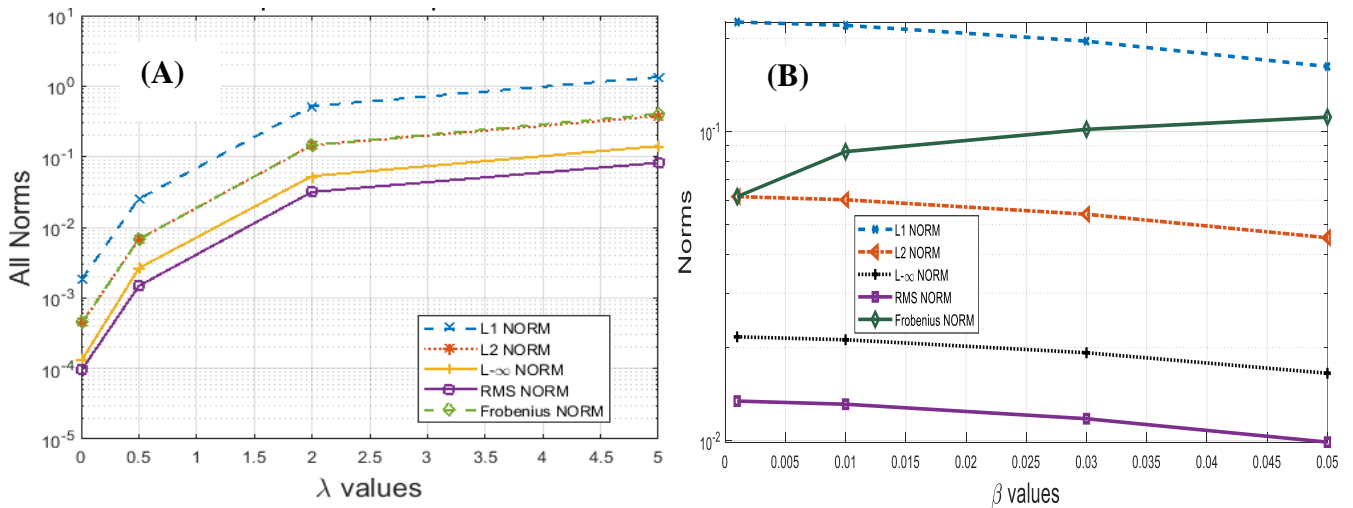


Figure 24: Other norms computation for the catalytic reaction problem when (A) $\gamma = 1, \beta = 0.2$; (B) $\gamma = 5, \lambda = 1$

Figure 24(A) shows when λ is increasing norm values are also increase. Figure 24(B) shows when β increasing norm values are decrease.

3.1.1.3 Temperature Distribution in Straight Fins with Temperature Dependent Thermal Conductivity

As mentioned the algorithm on Chapter 2, section 2.6 for temperature distribution in straight fins with temperature dependent thermal conductivity (2.4 eq. 32) , here we experiment the subdomain weighted residual method for this BVP. The exact solution of the equation is taken from [47]. Based on Algorithm 3 on Chapter 2, and section 2.6.2.3 , we seen the trial/approximate solution for the general application of weighted residual method.

The subdomain's formulation of the temperature distribution in straight fins with temperature dependent thermal conductivity (2.4 eq. 32) equation is as per Algorithm 3 , as the same as the other BVPs here, let us choose another middle limit ($c = 0.5$) between the upper ($b = 1$) and lower ($a = 0$) and we integrate them separately.

Integrating the residual function (2.4 eq. 42) using the middle limit $c = 0.5$ and lower limit $a = 0$, we have;

$$\int_0^{0.5} R dx \quad (3.1 \text{ eq. } 7)$$

And again, integrate the residual using the middle limit $b = 1$ and middle limit $c = 0.5$, we have;

$$\int_{0.5}^1 R dx \quad (3.1 \text{ eq. } 8)$$

The integration of the residue using the upper limit $b = 1$ and lower limit $a = 0$ is

$$\int_0^1 \left[2c_3 + \beta(1 - c_3 + c_3 x^2) 2c_3 + \beta(2c_3 x)^2 - \psi^2(1 - c_3 + c_3 x^2) \right] dx \quad (3.1 \text{ eq. } 9)$$

Based on the algorithm, we written a user defined computer program for the above equation (3.1 eq. 9) for subdomain weighted residual method by using MATLAB version Matlab R2019b v9.7.0. The results are presented in plots. For the numerical experiment we take fixed parameters *when*: $\psi = 0.5$ and $\beta = 0.1, 0.2, 0.3, 0.4$ and *when*: $\beta = 0.4$ and $\psi = 0.5, 1, 1.5$.

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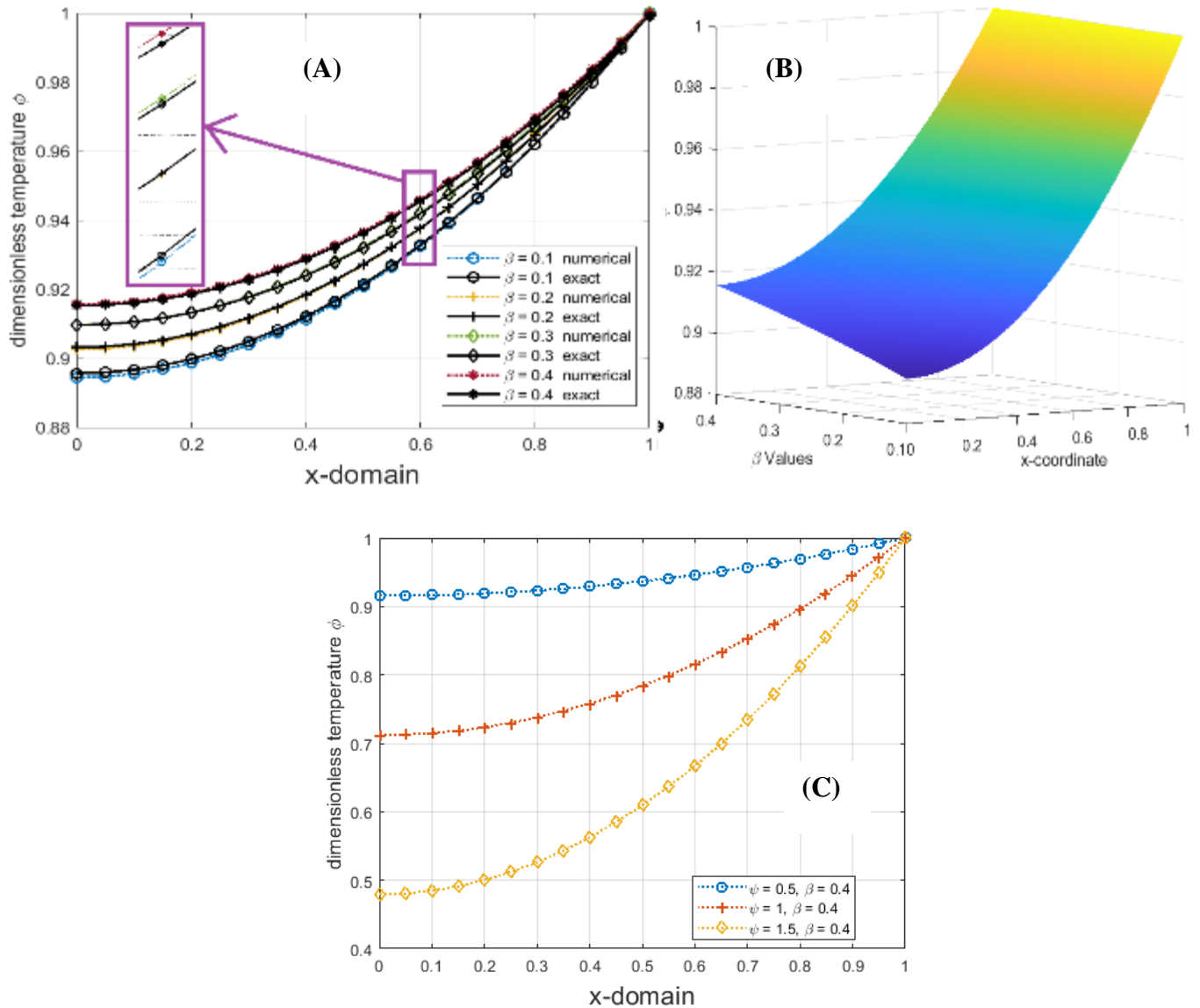


Figure 25: Solution for solving temperature distributions using subdomain WRM

The dimensionless temperature distributions along the fin surface with β varying from 0.1 to 0.4 are depicted in Figure 25 (A) for when $\psi = 0.5$. It will be seen that, if the thermal conductivity of the fin's material increases with the temperature, the mean temperature increases. Figure 25 (B) show that 3D plot for dimensionless temperature ϕ when various values of β when $\psi = 0.5$. From the Figure 25 (C), it is seen that when thermo-geometric ψ increases (i.e., the fin length increases or the cross-sectional area of the fin decreases), the dimensionless temperature ϕ decreases at the wall. This implies that the temperature of the wall is directly affected by the increase or decrease of the thermo-geometric fin parameter ψ , and in this case the non-dimensional parameter $\beta = 0.4$ is remains fixed.

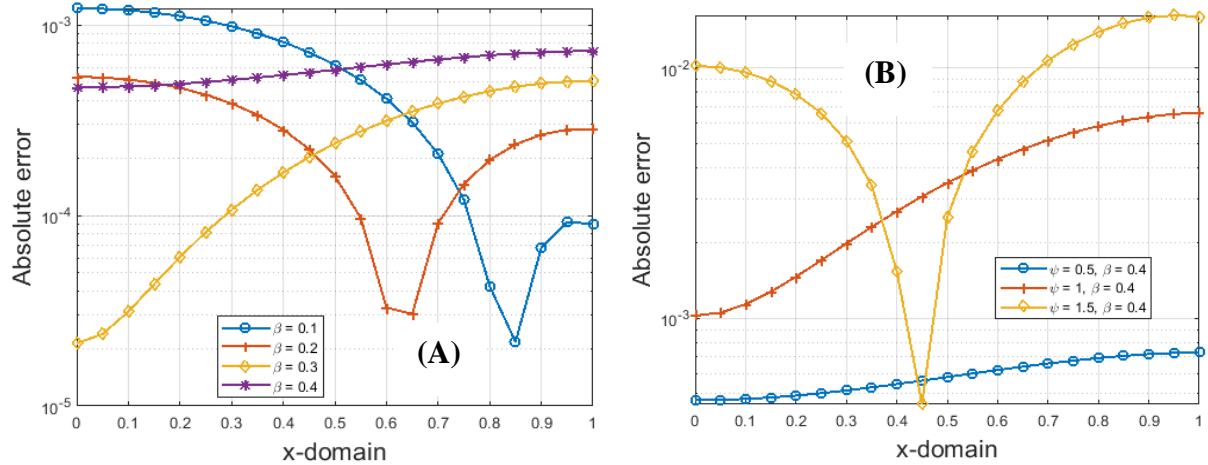


Figure 26: Absolute error for heat transfer problem

The accuracy of the numerical solution is calculated using absolute error and depicted in Figure 26 (A) various values of thermal conductivity parameter β when $\psi = 0.5$ and (B) various values of thermogeometric parameter ψ when $\beta = 0.4$, respectively.

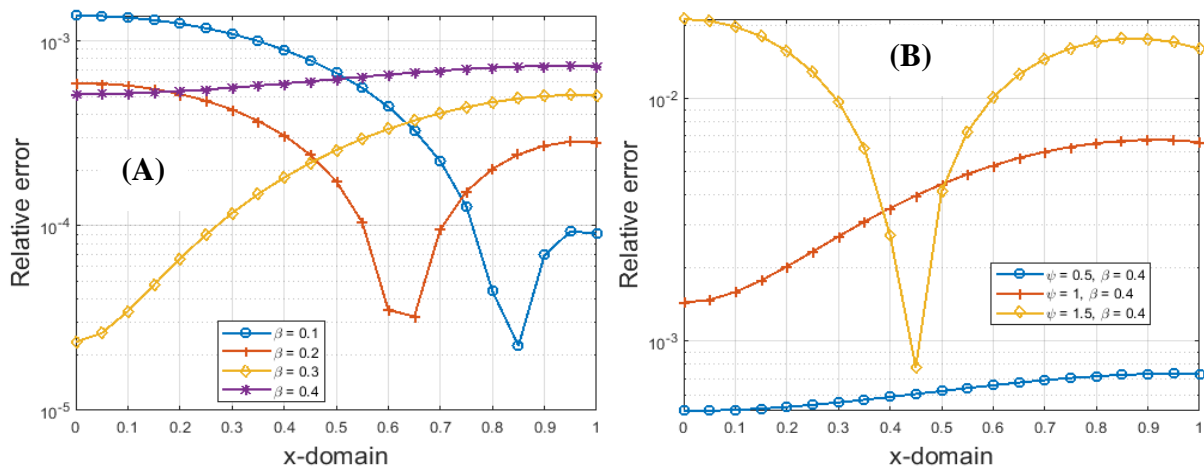


Figure 27: Relative error for heat transfer problem

The above Figure 27 shows relative errors for our computations (A) various values of β and when $\psi = 0.5$ (B) various values of ψ and when $\beta = 0.4$. The relative errors are decreasing as values of β and ψ increases.

Figure 28 illustrate the plots of L_2 - norm, L-infinity norm, root mean square (RMS), L_1 -norm and frobenius norm of the numerical solution of dimensionless temperature distribution in straight fin for the various values of β when $\psi = 0.5$.

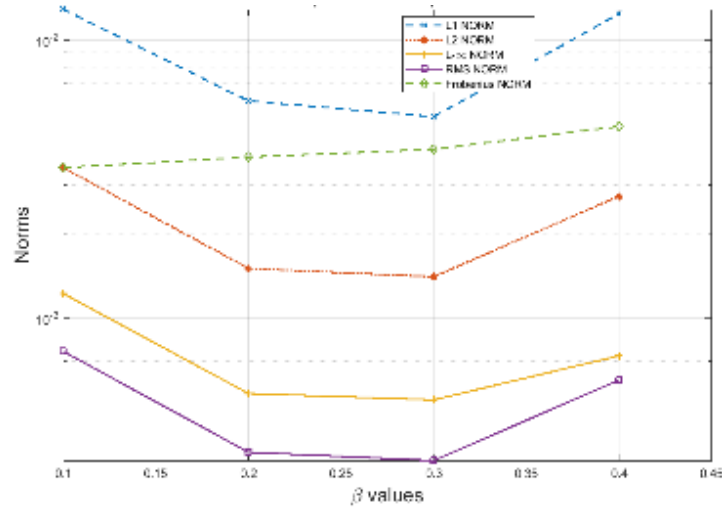


Figure 28: Other norms computation for heat transfer problem

From Figure 28 we observe that at the beginning of the simulations, L_2 and Frobenius norm seems like the same plots, indeed due to their characteristics they are the same at the beginning but they are not the same after their second vary parameter respectively since Frobenius norm is a matrix norm. In addition, L_1 , L_2 and Frobenius norm are larger than infinity norm and RMS, the infinity norm is also larger than root mean square (RMS). for various values of β and when $\psi = 0.5$.

Table 3: Comparisons of SDWRM, HAM, DTM for heat transfer problem

x	Subdomain-present	Semi-analytic [44]	DTM [45]	HPM [43]
0.00	0.902652	0.90318742	0.90344718	0.90313
0.05	0.902896	0.90342649	0.90368630	0.90314
0.10	0.903626	0.90533945	0.90559973	0.90539
0.20	0.906546	0.90701388	0.90727457	0.90707
0.20	0.908737	0.90916755	0.90942876	0.90912
0.30	0.911414	0.91180106	0.91206291	0.91190
0.35	0.914577	0.91491517	0.91517778	0.91492
0.40	0.918228	0.91851075	0.91877424	0.91857
0.45	0.922365	0.92258884	0.92285332	0.92285
0.50	0.926989	0.92715059	0.92741617	0.92711
0.55	0.932100	0.93219728	0.93246408	0.93216

0.60	0.937698	0.93773033	0.93799847	0.93779
0.65	0.943782	0.94375130	0.9440209	0.94373
0.70	0.950353	0.95026186	0.95053303	0.95023
0.75	0.957410	0.95726383	0.9575367	0.95723
0.80	0.964955	0.96475914	0.9650338	0.96303
0.85	0.972986	0.97274986	0.97302644	0.97282
0.90	0.981504	0.98123818	0.9815168	0.98121
0.95	0.990509	0.99022641	0.99050716	0.99030
1.00	1.000000	0.99991699	0.99999999	0.99999

Other norms computation for heat transfer problem

From Figure 28 we observe that at the beginning of the simulations, L_2 and Frobenius norm seems like the same plots, indeed due to their characteristics they are the same at the beginning but they are not the same after their second vary parameter respectively since Frobenius norm is a matrix norm. In addition, L_1 , L_2 and Frobenius norm are larger than infinity norm and RMS, the infinity norm is also larger than root mean square (RMS). for various values of β and when $\psi = 0.5$.

Table 3 gives a comparison of the Subdomain-present, DTM (A.A. Joneidi, D.D. Ganji, M. Babaelahi [45]), HPM (Pinar Mert Cuce, Erdem Cuce and Cemalettin Aygun [43]) and Semi-exact [44] for $\beta = 0.2$, $\psi = 0.5$. The Subdomain agrees excellently well with the HAM, DTM and the exact solution.

3.1.1.4 Thermal Explosion Problem

We experiment here the thermal explosion problem (2.4 eq. 22) with the boundary conditions in (2.4 eq. 23) using its algorithm for subdomain WRM on section 2.2.6.1 for comparison, the exact solution of the equation is taken from [39].

We saw the trial/approximate solution for the general application of weighted residual method. Based on Algorithm 3 on Chapter 2, and section 2.6.1.3, the subdomain's formulation of the thermal explosion equation, We have to have another middle limit ($c = 0.5$) between the upper ($b = 1$) and lower ($a = 0$) and we integrate them separately. Integrating the residual function (2.4 eq. 31) using the middle limit $c = 0.5$ and lower limit $a = 0$, we have;

$$\int_0^{0.5} R dx \quad (3.1 \text{ eq. } 10)$$

And again, integrate the residual function (2.4 eq. 31) using the middle limit $b = 1$ and lower limit $c = 0.5$, we have;

$$\int_{0.5}^1 R dx \quad (3.1 \text{ eq. 11})$$

We finally get the integration of the residue using the upper limit $b = 1$ and lower limit $a = 0$

$$\int_0^1 \left[2c_3 + \lambda e^{(-c_3+c_3x^2)} \right] dx \quad (3.1 \text{ eq. 12})$$

then we compute and solve the above equation (3.1 eq. 12), based on the above Algorithm 3 on Chapter 2, page 15, we developed a user defined computer program for solving exothermic explosion problem for Subdomain method by us by using MATLAB version R2019b v9.7.0.

Here, we validate the Subdomain weighted residual method is carried out by using its algorithm for the thermal explosion problem. we define here $\lambda = 0.1, 0.2, 0.3, 0.4$, for the numerical experiment. The following results show the solutions for subdomain weighted residual method with the analytic solution, absolute errors, L_2 norm for thermal explosion problem.

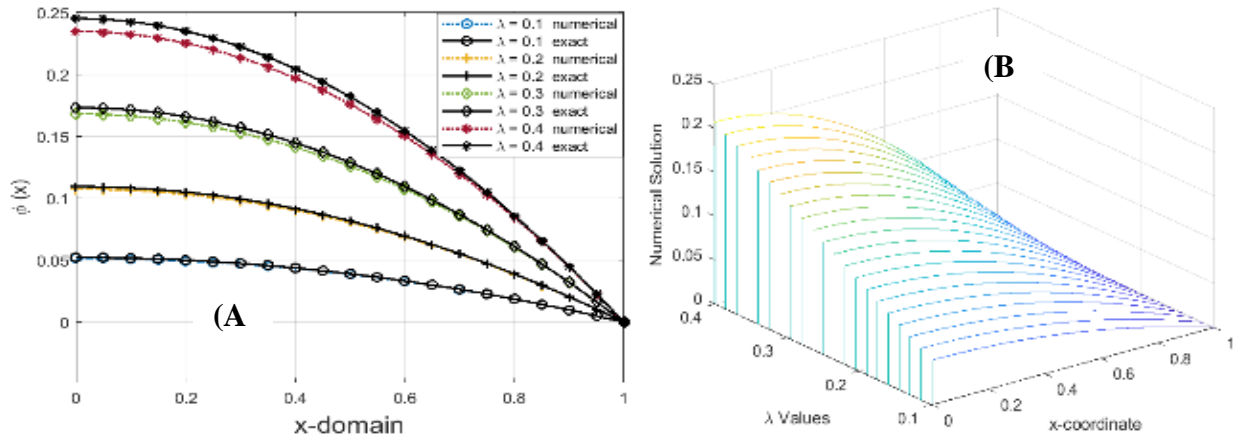


Figure 29: Solution for solving thermal explosion problem using Subdomain WRM

We observe from Figure 29 (A) the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless distance x obtained from (2.4 eq. 22) and (2.4 eq. 23). From these figures it is clear that the concentration (ϕ) increases for the different values of λ . Figure 29 (B) shows the 3D plot for the influence of the parameter (λ) values with dimensionless distance x on the dependent variable (ϕ) or solution.

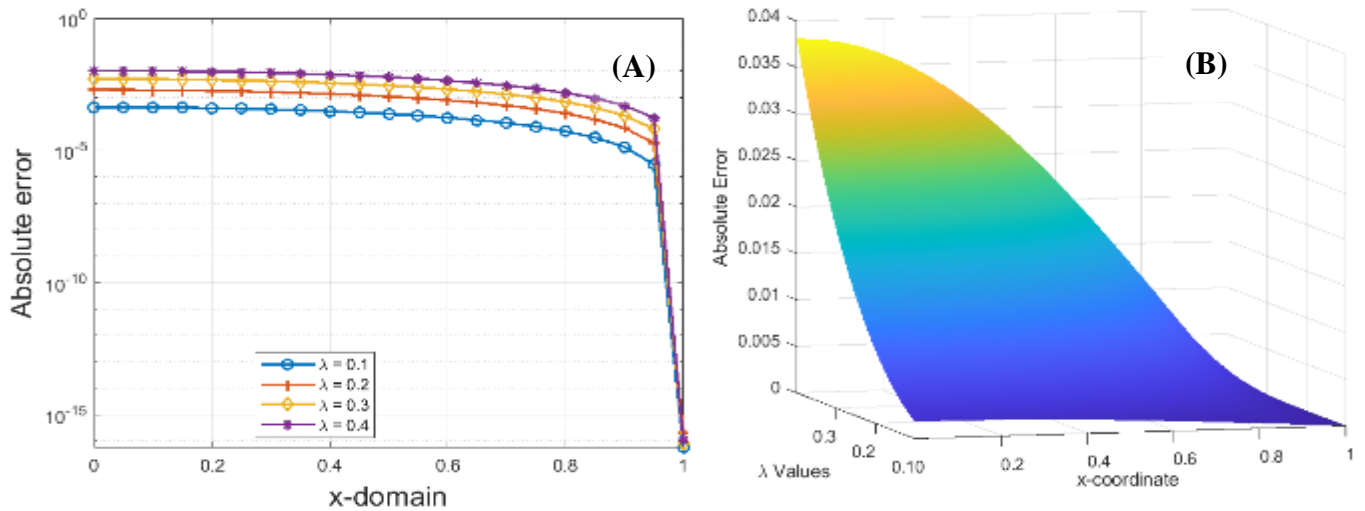


Figure 30: Absolute error for solving thermal explosion problem

From Figure 30 (A), 2D(absolute vs x -domain) and Figure 30 (B), 3D(absolute vs x -domain with λ values) respectively, it is clear that the absolute error is decrease to the right boundary for all dimensionless parameter λ values(e.g. for $\lambda = 0.2$ when $x = 0.00$ abs error = 0.007787 and when $x = 0.95$, abs error = 0.000587). From these figures, it is evident that our numerical solution very close to the exact solution and it is very accurate.

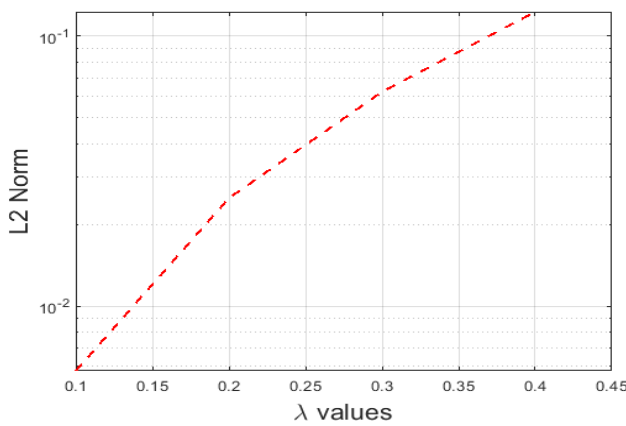


Figure 31: L2 norm for the thermal explosion problem

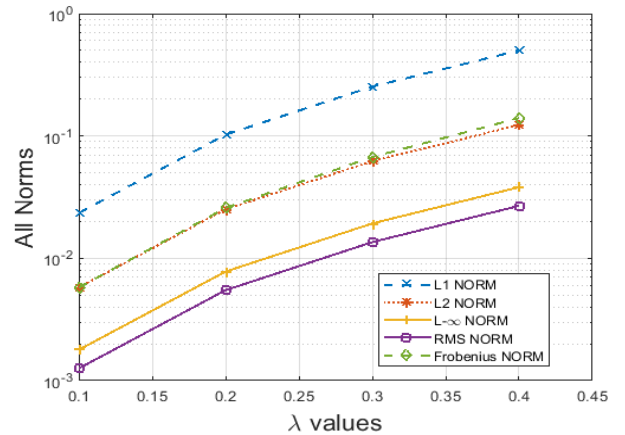


Figure 32: norms Vs λ comparisons for the thermal explosion problem

L_2 norm versus the dimensionless parameter λ is plotted in Figure 31 it show us L_2 norm is increasing as the λ values increases. We observe from Figure 32 L_1 , L_2 and frobenius norms are larger than infinity norm and RMS, the infinity norm is also larger than root mean square (RMS).

3.1.1.5 Troesch Problem

In this section, based on the algorithm 2.2.6.1 on Chapter 2 ,section 2.2, we analyzed the subdomain and the Galerkin weighted residual methods for the cases of troesch problem (2.4 eq. 43) with the boundary conditions in (2.4 eq. 23). The semi analytic solution of the equation is taken from (2.4 eq. 45).

we saw the trial/approximate solution for the general application of weighted residual method. The Subdomain's formulation of the thermal explosion equation is

we chose another middle limit($c = 0.5$) between the upper ($b = 1$) and lower ($a = 0$) and we integrate them separately. Integrating the residual function (2.4 eq. 53) using the middle limit $c = 0.5$ and lower limit $a = 0$, we have;

$$\int_0^{0.5} Rdx \quad (3.1 \text{ eq. } 13)$$

And again, integrate the residual function (2.4 eq. 53) using the middle limit $b = 1$ and lower limit $c = 0.5$, we have;

$$\int_{0.5}^1 Rdx \quad (3.1 \text{ eq. } 14)$$

We finally get the integration of the residue using the upper limit $b = 1$ and lower limit $a = 0$

$$\int_0^1 2c_3 - \lambda \sinh(\lambda(x - c_3x + c_3x^2))dx \quad (3.1 \text{ eq. } 15)$$

Then we used computational techniques to compute and solve the above equation (3.1 eq. 15), based on the above Algorithm 3 on Chapter 2, we developed a user defined computer program for solving Troesch problem for subdomain method by using MATLAB version R2019b v9.7.0.

Here, we validate the subdomain weighted residual method are carried out by using its algorithm for the Troesch problem. We define here $\lambda = 0.0001, 1, 1.3, 1.8$, for the numerical experiment. The following results show the numerical and analytic solutions, absolute errors, relative error, L_2 norm.

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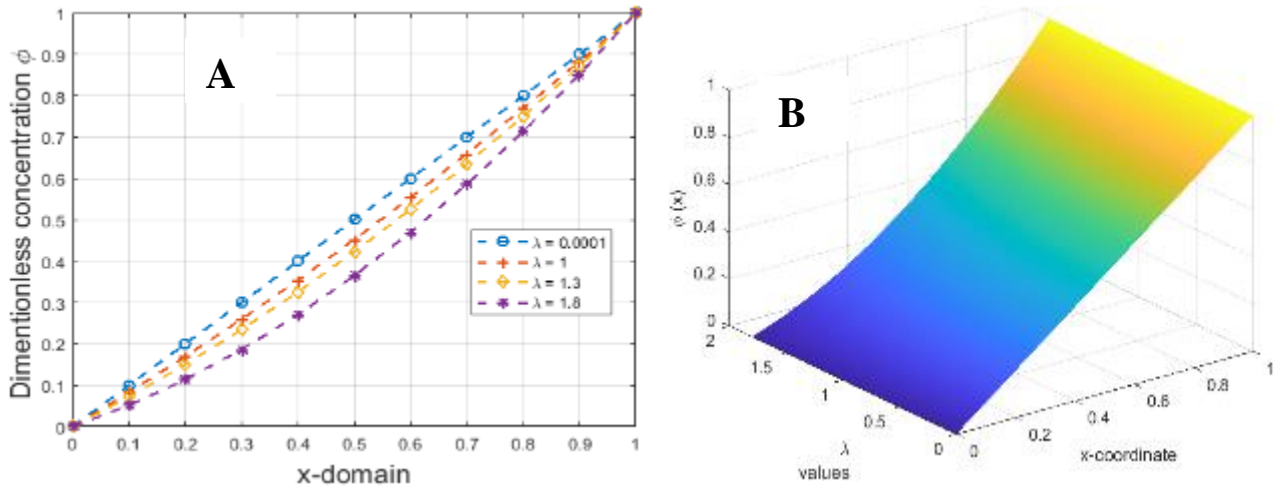


Figure 33: Subdomain weighted residual method for solving Troesch problem

We observe from Figure 33 (A) that the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless distance x obtained from (2.4 eq. 43) and (2.4 eq. 45). From these figures it is clear that the concentration (ϕ) increases for the different values of λ . Figure 33 (B) 3D plot for the influence of the parameter (λ) values with dimensionless distance x on the dependent variable (ϕ) or solution

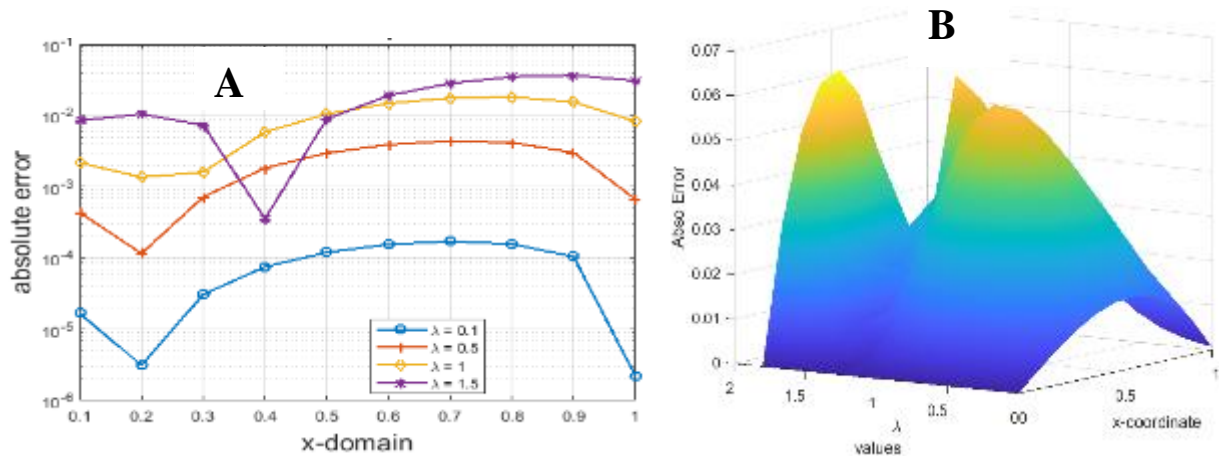


Figure 34: Absolute errors for solving troesch problem using Subdomain WRM

From Figure 34 (A and B) we learn the accuracy of our numerical solutions by computing absolute error, it tells us the absolute error is decrease from left to the right boundary for all lambda values. Figure 34 (A) shows for absolute error for subdomain method. Figure 34 (B) draws three-dimensional diagram for absolute error by taking the dependent variable (absolute

error) vs the independent variables (x-domain with λ values)). From these figures, it is evident that our numerical solution very close to the exact solution and it is very accurate.

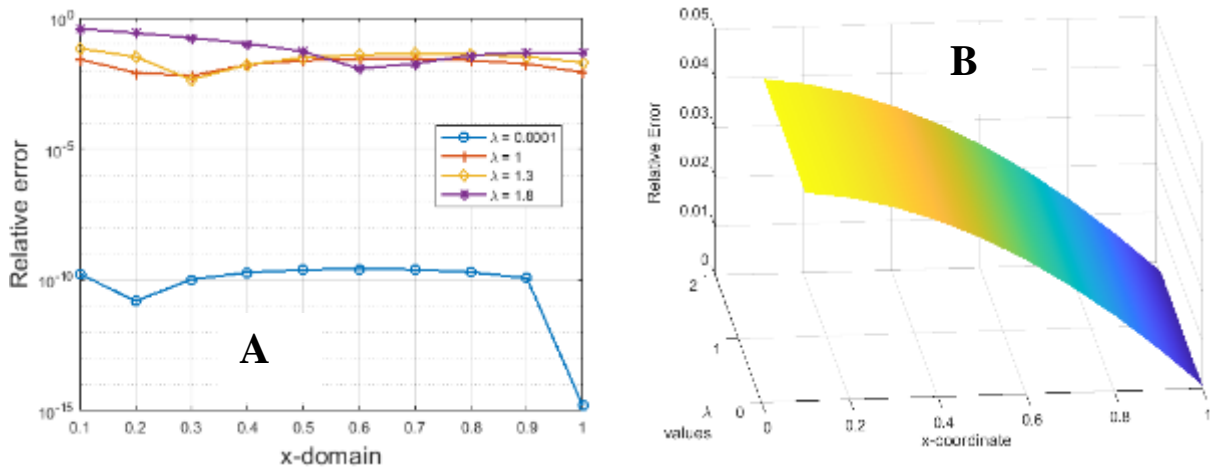


Figure 35: Relative errors for solving Troesch problem using Subdomain WRM

Since our exact solution is semi analytic, we computed the relative error on each grid point. Thus, Figure 35 (A) presents relative error for subdomain method, We learnt from Figure 35 (B) the influence of the independent variables (λ and x) on the dependent (relative error) by plotting 3D.

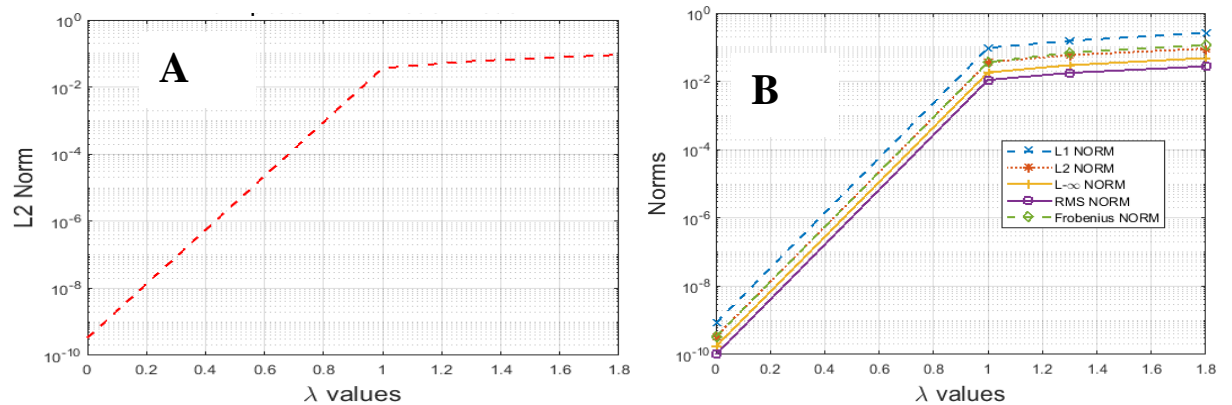


Figure 36: Norms for the Troesch problem

L_2 norm versus the dimensionless parameter λ is plotted in Figure 36 (A) for subdomain We observe from Figure 36 (B) for the subdomain about L_1 , L_2 and Frobenius norms are larger than infinity norm and RMS, the infinity norm is also larger than root mean square (RMS). Figure 36 (A & B) they show us L_2 norm is increasing as the λ values increases for both methods.

3.2 Galerkin Method

As we seen the method and algorithm for GRKWRM on section 2.2.5 based on that in this section, we validate the Galerkin weighted residual method for the experimented boundary value problems on section 2.6.

3.2.1 Numerical Experiments

3.2.1.1 Exothermic Chemical Reaction in a Slab of Combustible Material

Based on Algorithm 2 above on Chapter 2 and section 2.6.1.2 , we seen the trial/approximate solution for the general application of weighted residual method. In this section, the Galerkin weighted residual method is carried out by using its algorithm for the cases of Exothermic thermal explosion problem (2.4 eq. 1) with the boundary conditions in (2.4 eq. 2). The exact solution of the equation is taken from equation (2.4 eq. 3). The Galerkin's formulation of the Exothermic thermal explosion (2.4 eq. 1) equation is:

Integrating the residual function (2.4 eq. 10) using the upper $b = 1$ and lower limit $a = 0$, we have;

$$\int_0^1 N_i(x) R(x) dx \quad (3.2 \text{ eq. 1})$$

Substituting the weight function in equation (2.4 eq. 7) to equation (3.2 eq. 1), we have;

$$\int_0^1 (-1 + x^2) R(x) dx \quad (3.2 \text{ eq. 2})$$

On substituting the corresponding terms weighted function from equation (2.4 eq. 7) and the residual function (2.4 eq. 10) into equation (3.2 eq. 2), it was found that

$$\int_0^1 (-1 + x^2) \left[2c_3 + \lambda \left[(1 + \varepsilon(c_3 + c_3 x^2))^m e^{\left(\frac{c_3 + c_3 x^2}{1 + \varepsilon(c_3 + c_3 x^2)} \right)} - \delta(c_3 + c_3 x^2) \right] \right] dx \quad (3.2 \text{ eq. 3})$$

Now to we compute and solve the above equation (3.2 eq. 3), based on Algorithm 2 above on Chapter 2 , page 14, we developed a user defined computer program for solving exothermic explosion problem for Galerkin method by us by using MATLAB version R2019b v9.7.0, for the numerical experiment, we defined parameters in the above Table 1, row 1. The results are

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presented in plots and shows the solutions for galerkin weighted residual method with the analytic solution and also absolute and on each grid points.

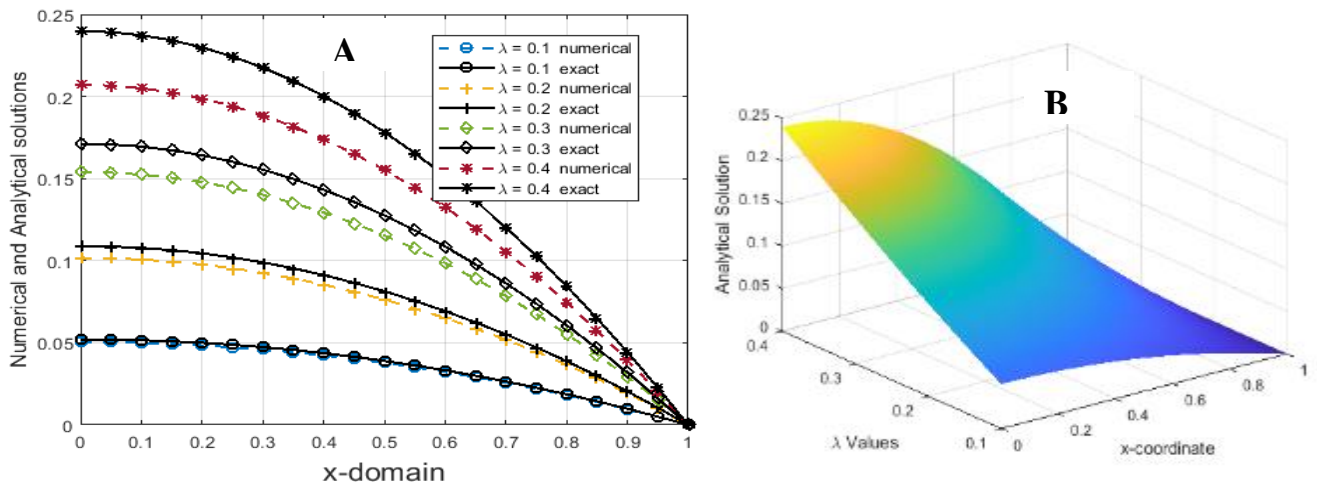


Figure 37: Solution for exothermic thermal explosion problem using Galerkin WRM when $m = 0.5, \varepsilon = 0.1, \delta = 0.1$

We learn from Figure 37 the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless coordinate x .

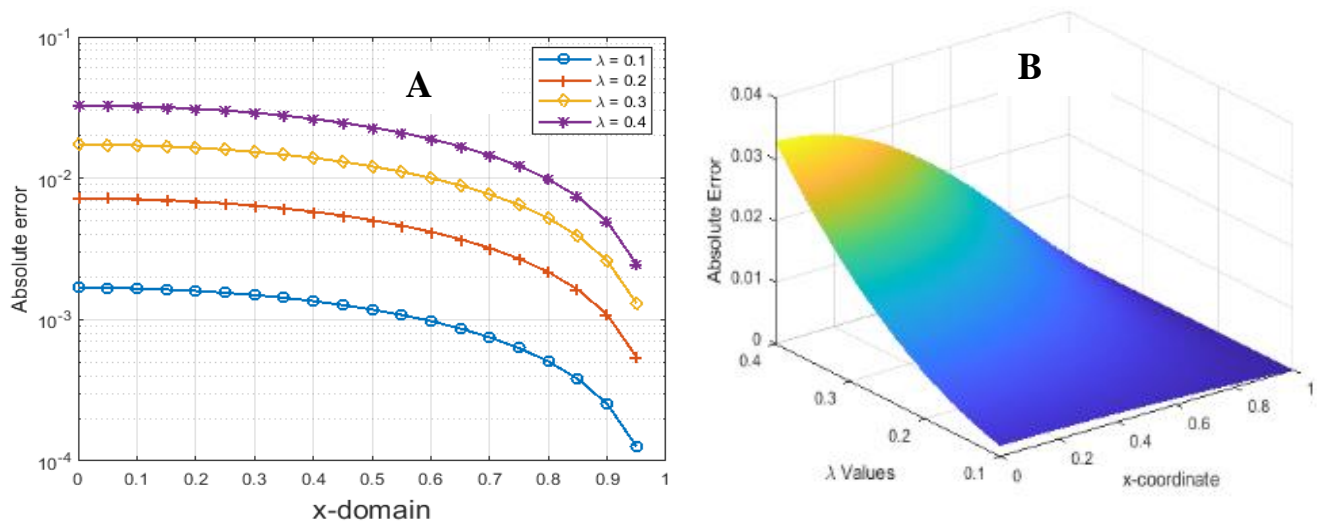


Figure 38: Absolute Error for solving Exothermic Explosion problem when $\lambda = \text{vary}$ and $m = 0.5, \varepsilon = 0.1, \delta = 0.1$

Figure 38 shows that the absolute error versus the dimensionless distance x and our solution is very close to the exact, the absolute error is decrease from left to the right boundary.

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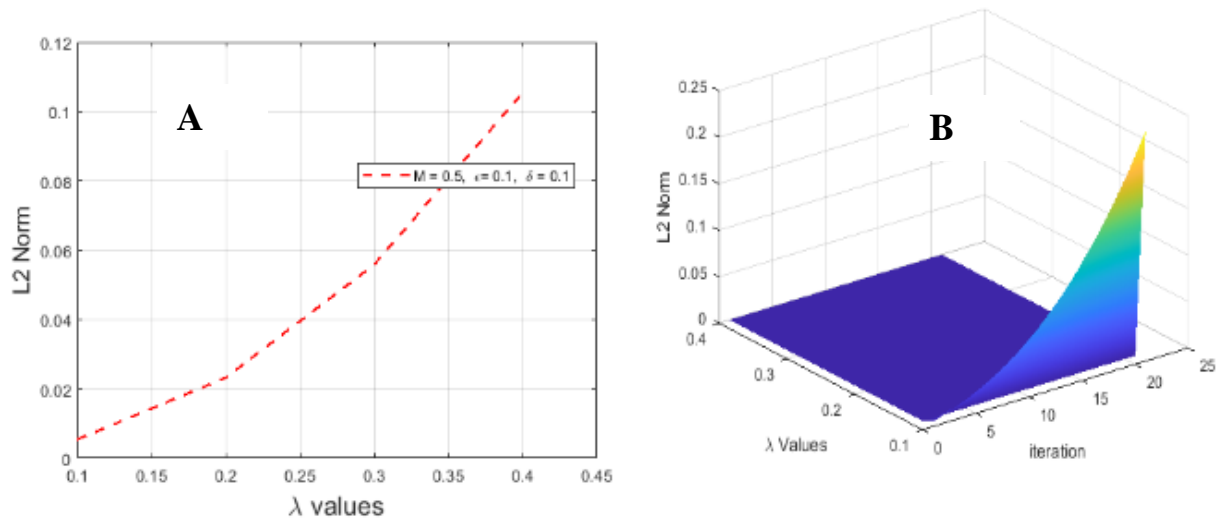


Figure 39: L2 Norm when $m = 0.5$, $\epsilon = 0.1$, $\delta = 0.1$

We can easily observe from Figure (A) and (B) L₂ norm is increasing as the dimensionless parameter increases.

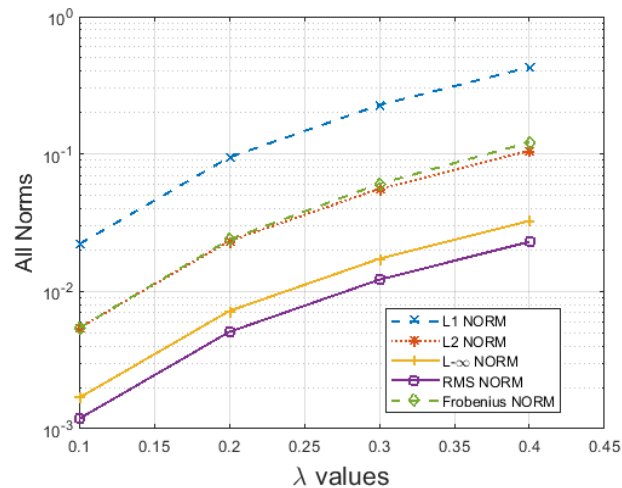


Figure 40: Other norms comparisons for the exothermic explosion problem using GWRM when $m = 0.5$, $\epsilon = 0.1$, $\delta = 0.1$

Figure 40 show us comparisons among norms, L-infinity and RMS norms are lower than the L2, L1 norms.

3.2.1.2 Catalytic Reaction Problem

we validate here the Galerkin weighted residual method for the cases of catalytic reaction problem (2.4 eq. 11) with the boundary conditions in (2.4 eq. 12). The exact solution of the

equation is taken from (2.4 eq. 13). By using its algorithm and physically realistic values of various embedded parameters that we defined in the above Table 2, for the numerical experiment. Based on Algorithm 3 on Chapter 2, and section 2.6.2.3 , we seen the trial/approximate solution for the general application of weighted residual method.

The domain limits are upper ($b = 1$) and lower ($a = 0$) and residual function (2.4 eq. 21). Thus, the Galerkin's formulation of the catalytic reaction problem (2.4 eq. 11) equation is

$$\int_0^1 N_i(x) R(x) dx \quad (3.2 \text{ eq. } 4)$$

Substituting the weight function in equation (2.4 eq. 18) to equation (3.2 eq. 4) ,we have;

$$\int_0^1 (1+x^2) R(x) dx \quad (3.2 \text{ eq. } 5)$$

On substituting the corresponding terms residual function (2.4 eq. 21) into equation (3.2 eq. 5), it was found that

$$\int_0^1 (1+x^2) \left[2c_3 - \lambda(1-c_3 + c_3 x^2) e^{\left[\frac{\gamma\beta(1-(1-c_3+c_3 x^2))}{1+\beta(1-(1-c_3+c_3 x^2))} \right]} \right] dx \quad (3.2 \text{ eq. } 6)$$

we developed a user defined computer program for solving catalytic reaction problem for galerkin method by us using MATLAB version R2019b v9.7.0 to compute and solve the above equation (3.2 eq. 6), based on Algorithm 3 on Chapter 2, page 15, for the numerical experiment, we defined parameters in the above Table 2, row 1. The results are presented in plots.

The algorithm and procedures above are applied and we validate the galerkin weighted residual method and physically realistic values of various embedded parameters that we defined in the above Table 2: catalytic reaction problem parameter definition, row 1, for the numerical experiment and we obtained the results as shown in the following figures below:

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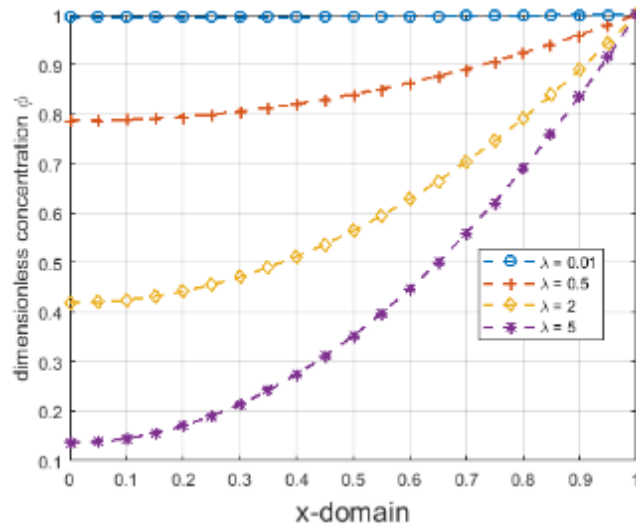


Figure 41: solution for solving catalytic problem using Galerkin WRM

Figure 41 shows the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless distance down the reactor x .

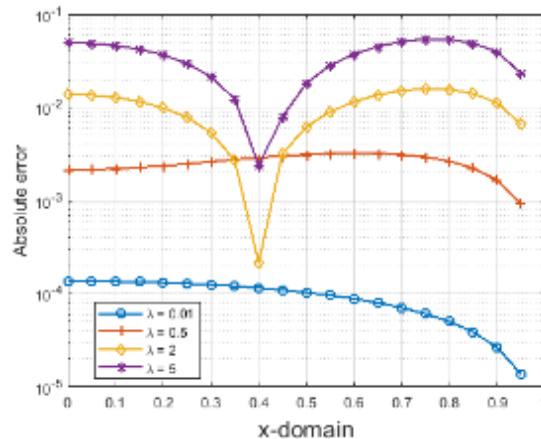


Figure 42: absolute error versus the dimensionless distance down the reactor x

we observe from Figure 42 shows the absolute error versus the dimensionless distance x and our solution is very close to the exact, the absolute error is decrease from left to the right boundary.

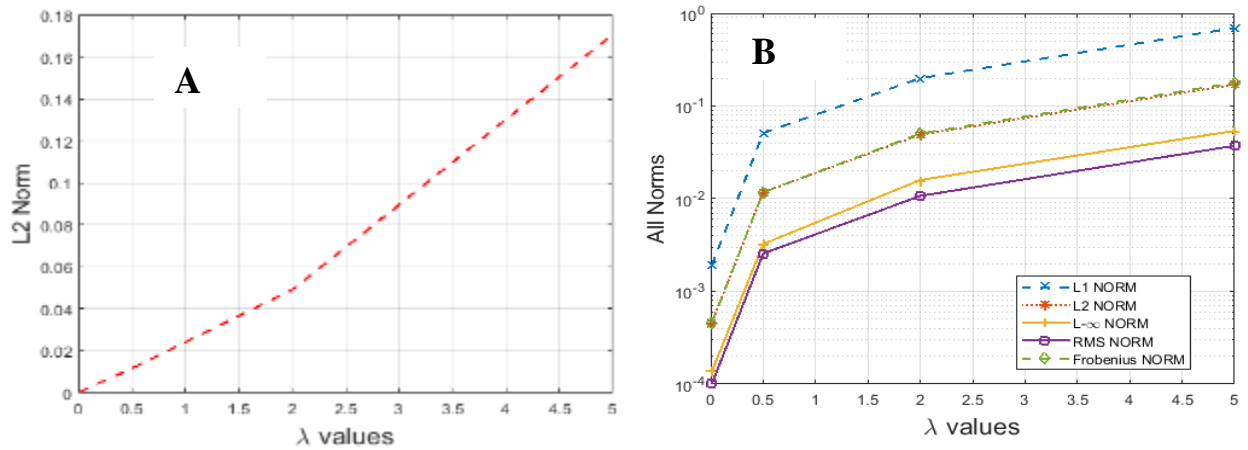


Figure 43: Norm computation for solving catalytic problem using Galerkin WRM

Figure 43 (A) L_2 norm is increasing as the dimensionless parameter increases. Figure 43 (B) show us comparisons among norms, L -infinity and RMS norms are lower than the L_2 , L_1 norms.

3.2.1.3 Thermal Explosion Problem

As we identified the algorithm on Chapter 2, section 2.2.5, we developed a user defined computer program by using MATLAB version Matlab R2019b v9.7.0 by us for the numerical solution for solving thermal explosion problem (2.4 eq. 22) with the boundary conditions in (2.4 eq. 23) of the Galerkin weighted residual method. The results are presented in plots. The exact solution of the equation is taken from [39].

We identified the algorithm on Chapter 2, section 2.2.5 for the numerical solution for solving thermal explosion problem (2.4 eq. 22) with the boundary conditions in (2.4 eq. 23) of the Galerkin weighted residual method. The exact solution of the equation is taken from [39].

We also saw the trial/approximate solution for the general application of weighted residual method. Based on the algorithm 2 on Chapter 2, the Galerkin's formulation of the thermal explosion equation is

The domain limits are upper ($b = 1$) and lower ($a = 0$) and residual function (2.4 eq. 31). Thus, the Galerkin's formulation of the thermal explosion problem (2.4 eq. 11) equation is

$$\int_0^1 N_i(x) R(x) dx \quad (3.2 \text{ eq. } 7)$$

Substituting the weight function in equation (2.4 eq. 28) to equation (3.2 eq. 7), we have;

$$\int_0^1 (-1+x^2) R(x) dx \quad (3.2 \text{ eq. } 8)$$

The integration of the residual function (2.4 eq. 31) using the upper limit $b = 1$ and lower limit $a = 0$

$$\int_0^1 (-1+x^2) \left[2c_3 + \lambda e^{(-c_3+c_3x^2)} \right] dx \quad (3.2 \text{ eq. } 9)$$

then we compute and solve the above equation (3.2 eq. 9), based on the above algorithm 2 on Chapter 2, page 15, we developed a user defined computer program for solving exothermic explosion problem for Subdomain method by us by using MATLAB version R2019b v9.7.0 .

Here, we validate the Galerkin weighted residual method is carried out by using its algorithm for the thermal explosion problem. We define here $\lambda = 0.1, 0.2, 0.3, 0.4$, for the numerical experiment. The following results show the solutions for Galerkin weighted residual method with the analytic solution, absolute errors, L_2 norm for thermal explosion problem.

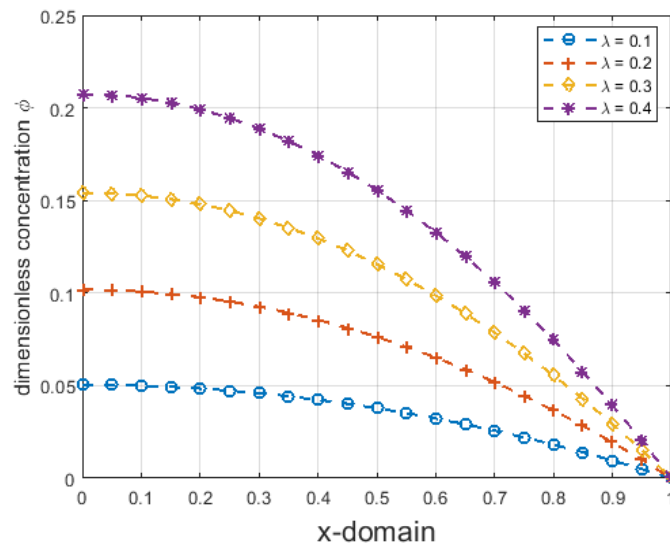


Figure 44: dimensionless concentration ϕ versus the dimensionless coordinate x

Figure 44 shows that dimensionless concentration (ϕ) increases as λ values increase in the dimensionless coordinate x .

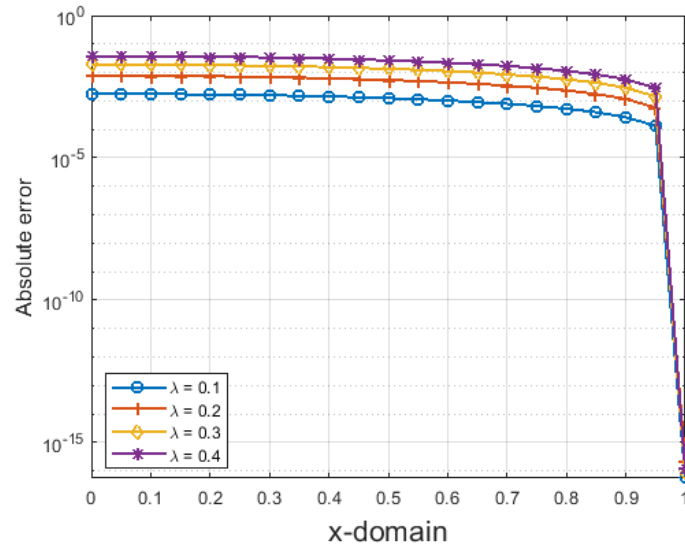


Figure 45: Absolute error versus the dimensionless coordinate x

We observe from Figure 45 the computation of absolute error in the grid points for different λ values, and the absolute error is decrease to the right boundary.

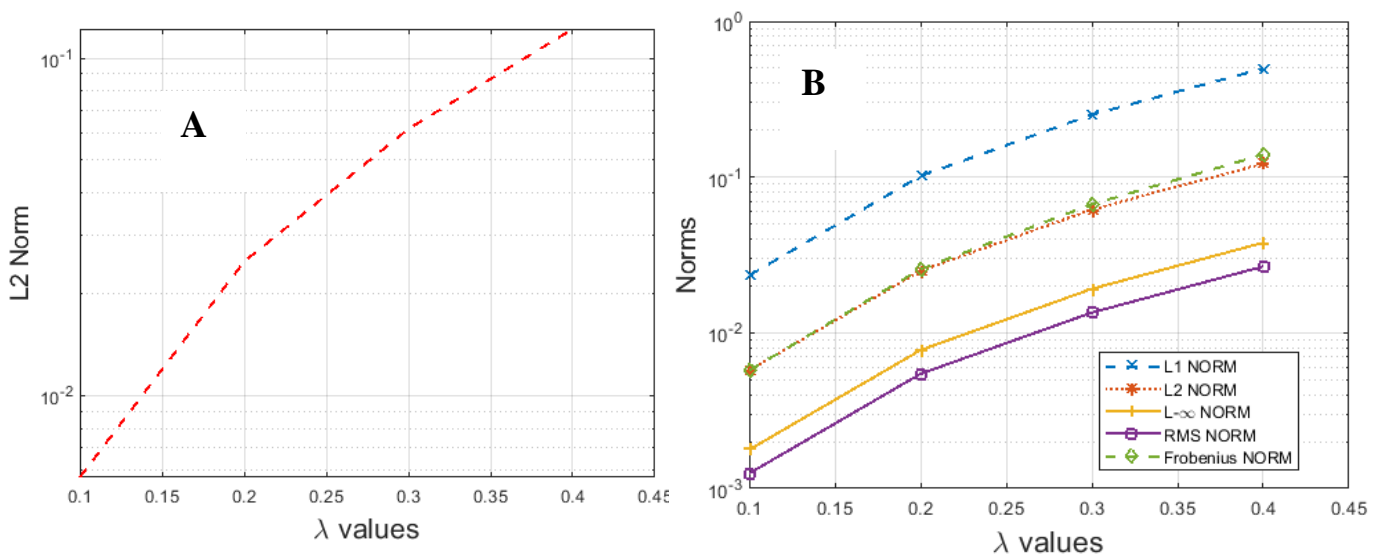


Figure 46: Norms for solving thermal explosion problem using Galerkin WRM

Figure 46 (A) tells us L_2 norm is increasing as the dimensionless parameter increases. Figure 46(B) show us comparisons among norms, L_2 and L_1 norms are higher than L -infinity and RMS norms.

3.2.1.4 Troesch Problem

In this section, based on the algorithm 2.2.5.1 on Chapter 2 ,section 2.2, we analyzed the subdomain and the Galerkin weighted residual methods for the cases of Troesch problem (2.4 eq. 43) with the boundary conditions in (2.4 eq. 23). The semi analytic solution of the equation is taken from (2.4 eq. 45).

we saw the trial/approximate solution (2.4 eq. 49) for the general application of weighted residual method. The Galerkin's formulation of the thermal explosion equation is

The domain limits are upper ($b = 1$) and lower ($a = 0$) and residual function (2.4 eq. 53). Thus, the Galerkin's formulation of the Troesh problem (2.4 eq. 43) equation is

$$\int_0^1 N_i(x) R(x) dx \quad (3.2 \text{ eq. } 10)$$

Substituting the weight function in equation (2.4 eq. 50) to equation (3.2 eq. 7) ,we have;

$$\int_0^1 (x + x^2) R(x) dx \quad (3.2 \text{ eq. } 11)$$

The integration of the residual function(2.4 eq. 53) using the upper limit $b=1$ and lower limit $a=0$

$$\int_0^1 (x + x^2) [2c_3 - \lambda \sinh(\lambda(x - c_3x + c_3x^2))] dx \quad (3.2 \text{ eq. } 12)$$

Then we used computational techniques to compute and solve the above equation (3.1 eq. 15) , based on the above Algorithm 3 on Chapter 2, we developed a user defined computer program for solving Troesch problem for Galerkin method by using MATLAB version R2019b v9.7.0.

Here, we validate the Galerkin weighted residual method are carried out by using its algorithm for the Troesch problem. We define here $\lambda = 0.0001, 1, 1.3, 1.8$, for the numerical experiment. The following results show the numerical and analytic solutions, absolute errors, relative error, L_2 norm. We observe from Figure 47 the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless distance x obtained from (2.4 eq. 43) and (2.4 eq. 45). From these figures it is clear that the concentration (ϕ) increases for the different values of λ .

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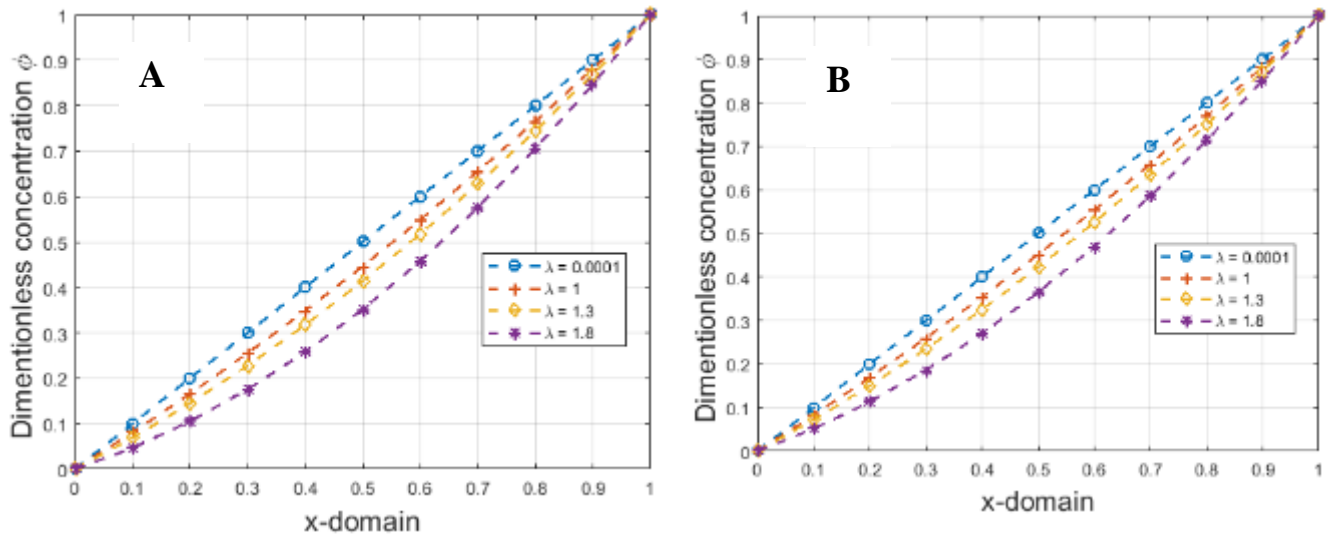


Figure 47: Galerkin and Subdomain WRMs for solving Troesch problem

Figure 47 (A) presents solution for the Galerkin weighted residual method and Figure 47 (B) illustrates for the subdomain weighted residual method.

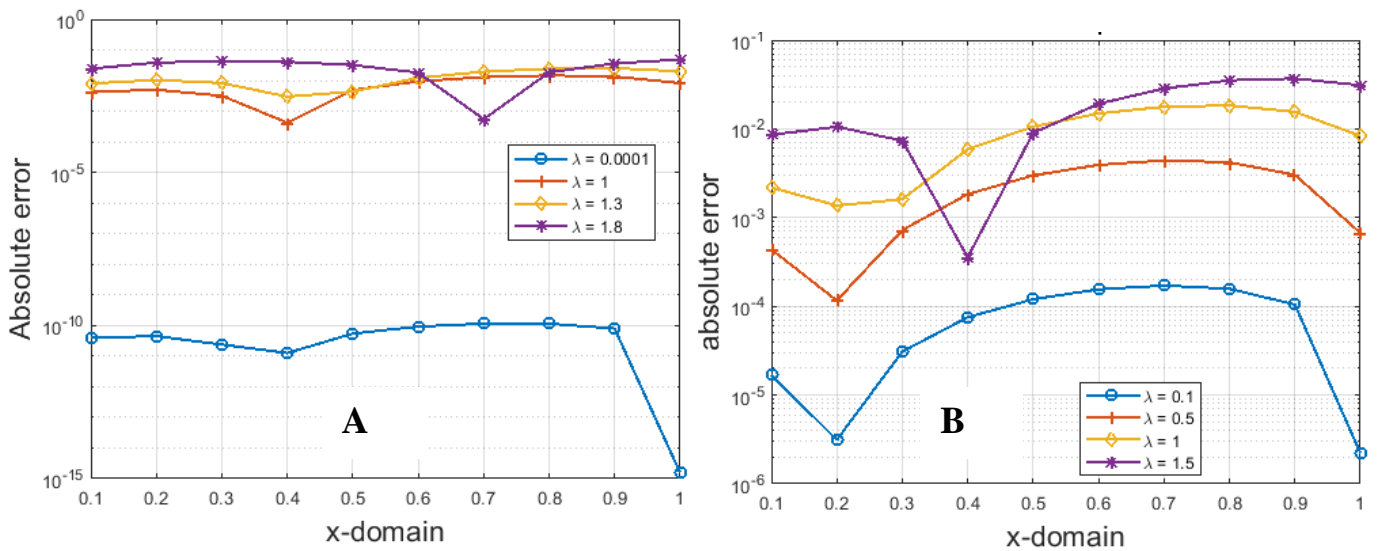


Figure 48: Absolute errors for solving troesch problem using SDWRM and GRKWRM

From Figure 48 (A and B) we learn the accuracy of our numerical solutions by computing absolute error, it tells us the absolute error is decrease from left to the right boundary for all lambda values. Figure 48 (A) shows for absolute error for galerkin method and Figure 48 (B) absolute error for the subdomain method. From these figures, it is evident that our numerical solution very close to the exact solution and it is very accurate.

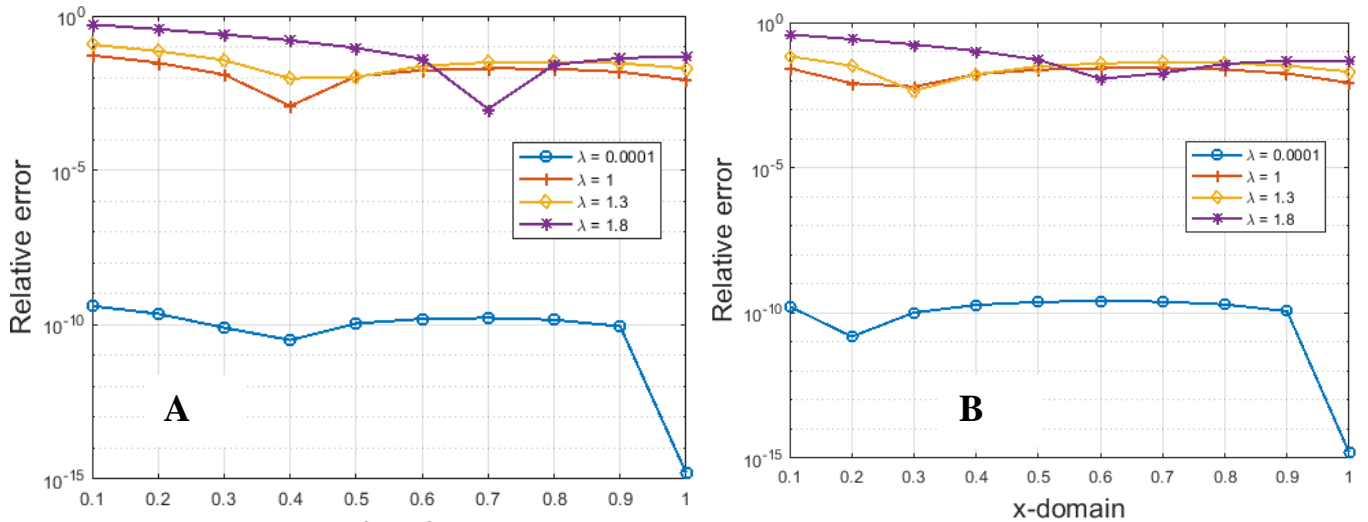


Figure 49: Relative errors for solving troesch problem using SDWRM and GRKW RM

Since our exact solution is semi analytic, we computed the relative error on each grid point. Thus, Figure 49 (A) presents relative error for galerkin method, Figure 49 (B) shows relative error for subdomain method

L_2 norm versus the dimensionless parameter λ is plotted in Figure 50 (A & B) they show us L_2 norm is increasing as the λ values increases for both methods Figure 50 (A) for Galerkin and Figure 50 (B) for subdomain.

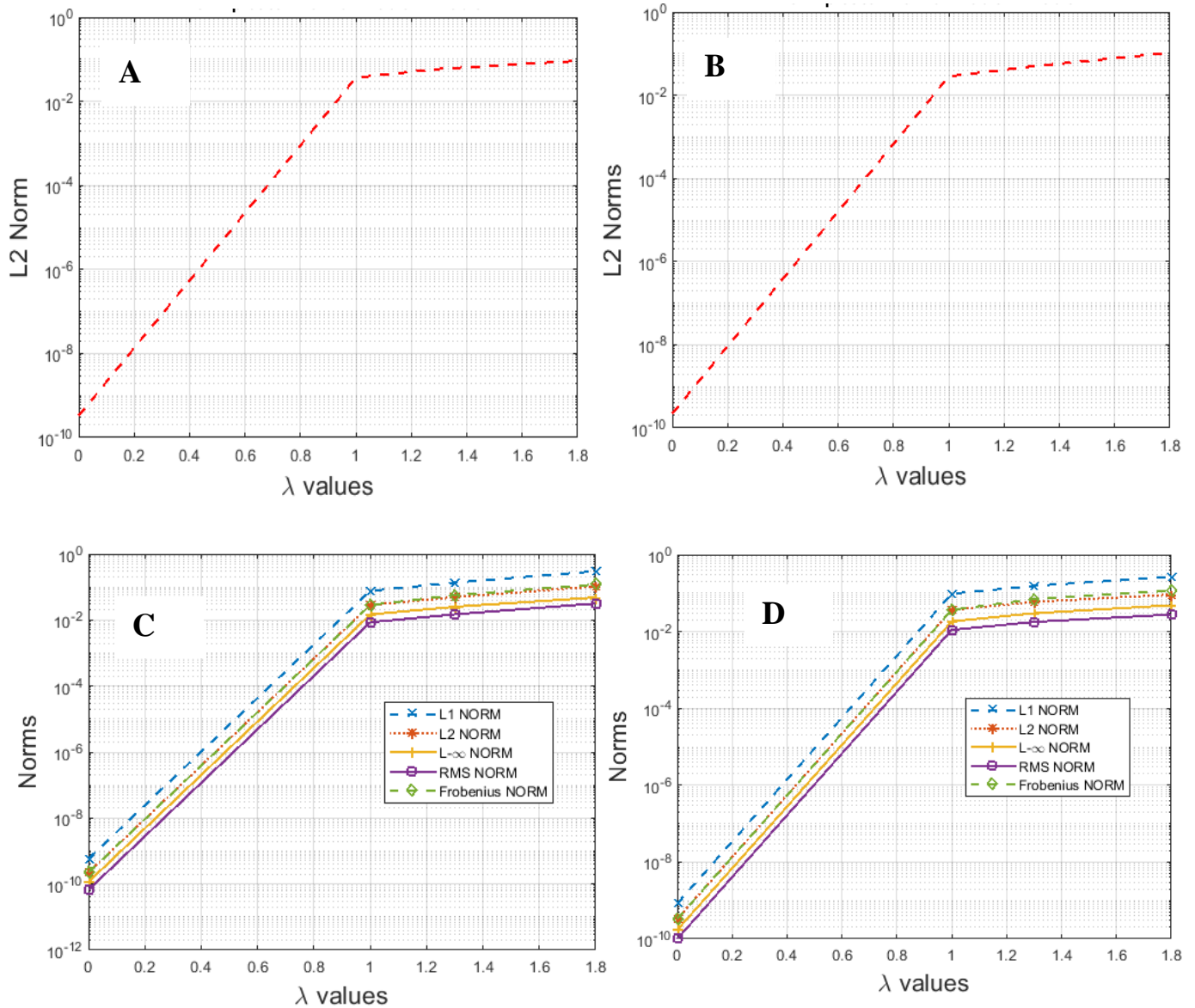


Figure 50: Norms for the Troesch problem

We observe from Figure 50 (C) for the Galerkin and Figure 50 (D) for subdomain methods about L_1 , L_2 and Frobenius norms are larger than infinity norm and RMS, the infinity norm is also larger than root mean square (RMS).

3.3 Collocation Method

we described the method and algorithm for collocation weighted residual method on section 2.2.7 based on that in this section, we validate the collocation weighted residual method for the experimented boundary value problems on section 2.6.

3.3.1 Numerical Experiments

3.3.1.1 Exothermic Chemical Reaction in a Slab of Combustible Material

In this section, the collocation weighted residual method is carried out using its algorithm to for the cases of Exothermic thermal explosion problem. As we define in the above Table 1: exothermic explosion problem parameter definition row 1. The collocation's of the exothermic thermal explosion (2.4 eq. 1) equation formulated as per Algorithm 3 let us choose an arbitrary location of x

$$x_n = 0.5 \quad (3.3 \text{ eq. } 1)$$

where n is any arbitrary point

we have the functional form of the approximate solution in (2.4 eq. 6) and we also chosen the arbitrary x (3.3 eq. 1). Thus, on substituting the arbitrary x_n into the residual function in (2.4 eq. 10), we got the new residual

$$R = 2c_3 + \lambda \left[(1 + \varepsilon(-c_3 + c_3(0.5)^2))^m e^{\left(\frac{-c_3 + c_3(0.5)^2}{1 + \varepsilon(-c_3 + c_3(0.5)^2)}\right)} - \delta(-c_3 + c_3(0.5)^2) \right] \quad (3.3 \text{ eq. } 2)$$

Then set (3.3 eq. 2) equal to zero. The overall computation is done for the above equation (3.3 eq. 2) using our user defined computer program for solving exothermic explosion problem for collocation method using MATLAB version R2019b v9.7.0, based on the above Algorithm 3 on Chapter 2, page 15, for the numerical experiment, we defined parameters in the above Table 1, row 1.

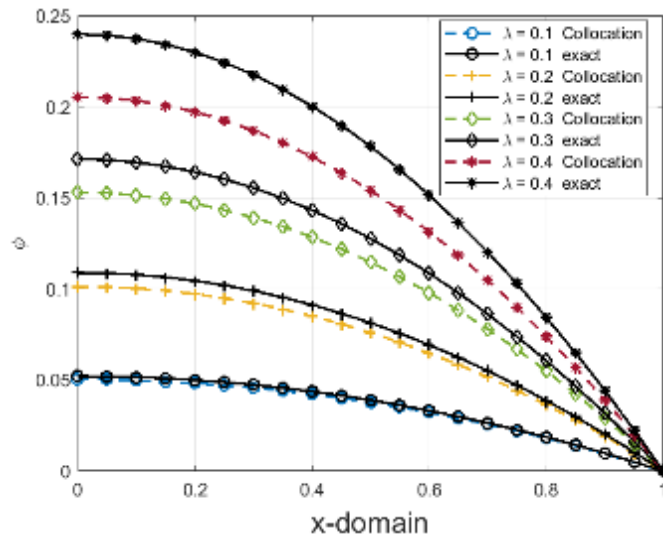


Figure 51: Solution for solving exothermic explosion problem using COLWRM

when $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Figure 51 presents the numerical solution that temperature increases with an increase in the parameter values of λ , whereas activation energy (ε), heat loss (δ), numerical exponent (m) parameters remains fixed.

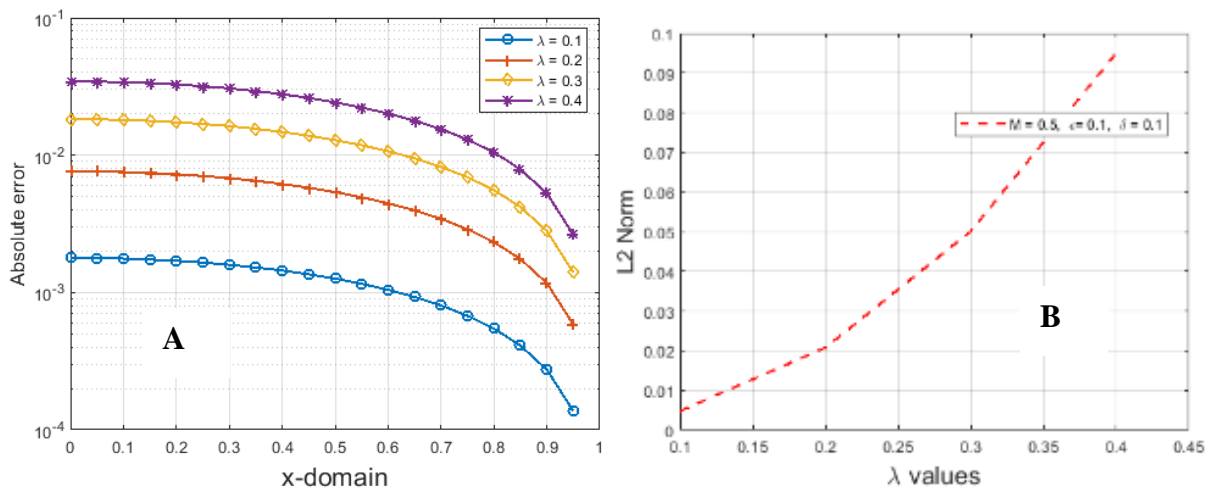


Figure 52: Absolute error and L_2 norm for solving exothermic explosion problem

when $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Figure 52 (A) illustrate the absolute error vs the dimensionless coordinate x for the collocation WR method, the absolute error decrease to the right boundary. Figure 52 (B) shows the L_2 norm increase as the dimensionless parameter λ increase.

3.3.1.2 Catalytic Reaction Problem

we validate here the galerkin weighted residual method for the cases of catalytic reaction problem (2.4 eq. 11) with the boundary conditions in (2.4 eq. 12). The exact solution of the equation is taken from (2.4 eq. 13). By using its algorithm and physically realistic values of various embedded parameters that we defined in the above Table 2, for the numerical experiment. Based on Algorithm 3 on Chapter 2, and section 2.6.2.3 , we seen the trial/approximate solution for the general application of weighted residual method.

The collocation's of the exothermic thermal explosion (2.4 eq. 11) equation formulated. As per Algorithm 3 let us choose an arbitrary location of x

$$x_n = 0.5 \quad \text{where } n \text{ is any arbitrary point} \quad (3.3 \text{ eq. } 3)$$

we have the functional form of the approximate solution in (2.4 eq. 17) and we also chosen the arbitrary x (3.3 eq. 3). Thus, on substituting the arbitrary x_n into the residual function in (2.4 eq. 21) , we got the new residual

$$R = 2c_3 - \lambda(1 - c_3 + c_3(0.5)^2) e^{\left[\frac{\gamma\beta(1-(1-c_3+c_3(0.5)^2))}{1+\beta(1-(1-c_3+c_3(0.5)^2))} \right]} \quad (3.3 \text{ eq. } 4)$$

Then set (3.3 eq. 4) equal to zero. The overall computation is done for the above equation (3.3 eq. 4) using our user defined computer program for solving exothermic explosion problem for collocation method using MATLAB version R2019b v9.7.0, based on the above Algorithm 3 on Chapter 2, page 15, for the numerical experiment, we defined parameters in the above table 2, row 1. The algorithm above are applied and we validate the collocation weighted residual method and physically realistic values of various embedded parameters that we defined in the above Table 2: catalytic reaction problem parameter definition, row 1, for the numerical experiment and we obtained the results as shown in the following figures below:

Figure 54 shows the dimensionless concentration (ϕ) versus the dimensionless coordinate x and the influence of λ on it.

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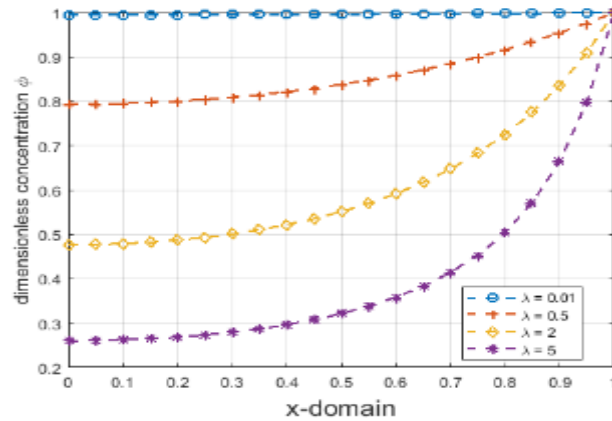


Figure 53: solution for solving catalytic problem using collocation WRM

We observe from Figure 53 our solution is very close to the exact, the absolute error is decrease to the boundary for every λ values and when $\gamma = 1$, $\beta = 0.2$.

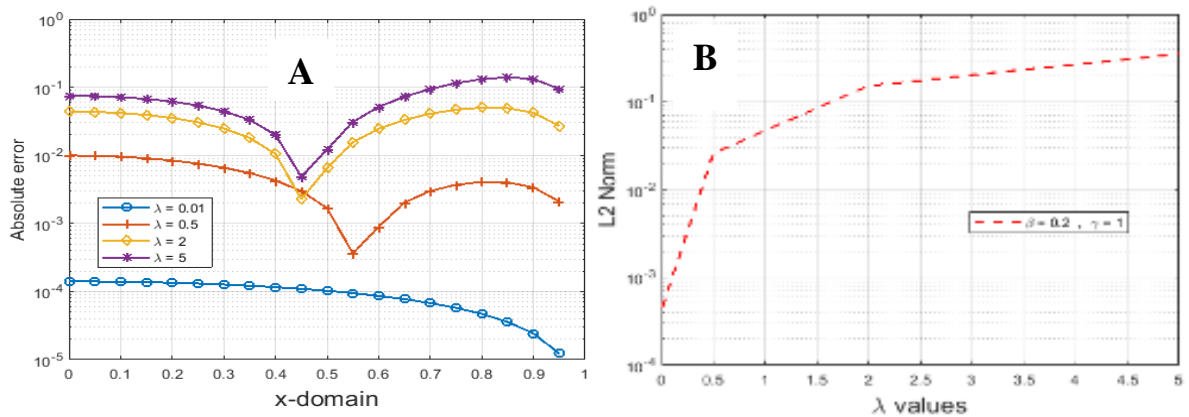


Figure 54: Absolute error & L_2 norm for solving catalytic reaction problem using collocation

Figure 54 (A) presents the accuracy by computing absolute errors decrease to right boundary. Figure 54 (B) are tells us L_2 norm is increasing as the dimensionless parameter λ increases.

3.3.1.3 Thermal explosion problem

we identified the algorithm on Chapter 2, section 2.2.7.1 for the numerical solution for solving thermal explosion problem (2.4 eq. 22) with the boundary conditions in (2.4 eq. 23)the collocation's of the exothermic thermal explosion (2.4 eq. 11) equation formulated. The exact solution of the equation is taken from [39]. We chose an arbitrary location of x

$$x_n = 0.5 \quad \text{where } n \text{ is any arbitrary point} \quad (3.3 \text{ eq. } 5)$$

We have the functional form of the approximate solution in (2.4 eq. 27) and we also chosen the arbitrary x (3.3 eq. 5). Thus, on substituting the arbitrary x_n into the residual function in (2.4 eq. 31), we got the new residual

$$R = 2c_3 + \lambda e^{(1-c_3+c_3(0.5)^2)} \quad (3.3 \text{ eq. 6})$$

Then set (3.3 eq. 6) equal to zero. The overall computation is done for the above equation (3.3 eq. 6) using our user defined computer program for solving thermal explosion problem for collocation method using MATLAB version R2019b v9.7.0.

Here, we validate the collocation weighted residual method is carried out by using its algorithm for the thermal explosion problem. We define here $\lambda = 0.1, 0.2, 0.3, 0.4$, for the numerical experiment. The following results show the solutions for collocation weighted residual method with the analytic solution, absolute errors and L_2 norm for thermal explosion problem.

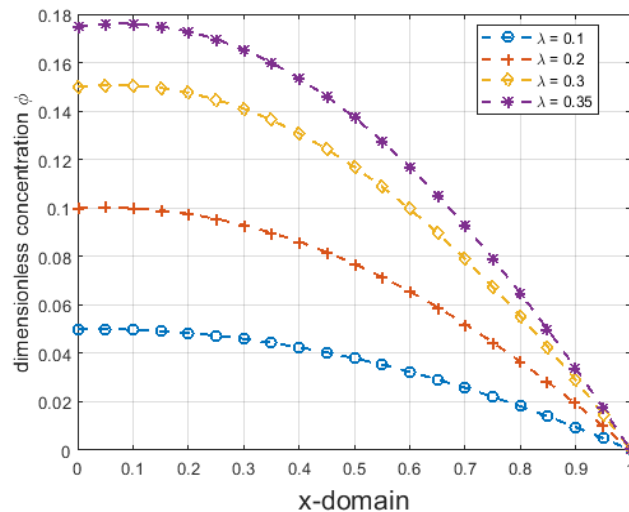


Figure 55: Solution for thermal explosion problem using collocation WRM

We learn from Figure 57Figure 55 dimensionless concentration (ϕ) increases as λ values increase in the dimensionless coordinate x .

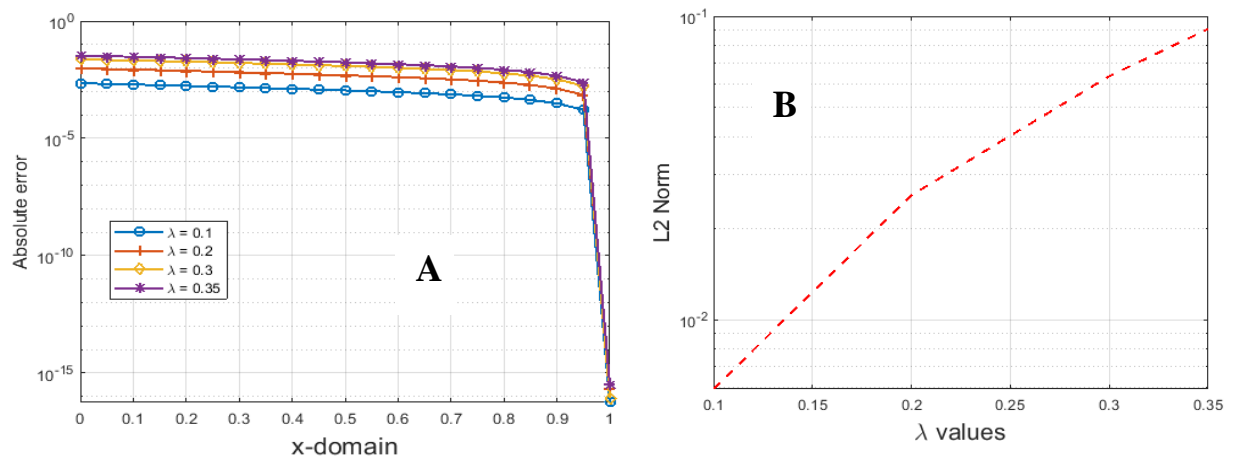


Figure 56: Absolute error and L_2 norm for solving thermal explosion problem

We observe from

Figure 56 (A) the computation of absolute error in the grid points for different λ values, and the absolute error is decrease to the right boundary (e.g. at $\lambda = 0.2$, absolute error at $\phi(0.05) = 0.009058$ and at $\phi(0.95) = 0.000713$).

Figure 56 (B) tells us L_2 norm is increasing as the dimensionless parameter λ increases.

3.3.1.4 Reaction Diffusion Equation

We apply the collocation weighted residual method for solving reaction diffusion equation (2.4 eq. 54) with the boundary conditions in. The exact solution of the equation is taken from [36]. Based on the algorithm we defined on 2.2.7.1, Chapter 2, section 2.2 **Error! Reference source not found.** The collocation's of the exothermic thermal explosion (2.4 eq. 1) equation formulated. We pointed an arbitrary location of x

$$x_n = 0.5 \quad \text{where } n \text{ is any arbitrary point} \quad (3.3 \text{ eq. } 7)$$

we have the functional form of the approximate solution in (2.4 eq. 60) and we also chosen the arbitrary x (3.3 eq. 7). Thus, on substituting the arbitrary x_n into the residual function in (2.4 eq. 64), we got the new residual

$$R = 2c_3 + \lambda e^{\left(\frac{(-c_3(0.5) + c_3(0.5)^2)}{(1 + \alpha(-c_3(0.5) + c_3(0.5)^2))} \right)} \quad (3.3 \text{ eq. } 8)$$

Then set (3.3 eq. 8) equal to zero. The overall computation is done for the above equation (3.3 eq. 8) using our user defined computer program for solving exothermic explosion problem for collocation method using MATLAB version R2019b v9.7.0, based on the above Algorithm 3 on Chapter 2 for the numerical experiment, we defined parameters. The results are presented in plots.

we validate the collocation weighted residual method is carried out using its algorithm for the reaction diffusion equation. we define here $\alpha = 0.0001$, $\lambda = 0.3$ and $\alpha = 30$, $\lambda = 0.3$, for the numerical experiment. The following results shows the solutions for collocation weighted residual method with the analytic solution, absolute errors and L_2 norm.

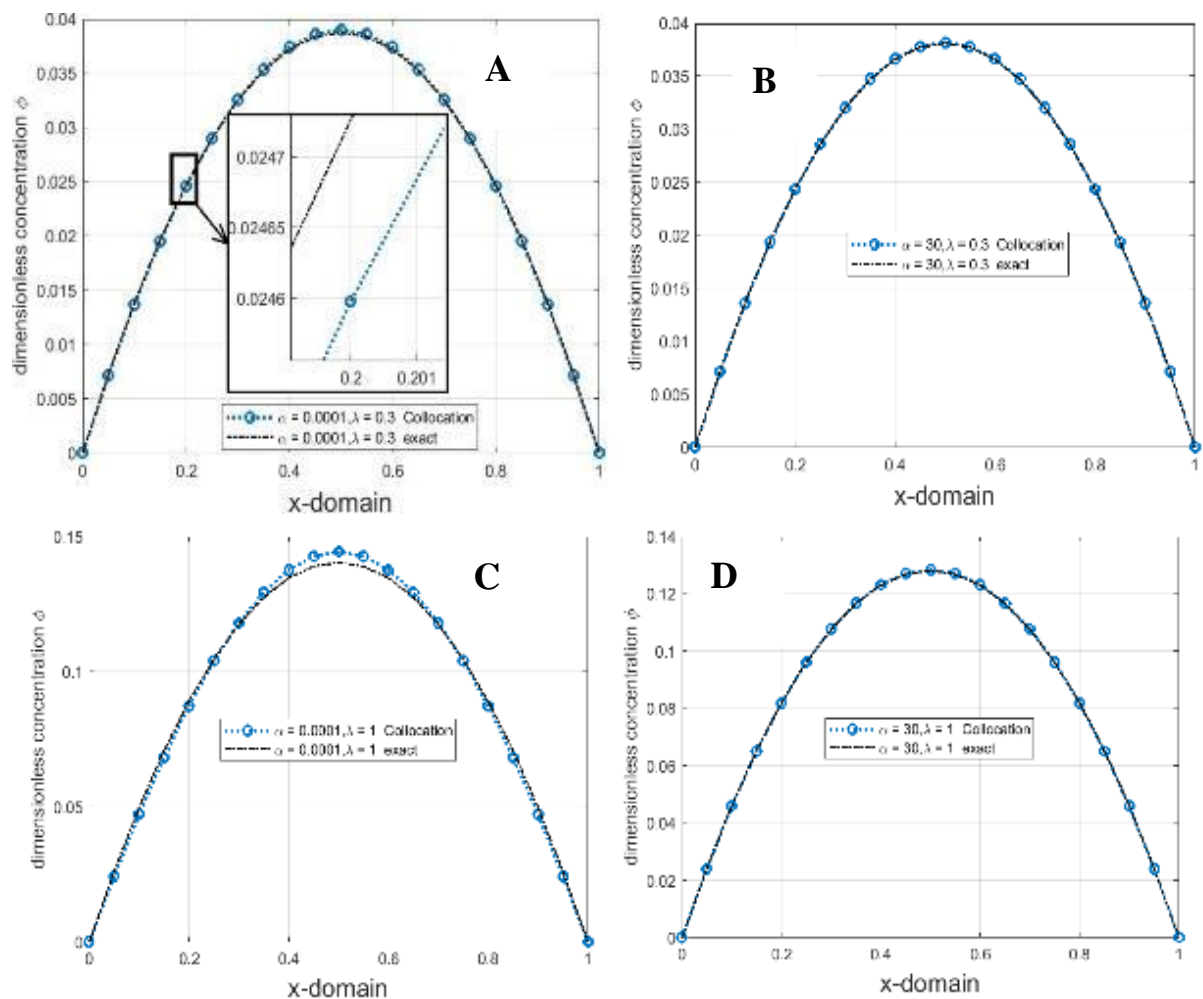


Figure 57: Dimensionless concentration ϕ versus the dimensionless coordinate x

We observe from the Figure 57 (A-D), the influence of α and λ on the dimensionless concentration $\phi(x)$ and its decreases as the dimensionless parameter α increase (Figure 57 (A)

when $\alpha = 0.0001$ and Figure 57 (B) at $\alpha = 30$), for both λ is fixed $\lambda = 0.3$. And also dimensionless concentration $\phi(x)$ decreases as the dimensionless parameter λ increase (Figure 57 (C) when $\lambda = 1$ for (B and C) both α is fixed $\alpha = 0.0001$. Figure 57 (D) when $\alpha = 30$ and $\lambda = 1$), for both λ is fixed $\lambda = 0.3$. It is clear that the numerical solution is very close to the analytical solution.

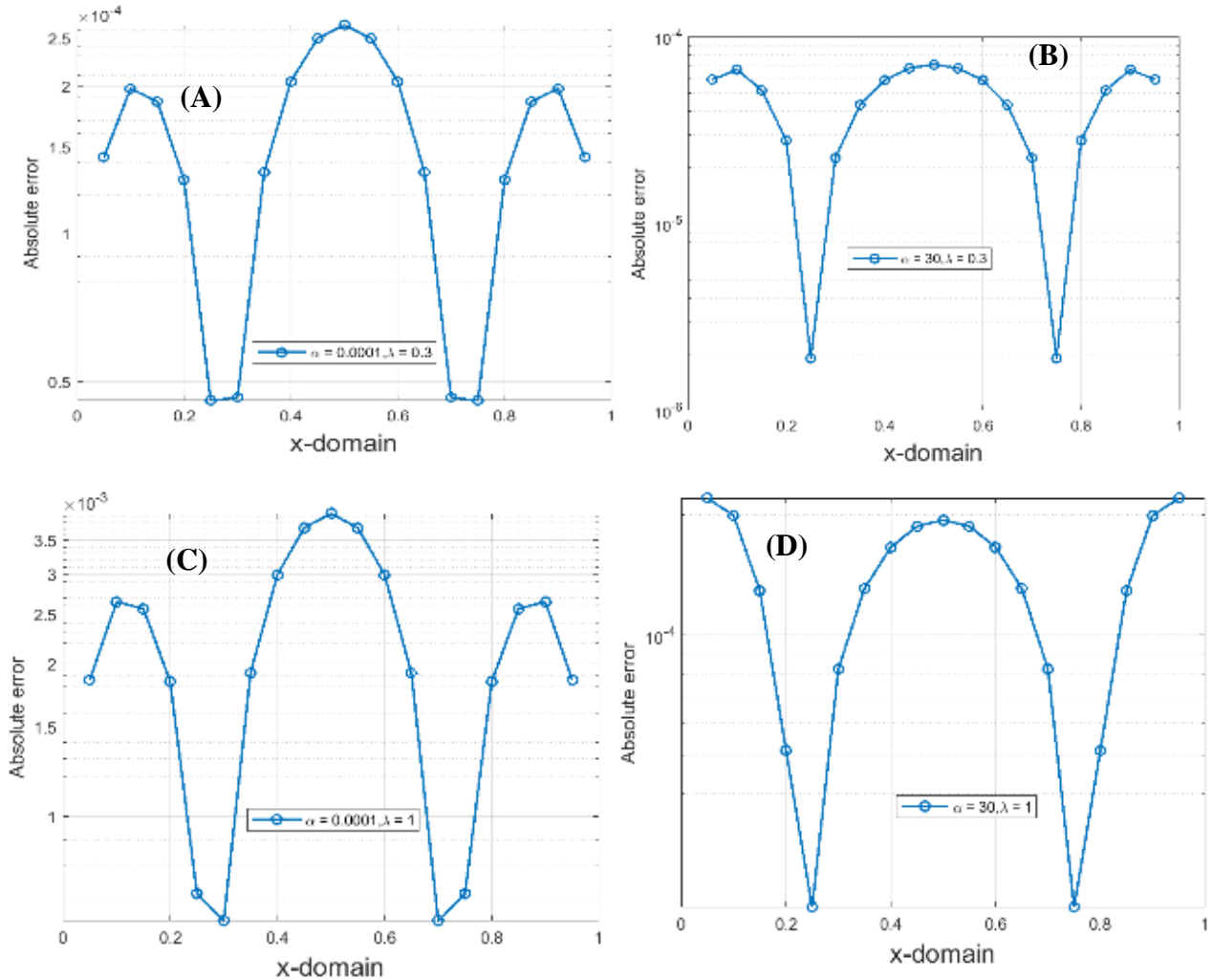


Figure 58: Absolute error versus the dimensionless coordinate x

Figure 58 (A-D) represents the accuracy of collocation weighted residual method by computing absolute error (A) when $\alpha = 0.0001$ and $\lambda = 0.3$, (Figure 58 B) when $\alpha = 30$ and $\lambda = 0.3$, (Figure 58 C) when $\alpha = 0.0001$ and $\lambda = 1$, (Figure 58 D) when $\alpha = 30$ and $\lambda = 1$. Absolute error is very small to the left boundary as well as to the right (e.g. from arbitrary figures of Figure 58 for (B) when $x=0.05$, absolute error is 0.000059 and when $x=0.95$, absolute error is 0.000059). So, it is confirming that our solution is accurate.

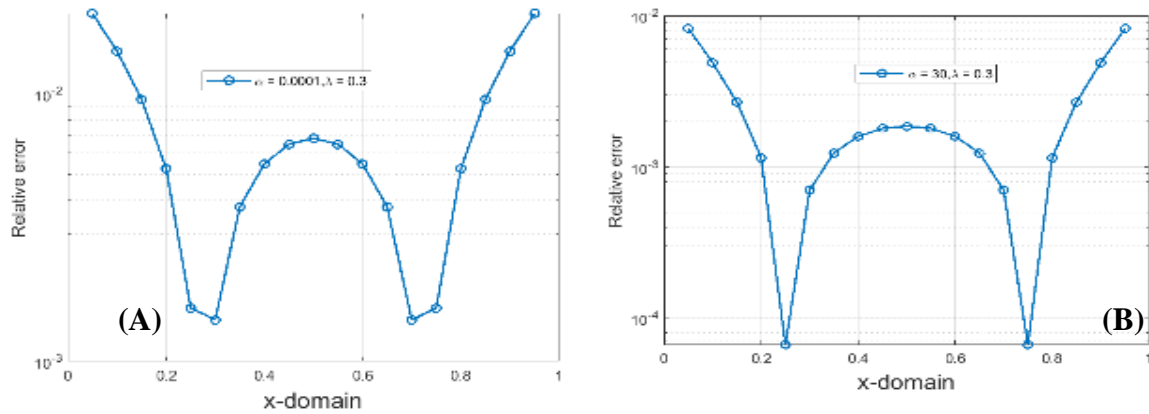


Figure 59: Relative error versus the dimensionless coordinate x

Figure 59 (A) and (B) shows relative errors over the dimensionless coordinate x . (Figure 59 A) when $\alpha = 0.0001$ and (Figure 59 B) when $\alpha = 30$.

3.4 Comparisons for the Application of WRM to the BVP

In this section, we present the solutions for sub domain, Galerkin and collocation weighted residual methods for comparison on selected equally spaced grid points for the experimented BVPs.

3.4.1 Exothermic Thermal Explosion

For the cases of Exothermic explosion problem. As we define on Table 1: exothermic explosion problem parameter definition row 1.

3.4.1.1 Result Comparisons

We observe from Table 4 as per the parameters we defined on Table 1, row 1 above, the collocation WR method gives better result to the near left boundary, at the middle and to the near right boundary for equally spaced x -domain points.

Table 4: Comparisons among WRM results of for exothermic thermal explosion problem

X	Subdomain	Galerkin	Collocation	Exact [35]
0.25	0.047265	0.047276	0.047442	0.048824
0.50	0.037812	0.037820	0.037953	0.038999
0.75	0.022057	0.022062	0.022139	0.022691

Errors Comparisons and Analysis Table 5 shows the comparisons for absolute and relative errors for each λ values and on selected equally spaced grid points.

Table 5: Absolute errors comparisons for exothermic thermal explosion problem

Absolute Error			
X	Subdomain	Galerkin	Collocation
0.25	0.001559	0.001549	0.001382
0.50	0.001187	0.001179	0.001046
0.75	0.000634	0.000629	0.000552

3.4.2 Catalytic Reactions in A Flat Particle

3.4.2.1 Result comparisons

Results for sub domain, galerkin and collocation weighted residual methods on equally spaced x-domain points is presented for the cases of catalytic reaction problem. This is useful to compare our numerical solution with the exact solution. We presented the absolute and relative errors to our numerical solutions for comparisons on selected equally spaced grid points.

We learnt from Table 6 as per the parameters we defined on Table 2,row 1 above, the subdomain WR solution is close to the exact solution for equally spaced x-domain points.

Table 6: Comparisons among the results of WRM & analytic results for catalytic reaction

when $\lambda = 0.01$, $\beta = 0.2$, $\gamma = 1$

X	Subdomain	Galerkin	Collocation	Exact [36]
0.25	0.995325	0.995327	0.995330	0.995199
0.50	0.996260	0.996262	0.996261	0.996159
0.75	0.997818	0.997819	0.997816	0.997759

3.4.2.2 Errors Comparisons and Analysis

Table 7: Comparisons among the results of absolute errors when $\lambda = 0.01, \beta = 0.2, \gamma = 1$

Absolute Error			
X	Subdomain	Galerkin	Collocation
0.25	0.000126	0.000128	0.000131
0.50	0.000101	0.000103	0.000102
0.75	0.000060	0.000061	0.000058

Table 8: Comparisons among the results of relative Errors when $\lambda = 0.01, \beta = 0.2, \gamma = 1$

Relative Error			
X	Subdomain	Galerkin	Collocation
0.25	0.000127	0.000129	0.000132
0.50	0.000102	0.000104	0.000103
0.75	0.000060	0.000061	0.000058

Table 7 and Table 8 shows that comparisons for absolute and relative errors for our weighted residual solutions on selected grid points.

3.4.3 Thermal Explosion Problem

3.4.3.1 Result comparisons

Table 9: Comparisons among results of WRM & analytic for thermal explosion problem when $\lambda = 0.01, \beta = 0.2, \gamma = 1$

X	Subdomain	Galerkin	Collocation	Exact [36]
0.25	0.047286	0.047297	0.047321	0.048934
0.50	0.037828	0.037838	0.037978	0.039083
0.75	0.022067	0.022072	0.022083	0.022737

Table 9 show that the solutions for sub domain, galerkin and collocation weighted residual methods and the exact solutions on equally spaced x-domain points for thermal explosion problem.

3.4.3.1 Errors Comparisons and Analysis

comparisons for absolute and relative errors for our weighted residual solutions on selected grid points are presented on Table 10 and Table 11 and Table 8 respectively.

Table 10: Comparisons among the results of absolute error when $\lambda = 0.01$, $\beta = 0.2$, $\gamma = 1$

Absolute Error			
X	Subdomain	Galerkin	Collocation
0.25	0.001648	0.001637	0.001613
0.50	0.001255	0.001246	0.001105
0.75	0.000670	0.000665	0.000654

Table 11: Comparisons among the results of relative error when $\lambda = 0.01$, $\beta = 0.2$, $\gamma = 1$

Relative Error			
X	Subdomain	Galerkin	Collocation
0.25	0.034855	0.033448	0.034086
0.50	0.033167	0.031869	0.029106
0.75	0.030372	0.029243	0.029607

3.4.4 Troesch Problem

3.4.4.1 Result comparisons

Table 12 show that the comparisons among the solutions for sub domain and galerkin weighted residual methods and the HPM with exact solutions on equally spaced x-domain points for Troesch problem. The table shows that both numerical solutions are very close to analytical solution. This further confirms that numerical solutions are very close to analytic solution.

Table 12: Comparisons among the results of WRM & analytic results when $\lambda = 0.5$

X	Subdomain	Galerkin	HPM solution [47]	Exact [49]
0.0	0.000000	0.000000	0.000000	0.000000
0.1	0.095511	0.094941	0.095948	0.095177
0.2	0.192020	0.191007	0.192136	0.190634
0.3	0.289526	0.288197	0.288805	0.286653
0.4	0.388029	0.386511	0.386197	0.383522
0.5	0.487531	0.485948	0.484560	0.481537
0.6	0.588029	0.586511	0.584143	0.581001
0.7	0.689526	0.688197	0.685201	0.682235
0.8	0.792020	0.791007	0.787992	0.785571
0.9	0.895511	0.894941	0.892784	0.891366
1.0	1.000000	1.000000	0.999848	0.999968

We observed from Table 12 the results of WRM are very close to HPM and to the exact solution

3.4.4.2 Errors Comparisons and Analysis

For subdomain and galerkin WR methods the absolute and relative errors are very small at the left boundary and absolute and relative errors are also decrease to the right boundary. comparisons on selected grid points are presented on Table 14 and Table 13 respectively.

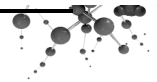
Table 14: Comparisons among the results of absolute error when $\lambda = 0.5$

Absolute Error			
X	Subdomain	Galerkin	HPM solution [47]
0.3	0.000721	0.000608	0.002152
0.6	0.003886	0.002368	0.004200
0.9	0.002727	0.002157	0.003418

Table 13: Comparisons among the results of relative error when $\lambda = 0.5$

Relative Error		
X	Subdomain	Galerkin
0.3	0.002491	0.002110
0.6	0.006609	0.004037
0.9	0.003045	0.002410

Chapter 4



APPLICATION OF ORTHOGONAL COLLOCATION FINITE ELEMENT FOR SOLVING NONLINEAR BVPs

This chapter presents application of OCFE for solving for the steady state exothermic chemical reaction in a slab of combustible material, thermal explosion in a vessel, catalytic reactions in a flat particle, reaction-diffusion equation.

4.1 Numerical Experiments

Consider the differential equations on chapter 2, on section 2.6 for different boundary value problems. We have seen the approximate solutions obtained by using weighted residual methods with exact solution on the above Chapter 2 and sections 2.6.1.2. In this section we solve these BVPs using the OCFE method based on their algorithms on Chapter 2, page 15.

Let us recall some notes from chapter three, OCFE method section using the transformation on chapter 2 .algorithm 5, (2.3 eq. 2), we obtained V , and by using a polynomial of order $N = 3$ for the trial solution, we write

$$\phi^i(v) = \sum_{k=1}^4 c_k^j I_k(v), \quad i = 1, 2 \quad (4.1 \text{ eq. } 1)$$

Since we require two collocation points per element, they will be chosen as the roots of an orthogonal polynomial of order two, namely v_2^c and v_3^c . Together with the boundary points $v_1 = 0$ and $v_4 = 1$, we have four nodes: $v_1 = 0$, v_2^c , v_3^c and $v_4 = 1$. We satisfy the residual equation for each element at the collocation points v_2^c and v_3^c to obtain

$$R^i(v_j^c) = 0, \quad i = 1, 2. \quad j = 2, 3 \quad (4.1 \text{ eq. } 2)$$

Due to the total number of unknowns, we have additional equations for a unique solution. These are obtained from the continuity ϕ conditions. $\phi^1(x_2) = \phi^2(x_2)$ and $\left. \frac{d\phi^1}{dx} \right|_{x_2} = \left. \frac{d\phi^2}{dx} \right|_{x_2}$ which are equivalent to $\phi^1(v_4) = \phi^2(v_1)$ and $\left. \frac{d\phi^1}{dv} \right|_{v_4} = \left. \frac{d\phi^2}{dv} \right|_{v_1}$ in the variable v . The continuity of the function's yields

$$\sum_{k=1}^4 c_k^1 I_k(v_4) = \sum_{k=1}^4 c_k^2 I_k(v_1) \quad (4.1 \text{ eq. 3})$$

Which simplifies to

$$c_4^1 - c_1^2 = 0 \quad (4.1 \text{ eq. 4})$$

And the continuity of the derivatives yields

$$\sum_{k=1}^4 \left[c_k^1 \frac{I_k'(v_4)}{h_1} - c_k^2 \frac{I_k'(v_1)}{h_2} \right] = 0 \quad (4.1 \text{ eq. 5})$$

Based on (4.1 eq. 2), (4.1 eq. 3), (4.1 eq. 4), (4.1 eq. 5), we have now a system of equations.

This yields a matrix vector form $A\mathbf{c} = \mathbf{b}$.

4.1.1 Exothermic Thermal Explosion Problem

In this section we try to solve the differential equation with its boundary conditions which we mentioned on (2.4 eq. 1) with the boundary conditions (2.4 eq. 2) using OCFEM

The above (4.1 eq. 1) approximate solution satisfies the differential equation

$$\frac{d^2 \phi^i}{dv^2} = -\lambda \left[(\mathbf{1} + \varepsilon \phi)^m e^{\left(\frac{\phi}{1 + \varepsilon \phi} \right)} - \delta \phi \right], \quad i = 1, 2, \quad (4.1 \text{ eq. 6})$$

Substituting the approximate solution in equation (4.1 eq. 1) into the differential equation (4.1 eq. 6) gives the residual in the i th element.

$$\mathbf{R}^i(\mathbf{v}) = \sum_{k=1}^4 \left[c_k^i I_k''(\mathbf{v}) \right] + \lambda \left[(\mathbf{1} + \varepsilon c_k^i I_k(\mathbf{v}))^m e^{\left(\frac{c_k^i I_k(\mathbf{v})}{1 + \varepsilon c_k^i I_k(\mathbf{v})} \right)} - \delta c_k^i I_k(\mathbf{v}) \right], \quad i = 1, 2, \dots \quad (4.1 \text{ eq. 7})$$

We satisfied the residual equation (4.1 eq. 2) for each element at the collocation points v_2^c and v_3^c to obtain Residual (4.1 eq. 2). The left boundary condition falls in element one, hence $\phi^1(x_1) = \phi^1(v_1) = 0$. These yields

$$c_1^1 = 0 \quad (4.1 \text{ eq. 8})$$

Similarly, the right boundary condition falls in element two, hence $\phi^2(x_3) = \phi^2(v_4) = 0$. These yields

$$c_4^2 = 0 \quad (4.1 \text{ eq. } 9)$$

Since we have a total of eight unknowns, we need two more additional equations. Based on the continuity conditions above, we use the continuity function's (4.1 eq. 3) and the continuity of the derivatives (4.1 eq. 5). We have now a system of equations. This yields a matrix vector form $Ac = b$.

Firstly, we use two equally spaced elements with sub-domains $[0,0.5]$ and $[0.5,1]$ then the interpolation points are $v_1 = 0$, $v_2 = \left(\frac{1}{\sqrt{1.5+2}}\right)/5$, $v_3 = \left(\frac{1}{\sqrt{1.5+2}}\right)/5$, $v_4 = 1$ where v_1 and v_2 are selected as the roots of T_2 . Thus, the collocation points $v_2^c = \left(\frac{1}{\sqrt{2+2}}\right)/4$, $v_3^c = \left(\frac{1}{\sqrt{2+3}}\right)/4$ are chosen as the roots of the Legendre polynomial.

4.1.1.1 Two Finite Elements

Let us consider number of elements are two ($N_e = 2$) with Subdomain $[x_1, x_2]$ and $[x_2, x_3]$ each element is applied to the domain $[0,1]$. Accordingly, after we computed by using MATLAB version Matlab R2019b v9.7.0, it gives the following matrix $Ac = b$. where A is a $4N_e \times 4N_e$ matrix and b is a $4N_e \times 1$ vector.

$$\begin{bmatrix} -7.63 & 8.43 & -3.15 & 2.36 & 0 & 0 & 0 & 0 \\ 2.25 & -0.10 & -25.47 & 23.32 & 0 & 0 & 0 & 0 \\ -1.81 & 6.07 & -37.18 & 32.92 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.25 & -0.10 & -25.47 & 23.32 \\ 0 & 0 & 0 & 0 & -1.81 & 6.07 & -37.18 & 32.92 \\ 0 & 0 & 0 & 0 & -1.00 & 0 & 0 & 0 \\ -0.85 & 1.57 & -28.63 & 27.91 & 15.27 & -16.85 & 6.31 & -4.73 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0.0589 \\ 0.0586 \\ 0.0482 \\ 0.0456 \\ 0.0456 \\ 0.0395 \\ 0.0053 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -0.037 \\ -0.041 \\ -0.037 \\ -0.041 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

In this section, we validate the orthogonal collocation finite element method by using its algorithm and physically realistic values of various embedded parameters that we defined in the above Table 1: exothermic explosion problem parameter definition, for the numerical experiment.

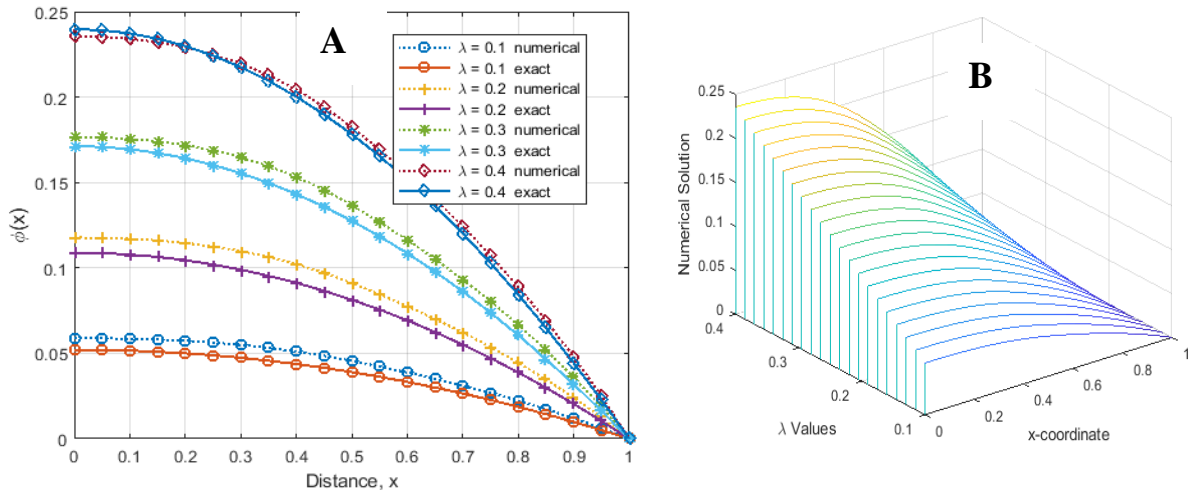


Figure 60: Solution for exothermic thermal explosion problem using OCFEM

when $N_e = 2$ and $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

As per the parameters we define in the above Table 1, row 1, For $N_e = 2$, we observe from Figure 60 (A) As the Frank-Kamenetskii parameter (λ) increases, and whereas activation energy(ε), heat loss(δ), numerical exponent(m) parameters remains fixed, the numerical and analytic solutions that temperature increases with an increase in the parameter values of λ , then the internal heat generation due to exothermic reaction increases, this invariably leads to an elevation in the temperature. Figure 60 (B) shows the 3D plot for the influence of the parameter (λ) values with the independent variable on the dependent variable (ϕ) or solution.

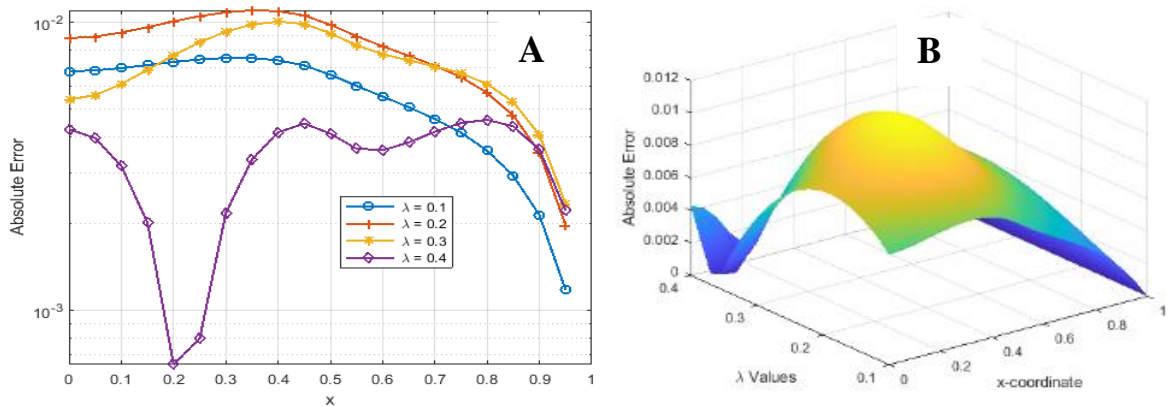


Figure 61: Absolute error for solving exothermic explosion problem using OCFEM

when $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Figure 61 (A) shows that the accuracy of our numerical method by computing the absolute error, the *absolute errors* are decreasing from left boundary to the right for all lambda values. And also, as lambda vary and m, ε, δ keeps fixed and the error is decreasing. Figure 61 (B) shows us the 3D view of the error plot as λ and x are going increasing.

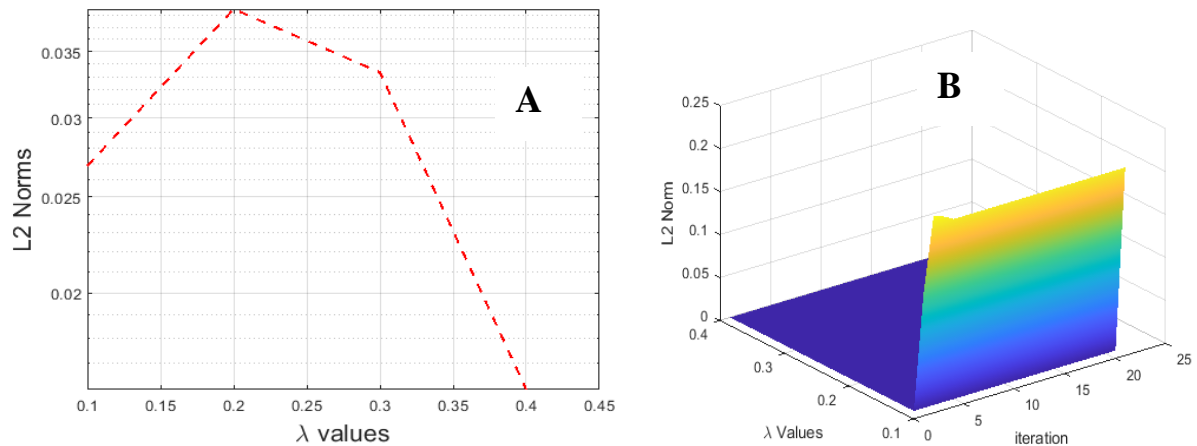


Figure 62: L2 Norm for solving exothermic explosion problem using OCFEM

when $\lambda = 0.1$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Figure 62 (A) is also show us the accuracy of our numerical method by computing L2 norm, L2 norm is decreasing with an increase in the parameter values of λ . We observe from Figure 62 (B) the effect of the L2 norm with an decrease in λ values and the iteration by using 3D graph (e.g. we observe there is the highest L2 norm at 1st iteration & $\lambda = 0.1$, and there is the lowest L2 norm at 21st iteration & $\lambda = 0.4$).

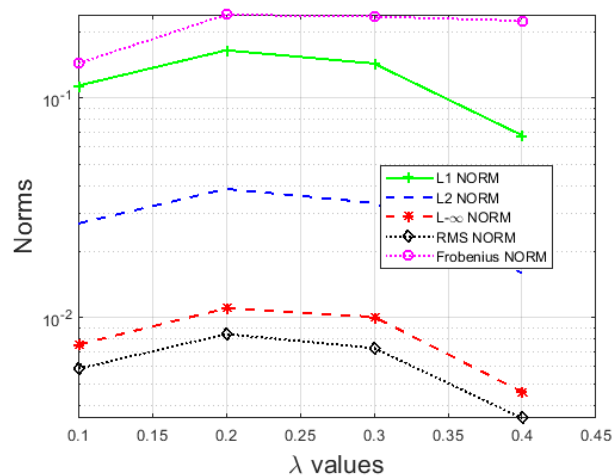


Figure 63: Other norms comparison for the exothermic explosion problem using OCFEM

when $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Figure 63 illustrate the plots of L_2 - norm, L-infinity norm, root mean square (RMS), L_1 -norm and frobenius norm of the numerical solution of (2.4 eq. 1) for the parameter values of $\lambda, m, \varepsilon, \delta$. All norms are decreasing as λ values are increase.

4.1.1.2 More Finite Elements

On section 4.1.1.1 the results show our OCFE method when the number of elements are two. However, by using more elements ($N_e > 2$), we can improve the accuracy of the results. In this section we see the accuracy of our numerical method as we increase the number of elements. As we increase the number of elements, the approximate solution tends to converge to the exact solution as shown in Figure 64 when $N_e = 3, 4, 5, 6$

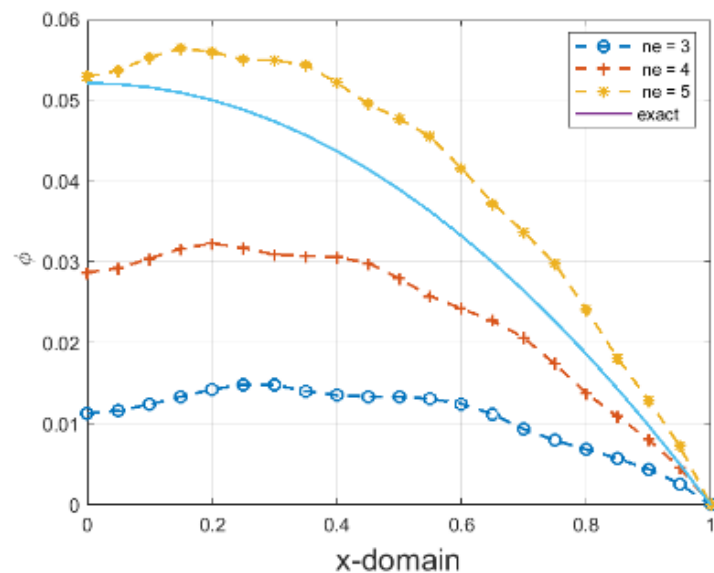


Figure 64: Solution for exothermic thermal explosion problem, using OCFEM
when $N_e > 2$ and $\lambda = 0.1, m = 0.5, \varepsilon = 0.1, \delta = 0.1$

We discussed above about the convergence of orthogonal collocation finite element method to the exact solution as we use a greater number of elements (N_e). Thus, Figure 64 shows we get very close solution to the exact if we use five number of elements than three for a single parameter $\lambda = 0.1$.

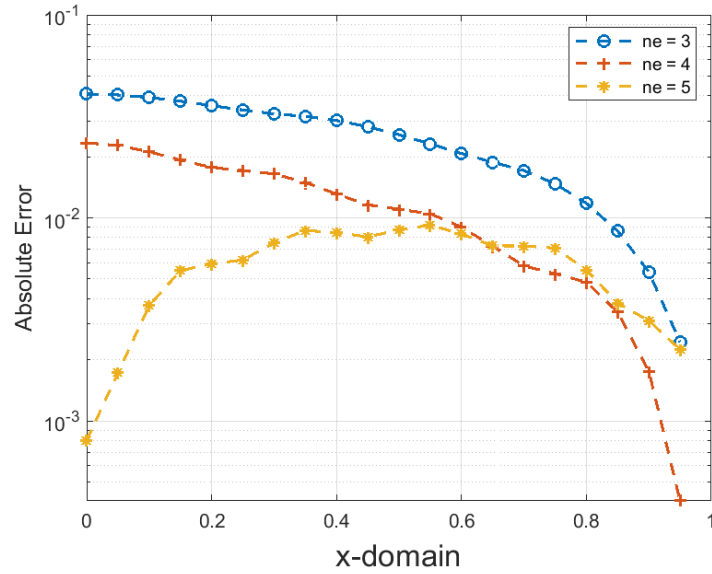


Figure 65: Absolute error for the Exothermic Explosion problem

when $N_e > 2$ and $\lambda = 0.1$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

The corresponding error plots are given in Figure 65 the error plots when number of elements are three, four, five ($N_e = 3$, $N_e = 4$, $N_e = 5$), for more elements are given in Figure 65. Observe the gradual decrease in the error as we increase the number of elements.

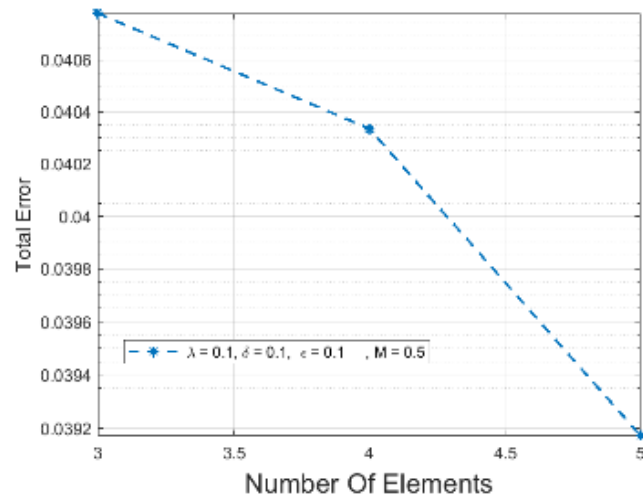


Figure 66: Total error for the exothermic explosion problem

when $N_e > 2$ and $\lambda = 0.1$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Figure 66 tells the total error is decreasing as we use more number of elements in this case number of elements are three, four, five ($N_e = 3, N_e = 4, N_e = 5$).

4.1.2 Catalytic reaction problem

We mentioned the differential equation with its boundary conditions on (2.4 eq. 11) and (2.4 eq. 12). Here, we try to solve this equation using orthogonal collocation finite element method. Thus, the above (4.1 eq. 1) approximate solution satisfies the differential equation.

$$\frac{d^2 \phi^i}{dv^2} = \lambda \phi e^{\left[\frac{\gamma \beta (1-\phi)}{1+\beta(1-\phi)} \right]}, \quad i = 1, 2, \quad (4.1 \text{ eq. } 10)$$

Substituting the approximate solution in equation (4.1 eq. 1) into the differential equation (4.1 eq. 10) gives the residual in the i^{th} element.

$$R^i(v) = \sum_{k=1}^4 [c_k^i I_k''(v)] - \lambda c_k^i I_k(v) e^{\left[\frac{\gamma \beta (1-c_k^i I_k(v))}{1+\beta(1-c_k^i I_k(v))} \right]}, \quad i = 1, 2, \quad (4.1 \text{ eq. } 11)$$

We satisfied the residual equation (4.1 eq. 2) for each element at the collocation points v_2^c and v_3^c to obtain Residual (4.1 eq. 2). The left boundary condition falls in element one, hence $\phi^1(x_1) = \phi^1(v_1) = 0$. These yields

$$c_1^1 = 0 \quad (4.1 \text{ eq. } 12)$$

Similarly, the right boundary condition falls in element two, hence $\phi^2(x_4) = \phi^2(v_4) = 1$. These yields

$$c_4^2 = 1 \quad (4.1 \text{ eq. } 13)$$

Since we have a total of eight unknowns, we need two more additional equations. Based on the continuity conditions above, we use the continuity function's (4.1 eq. 3) and the continuity of the derivatives (4.1 eq. 5). we have now a system of equations. This yields a matrix vector form $Ac = b$.

Firstly, we use two equally spaced elements with sub-domains $[0,0.5]$ and $[0.5,1]$ then the

interpolation points are $v_1 = 0, v_2 = \frac{\left(\frac{1}{\sqrt{1.35} + 1} \right)}{2}, v_3 = \frac{\left(\frac{-1}{\sqrt{1.21} + 1} \right)}{2}, v_4 = 1$. where v_1 and v_2 are

.....

selected as the roots of T_2 . Thus, the collocation points $v_2^c = \frac{\left(\frac{1}{\sqrt{1.18+1}}\right)}{2}$, $v_3^c = \frac{\left(\frac{-1}{\sqrt{1.38+1}}\right)}{2}$ are chosen as the roots of the Legendre polynomial.

4.1.2.1 Two Finite Elements

In this section, we validate the OCFE method when number of elements are two ($N_e = 2$) by using the algorithm and for the numerical experiment we defined in the above Table 2: catalytic reaction problem parameter definition, physically realistic values of various embedded parameters are defined. Thus, we developed a computer program by us using MATLAB R2019b version v9.7.0. for solving catalytic reaction problem (2.4 eq. 11) with the boundary conditions in (2.4 eq. 12) numerically. The results are presented in plots. The exact solution of the equation is taken from (2.4 eq. 13).

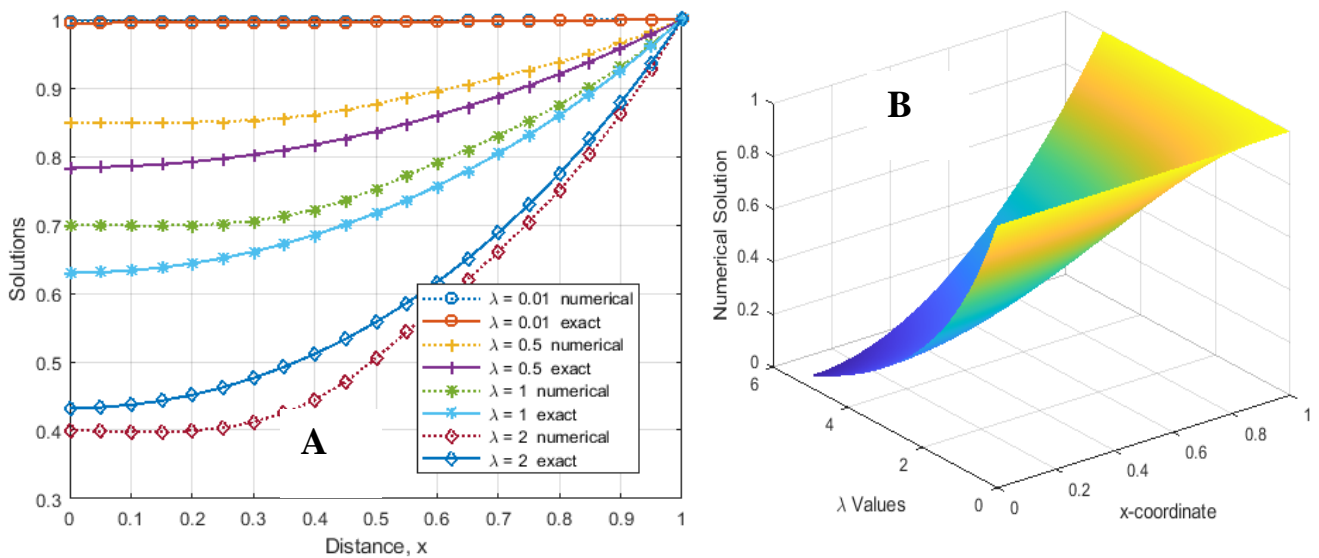


Figure 67: Solution for solving catalytic problem using OCFEM
when $N_e = 2$ and $\gamma = 1$, $\beta = 2$ and $N_e = 2$

From Figure 67 (A) it is clear that the concentration (ϕ) decreases for the fixed values of β and γ for the different values of λ due to the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless distance down the reactor x obtained from Equations (2.4 eq. 11) Table 2, row 1. Figure 67 (B) shows the 3D plot for the influence of the parameter (λ) values with the independent variable on the dependent variable (ϕ) or solution.

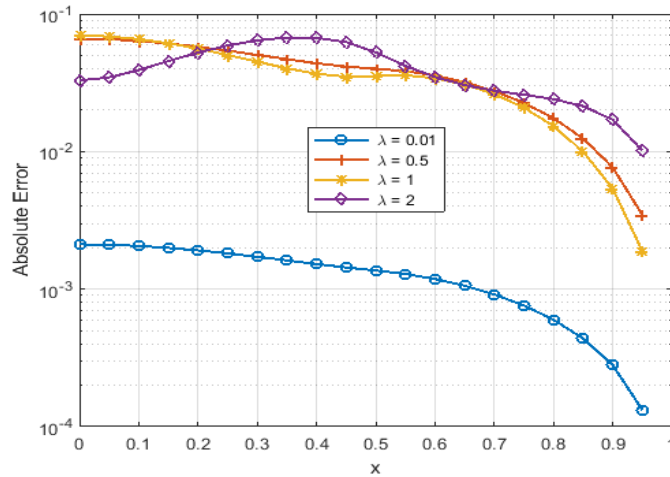


Figure 68: Absolute errors for solving catalytic reaction problem

when $N_e = 2$ and $\gamma = 1$, $\beta = 0.2$

We learn from Figure 68 the accuracy of OCFE method using computation of absolute error. The numerical results are very close to the analytic solution for parameter values mentioned on Table 2, row 1 and row 2 respectively.

4.1.2.2 More Finite Elements

Here, we see the accuracy of our numerical method when we increase number of elements ($N_e > 2$). As we increase the number of elements, the approximate solution tends to converge to the exact solution as shown in Figure 69 when $N_e = 3, 4, 5, 6$. Thus, we can improve the accuracy of our numerical results.

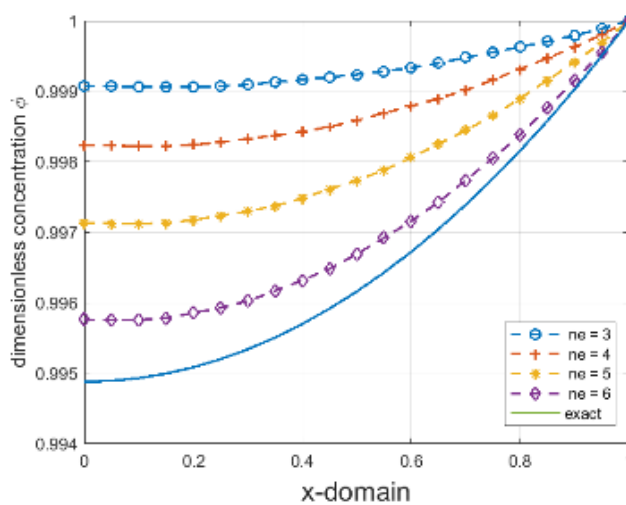


Figure 69: OCFEM for solving catalytic problem

when $N_e > 2$ and $\lambda = 0.01$, $\gamma = 1$, $\beta = 2$

We learnt above about the computation of orthogonal collocation finite element using more elements is very important, because it gives better solutions as we compute it using increase number of elements (N_e). Thus, Figure 69 shows we get very close solution to the exact when we use six number of elements ($N_{e=6}$). than two ($N_{e=2}$). for a single parameter $\lambda = 0.1$ and fixes parameters of $\gamma = 1$, $\beta = 0.2$

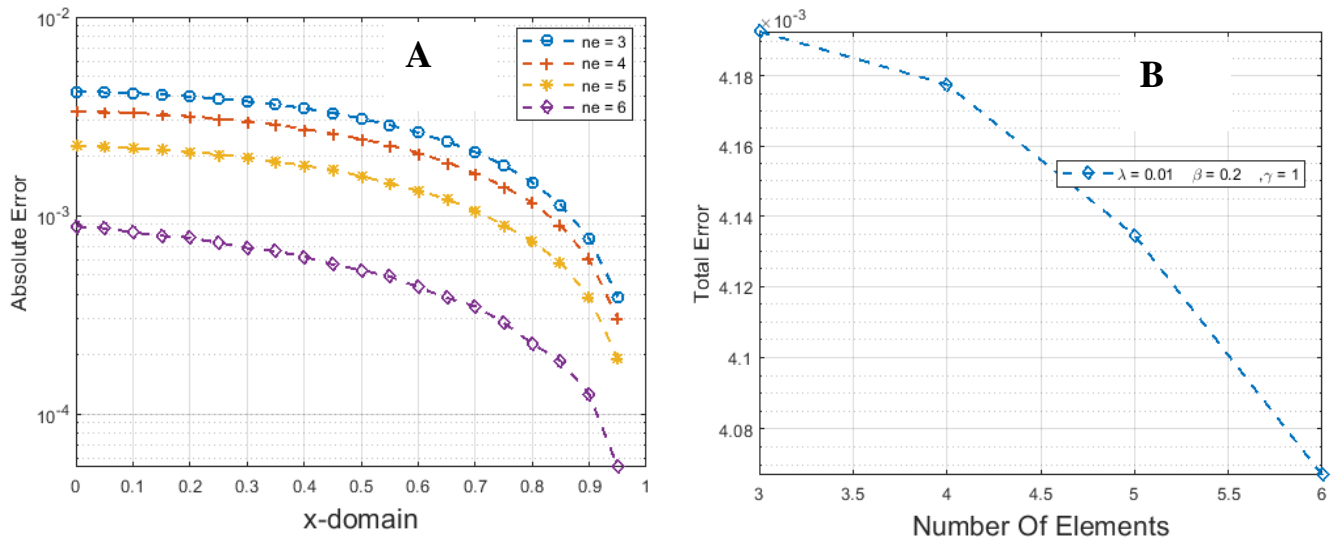


Figure 70: Absolute and total errors for solving catalytic reaction problem

when $N_e > 2$ and $\gamma = 1$, $\beta = 0.2$

The appropriate error plots are given in Figure 70 (A) the error plots when number of elements are three, four, five and six ($N_e = 3, 4, 5, 6$), for more elements are given in Figure 70 (A). Observe the gradual decrease in the error as we increase the number of elements. We observe from Figure 70 (B) the total error is decreasing levels off at 0.004067 ($N_e = 6$) which is better than the corresponding total error of 0.004193 ($N_e = 3$).

4.1.3 Thermal Explosion Problem

we try to solve the differential equation with its boundary conditions which we mentioned on (4.1 eq. 14). The above (4.1 eq. 1) approximate solution satisfies the differential equation

$$\frac{d^2 \phi^i}{dv^2} = \lambda e^{(\phi)}, \quad i = 1, 2, \quad (4.1 \text{ eq. } 15)$$

Substituting the approximate solution in equation (4.1 eq. 1) into the differential equation (4.1 eq. 15) gives the residual in the i^{th} element.

$$\mathbf{R}^i(\mathbf{v}) = \sum_{k=1}^4 \left[\mathbf{c}_k^i \mathbf{I}_k''(\mathbf{v}) \right] - \lambda e^{(c_k^i I_k(\mathbf{v}))}, \quad i = 1, 2, \quad (4.1 \text{ eq. } 16)$$

We satisfied the residual equation (4.1 eq. 2) for each element at the collocation points v_2^c and v_3^c to obtain Residual (4.1 eq. 2)

The left boundary condition falls in element one, hence $\phi^1(x_1) = \phi^1(v_1) = 0$. These yields

$$c_1^1 = 0 \quad (4.1 \text{ eq. } 17)$$

Similarly, the right boundary condition falls in element two, hence $\phi^2(x_4) = \phi^2(v_4) = 1$. These yields

$$c_4^2 = 1 \quad (4.1 \text{ eq. } 18)$$

Since we have a total of eight unknowns, we need two more additional equations. Based on the continuity conditions above, we use the continuity function's (4.1 eq. 3) and the continuity of the derivatives (4.1 eq. 5). We have now a system of equations. This yields a matrix vector form $\mathbf{A}\mathbf{c} = \mathbf{b}$.

Firstly, we use two equally spaced elements with sub-domains $[0,0.5]$ and $[0.5,1]$ then the interpolation points are $v_1 = 0, v_2 = 0.1802741786, v_3 = 0.9147870929, v_4 = 1$. where v_1 and v_2 are selected as the roots of T_2 . Thus, the collocation points $v_2^c = 0.606455532, v_3^c = 0.708206781$ are chosen as the roots of the Legendre polynomial.

4.1.3.1 Two Finite Elements

We apply here two elements in the domain $[0,1]$. We discussed in section 2.3.3 the procedures and the method of OCFE. Accordingly, for thermal explosion problem (2.4 eq. 22) with the boundary conditions in (2.4 eq. 23). For computational analysis we developed a computer program by using MATLAB version R2019b v9.7.0. we present the results in plots. The exact solution of the equation is taken from [39]. The following results shows the solutions for OCFE method with the analytic solution, absolute errors, L_2 norm for thermal explosion problem.

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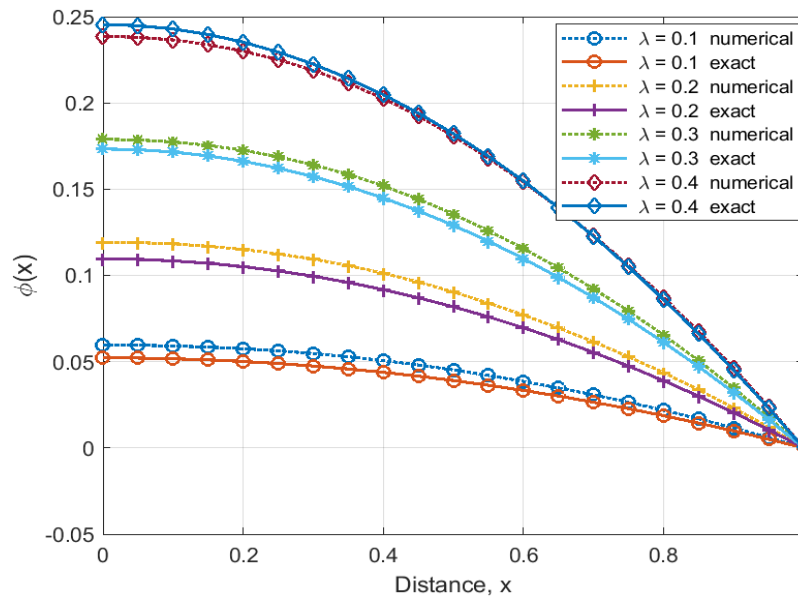


Figure 71: Solution for solving thermal explosion problem using OCFEM when $N_e = 2$

Figure 71 shows that the influence of λ on the dimensionless concentration (ϕ) versus the dimensionless distance x for both numerical and analytical solutions from these figures it is clear that the concentration (ϕ) increases for the different values of λ .

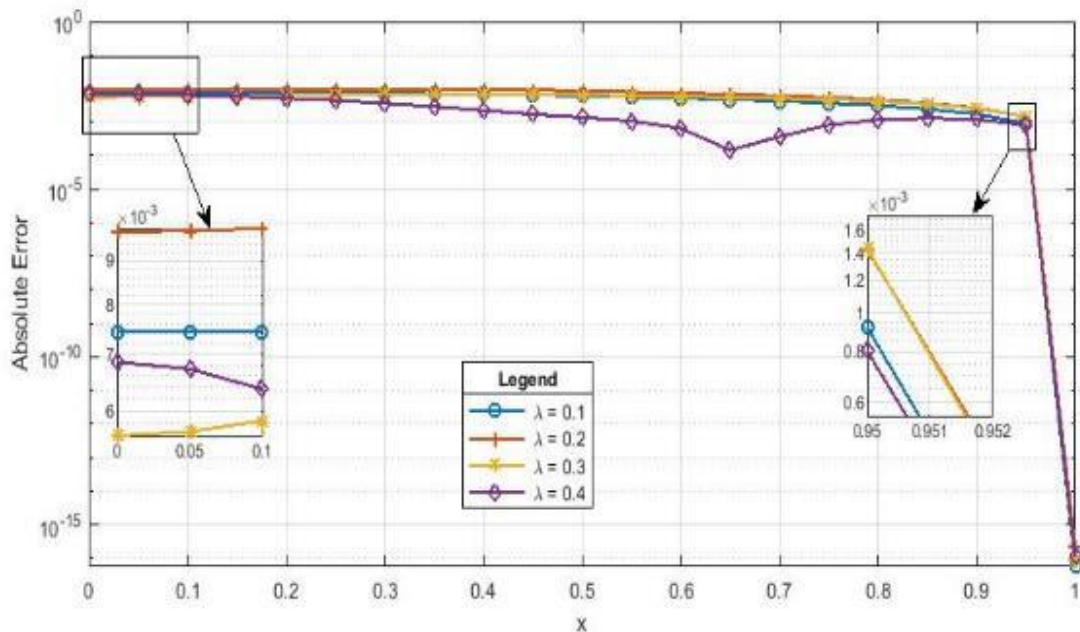


Figure 72: Absolute error thermal explosion problem using OCFEM when $N_e = 2$

Figure 72 illustrates absolute errors vs x-domain, it is clear that the absolute error is decrease to the right boundary for all dimensionless parameter λ values (e.g. for $\lambda = 0.1$ when $x = 0.00$,

absolute error = 0.007421 and when $x = 0.95$, *absolute error* = 0.000919). From these figures, it is evident that our numerical solution very close to the exact solution and it is very accurate

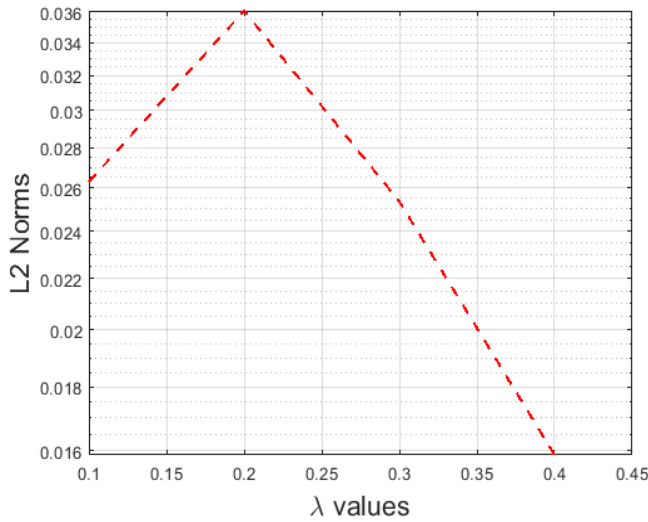


Figure 73: L2 norm for the thermal explosion problem

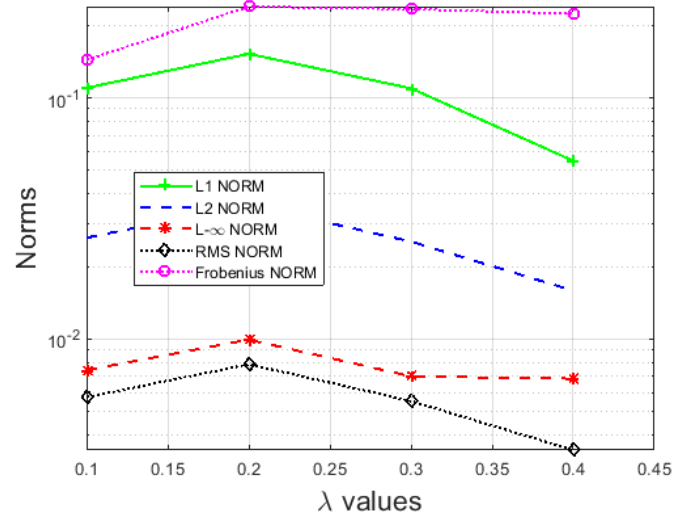


Figure 74: All norms Vs lambdas comparisons for the thermal explosion problem

L_2 norm versus the dimensionless parameter λ is plotted in Figure 73 it shows us L_2 norm is increasing as the λ values increases. We observe from Figure 74 L_1 , L_2 and Frobenious norms are larger than infinity norm and RMS, the infinity norm is also larger than root mean square (RMS).

4.1.4 Reaction Diffusion Equation

We apply the orthogonal collocation finite element method for solving reaction diffusion equation with its boundary condition. Based on the algorithm we defined on 2.3.32.2.7.1, Chapter 2, section 2.3, we developed a user defined computer program by using MATLAB version Matlab R2019b v9.7.0 by us for the numerical solution for solving reaction diffusion equation (2.4 eq. 54) with the boundary conditions in (2.4 eq. 55). The results are presented in plots. The exact solution of the equation is taken from [36].

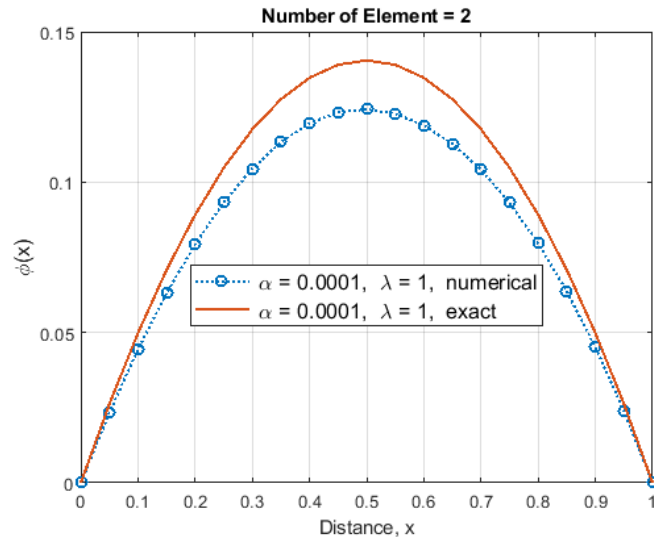


Figure 75: Solution for reaction diffusion equation using OCFEM when $N_e = 2$

We consider number of elements are two ($N_e = 2$) and parameters, $\alpha = 0.0001$, and $\lambda = 1$. hence, Figure 75 shows that the result of OCFE Method for reaction diffusion equation the numerical solution is very close to analytical solution.

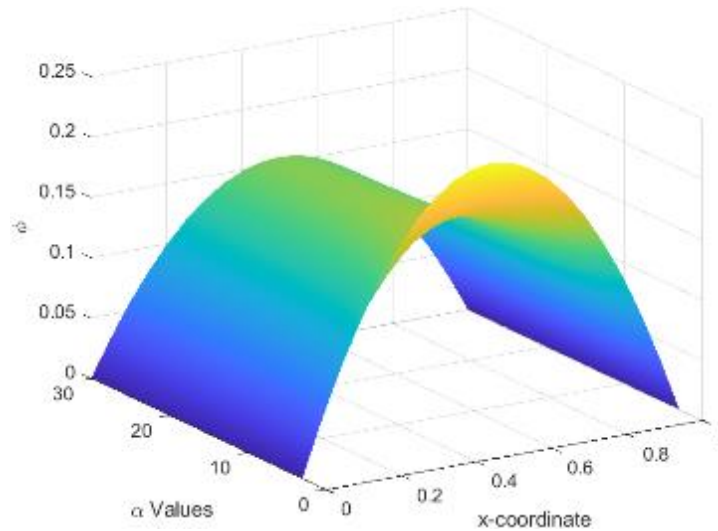


Figure 76: 3D plot for OCFEM for solving reaction diffusion equation

We saw the solutions of ϕ when the values of α is 0.0001 on Figure 75, and Figure 76 presents the 3 dimensional diagram (the independent variables α and x Vs the dependent ϕ) when the values α starting from 5 up to 30. We observe here the method is stable even the values of α is varying and go to highest numbers like 30.

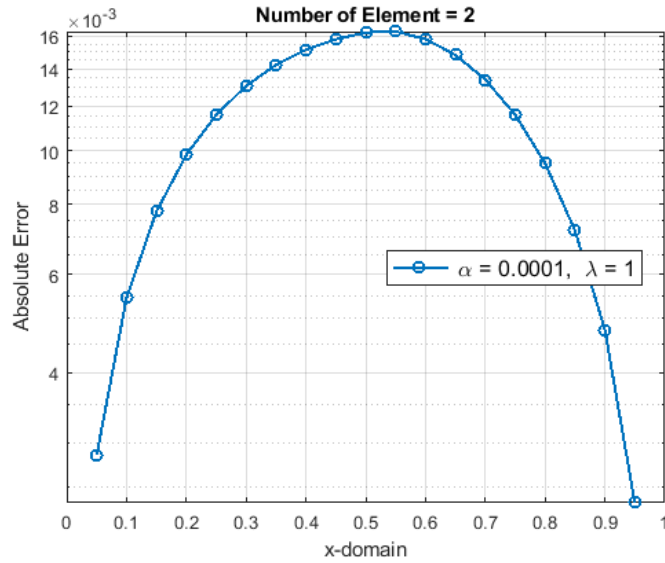


Figure 77: Absolute error for solving reaction diffusion equation using OCFEM

Figure 77 presents the accuracy of the numerical solution by computing absolute error when number of elements are 2.

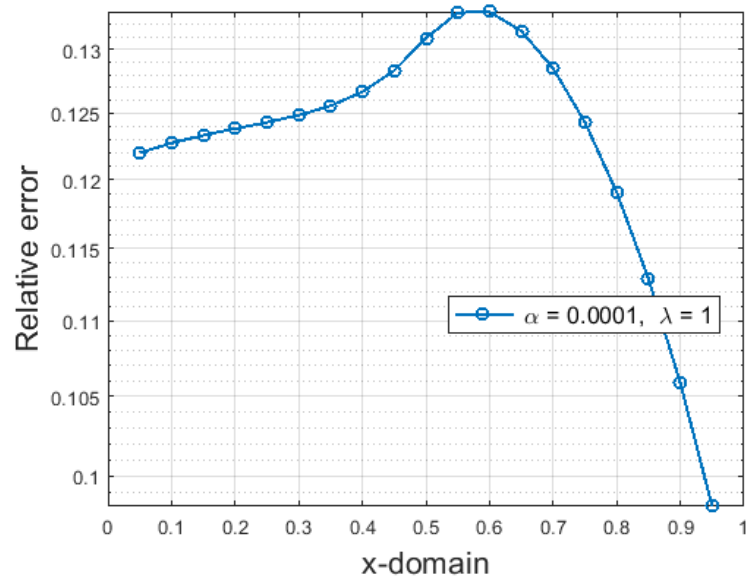


Figure 78: Relative error for solving reaction diffusion equation using OCFEM

Figure 78 presents relative error when number of elements are 2 and the value of α is 0.0001.

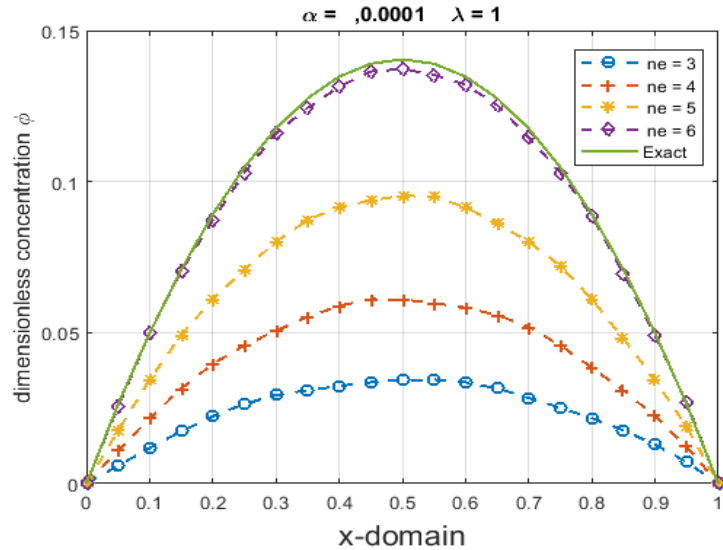


Figure 79: Solution for solving reaction diffusion equation using OCFEM when $N_e > 2$

By using more elements ($N_e > 2$), we can improve the accuracy of the results, as we increase the number of elements, the approximate solution tends to converge to the exact solution as shown in Figure 79 when $N_e = 6$, it's very close to analytic.

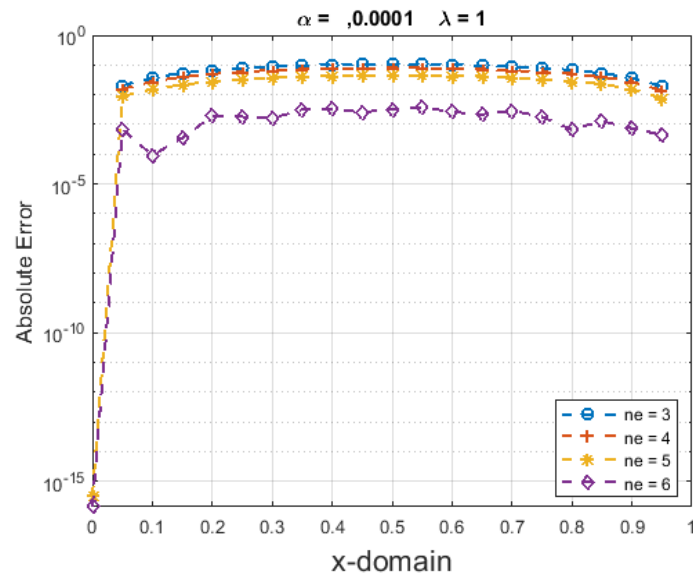


Figure 80: Absolute error for reaction diffusion equation using OCFEM when $N_e > 2$

We observe from Figure 80 absolute errors are very converging to the boundary conditions. When $N_e = 3, 4, 5, 6$.

4.1.5 Comparisons for the Application of OCFEM Vs WRMs to the Nonlinear BVP

We learnt methods and applications of weighted residuals on Chapter 3 and in this chapter, we discussed about orthogonal collocation finite element method, we check their accuracy, we compared numerical solutions among themselves. In this section, we present the comparisons between the methods of orthogonal collocation finite element when number of elements is two ($N_e = 2$) and weighted residuals for the nonlinear boundary value problems.

4.1.5.1 Exothermic Thermal Explosion

4.1.5.1.1 Result Comparisons

As we define in the above Table 1 , row 1 and discussed exothermic thermal explosion problem weighted residuals and orthogonal collocation finite element method.

Table 15: Comparisons among WRMs and OCFEM for exothermic explosion problem

when ($N_e = 2$) and $\lambda = 0.1$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$					
X	OCFE	Subdomain	Galerkin	Collocation	Exact [35]
0.25	0.056274	0.047265	0.047276	0.047442	0.048824
0.50	0.045592	0.037812	0.037820	0.037953	0.038999
0.75	0.026834	0.022057	0.022062	0.022139	0.022691

In this section, we present comparisons among OCFE method and sub domain, Galerkin and collocation weighted residual methods. For the comparison, we selected equally spaced grid points. We observe from Table 15 the results are very close to each other and to analytic solutions as well. OCFE method and all WR methods give better result to the near left boundary, at the middle and fast convergence to the near right boundary for equally spaced x-domain points.

4.1.5.1.2 Errors Comparisons and Analysis

Table 16: Absolute error comparisons when $\lambda = 0.1$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

X	OCFE	Subdomain	Galerkin	Collocation
0.25	0.007449	0.001559	0.001549	0.001382
0.50	0.006593	0.001187	0.001179	0.001046
0.75	0.004142	0.000634	0.000629	0.000552

Table 17: Relative error comparisons when $\lambda = 0.1$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

X	OCFE	Subdomain	Galerkin	Collocation
0.25	0.132380	0.032992	0.031717	0.029139
0.50	0.144599	0.031399	0.030222	0.027552
0.75	0.154375	0.028760	0.027734	0.024923

Table 16 shows the comparisons for absolute among WRMs and OCFEM ($N_e = 2$). On the other hand Table 17 presents relative errors among WRMs Vs OCFEM ($N_e = 2$) for a single λ value and on selected equally spaced grid points.

4.1.5.1.3 Computational Cost Comparison

We analyzed the computational cost in terms of time in each iteration to solve numerical solutions using OCFE and weighted residual methods for solving exothermic thermal explosion problem. We observe from Table 18 and Table 19 orthogonal collocation finite element method requires less computational cost than the others on each iteration and on each lambda values.

Table 18: Elapsed time comparison among OCFEM and WRM for exothermic thermal problem

when $\lambda = [0.1, 0.2, 0.3, 0.4]$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

Elapsed Time in Seconds				
Iteration	OCFE	Subdomain	Galerkin	Collocation
1	0.064	33.248	33.592	7.921
2	0.110	65.946	68.242	15.595
3	0.125	100.005	103.052	24.108
4	0.133	134.545	137.928	31.508

Table 18 tells the total duration of time to complete the numerical solutions.

Table 19: CPU time comparisons among OCFE and weighted residual methods

When $\lambda = [0.1, 0.2, 0.3, 0.4]$, $m = 0.5$, $\varepsilon = 0.1$, $\delta = 0.1$

CPU Time in Seconds				
Iteration	OCFE	Subdomain	Galerkin	Collocation
1	0.063	36.328	33.625	7.906
2	0.094	70.172	68.813	15.734
3	0.109	105.047	105.484	24.328
4	0.109	140.016	140.375	32.328

Table 19 presents CPU time for the numerical solutions.

4.1.5.2 Catalytic Reactions in a Flat Particle

4.1.5.2.1 Result Comparisons

Results for OCFE, sub domain, Galerkin and collocation weighted residual methods on equally spaced x-domain point is presented for the cases of catalytic reaction problem. This is useful to compare our numerical solution with the exact solution. We presented the absolute and relative errors to our numerical solutions for comparisons on selected equally spaced grid points. Note the number of elements that we used here is six ($N_e = 6$).

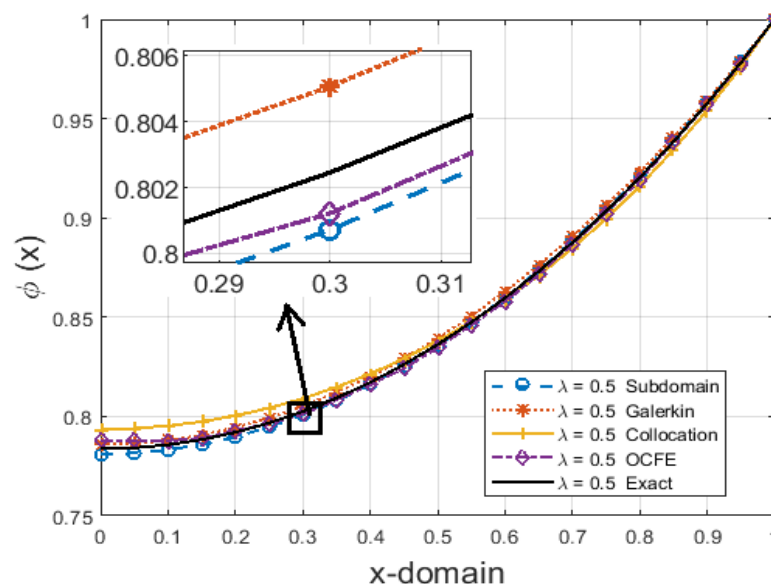


Figure 81: WRM Vs OCFEM results comparisons for catalytic reaction problem

We learnt from Figure 81 as per the parameters we defined on Table 2, row 1 above, the subdomain WR solution is close to the exact solution for equally spaced x-domain points. Figure 83 depicts results of SDWRM, GRKWRM, COLWRM and OCFEM for catalytic reaction problem when $\lambda = 0.5$. Thus, OCFEM and SDWRM are close to the exact solution.

4.1.5.2.2 Errors Comparisons and Analysis

Comparisons among WRMs and OCFEM is presented for absolute error in Table 20 and for relative errors in Table 21 on selected grid points.

Table 20: Absolute error comparisons when
 $\lambda = 0.5, \beta = 0.2, \gamma = 1$

X	OCFE	Subdomain	Galerkin	Collocation
0.25	0.000291	0.001996	0.002477	0.007570
0.50	0.001720	0.000453	0.003127	0.001674
0.75	0.000987	0.000848	0.002936	0.003698

Table 21: Relative error comparisons when
 $\lambda = 0.5, \beta = 0.2, \gamma = 1$

X	OCFE	Subdomain	Galerkin	Collocation
0.25	0.000365	0.002512	0.003110	0.009412
0.50	0.002061	0.000541	0.003739	0.001998
0.75	0.001094	0.000938	0.003250	0.004110

4.1.5.2.3 Computational Cost Comparison

We analyzed the computational cost in terms of time in each iteration to solve numerical solutions using weighted residual methods for solving catalytic reaction in a flat particle. We observe from Table 22 collocation weighted residual method requires less computational time than the others on each iteration and on each lambda values.

Table 22: Elapsed time comparisons WRMs for catalytic reaction problem
when $\lambda = [0, 0.5, 1, 5]$, $\beta = 0.2, \gamma = 1$

Elapsed Time in Seconds				
Iteration	OCFE	Subdomain	Galerkin	Collocation
1	0.108	46.998	35.881	21.045
2	0.167	84.963	73.050	43.549
3	0.179	118.401	109.604	64.717
4	0.188	151.094	139.991	86.960

4.1.5.3 Thermal Explosion Problem

4.1.5.3.1 Result Comparisons

We observe from Figure 82 our numerical solutions are very close to the exact and they have fast convergence to the right boundary. For OCFE ($N_e = 2$) and for sub domain, Galerkin and collocation weighted residual methods and the exact solutions on equally spaced x-domain points for thermal explosion problem.

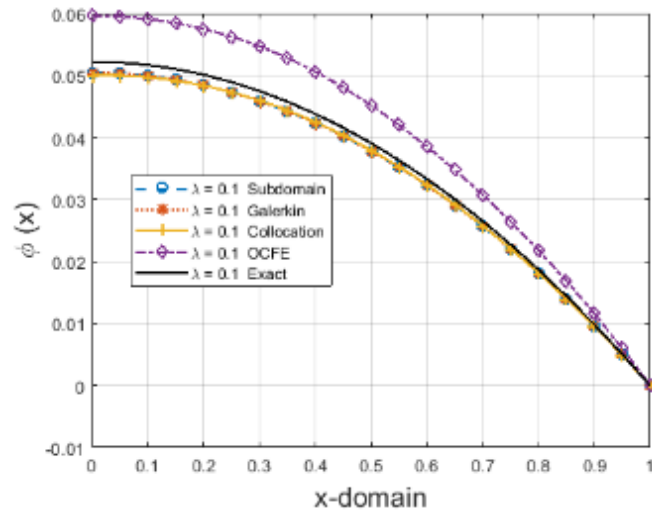


Figure 82: WRM Vs OCFEM results comparisons for thermal explosion problem

4.1.5.3.2 Errors Comparisons and Analysis

Table 23 tells absolute error comparisons and in Table 24 relative errors comparison among WRMs and OCFEM on selected grid points are presented respectively.

Table 23: Absolute error comparisons when

$$\lambda = 0.1$$

X	OCFE	Subdomain	Galerkin	Collocation
0.25	0.007335	0.001648	0.001637	0.001613
0.50	0.006119	0.001255	0.001246	0.001111
0.75	0.003709	0.000670	0.000665	0.000654

Table 24: Relative error comparisons when

$$\lambda = 0.1$$

X	OCFE	Subdomain	Galerkin	Collocation
0.25	0.130357	0.034855	0.033448	0.034086
0.50	0.135370	0.033167	0.031869	0.029106
0.75	0.140251	0.030372	0.029243	0.029607

4.1.5.3.3 Computational Cost Comparison

We analyzed the computational cost in terms of time in each iteration to solve numerical solutions using weighted residual methods for solving catalytic reaction in a flat particle. We learn from Table 25 OCFEM requires less computational time than weighted residual methods and among WRMs collocation WR method is computed less time than the others on each iteration and on each lambda values.

Table 25: Elapsed time comparisons WRMs and OCFEM for thermal explosion problem

when $\lambda = [0.1, 0.2, 0.3, 0.4]$

Elapsed Time in Seconds				
Iteration	OCFE	Subdomain	Galerkin	Collocation
1	0.108	46.998	35.881	21.045
2	0.167	84.963	73.050	43.549
3	0.179	118.401	109.604	64.717
4	0.188	151.094	139.991	86.960

Chapter 5



SUMMARY, CONCLUSION AND FURTHER RESEARCH

This chapter presents the summary, the conclusion of the thesis and recommendations for further research.

5.1 Summary

The main objective of this study is application of weighted residual and orthogonal finite element computational techniques to nonlinear boundary value problems. Thus, we aimed to study the application of subdomain weighted residual method, Galerkin weighted residual method, collocation weighted residual method and orthogonal collocation finite element method for the nonlinear boundary value problems.

To this end, the study focused to find out the numerical solutions of the model equations, namely for the steady state exothermic chemical reaction in a slab of combustible material, thermal explosion in a vessel, catalytic reactions in a flat particle, temperature distribution in straight fins with temperature dependent thermal conductivity, reaction-diffusion equation, Troesch boundary value problem for temperature distribution. The summaries of the major findings of this study are presented below.

We find out the accuracy of SDWRM, GRKWRM, COLWRM and OCFEM for exothermic thermal explosion problem by measuring absolute errors. The absolute errors are very small ($10^{-6} < \text{absolute error} < 10^{-2}$) in the grid point due to the influence of the varying parameters, frank-Kamenetskii (λ) or heat loss (δ) parameters, which are in acceptable range.

We investigate catalytic reaction has small absolute errors ($10^{-5} < \text{absolute error} < 10^{-1}$) for SDWRM, GRKWRM, COLWRM and OCFEM for the defined (λ) parameter.

We prove absolute errors for thermal explosion problem are drastically decreasing to the right boundary ($< 10^{-15}$). Which is also reflected on when Kamenetskii (λ) going increasing.

We examine absolute error results for Troesch problem gives very small error 10^{-10} absolute error $< 10^{-15}$ for small values of (λ) and absolute is between 10^0 absolute error $< 10^{-5}$ For $\lambda > 1$.

We also prove absolute error for the SDWRM smaller than GRKWRM our WRM gives better

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absolute error than HPM solution [47] (e.g. at $x=0.3$ absolute for SDWR = **0.000721** ,for GRKWRM = **0.000608**, for HPM solution [47]=**0.002152**, at $x=0.6$ absolute for SDWR = **0.003886** ,for GRKWRM = **0.002368**, for HPM solution [47]=**0.004200**).

We experiment reaction diffusion equation using OCFEM and COLWRM, our numerical solution has very small absolute errors on the grid points for different parameters of α, λ (e.g. when $\alpha=0.0001$, $\lambda=1$ from random pick point at $x=0.25$ absolute error for COLWRM = 0.000705 & for OCFEM 0.011580, at $x=0.5$ absolute error for COLWRM = 0.003956 & for OCFEM 0.016261).

We look into the accuracy of the numerical solution for temperature distribution in straight fins with temperature dependent thermal conductivity by calculating absolute error. Absolute errors are decreasing drastically from left to right boundary for all values of β . Due to thermal conductivity parameter β , absolute errors are very small initially at the left boundary for highest values of β (absolute error is between $10^{-5} < absolute\ error < 10^{-4}$ for $\beta=0.3, 0.4$) and (absolute error is between $0.000535 < absolute\ error < 0.001224$ for $\beta=0.1, 0.2$) but absolute error for lower values of $\beta=0.1, 0.2$ going decreasing to the right boundary ($absolute\ error = 0.000092$) and absolute error of high values of $\beta=0.3, 0.4$ going increase to the right boundary (absolute error = 0.000727).

We highlight the computational cost in terms of seconds to compute exothermic thermal explosion problem for parameters $\lambda=[0.1, 0.2, 0.3, 0.4]$, $m=0.5$, $\varepsilon=0.1$, $\delta=0.1$ using SDWRM, GRKWRM, COLWRM and OCFEM. Hence, for the first iteration OCFEM takes 0.064 sec, SDWRM takes 33.248 sec, GRKWRM 33.592 sec, COLWRM 7.921sec for the last iteration OCFEM takes 0.133, SDWRM takes 134.545, GRKWRM 137.928 COLWRM 31.508.

We indicate the computational cost for the numerical solution of catalytic reaction equation for parameter definition $\lambda=[0, 0.5, 1, 5]$, $\beta=0.2$, $\gamma=1$. To compute and finish the first iteration, OCFEM takes 0.108 seconds, SDWRM takes 46.998, GRKWRM takes 35.881 sec, COLWRM takes 21.045 sec. And for the last iteration OCFEM takes 0.188 sec, SDWRM takes 151.094 sec, GRKWRM takes 139.991sec, COLWRM takes 86.960 sec. Based on this we draw the following conclusion.

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Application of weighted residual and Orthogonal Finite Element Computational Techniques to
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5.2 Conclusion

In Chapter 2, we described the algorithms, concepts and methods of weighted residuals and orthogonal collocation finite element method and on section 2.6 we experimented different types of boundary value problems with different boundary conditions (mixed BC and Dirichlet BC type), namely the steady state exothermic chemical reaction in a slab of combustible material, the catalytic reactions in a flat particle, the thermal explosion in a vessel, Troesch boundary value problem for temperature distribution, reaction-diffusion equation, temperature distribution in straight fins with temperature dependent thermal conductivity numerically with respect to the different parameters. We also reported their analytic or semi analytic solutions for each defined BVPs from different literatures.

In chapter 3, we investigated and applied the application of weighted residual methods, namely subdomain, Galerkin, collocation weighted residual methods algorithm for the solution of for the steady state exothermic chemical reaction in a slab of combustible material, the catalytic reactions in a flat particle, the thermal explosion in a vessel, Troesch boundary value problem for temperature distribution, reaction-diffusion equation, temperature distribution in straight fins with temperature dependent thermal conductivity numerically with respect to the parameters. We compared the numerical solution with the analytical solution, we checked the accuracy by computing absolute errors and norms. Thus, we saw that the weighted residual methods were accurate and generates numerical solutions that are stable and physically reasonable for the nonlinear BVPs.

We studied in chapter 4, the application Orthogonal Collocation Finite Element method procedures for solving the steady state exothermic chemical reaction in a slab of combustible material, the catalytic reactions in a flat particle and thermal explosion in a vessel and reaction-diffusion equation. The OCFE applied to an ODE using N_e equally spaced elements, the $4N_e \times 4N_e$ matrix A is sparse and only involves 16 different entries to be evaluated and OCFEM applied using an increased number of elements ($N_e=3,4,5,6$) in the domain to be analyzed. We compared results, absolute error, norms and computational time of orthogonal collocation finite element method with weighted residual methods. We proved that the method was accurate and generates numerical solutions that are stable and physically reasonable for the nonlinear BVPs.

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To conclude the highlights of our findings, in chapter 3 and 4, we tested six nonlinear BVPs with respect to their mixed boundary conditions and different parameters using WRM and OCFEM.

Accordingly, the steady state exothermic chemical reaction in a slab of combustible material is considered. The nonlinear ordinary differential equation governing the problem was formulated and solved numerically using the subdomain, Galerkin, Collocation and Orthogonal Collocation Finite Element techniques.

An increase in the parameter value of λ indicates increasing rate of exothermic chemical kinetics. As parameter δ increases in value ($\delta > 0$), the rate of heat loss to the ambient increases as well as the thermal explosion criticality values. This invariably enhances the thermal stability of the reacting slab by preventing the occurrence of thermal runaway.

We have considered a nonlinear boundary value problem describing the onset of a thermal explosion in a vessel. Numerical experiments show that to solve the thermal explosion model (2.4 eq. 22) Subdomain is suitable from weighted residual method and OCFE method is preferable if we use increase number of elements and it requires least computational cost.

We proved the influence of λ on the concentration (ϕ) of catalytic reactions in a flat particle and dimensionless distance down the reactor x obtained from Equations (2.4 eq. 11) Table 2, row 1. That shown the concentration (ϕ) decreases for the fixed values of β and γ .

The method of OCFE which combines the features of the orthogonal collocation method with the finite element method was found to be more numerically stable and reliable than the orthogonal collocation method. The orthogonal collocation method provides the accuracy whereas the finite element provides the stability to the numerical results. The computational time is compensated for by the accuracy achieved by using more elements.

One could concentrate elements in regions with steep gradients by noting that the essence of all weighted residual methods is to make the residual close to zero as much as possible. Hence, we try to insert more elements in regions with large residuals, thus forcing the residual to zero at those points and making the solution converge faster. This implies that the residual has to be forced to zero over each element.

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We analyzed computational costs by comparing elapsed time in seconds for the application of subdomain WRM, Galerkin WRM, collocation WRM and Orthogonal Collocation Finite Element methods for the nonlinear BVPs on Chapter 4, section 4.1.5. Thus, we verified that OCFEM requires less computational time than the WRM to compute nonlinear BVPs. We also confirmed subdomain and collocation methods have better accuracy as reported on absolute error comparisons among subdomain, Galerkin, Collocation Weighted Residual methods and Orthogonal Collocation Finite Element method.

5.3 Further Research

we shall state the following future research areas or sections.

- ✍ Robin boundary conditions for nonlinear boundary value problems included for future studies and research.
- ✍ Dynamics analysis or qualitative analysis for BVPs.
- ✍ For further study including
- ✍ Least square WRM, Rayleigh ritz WRM and Method of moment WRM for nonlinear boundary value problems included for future studies and research.
- ✍ For further study including
- ✍ Application of orthogonal collocation on finite elements to nonlinear PDE

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