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Solving linear and nonlinear transient diffusion problems with the Laplace Transform Dual Reciprocity Method

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Solving Linear And Nonlinear Transient Diffusion Problems With The Laplace Transform Dual Reciprocity Method

A thesis submitted in fulfilment of the requirements for the award of the degree of

Doctor of Philosophy

from

The University of Wollongong

by

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1996
This thesis is submitted to the University of Wollongong, and has not been submitted for a degree to any other University or Institution.

Pornchai Satravaha

March, 1996
The very first two teachers of mine are my dearest father and mother,

*Vichit and Darunee Satravaha,*

and the present one is my supervisor,

*Dr. Songping Zhu.*

I am most grateful to all of my teachers
from whom I have acquired gigantic knowledge.

This thesis is dedicated to them all.
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Abstract

In this thesis, a new numerical method, with the Laplace Transform and the Dual Reciprocity Method (DRM) combined into the so called Laplace Transform Dual Reciprocity Method (LTDRM), is proposed and applied to solve linear and non-linear transient diffusion problems. The method comprises of three crucial steps. Firstly, the Laplace transform is applied to the partial differential equation and boundary conditions in a given differential system. Secondly, the dual reciprocity method is employed to solve the transformed differential system. Thirdly, a numerical inversion is utilised to retrieve the solution in the time domain.

The LTDRM is first applied for the solution of the linear transient diffusion equation. A time-free and boundary-only integral formulation is produced due to the first and second steps of the method. In this work, only the fundamental solution of the Laplace’s equation is utilised in the dual reciprocity method. That is, the Laplacian operator is treated as the main operator and the nonhomogeneous terms, such as those obtained from the Laplace transform of the temporal derivative, sources or sinks, or other terms, are left to a domain integral. The DRM technique then requires all these terms be approximated by a finite sum of interpolation functions that will allow the domain integral to be taken onto the boundary.

Several problems are then analysed to demonstrate the efficiency and accuracy of the LTDRM. A numerical inversion due to the Stehfest’s algorithm is examined and found to be satisfactory in terms of the numerical accuracy, efficiency and ease of implementation.

Next, the LTDRM is extended to the solution of the diffusion problems with nonlinear source terms. A linearisation of the nonlinear governing equation is required before the LTDRM can be applied. Two linearisation techniques are adopted. The convergence of solution of the linearised differential system to the true solution of the original nonlinear system is studied and found to be quite
satisfactory. Then, the LTDRM is applied to solve some practical nonlinear problems of microwave heating process and spontaneous ignition.

Finally, the diffusion problems with nonlinear material properties and nonlinear boundary conditions are solved by the LTDRM. Three integral formulations are presented; one of them is based on the use of the Kirchhoff transform to simplify the governing differential system before the LTDRM is applied while the other two are based on the direct approach with the LTDRM being applied directly to the governing differential system. Due to the presence of spatial derivatives in two of these formulations, another set of interpolation functions, which is different from that used to cast the domain integral into the boundary integrals, is employed to approximate these derivative terms. These formulations are applied to solve a variety of problems, and their advantages and disadvantages are discussed.

It may be noteworthy that for all the cases, a time-free and boundary-only integral formulation is produced. As a result of both step-by-step calculation in the time domain and computation of domain integrals being eliminated, the dimension of the problem is virtually reduced by two. The results of numerical examples presented throughout these research projects demonstrate the efficiency and accuracy of the LTDRM. For linear problems, the LTDRM is shown to be very efficient when a solution at large time is required. In addition, solutions at both small time and large time can be obtained with the same level of accuracy. Similar conclusions can be drawn for nonlinear cases. As stated before, the LTDRM is shown to possess good convergence properties for nonlinear problems presented herein.
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Chapter 1

Introduction

1.1 Background

There are numerous scientific, engineering and technological processes that can be mathematically modelled by transient diffusion equations such as smelting of metal, sintering of ceramics, and joining (welding) of polymers by microwave radiation, spontaneous ignition of a reactive solid, heat transfer in nuclear reactor components, mass transport in groundwater, etc. The study of these diffusion problems is thus of fundamental importance.

In the past two decades, the Boundary Element Method (BEM) has become increasingly attractive to scientists and engineers as an alternative numerical method to the more established ones such as the Finite Difference (FDM) and Finite Element (FEM) Methods, for solving diffusion problems. In many aspects, the BEM proves to be advantageous over the FDM and FEM. Its major advantageous and attractive characteristic is its ability in reducing the dimension of the problem by one. In other words, it provides a complete solution to the problem with the effort of solving an integral equation on the boundary of the computational domain only. In obtaining a boundary-only integral equation, the BEM makes use of the fundamental solution (Green’s function) of the partial differential equation (PDE), and the reciprocity theorem (Green’s second identity). This equation is then applied, in a discretised form, to a certain number of nodal points
on the boundary (e.g., by using a collocation technique), resulting in a system of algebraic equations. Once all the unknowns on the boundary are found, the solution at any interior point can be easily obtained with a high accuracy using only the computed boundary values.

Generally, the treatment of transient diffusion problems with the BEM can be categorised into two main approaches. The first one solves the problem directly in the time domain, and we shall call it a “time-domain” approach. The second one solves the problem in a transformed domain (usually, the Laplace-transformed domain), and we shall call it a “Laplace-transform” approach. It is advantageous at this point to summarise previous BEM-based methods for the solution of transient diffusion equations.

1.1.1 The time-domain method

The formulations based on the boundary integral equation method for solving transient diffusion problems in the time domain can be traced back to the early seventies. Butterfield and Tomlin [14, 95] applied the indirect (source) formulation for the analyses of zoned orthotropic media in geotechnical engineering. Transient solutions were generated by distributing instantaneous sources over the problem region at zero time to reproduce the initial conditions and continuous sources over the region boundaries and interfaces, satisfying the prescribed boundary and interface conditions.

Chang et al. [16] proposed a direct formulation with the time-dependent fundamental solutions for the solution of two-dimensional heat conduction problems in isotropic and anisotropic media. The discretisation of the boundary integral equation was carried out using constant variations of space and time variables. The conditions for the method to maintain reasonable accuracy were also discussed. A similar approach was employed by Shaw [81] to formulate a Neumann problem for three-dimensional heat conduction in solids. However, an emphasis was given to the analytical rather than numerical aspects of the method. This formulation was later extended by Liggett and Liu [49] to Neumann and mixed
boundary conditions for groundwater problems, and by Wrobel and Brebbia [99] in order to allow higher-order space and time interpolation functions to be included, thus making the analysis of more practical problems possible.

The time-dependent fundamental-solution approach was later applied to complex physical problems such as viscous flows [83], natural convection problems [63], phase change problems [97], plasma arch heating for machining of cast iron cylinders [84], and heat transfer problems with moving heat sources [33]. However, this formulation has lost the "boundary-only" characteristic of the boundary element method due to the presence of a domain integral associated with the initial condition. Moreover, since the time variation of the unknown function and its normal derivative is not known a priori, a time-marching scheme has to be introduced.

Two available time-stepping schemes were discussed in detail by Brebbia et al. [12]. The first scheme requires computation of the values of the unknown function at a sufficient number of internal points which are treated as pseudo-initial values for the next timestep. In addition, care must be taken in the choice of timestep size since a singularity may occur in the argument of the Green's function (fundamental solution) in the temporal direction which may lead to deterioration of the accuracy of the solution [27]. Stability analysis of this scheme was later discussed by Sharp [80] who produced, for limited cases, a condition to guarantee the stability. There are other variants of this scheme, and they can be found, for example, in [90]. In the second scheme [100], all time integrations are always restarted from the initial time which leads to repeated boundary integrations over the same contour path, but domain integration can be avoided if the initial condition is harmonic. A mathematical proof of the uniform convergence and stability of this scheme used in conjunction with the BEM as applied to linear two-dimensional transient heat conduction problems was reported in [62]. Although mathematically elegant, this technique may be time consuming if the number of timesteps in the problem is too large. Apart from these limitations, the method requiring an analytic Green's function in both space and time also
restricts its applicability to the problems where the appropriate Green’s functions are available.

Other alternative integral formulations for the solution of transient problems include the coupled boundary element–finite difference method [13, 28] and the potential method of Curran et al. [29, 30]. The former utilises a finite difference to approximate the temporal derivative, and very small timesteps again have to be adopted if the formulation is to produce good results [28]. The latter is an indirect version of the time-dependent Green’s function method.

During the mid-eighties, there was a trend towards the use of time-independent fundamental solution [98], as can be noted in the works of, amongst many others, Ingber and Mitra [45], Taigbenu and Liggett [91, 92], Aral and Tang [3, 4], Loeffler and Mansur [50], and Wrobel et al. [102]. The main operator used in this approach is part of the governing equation, excluding the temporal derivative term, where its fundamental solution is readily available. The Green’s second identity is then utilised to cast this part of the governing equation into boundary integrals, while the remaining terms stay in a domain integral. However, a simplification of the temporal derivative by finite differences offers a variety of schemes, e.g., fully explicit, fully implicit or Crank-Nicolson scheme, to be incorporated into the formulation. Thus, the resulting formulation from this approach eliminates the previous complexity associated with the time integration.

With this approach, the method adopted by Ingber and Mitra [45], and Taigbenu and Liggett [91, 92] involves a domain discretisation by the use of triangular elements, with the temporal derivative assumed constant within each element [45] or to vary linearly between nodes [91, 92]. The main disadvantages of these formulations are evidently the need of a domain discretisation and the calculation of results at internal points. The approach adopted by Aral and Tang [3, 4], the so-called secondary reduction process, makes use of the idea of Brebbia and Nardini [11] of approximating temporal derivative at any point inside the domain by a finite sum of interpolation\(^1\) functions weighted by a set of unknown coefficients.

\(^1\)Sometimes referred to as coordinate functions [101] or approximating functions [70].
which are dependent on time. Although domain integration is still required, no internal unknowns are present and the resulting formulation is considered to be of "boundary-only" type.

However, an unavoidable process of domain integration required for all the above mentioned formulations prohibited these formulations from becoming "purely" boundary-only; the elegance of the boundary element method was therefore lost. Moreover, not only does it reduce the efficiency of the method as pointed out by Ingber and Phan-Thien [46] that the evaluation of the domain integral can sometimes consume more than 60% of the total CPU time, but it can also affect the accuracy of the solutions as the domain integration could be a major source of error if it is not evaluated properly [90].

In summary, the BEM-based formulations for solving problems in the time domain suffer from two deficiencies. The first one is that the timestep size adopted in these formulations has to be relatively small in order to obtain accurate results or avoid instability. Thus, it is time consuming when results at large time are required. The second one is due to the domain integration, which prevents these formulations from retaining purely boundary-only characteristic of the BEM. This latter deficiency can be shunned by the use of the so-called dual reciprocity method, which will be discussed later on. To remove the restrictions on the timestep size altogether, the Laplace transform is a natural solution.

1.1.2 The Laplace-transform method

It is quite interesting to notice that the first BEM-based formulation for the solution of transient diffusion equations was actually based on a Laplace-transform approach [76]. The main attraction of the Laplace-transform BEM method is the removal of the time variable so that the parabolic equation (transient diffusion equation) is transformed to an elliptic one which can then be solved more easily in the transformed space with the boundary element method.

The first BEM formulation utilising the Laplace-transform approach was proposed by Rizzo and Shippy [76] for the solution of heat conduction problems in
solids. This technique was extended by Liggett and Liu [49] to the unsteady flows in confined aquifers, and by Taigbenu et al. [89] to the solution of seawater intrusion in coastal aquifers.

To retrieve the solution in time domain, a numerical Laplace inversion must then be adopted, which usually requires solving the problem in the transformed space for a number of times, using different values of the Laplace parameter. In the early works, the solution of the original problem was recovered from the solutions in the Laplace-transformed space via a method of Schapery [78]. This method is essentially a curve-fitting process and it requires the determination of a certain number of coefficients which are obtained from the solution of a system of simultaneous equations. A disadvantage of using this inversion is that the general temporal behaviour of the solution has to be known a priori. Furthermore, the values of the Laplace parameter are also chosen arbitrarily. It is thereby difficult, without using an adaptive scheme, to decide the optimal values of the Laplace parameter; choosing too many of them would result in unstable solutions while too few may not represent the curve sufficiently and thus reduce the accuracy of the solutions [49]. In addition, problems with time-dependent boundary conditions will pose a great computational difficulty [48] which makes this inversion method impractical. Because of these limitations, the Laplace-transform-based BEM had only moderate successful applications to the solution of diffusion equations before the mid-eighties.

Not long afterwards, the Laplace-transform approach regained the attention of researchers, as many numerical Laplace inversions became available in the literature after Schapery proposed his method. These numerical inversions can be used to avoid the disadvantages which occurred when using the Schapery's method. For example, the so-called multidata method [24], which is a modified Schapery's technique, has been successfully applied with the Laplace-transform-based BEM formulation to poroelastic problems by Cheng and Detournay [23]. This technique was later extended to three-dimensional problems by Badmus et al. [7]. The Laplace-transform technique has also been successfully applied
in conjunction with different numerical methods such as finite difference and finite element methods for the solution of groundwater flow and solute transport problems, e.g., Sudicky [88], and Moridis and Reddell [54, 55, 56], and heat conduction problems, e.g., Chen and Chen [18, 19], and Chen and Lin [20, 21]. In these works, different Laplace inversion algorithms such as those of Stehfest [87], Talbot [93], Dubner and Abate [34], Durbin [35], and Crump [25], etc., were used with the advantages of each algorithm, e.g., its efficiency and accuracy, being pointed out. A detailed review and comparison of these algorithms can be found in Davies and Martin [31].

Recently, Moridis and Reddell [57] employed Stehfest’s algorithm to recover the solution in the time domain after the problem had been solved in the Laplace-transformed space by the BEM. Their formulation is of the same form as that described in [12] with the inclusion of source or sink terms. Apart from a demonstrated higher efficiency over the time-domain BEM, this approach involves domain integrals, which cannot be converted into boundary integrals unless the kernels are of special types such as those satisfying Laplace’s or Poisson’s equation [48, 56]. Cheng et al. [22] also used the BEM to solve axisymmetric diffusion problems in the Laplace-transformed space, without having a domain integral involved. However, their calculations, based on the pre-tabulated Green’s function, are not general and convenient enough in computation, since zero initial conditions have to be assumed and the Green's function needs to be discretised and pre-tabulated in advance. Although the domain integrals introduced in the Laplace-transform-based BEM do not give rise to any new unknowns, they have certainly eclipsed the elegance of the BEM. Nevertheless, Moridis and Reddell and Cheng et al. showed that the Stehfest’s algorithm for the numerical inversion of the Laplace transform employed in their formulations no longer causes problems as appeared in the earlier works.

It has been demonstrated that if solutions for a range of time are required, the Crump’s technique or Honig-Hirdes’ scheme [44], which is based on the methods of Dubner-Abate and Durbin, is suitable [18, 88]. On the other hand, if solutions
at some specific times are needed, the technique of Stehfest is very efficient [22, 57, 74].

However, the disadvantage of the Laplace-transform BEM which is in common with the time-domain BEM is due to the domain integrations. Such a disadvantage can be overcome by the use of a domain-integration-free method, the dual reciprocity method.

1.1.3 The Dual Reciprocity Method

In the literature, there have been several techniques such as Galerkin Vector Method [26], Fourier Expansion Technique [94], Dual Reciprocity Method [58], Multiple Reciprocity Method [60, 61], Particular Integral Approach [1], and Atkinson's Method [5], among others, proposed to deal with domain integrals that arise in the BEM analysis. However, the best method so far is the so-called Dual Reciprocity Method (DRM), proposed by Nardini and Brebbia [58], with which one is able to convert domain integrals in the BEM analysis into equivalent boundary integrals by using a set of particular solutions and the reciprocity theorem twice. Thus, a "purely" boundary-only integral formulation is obtained. The DRM was further extended by many authors, e.g., Nardini and Brebbia [59], Partridge and Brebbia [68, 69] and Partridge and Wrobel [71], and its application to a wide variety of problems can be found in [70]. Similar to the DRM, the particular integral approach, adopted by Ahmad and Banerjee [1], uses particular solutions to eliminate a domain integral and was extended by Herry and Banerjee [41, 40] and Ingber and Phan-Thien [46]. Another method similar to the DRM is Atkinson's method which allows domain integrals to be computed without explicit discretisation of the domain. This method was further improved by Goldberg and Chen [38]. In fact, Polyzos et al. [72] and Goldberg and Chen [39] respectively showed that the particular integral approach and Atkinson's method are equivalent to the dual reciprocity method.

Wrobel et al. [102, 103] derived a formulation using the dual reciprocity method, with the time-independent fundamental-solution approach, for transient
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heat conduction and axisymmetric diffusion problems. Loeffler and Mansur [50] also used the DRM to study problems in an infinite domain.

The method used by Wrobel et al. [102] was later extended to nonlinear problems. For example, among many others, Wrobel and Brebbia [101] applied the method to the solution of transient heat conduction problems in which the thermal conductivity, density and specific heat are all functions of temperature. Partridge and Wrobel [71] used the DRM to solve spontaneous ignition problems where the reaction-heating term appearing in the governing equation is of exponential form. Recently, Zhu et al. [107] employed this technique to solve microwave heating problems with nonlinear heat source term being a power function of temperature. As the problems are nonlinear, a solution procedure requires some sort of nonlinear iterations, e.g., a direct iteration [71, 107] or Newton-Ralphson algorithm [101]. Despite its success, the formulation based on using the DRM with a "finite-difference time-integration" is not without drawbacks. Since a number of iterations needs to be performed at each timestep, this approach can be computationally expensive if the number of timesteps is large.

1.2 The Current Research Projects

It can be clearly seen from the above literature review that a Laplace-transform method has certain advantages over a time-domain method, one of which resides in the fact that the Laplace-transform method allows an unlimited timestep size to be taken, which, in other words, permits a solution at any desired observation time to be obtained in just a single timestep! Although the Laplace-transform method requires solving problem several times in the transformed space, it can still easily outpace the time-domain method, especially when a solution at a large time is required.

Another advantage is evident when solving nonlinear problems. Since an additional iterative process is required in the solution procedure, any time-domain method is generally very expensive as not only is a large number of timesteps
needed but iterations are also required at each timestep. On the other hand, the Laplace-transform method can be used to save a large amount of computational time because iterations are only required for a single timestep.

Another important part of a solution procedure in both time-domain and Laplace-transform methods is to solve a boundary value problem at each timestep regardless of how many timesteps are needed in the calculation. When the traditional boundary element method is utilised, domain integrals usually appear in the formulation. These undesirable domain integrals reduce the efficiency of the BEM. However, they can be avoided by the use of the dual reciprocity method; a boundary-only integral formulation can then be obtained.

To recapitulate, the elegance of the BEM, i.e., the dimensionality reduction of the problem by one, is well preserved by the use of the DRM, and a further reduction in dimension, i.e., the time dimension, can be achieved by the application of the Laplace transform. From these advantages, the idea of using these two techniques, in a combined form, to solve the transient diffusion problems naturally emerged and is presented in this thesis. The new method, combining the Laplace transform and the dual reciprocity method, proposed herein will be called the Laplace Transform Dual Reciprocity Method (LTDRM).

This thesis is divided into 5 chapters, with the background of the research outlined in Chapter 1.

In Chapter 2, the LTDRM is first developed and applied to solve a linear transient diffusion equation. It is in this first stage of the current research projects that the most important features of the LTDRM are clearly demonstrated.

The method comprises of three major steps: 1) the Laplace transform is applied to the governing partial differential equation and boundary conditions in a given differential system; 2) the transformed differential system is then solved with the dual reciprocity method; and 3) the solutions obtained in the Laplace-transformed space are numerically inverted to yield the results in the original domain.

As a result of steps one and two, a “time-free and boundary-only” integral
formulation is produced. It should be noted that whether the LTDRM, or in fact any other Laplace-transform method, is to be successful depends vitally on the effectiveness of the numerical inversion employed in the third step. It has been shown that a solution at any specific time can be obtained via the Stehfest’s algorithm [87] with the computation of only four to six terms of solutions in the Laplace-transformed space [22, 57, 74]. Moreover, solutions at both small and large time can be obtained with the same level of accuracy. Due to its efficiency, accuracy and ease of implementation, the Stehfest’s algorithm is therefore chosen in these research projects.

Several examples of linear diffusion problems are provided which illustrate the efficiency and accuracy of the LTDRM.

In Chapter 3, the LTDRM is then extended to the nonlinear regime. The transient diffusion equation with nonlinear source terms is first chosen for such an extension. The reason for choosing this type of equations is that it is simple, yet nonlinear, and also important in modelling many technological and environmental processes.

As the governing equation is now nonlinear, a linearisation of this equation is required so that the Laplace transform can be applied. The linearisation of the nonlinear governing equation is therefore crucial to the success of the extension of the LTDRM to the nonlinear regime.

In these research projects, two linearisation techniques are adopted, and the convergence of the solution of the linearised differential system to the true solution of the original nonlinear system is studied and found to be quite satisfactory. Accordingly, two LTDRM formulations are then formulated and applied to solve some practical nonlinear problems of microwave heating and spontaneous ignition. A comparison of these two formulations is also made.

In Chapter 4, the LTDRM is further extended to nonlinear transient diffusion problems with nonlinear material properties and nonlinear boundary conditions. These types of nonlinearities are two of the most important nonlinear features that arise in the problems encountered in engineering practice and applied science.
In extending the LTDRM to this type of nonlinear problems, a linearisation of both governing equation and boundary conditions needs to be carried out first. Once this has been done, the LTDRM can be applied and two integral formulations are obtained. Due to the presence of spatial derivatives in these formulations, another set of interpolation functions, which is different from that used to cast the domain integral into the boundary integrals, is employed to approximate these derivatives. Another integral formulation is also presented which is based on the use of the Kirchhoff transform to firstly simplify the governing differential system, followed by a linearisation and the LTDRM procedure. These three integral formulations are then applied to solve a variety of problems, and their advantages and disadvantages are discussed.

The major findings in these research projects are summarised in Chapter 5.
Chapter 2

Linear Diffusion Problems

Linear transient diffusion equations play a significant role in engineering and applied science. A large number of problems that occur in engineering practice and applied science such as heat transfer problems [64], heat conduction in solids [15, 76, 81], unsteady flow in confined aquifers [49], etc., can be modelled by this type of equations as the governing differential equation. Efficiently and accurately solving linear diffusion equations is a usual task faced by scientists and engineers.

If a problem is defined on a regular domain, the linear equations can often be solved analytically [15, 64]. However, most of the practical problems encountered in engineering are posed on an irregular domain, and the analytical solutions are either very difficult or impossible to find; numerical approaches are therefore resorted to. The Boundary Element Method (BEM) is one of the numerical methods which has been successfully applied for the solution of transient diffusion problems. Compared to other numerical methods, one of the important features of the BEM is its operation on the boundary of a given computational domain, which consequently results in a high numerical efficiency. However, such an advantage usually disappears as a domain integral needs to be carried out when the BEM is used in conjunction with the Laplace transform so that the solution of a linear transient diffusion equation, particularly at large time, can be found efficiently. Naturally, combining the Laplace transform and dual reciprocity method to form a new approach for the linear transient diffusion equations should lead
to improved numerical efficiency. The study of a newly proposed boundary element method, the Laplace Transform Dual Reciprocity Method (LTDRM), is the subject of this chapter.

The LTDRM is first developed for the solution of linear transient diffusion equations. The application of the LTDRM to linear problems is important due to the fact that there are many analytical solutions available for the LTDRM solutions to be compared with and therefore, the numerical accuracy of the LTDRM solutions can be evaluated and demonstrated. Furthermore, as most nonlinear problems are solved iteratively after some sort of linearisation, once the LTDRM is established for the linear problems, it can then be extended to nonlinear problems which will be presented in the latter chapters.

The LTDRM comprises of three crucial steps. The Laplace transform is first applied to the governing differential system and the dual reciprocity method is then employed to solve the transformed differential system. The result obtained from these two steps is a time-free and boundary-only integral equation.

Once this integral equation is solved and solutions are obtained, a numerical inversion of the Laplace transform is needed to bring these solutions back to the original time domain, and the success of the LTDRM depends on, to a large extent, the effectiveness of the numerical inversion adopted in this step.

The efficiency and accuracy of the LTDRM are demonstrated via several numerical examples. The effectiveness of the numerical inversion of the Laplace transform is also discussed.

2.1 The Laplace Transform Dual Reciprocity Method (LTDRM)

We are seeking for an approximate solution to the problem governed by the diffusion equation of the form

\[ \nabla^2 u(x, t) = \frac{1}{k} \frac{\partial u(x, t)}{\partial t}, \quad x \in \Omega, \]

(2.1)
in which \( u(x,t) \) is the unknown function of spatial point \( x \) at time \( t \), and \( \Omega \) is a solution domain for \( u \). The interpretation of \( u \) depends upon the problem under consideration, which may be the temperature field in a heat conduction problem or the potential in a groundwater problem. In this thesis, however, \( u \) will be interpreted as a temperature field as we will consider problems of heat conduction most of the time unless stated otherwise. Accordingly, the term \( k \) in Equation (2.1) is interpreted as the thermal diffusivity of a substance and assumed to be constant in time and space here in this chapter.

Two types of boundary conditions are applied to Equation (2.1). The Dirichlet condition gives the values of \( u \),

\[
    u(x,t) = \bar{u}(x,t), \quad x \in \Gamma_1, \tag{2.2}
\]

and the Neumann condition provides the values of normal derivative of \( u \),

\[
    q(x,t) = \frac{\partial u(x,t)}{\partial n(x)} = \bar{q}(x,t), \quad x \in \Gamma_2, \tag{2.3}
\]

where \( \Gamma_1 \) and \( \Gamma_2 \) represent complementary segments of the boundary \( \Gamma \) of \( \Omega \), respectively, and \( n(x) \) is the unit outward vector normal to \( \Gamma \) at point \( x \). In addition to these boundary conditions, since the problem is time dependent, an initial condition at a specific time \( t_0 \) must also be prescribed,

\[
    u(x,t) = u_0(x,t_0), \quad x \in \Omega. \tag{2.4}
\]

Without loss of generality, we shall let \( t_0 = 0 \).

It should be noted that if there are additional terms, such as sources or sinks, in Equation (2.1), there will be only a minor change to the integral formulation described below so long as these terms are also linear. Equation (2.1) with nonlinear source terms will be discussed later on in Chapter 3.
2.1.1 The Laplace transform of a linear differential system

In order to make use of the Laplace transform, let us first define the Laplace transform of a function \( u(x, t) \) when it exists by

\[
\mathcal{L}[u(x, t)] = U(x, p) = \int_0^\infty u(x, t)e^{-pt}\,dt,  \tag{2.5}
\]

where \( p \) is the Laplace parameter. By integration by parts, one can show that

\[
\mathcal{L}\left[\frac{\partial u(x, t)}{\partial t}\right] = pU(x, p) - u_0(x, t_0).  \tag{2.6}
\]

After taking the Laplace transform with respect to \( t \), Equation (2.1) becomes

\[
\nabla^2 U(x, p) = \frac{1}{k}\{pU(x, p) - u_0(x, t_0)\},  \tag{2.7}
\]

with the boundary conditions

\[
U(x, p) = \overline{U}(x, p), \quad x \in \Gamma_1,  \tag{2.8}
\]

\[
Q(x, p) = \frac{\partial U(x, p)}{\partial n(x)} = \overline{Q}(x, p), \quad x \in \Gamma_2.  \tag{2.9}
\]

Note that Equation (2.7) is nonhomogeneous and solving it with the traditional BEM leads to an integral equation with a domain integral containing initial conditions as shown by Moridis and Reddell [57]. For some special initial conditions such as those commonly encountered in engineering and applied mathematics with \( u_0 \) satisfying Laplace's or Poisson's equation, the domain integral can be transformed into equivalent boundary integrals by using the so-called Galerkin vector [48, 56]. However, an efficient method which deals with an arbitrary initial condition is sought after for the following three reasons. First of all, the condition attached to the Galerkin vector technique is too restrictive to be applied for general initial conditions, which may be encountered in modelling a complex physical process. Secondly, if there are heat sources inside a computational domain [52], an extra term would appear in the governing differential equation; hence the calculation of a domain integral becomes unavoidable. Thirdly, even for a regular
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heat transfer problem or diffusion problem governed by a diffusion equation like (2.1) without source terms and with simple initial conditions so that the Galerkin vector technique can be adopted, Zhu and Zhang [106] showed that a mapping may be useful to convert an exterior problem into an interior problem so that a solution similar to the optimised solution of Loeffler and Mansur [50] is naturally obtained; such a mapping leads to an artificial "heat source" in the transformed governing differential equation. In any case, we must face volume integrals that arise in the formulation.

2.1.2 Application of the DRM in Laplace-transformed space

The most powerful and elegant approach so far in converting volume integrals into boundary integrals is the dual reciprocity method and its application to the current formulation in the Laplace-transformed space is described as follows.

First of all, the right-hand side of Equation (2.7) is approximated by a finite sum of interpolation functions \( f_j \), i.e.,

\[
\frac{1}{k} \left\{ pU(x,p) - u_0(x,t_0) \right\} = \sum_{j=1}^{N+L} f_j \alpha_j,
\]

where \( \alpha_j \) are the coefficients to be determined by the collocation method with \( N \) boundary collocation points and \( L \) interior collocation points (see Figure 2.1).

As for the interpolation functions \( f_j \), Partridge and Brebbia [68] showed that the best results can be obtained if \( f_j \) takes the form \( \sum_{m=0}^{s} r_j^m \) where \( r_j \) is the distance from a source point \( j \) to a field point \((x,y)\). Moreover, they also pointed out that the use of \( s = 1 \) giving \( f_j = 1 + r_j \) is generally sufficient. Hence, we took only the simplest form of \( f_j = 1 + r_j \) in all of our numerical experiments so far completed.

It should be noticed that herein we intend to use the DRM with the Laplacian as the main operator and all the remaining terms are dealt with in the approximation in Equation (2.10). For diffusion problems, one could also use the Modified Helmhholtz operator, i.e., \( \nabla^2 - p/k \), as a whole in a DRM process where the fundamental solution is readily available [12, 57]. However, the resulting formulation
Figure 2.1: A sketch of boundary and internal nodes used in the DRM.
using this operator can be quite involved and difficult to extend to nonlinear problems. On the other hand, the DRM procedure using the Laplacian as the main operator is much simpler and the formulation obtained yields accurate results, as will be seen from examples presented later. Moreover, it is easier to extend this formulation to nonlinear problems. For these reasons, the Laplacian will be used as the main operator throughout this work.

Applying the usual boundary element technique, Equation (2.7) is multiplied by the fundamental solution of Laplace's equation, \( U^* \), with Equation (2.10) being utilised and integrated over domain \( \Omega \), i.e.,

\[
\int_{\Omega} (\nabla^2 U) U^* \, d\Omega = \sum_{j=1}^{N+L} \alpha_j \int_{\Omega} f_j U^* \, d\Omega. \tag{2.11}
\]

Replacing \( f_j \) in Equation (2.11) by \( \nabla^2 \hat{U}_j \), i.e., by demanding \( \hat{U}_j \) to be a particular solution of the equation \( \nabla^2 \hat{U}_j = f_j \) (such a solution can be easily found, e.g. \( \hat{U}_j = r_j^2/4 + r_j^3/9 \) for \( s = 1 \)), one can then transform the domain integrals in Equation (2.11) to the corresponding boundary integrals. The integration by parts twice produces

\[
c_\xi U_\xi - \int_\Gamma U^* Q \, d\Gamma + \int_\Gamma Q^* U \, d\Gamma = \\
\sum_{j=1}^{N+L} \left\{ \alpha_j \left( c_\xi \hat{U}_{\xi j} - \int_\Gamma U^* \hat{Q}_j \, d\Gamma + \int_\Gamma Q^* \hat{U}_j \, d\Gamma \right) \right\}, \tag{2.12}
\]

where \( \xi \) is a source point of \( U^* \) which can be any point within the domain or on the boundary; \( U_\xi \) and \( \hat{U}_{\xi j} \) are the values of \( U \) and \( \hat{U}_j \) on point \( \xi \), respectively; and \( Q, Q^* \) and \( \hat{Q}_j \) are the normal derivatives of \( U, U^* \) and \( \hat{U}_j \), respectively. The value of \( c_\xi \) in Equation (2.12) depends upon the location of the source point \( \xi \). It can be shown [12] that

\[
c_\xi = \begin{cases} 
\frac{\alpha(\xi)}{2\pi} & \text{if } \xi \text{ is a boundary point;} \\
1 & \text{if } \xi \text{ is an interior point},
\end{cases} \tag{2.13}
\]

where \( \alpha(\xi) \) denote the internal angle of the boundary at \( \xi \). The discretised form of Equation (2.12) is then

\[
c_\xi U_\xi - \sum_{k=1}^{N} Q_k g_{\xi k} + \sum_{k=1}^{N} U_k h_{\xi k} = \sum_{j=1}^{N+L} \left\{ \alpha_j \left( c_\xi \hat{U}_{\xi j} - \sum_{k=1}^{N} \hat{Q}_{jk} g_{\xi k} + \sum_{k=1}^{N} \hat{U}_{jk} h_{\xi k} \right) \right\}. \tag{2.14}
\]
After applying Equation (2.14) to all collocation points, one obtains a linear system of order $(N + L)$ as

$$c_i U_i - \sum_{k=1}^{N} Q_k g_{ik} + \sum_{k=1}^{N} U_k h_{ik} = \sum_{j=1}^{N+L} \left\{ \alpha_j \left( c_i \hat{U}_{ij} - \sum_{k=1}^{N} \hat{Q}_{jk} g_{ik} + \sum_{k=1}^{N} \hat{U}_{jk} h_{ik} \right) \right\},$$

(2.15)

which can be written in a matrix form as

$$H U - G Q = (H \hat{U} - G \hat{Q}) \alpha,$$

(2.16)

where $H$ and $G$ are matrices with their elements being $h_{ik}$ and $g_{ik}$ respectively and the coefficients $c_i$ have been incorporated into the principal diagonal elements of the matrix $H$ on both sides of the equation. $\hat{U}$ and $\hat{Q}$ in Equation (2.16) are matrices with the $j$th column being vectors $\hat{U}_j$ and $\hat{Q}_j$, respectively. Note that the coefficient $c_i$ can be determined either from Equation (2.13) according to the location of the source point, or it can also be determined from, as pointed out by Partridge and Brebbia [69],

$$c_i = -\sum h_{ij}, \quad i \neq j.$$  

(2.17)

If constant boundary elements are employed, $c_i$ is simply $1/2$.

After applying Equation (2.10) to each node $i$, one obtains

$$\frac{1}{k} [pU(x, p) - u_0(x, t_0)]_i = \sum_{j=1}^{N+L} f_{ij} \alpha_j,$$

(2.18)

in which the subscript $i$ on the left-hand side indicates that the terms within the bracket are being evaluated at node $i$, $f_{ij} = 1 + r_{ij}$, and $r_{ij}$ is the distance from node $i$ to node $j$. By writing Equation (2.18) in matrix form and inverting, one obtains

$$\alpha = F^{-1} \frac{1}{k} (pU - u_0).$$

(2.19)

After substituting Equation (2.19) into Equation (2.16), we obtain a system of simultaneous equations in matrix form as

$$H U - G Q = \frac{1}{k} S (pU - u_0),$$

(2.20)

where

$$S = (H \hat{U} - G \hat{Q}) F^{-1}.$$  

(2.21)
After rearranging terms in Equation (2.20), a final \((N + L) \times (N + L)\) linear system of equations
\[
\left( H - \frac{p}{k} S \right) U - GQ = -\frac{1}{k} Su_0,
\] (2.22)
is obtained. Upon imposing the appropriate boundary conditions, such a linear system can be readily solved.

### 2.1.3 Numerical Laplace inversion

After the solution for \(U(x, p)\) in the Laplace-transformed space is found numerically, the inverse of the Laplace transform is needed in order to obtain the solution for \(u(x, t)\) in the original physical domain. There are many Laplace inverse transform algorithms available in the literature. For example, Dubner and Abate [34], Durbin [35], Crump [25], Talbot [93] and many others all give reasonably good Laplace inverse transform algorithms. A comprehensive review has been provided by Davies and Martin [31], who compared 14 different methods by applying them to 16 different test functions. In terms of numerical accuracy, computational efficiency and ease of implementation, Davies and Martin showed that Stehfest’s algorithm [87] gives good accuracy on a fairly wide range of functions. Furthermore, Moridis and Reddell [57] and Cheng et al. [22] also reported successful utilisation of Stehfest’s algorithm, which was therefore also chosen for our numerical inversion.

As required by the algorithm, one needs to calculate a set of solutions in the Laplace-transformed space, corresponding to different values of parameter \(p\), in order to allow the solution in the physical domain to be accurately restored from such solutions in the Laplace-transformed domain. For any observation time \(t\) at which a solution is required, \(N_p\) discrete solutions need to be calculated in the Laplace-transformed space with the corresponding \(p\) values given as [87]
\[
p \nu = \frac{\ln 2}{t} \cdot \nu, \quad \nu = 1, 2, \ldots, N_p,
\] (2.23)
in which \(N_p\) must be taken as an even number. The system of linear equations in Equation (2.22) is now solved \(N_p\) times in the Laplace-transformed space, which
results in a set of $N_p$ vectors of the unknowns $U(p)$ and/or $Q(p)$. To obtain a solution for any interior point $\xi$ at any time $t$, a set of $U(\xi)$ is needed and can be evaluated from

$$c_\xi U(\xi) - \sum_{k=1}^{N} Q_k(p) g_{\xi k} + \sum_{k=1}^{N} U_k(p) h_{\xi k} = \sum_{j=1}^{N+L} \left\{ \alpha_j \left( c_\xi \hat{U}_j - \sum_{k=1}^{N} \hat{Q}_j g_{\xi k} + \sum_{k=1}^{N} \hat{U}_j h_{\xi k} \right) \right\}. \quad (2.24)$$

Now, the function value of $u$ at any interior point $\xi$ can be calculated by summing up $N_p$ values of $U(\xi)$ in the way suggested in the Stehfest's algorithm as follows:

$$u(\xi(t)) = \frac{\ln 2}{t} \sum_{\nu=1}^{N_p} W_\nu \cdot U(\xi(\nu)), \quad (2.25)$$

with weights $W_\nu$ being defined as

$$W_\nu = (-1)^{N_p + \nu} \sum_{\kappa=[\nu+1]^{\frac{N_p}{2}}}^{\min\{\nu, \frac{N_p}{2}\}} \frac{\kappa^{\frac{N_p}{2}} (2\kappa)!}{\kappa! (\kappa - 1)! (\nu - \kappa)! (2\kappa - \nu)!}. \quad (2.26)$$

According to Stehfest [87], such a weighted summation leads to a satisfactory numerical inversion of the Laplace transform.

However, there is a minor deficiency associated with the Stehfest's algorithm. It is due to the selection of the value of $N_p$ with which the algorithm yields best results. Generally, there is no means to determine, a priori, the optimum value of $N_p$. Theoretically speaking, the solution is expected to be more accurate with increasing $N_p$. However, roundoff errors practically worsen the results if $N_p$ becomes too large. After applying his algorithm to 50 test functions with the known inverse Laplace transforms, Stehfest suggested that the optimum value of $N_p$ be 10 for single precision variables (8 significant figures) and 18 for double precision variables (16 significant figures). However, our experience showed that no significant difference was noticed when using the algorithm for $N_p$ between 6 and 16, but large errors were observed when using $N_p > 16$. In fact, accurate solutions may even be obtained for $N_p$ as small as 6. Thus, the choice of the optimal value of $N_p$ depends on the user's experience. Even so, this minor deficiency is overshadowed by the fact that the algorithm is very simple to implement and
yields satisfactorily accurate results. In addition, $W_\nu$ in Equation (2.26) can be calculated once and stored in a data file for next access or can even be placed in the main program as a block of data.

It is also important to acknowledge that there is no particular method suitable for the numerical inversion of the Laplace transforms of all functions. It was shown that the numerical inversion is generally unstable for functions of time that are of spike or periodic type [8]. To overcome this instability, Cheng et al. [22] utilised the influence function based on the Duhamel principal of superposition. Herein we shall adopt a simpler technique.

First of all, we shall examine a numerical inversion of the Laplace transform of a function of the types described above. Particularly, we shall take the function $\sin t$ as an example. We know that the Laplace transform of this function is

$$L[\sin t] = \frac{1}{1 + p^2}. \quad (2.27)$$

Now, let us assume that we want to obtain the value of $\sin t$ at $t = 5$, say, from the solutions in the Laplace-transformed space via Stehfest's algorithm. What we need is 6 values calculated from the expression (2.27), corresponding to 6 values of $p$ given by Equation (2.23). The reason for using $N_p = 6$ will be apparent later on. Plugging these computed values in the inversion in Equation (2.25), we obtain the value for "$\sin 5$" as -0.16198 while the actual value of $\sin 5$ is -0.95892; an inaccuracy is evident.

Now, if the function $\sin t$ appears in the boundary conditions, the Laplace transform of these conditions would essentially take the form as Equation (2.27). Note that functions of spatial coordinates are immaterial to the Laplace transform with respect to time. So, if we want a solution at time $t = 5$ and therefore supplied the values from the boundary conditions according to Equation (2.27) to the problem, it means that we have supplied incorrect boundary values to the problem, and so caused instability.

It should be noticed that in fact the boundary values are known exactly in the time domain at that particular time, i.e., $t = 5$. Thus, it will be more accurate if we provide boundary values in the Laplace-transformed space according to
(\sin 5)/p rather than 1/(1 + p^2) when a solution at \( t = 5 \) is being sought. This is because the numerical inversion handles well the Laplace transform of a constant function. To confirm this, 6 values calculated from \((\sin 5)/p\) are inverted by Equation (2.25) and the returned approximation to \(\sin 5\) is accurate up to 13 significant digits. Therefore, it is recommended that the Laplace transform of the boundary conditions in Equations (2.8) and (2.9) be taken the form

\[
U(x, p) = \frac{\overline{u}(x, t)}{p}, \quad x \in \Gamma_1, \tag{2.28}
\]

\[
Q(x, p) = \frac{\partial U(x, p)}{\partial n(x)} = \frac{\overline{q}(x, t)}{p}, \quad x \in \Gamma_2. \tag{2.29}
\]

### 2.2 Numerical Examples and Discussions

In this section, five numerical examples of heat conduction problems, to which the analytical solutions are available, are used to test the accuracy and efficiency of the LTDRM. In order to measure the accuracy of numerical solutions, a relative error \( E \) defined as

\[
E = \left| \frac{u_a(t) - u(t)}{u(t)} \right| \times 100, \tag{2.30}
\]

is used for all the test examples. In Equation (2.30), \( u_a \) denotes an approximate solution at a particular time \( t \) and \( u \) denotes the corresponding analytical solution.

#### 2.2.1 Heat flow in a glass square

The first test example was used in Moridis and Reddell [57] to test their Laplace Transform Boundary Element (LTBE) method. It represents the flow of heat in a glass square of size \(- a < x < a, - b < y < b\) where \( a = b = 0.2 \text{ m} \) with a uniform initial temperature of unity. The boundary of the glass square was suddenly cooled down to zero temperature at \( t = 0 \text{ sec} \) and maintained at this temperature for all the subsequent time. The analytical solution for the temperature distribution of such a problem was given by Carslaw and Jaeger [15]
as

\[ u(x, y, t) = \frac{16}{\pi^2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} L_{n,m} \cos \left( \frac{(2n+1)\pi x}{2a} \right) \cos \left( \frac{(2m+1)\pi y}{2b} \right) e^{-D_{n,m}t}, \tag{2.31} \]

where

\[ L_{n,m} = \frac{(-1)^{n+m}}{(2n+1)(2m+1)}, \tag{2.32} \]

and

\[ D_{n,m} = \frac{k\pi^2}{4} \left[ \frac{(2n+1)^2}{a^2} + \frac{(2m+1)^2}{b^2} \right]. \tag{2.33} \]

The quantity \( k \) in Equation (2.33), which corresponds to the term \( k \) in Equation (2.1), is the thermal diffusivity of the substance. Here, the value \( k = 5.8 \times 10^{-7} \text{ m}^2/\text{sec} \), as used by Moridis and Reddell [57], is taken.

In applying the LTDRM to this problem, the boundary was discretised into 24 equal-size linear elements and 25 internal nodes were placed inside the glass square, i.e., \( N = 24 \) and \( L = 25 \), as shown in Figure 2.2. The temperature distribution along the direction of \( z \)-axis at \( y = 0.025 \text{ m} \) at \( t_{\text{obs}} = 9000 \text{ sec} \) is plotted in Figure 2.3. With \( N_p \) in the Stehfest's algorithm being taken to be as small as 6, an excellent performance of the LTDRM in terms of numerical accuracy is clearly demonstrated in Figure 2.3; the temperature distribution resulting from the analytical solution in Equation (2.31) and that from the numerical solution (LTDRM) agree remarkably well with each other. The maximum relative error between the two solutions is less than 2%.

Furthermore, one of the distinct features of this problem is that there exists a discontinuity between initial and boundary conditions (the initial condition is \( u = 1 \) whereas the boundary condition is \( u = 0 \)). Methods proposed for generally solving linear diffusion problems in time domain, such as those of Ingber and Phan-Thien [46] and Curran et al. [28], have difficulty in dealing with such a discontinuity when applied to this type of problems. On the other hand, there is no such problem with the present LTDRM.

As far as the numerical efficiency is concerned, Moridis and Reddell [57] compared the efficiency of their LTBE method with the BEM in a time domain and pointed out that the good results from the conventional BEM were obtained
Figure 2.2: The boundary and internal nodes placed on the glass square.
Figure 2.3: Comparison of the LTDRM solution with the analytical solution at 
$t = 9000$ sec.
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when 9000 timesteps were used. They concluded that their LTBE method, while yielding accurate results, reduces the computational time taken to obtain results by a factor of 1500 compared to the traditional BEM applied in a time domain. The same conclusion can also be made when comparing the LTDRM with the time-domain BEM. Although the LTDRM is not better than the LTBE method for this particular problem since a domain integral associated with the initial condition can be avoided, the efficiency of the LTDRM is usually higher than that of the LTBE method since no domain integration whatsoever is needed in the LTDRM.

Now, if the method described in [98], using the DRM with a finite-difference time integration, had been employed to solve this problem, the final matrix equation would have needed to be solved at each timestep. Although the actual calculation that takes place is a multiplication of the once-inverted coefficient matrix, which is time independent, with a known vector from the previous timestep, the attempt of solving the problem in a time domain could still be time consuming when the unknown function values at a large observation time are needed. This is due to the fact that the timestep size cannot be chosen too large and the operational numbers for the multiplication of the once-inverted coefficient matrix with the known vector are amplified proportionally to the total number of timesteps. Furthermore, large numerical errors could be accumulated if the solution within a large range of time is required. In contrast, the LTDRM takes only one timestep to obtain the required solution and no error is accumulated. Thus, the advantage of the LTDRM over this time-domain method is clearly seen.

The efficiency and accuracy of the LTDRM also rely very much on the number of solutions, i.e., the value of $N_p$, needed in the Laplace-transformed domain. For the efficiency, it is obvious that the less the value of $N_p$ the more efficient the LTDRM. On the other hand, the effect of $N_p$ on the accuracy of the LTDRM is demonstrated by comparing the differences between analytical and numerical solutions corresponding to four different values of $N_p$. Such differences are shown in Figure 2.4. As can be seen from this figure, the difference between the an-
Figure 2.4: Effect of $N_p$ on the accuracy of the LTDRM for heat flow problem.
alytical and numerical solutions for $N_p$ being 6 is generally smaller than those corresponding to other values of $N_p$. Such a reduction of accuracy as $N_p$ becomes large is expected since roundoff errors are accumulated as too many terms are included in a calculation [87]. However, with the maximum of these differences less than 0.025, we can conclude that the accuracy of the LTDRM for this two-dimensional problem is practically insensitive to the value of $N_p$. As a matter of fact, the difference between analytical and LTDRM solutions is negligible for $N_p$ ranging between 6 and 16. In addition, the fact that the minimum difference was reached when $N_p = 6$ and increased for $N_p > 6$ led us to believe that a sufficiently accurate solution may be obtained by summing up only 6 terms in the algorithm given in Equation (2.25). This number is much smaller than $N_p = 18$ suggested by Stehfest [87] for double precision variables. Thus, summing up only 6 solutions in lieu of 18 solutions certainly leads to a considerable saving in CPU time and makes the LTDRM even more efficient than anticipated.

We have also solved this problem by the LTDRM with the boundary of the computational domain being discretised using constant elements. Solution obtained from using linear boundary elements is plotted in Figure 2.5 together with that obtained from using constant boundary elements. It can be observed from the figure that there is very little difference between the two solutions. Due to the simplicity of adopting constant elements, the results of this comparison led us to believe that using constant boundary elements in conjunction with the LTDRM is sufficient in carrying out the calculation for the rest of numerical examples.

2.2.2 Heat transfer in a circular cylinder

This example involves transient heat transfer in a circular cylinder of radius 1.0 m with a zero initial temperature and a uniform heat flux 1.0 K/m being suddenly applied. The analytical solution to the problem was provided by Carslaw and
Figure 2.5: Comparison of the LTDRM solutions using constant and linear boundary elements.
Jaeger [15] as

\[
    u(r, t) = 2kt + \frac{r^2}{2} - \frac{1}{4} - 2 \sum_{s=0}^{\infty} e^{-k\alpha_s^2t} \frac{J_0(\alpha_s r)}{\alpha_s^2 J_0(\alpha_s)},
\]

(2.34)

where \( k \) is the thermal diffusivity taken to be 1.0 m\(^2\)/sec, \( \alpha_s \) are the positive roots of

\[
    J_1(\alpha) = 0,
\]

(2.35)

and \( J_0 \) and \( J_1 \) are the Bessel functions of orders zero and one, respectively.

In this example, the boundary was evenly discretised, as shown in Figure 2.6, into 24 constant elements and 16, 12, 8, 4 and 1 internal nodes were placed on five circles with radii 0.85, 0.5, 0.3, 0.1 and 0, respectively. Such a discretisation results in a total of 24 boundary nodes (\( N = 24 \)) and 41 internal nodes (\( L = 41 \)). Figure 2.7 shows the time history of the temperature on the surface of the cylinder (\( r = 1 \)) computed by the LTDRM and the analytical solution plotted with a solid line. Once again, one can see an excellent agreement between the two solutions with a maximum relative error \( E \) less than 1%. The results shown in Figure 2.7 also demonstrate that solutions at small as well as large time can be obtained with the same level of accuracy.

### 2.2.3 A problem with time-dependent boundary conditions

Since the first two examples involve either a Dirichlet (example 1) or a Neumann (example 2) boundary condition, we have also artificially constructed a problem with a mixed boundary condition for the testing of the LTDRM. In addition, we wish to see how our LTDRM can deal with more complex boundary conditions, such as the time-dependent boundary conditions which are deliberately included in the current test example.

The problem chosen can be described as heat flow in a unit square with the analytical solution being set as

\[
    u(x, y, t) = \frac{4}{\pi^2} \sin(\frac{\pi x}{2}) \sin(\frac{\pi y}{2}) e^{-\frac{\pi^2 kt}{4}}.
\]

(2.36)
Figure 2.6: The boundary and internal nodes placed on the cylinder.
Figure 2.7: Time history of the temperature on the surface of the cylinder.
The Dirichlet (essential) boundary conditions are prescribed, according to the function values of Equation (2.36), on the boundaries $x = 0$ and $y = 0$ of the square while the Neumann (natural) boundary conditions are prescribed, according to the normal derivatives of the function values in Equation (2.36), on the boundaries $x = 1$ and $y = 1$. The boundaries were equally discretised into 24 constant elements and 25 internal nodes were uniformly placed inside the domain, as shown in Figure 2.8.

The problem was solved with the thermal diffusivity $k = 5.8 \times 10^{-7} \text{ m}^2/\text{sec}$ being used and a single observation time $t_{\text{obs}} = 9000 \text{ sec}$ was made. The temperature profile along the direction of $x$-axis at a cross-section $y = 0.3 \text{ m}$ at this instant was output and plotted in Figure 2.9, from which one can clearly see a good match between numerical and analytical solutions. With the maximum relative error $E$ being less than $2\%$ once again, the excellent performance of the LTDRM for calculating the solution at a large time is confirmed.

### 2.2.4 An exterior problem

In this example, a transient heat transfer problem defined on an exterior infinite domain is solved by the LTDRM. This problem is described on an infinite isotropic medium with a unit circular cavity. The initial temperature is assumed to be zero everywhere and a uniform heat flux (1.0 K/cm) is suddenly applied to the boundary of the cavity. Both Loeffler and Mansur [50] and Zhu and Zhang [106] solved this problem with the DRM in the time domain, for the temperature distribution in the medium at a sequence of time levels. They all compared their solutions with the analytical solution provided by Carslaw and Jaeger [15] with the thermal diffusivity being taken as $k = 1.0 \text{ cm}^2/\text{sec}$.

To solve this problem by the LTDRM, we follow Zhu and Zhang's approach, from which this exterior problem is transformed into an equivalent interior problem using a coordinate transformation $R = 1/r$ and $\Theta = \theta$. By applying the LTDRM to the transformed problem, Equation (2.22) in the previous section...
Figure 2.8: The boundary and internal nodes placed on the square.
Figure 2.9: Comparison of the LTDRM solution with the analytical solution at $t = 9000$ sec.
now becomes
\[(HR - pSW)U = G\dot{Q} - SKu_0,\] (2.37)

where
\[W = \left( K + F_1 \frac{\partial F}{\partial x} F^{-1} + F_2 \frac{\partial F}{\partial y} F^{-1} + F_3 \right),\] (2.38)
in which \(K, R, F_1, F_2, F_3\) are diagonal matrices containing values of \(1/k, R^4, 8R^2\eta, 8R^2\xi, 16R^2\), respectively, where \(\eta\) and \(\xi\) are cartesian coordinates corresponding to polar coordinates \(R\) and \(\Theta\). The vector \(\dot{Q}\), in Equation (2.37), can be written in terms of the values of the vector \(U\) which lie on the boundary, i.e., \(\dot{U}\), and its normal derivative \(Q\) as
\[\dot{Q} = 4\dot{U} + Q,\] (2.39)
in which each component of \(Q\) is \(1/p\). After some rearrangement, Equation (2.37) is solved for the unknown temperatures on the boundary and at the interior points.

After Zhu and Zhang's mapping, the domain of interest now becomes a unit disc. In order to compare our results with those obtained by previous investigators, we employed the same discretisation, i.e., the boundary was evenly discretised into 8 linear elements and 73 internal nodes were evenly placed on ten circles with radii \(0(0.1)0.9\), as shown in Figure 2.10. Due to the symmetry of the problem, only the variation of the temperature versus time at a point on the boundary of the cavity needs to be compared with the other solutions. In Figure 2.11, Carslaw and Jaeger's analytical solution, Loeffler and Mansur's solution with the optimal \(c\) value \((c \approx 70)\), Zhu and Zhang's solution with a special transformation and our new LTDRM solution are all plotted and compared. One can clearly see that the LTDRM solution has an excellent agreement with the analytical solution. With the maximum relative error between the LTDRM and analytical solutions being less than 1.3\%, the accuracy of the LTDRM is well demonstrated. Furthermore, it is quite interesting to have observed that the LTDRM yields more accurate results at small observation time than the time-domain methods \([50, 106]\). As far as numerical efficiency is concerned, the LTDRM is certainly superior to the
Figure 2.10: The boundary and internal nodes placed on a unit disc.
Figure 2.11: Comparison between the LTDRM, analytical and other two numerical solutions.
others since there is no need to march through the solution step by step. Thus, a great amount of CPU time can be saved, especially when solutions at large time are required.

### 2.2.5 A problem with the inclusion of source terms

In the last example, a Dirichlet problem is studied with a source term being included in the governing equation. The problem under consideration is governed by the equation

\[ \nabla^2 u = \frac{\partial u}{\partial t} - 2u - \sin x \sin y \cos t, \]  

(2.40)
on a unit square. The analytical solution to this problem is

\[ u(x, y, t) = \sin x \sin y \sin t. \]  

(2.41)

Application of the Laplace transform followed by the DRM yields the final matrix equation that needs to be solved, which is of the form

\[ (H - (p - 2)S)U - GQ = -S(u_0 + g), \]  

(2.42)

where \( g \) is a vector containing nodal values of the Laplace transform of the function \( \sin x \sin y \cos t \).

To discretise the square, 32 equal-size constant elements were placed on the boundary and 16 internal nodes were uniformly distributed inside the square. The numerical solutions obtained at three different time levels are compared with the analytical solution given in Equation (2.41), and the relative errors are graphically presented in Figure 2.12. From this figure, it is clear that the numerical solutions are very accurate with a maximum relative error of 0.15%. Moreover, Figure 2.12 also shows that solutions at different time levels can be obtained with the same level of accuracy and efficiency. As for the convergence of the numerical solution to the analytical one, the results shown in Figure 2.13, with 16 and 25 internal nodes being used, demonstrate convergence as the error is reduced with the increasing number of internal nodes.
Figure 2.12: Relative errors between the LTDRM and analytical solutions at three different time levels.
Figure 2.13: Relative errors between the LTDRM and analytical solutions at $t = 1000$ with different numbers of internal nodes being used.
2.3 Conclusions

In this chapter, the dual reciprocity method is applied in the Laplace-transformed domain to solve linear time-dependent diffusion equations. Five examples are analysed using the Laplace transform dual reciprocity method. The first and third problems are used to demonstrate the numerical efficiency and accuracy of the method when it is applied to find the solution at large time, whereas the second and fourth examples are mainly used to show that the solutions at small observation time can also be obtained with an equal efficiency and accuracy as those obtained at large time. In the fifth example, we have included the terms such as sources or sinks that give rise to domain integrals which cannot be avoided when using the traditional BEM, but can be well taken care of by the LTDRM. Through the presented numerical test examples, the accuracy and efficiency of the Laplace transform dual reciprocity method are well demonstrated.

From the computational point of view, the proposed scheme is not only more efficient than existing methods (especially in dealing with arbitrary initial conditions) but also easier to implement. From the accuracy point of view, a high level of accuracy is reached from this formulation and no error is accumulated. From the efficiency point of view, execution time is virtually reduced by several orders of magnitude since only calculations at the desired observation time are needed; this is especially true for the cases where the unknown function values at a large observation time need to be calculated. When comparing with the LTBE method, which applies the traditional BEM in the Laplace-transformed space, the LTDRM is still more efficient because no domain discretisation or integration is required; further savings not only on computer operating cost but also in data preparation have been achieved. As far as the data storage is concerned, 6 LTDRM solutions are required in the Laplace-transformed space for a single timestep. Such a disadvantage is however compensated by the fact that the LTDRM allows unlimited timestep size with no increase in computer storage and execution time.

As far as the numerical inversion of the Laplace transform is concerned, Ste-
hfest's algorithm utilised in the present study is found to be quite satisfactory in terms of its efficiency, accuracy and simplicity in implementation. It is also found from our examples that $N_p = 6$ is generally sufficient to accurately bring solutions in the Laplace-transformed domain back to the actual time domain. This number is the same as that reported by Moridis and Reddell [57] and Cheng et al. [22], but far smaller than $N_p = 18$ suggested in the Stehfest's original paper [87]. Such a reduction of the total number of solutions needed in the Laplace-transformed domain for a particular time makes the LTDRM even more efficient than expected and thereby more attractive.
Chapter 3

Diffusion Problems with Nonlinear Source Terms

In the previous chapter, the Laplace Transform Dual Reciprocity Method (LT-DRM) has been successfully applied to solve linear transient diffusion problems. In this chapter, the transient diffusion equations with nonlinear source terms are first chosen for the extension of the LTDRM to the nonlinear regime, not only because they are simple, but also because they are important as they appear as modelling equations of problems in many different fields of mathematical physics, applied science and engineering. Many technological and environmental processes such as microwave heating process [107], spontaneous ignition [71] and mass transport in groundwater [88] can be modelled by this type of equations.

However, the extension of the LTDRM to the nonlinear regime is far from trivial. First of all, a successful performance of the Laplace transform is crucial for the method to be applied. It is well known that the Laplace transform can be only applied to linear governing equations. Therefore, to cleverly construct a linearisation of the governing equations and an iterative process is a challenge and the key to the success of the extension of the LTDRM to nonlinear cases.

Two linearisation techniques are adopted, and their compatibility with the Laplace transform is investigated for the one-dimensional transient diffusion problems first. A linearisation scheme adopted is deemed to be successful if the solu-
tion of the linearised differential system, which is numerically converted from the solutions obtained from solving the linearised system in the Laplace-transformed domain, approaches the true solution of the original nonlinear differential system after a number of iterations. Through the tests conducted for the one-dimensional transient diffusion problems, the convergence rate of these two techniques are found to be quite satisfactory.

Two LTDRM formulations based on these two linearisation techniques for two-dimensional transient diffusion problems are then formulated and applied to solve some practical nonlinear transient problems involving microwave heating and spontaneous ignition. A comparison between these two formulations is also provided.

### 3.1 Nonlinear Governing Differential Equation and Its Linearisation

We consider first a nonlinear time-dependent diffusion problem in which nonlinearity arises from nonlinear source terms. The governing differential equation for this kind of problems is generally a diffusion-reaction equation of the form

\[
\nabla^2 u = a \frac{\partial u}{\partial t} - \beta g(u), \tag{3.1}
\]

in which \( a \) and \( \beta \) are given constants and \( g \) is a nonlinear function of \( u \). For heat conduction problems, \( a \) is interpreted as a reciprocal of the thermal diffusivity. The boundary conditions of the problems considered are assumed to be of the form

\[
\begin{align*}
  u &= \bar{u}, & \text{on } \Gamma_1, \\
  q &= \frac{\partial u}{\partial n} &= \bar{q}, & \text{on } \Gamma_2,
\end{align*}
\tag{3.2, 3.3}
\]

and the initial condition is of the form

\[
u = u_0, \tag{3.4}\]
where \( q \) is the flux; \( n \) is the unit outward normal; \( \bar{u}, \bar{q} \) are given functions; \( u_0 \) is a known function at the initial time \( t_0 \); and \( \Gamma_1 \cup \Gamma_2 \) is the boundary of the domain under consideration.

In the initial attempt to extend the LTDRM to the solution of the differential system (3.1) – (3.4), a great deal of difficulty was encountered with the nonlinearity appearing in the governing equation. It is well known that constructing some sort of linearisation and then performing suitable iterations are unavoidable in dealing with a nonlinear differential system. The success of extending the LTDRM to nonlinear cases therefore relies on the construction of an iteration scheme such that not only can the advantage of solving the problem in the Laplace-transformed space be kept intact, but also the nonlinearity can be dealt with efficiently. We realised that the ability to determine the solution at a particular observation time, especially at a large time, is a great advantage of the LTDRM. Thus, we naturally adopted the linearisation schemes presented below.

### 3.1.1 Linearisation schemes

#### A direct iteration scheme

If the solution of the unknown function is to be sought at a particular time, say \( t_1 \), a simple linearisation of Equation (3.1) can be of the form

\[
\nabla^2 u = a \frac{\partial u}{\partial t} - \beta \tilde{g}(\tilde{u}) u,
\]

in which \( \tilde{u} \) is the solution from the previous iteration.

#### A Taylor series expansion scheme

A more systematic linearisation scheme is based on the Taylor series expansion. This technique was used, for example, by Chen and Lin [20] in solving one-dimensional transient problems with nonlinear material properties and by Ramachandran [75] in solving one-dimensional nonlinear diffusion-reaction problems. Based on this approach, if the solution of the unknown function at a particular time, say \( t_1 \), is to be sought, the nonlinear source term can be linearised
by a first-order Taylor series expansion as

\[ g(u) = g_1(\tilde{u}) + g_2(\tilde{u})u, \]  

where

\[ g_1(\tilde{u}) = g(\tilde{u}) - \tilde{u} \left[ \frac{dg(u)}{du} \right]_{u=\tilde{u}}, \]

\[ g_2(\tilde{u}) = \left[ \frac{dg(u)}{du} \right]_{u=\tilde{u}}, \]

and thus Equation (3.1) can be written as

\[ \nabla^2 u = a \frac{\partial u}{\partial t} - \beta g_1(\tilde{u}) - \beta g_2(\tilde{u})u. \]  

3.1.2 Convergence tests

It should be noted that an important criterion for judging the success of a linearisation to a nonlinear equation is the convergence of the linearised system; the solution of the linearised system should approach the true solution of the original nonlinear system after several iterations. Thus, it is a necessary step to test our linearisation schemes on a simplified version of Equation (3.1) whose analytical solution can be found. A natural simplification without altering the type of the equations is to consider a one-dimensional problem with the Laplacian operator in Equation (3.1) being replaced by the second-order derivative in one spatial direction, say \( x \)-direction.

Ideally, it would be desirable to establish the convergence character of the linearisation schemes in Equations (3.5) and (3.9) for an arbitrary function \( g \) before they are adopted for transient two-dimensional diffusion problems. However, as there are only a few special forms of \( g \) for which nonlinear diffusion equations, even in one-dimension, have exact solutions available, such kind of tests seem to be almost impossible. Therefore, only two test cases are presented here.

**Test case 1**

The first test example considers the one-dimensional nonlinear diffusion equation

\[ \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} - u(1 - u)(u - \gamma), \]  

(3.10)
Chapter 3: Diffusion problems with nonlinear source terms

in which nonlinear source term is dependent on the temperature. Its exact solution is given by Satsuma [77] as

\[ u = \frac{e^{\eta_1} + \gamma e^{\eta_2}}{1 + e^{\eta_1} + e^{\eta_2}}, \tag{3.11} \]

where

\[ \eta_1 = \frac{1}{\sqrt{2}}[x - (\sqrt{2}\gamma - \frac{1}{\sqrt{2}})t], \tag{3.12} \]

\[ \eta_2 = \frac{\gamma}{\sqrt{2}}[x - (\sqrt{2} - \frac{\gamma}{\sqrt{2}})t]. \tag{3.13} \]

Using the linearisation described in Equation (3.5), we obtain a linearised version of Equation (3.10) as

\[ \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} + \{\gamma - (\gamma + 1)\dot{u} + \ddot{u}\}u. \tag{3.14} \]

After applying the Laplace transform with respect to \( t \), Equation (3.14) is reduced to an ordinary differential equation. However, the transformed equation still cannot be solved analytically. It is therefore solved numerically with the finite difference method in the Laplace-transformed space. The solution in the time domain is then obtained via a numerical inversion of the Laplace transform based on the algorithm proposed by Stehfest [87]. The solution for the unknown function \( u \) at the time level \( t_1 \) is obtained once the difference between two successive iterated solutions is sufficiently small.

The exact values of \( u \) between the interval \([0, 1]\) with \( \gamma \) being set to 3 are plotted in Figures 3.1(a–c). Using the essential boundary and initial conditions generated from Equation (3.11) by setting \( x = 0, 1 \) and \( t = 0 \) respectively, Equation (3.14) can be solved and iterated. The results obtained after 3, 8 and 12 iterations respectively at time \( t = 0.1, 1 \) and 5 are shown in Figures 3.1(a–c) as well for the comparison purpose. As can be seen, a reasonable agreement is found for a very small time level; there is only about 3% maximum relative error at \( t = 0.1 \). On the other hand, the maximum relative error is remarkably reduced as the time became larger. At \( t = 5 \), it is even less than 0.1%, which resulted in a perfect match between the exact solution of the original nonlinear equation and that of the corresponding linearised equation (3.14), as shown in Figure 3.1(c).
Now, if the Taylor series expansion scheme is adopted, Equation (3.10) is linearised as

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} + \{\gamma - 2(\gamma + 1)\bar{u} + 3\bar{u}^2\}u + \{(\gamma + 1)\bar{u}^2 - 2\bar{u}^3\}. \quad (3.15)$$

The solutions obtained from Equation (3.15) are also shown in Figures 3.1(a–c). The results at time $t = 0.1, 1$ and $5$ were obtained respectively after 2, 4 and 4 iterations; the convergence rate of the Taylor series expansion scheme is faster than that of the direct iteration scheme. It is seen from Figures 3.1(a–c) that numerical solutions from linearised equation (3.15) agree well with analytical solution from the original nonlinear equation (3.10). In addition, the maximum relative error of 2% is found at $t = 0.1$ and it is reduced to 0.001% at $t = 5$.

Another important task is to always make sure that the contribution from the nonlinear terms is significant, so that any doubt of such an excellent match between the two solutions at large time being attributed to the relative unimportance of the nonlinear terms cannot be cast at all. We have therefore dropped the nonlinear source terms in Equation (3.10) and solved the equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} + \gamma u, \quad (3.16)$$

subject to the same boundary and initial conditions generated for Equation (3.14). The numerical results are also depicted in Figures 3.1(a–c) with dots. Clearly, a maximum 32% of large difference between the solution of Equation (3.16) and the exact solution of Equation (3.10) is quite convincing in showing that the nonlinear terms do indeed play an important role in the governing equation and their effects have been correctly accounted for by the linearisations suggested in Equations (3.5) and (3.9).

**Test case 2**

The one-dimensional nonlinear diffusion equation considered in this example is of the form

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} - \alpha u \frac{\partial u}{\partial x} - \beta u(1 - u), \quad (3.17)$$
Figure 3.1: (a) Comparison of solutions at $t = 0.1$. 
Figure 3.1: (b) Comparison of solutions at $t = 1$. 
Figure 3.1: (c) Comparison of solutions at $t = 5$. 
and its exact solution is given by Satsuma [77] as
\[ u = \frac{1}{2} + \frac{1}{2} \tanh \frac{\alpha}{4} \left\{ x + \frac{1}{2} \left( \alpha + \frac{4\beta}{\alpha} \right) t \right\}. \] (3.18)

A distinguished feature of this equation is that not only does it have a nonlinear source term, but it also has a nonlinear convection term. In this case, both of these terms can be regarded as an integrated heat source term; the generation of heat then depends not only on the temperature but also on the gradient of the temperature. The values of \( \alpha \) and \( \beta \) for this problem are taken to be 1 and 3, respectively.

Using the direct iteration scheme, Equation (3.17) is linearised as
\[ \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} - \alpha \frac{\partial u}{\partial x} - \beta \hat{u}(1 - u). \] (3.19)

On the other hand, to use the Taylor series expansion scheme we need to rewrite the nonlinear convection term as
\[ \frac{\partial u}{\partial x} = \frac{1}{2} \frac{\partial u^2}{\partial x}. \] (3.20)

The term \( u^2 \) is nonlinear and is linearised as
\[ u^2 = 2\tilde{u}u - \tilde{u}^2. \] (3.21)

Thus, Equation (3.17) is linearised by the Taylor series expansion scheme in the form
\[ \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} - \alpha \frac{\partial u}{\partial x} - \beta (1 - 2\tilde{u})u + \beta \tilde{u}^2. \] (3.22)

After implementing similar procedure as that described in the previous test case, the convergence of the linearised equations was found to be excellent; for large time, the relative errors were all less than 0.1% while the relative errors were a little larger for extremely smaller time with a maximum relative error of 4%. These results are clearly demonstrated in Figure 3.2(a–c).

Again, to check the contribution of nonlinear terms towards the solution of diffusion equation (3.17), the nonlinear terms are dropped and the linear equation
\[ \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} - \beta u, \] (3.23)
Figure 3.2: (a) Comparison between relative errors of three solutions at $t = 0.1$. 

- **Differentiation with nonlinear source terms**
- Linear equation (3.23)
- Direct iteration
- Taylor series

![Graph showing relative errors comparison](image)
Figure 3.2: (b) Comparison between relative errors of three solutions at $t = 1$. 
Figure 3.2: (c) Comparison between relative errors of three solutions at \( t = 3 \).
is solved. The relative errors of the numerical solution obtained from solving this equation compared with the exact solution of Equation (3.17) are also plotted in Figure 3.2(a–c). Once again, the huge error (over 50%) confirms that the nonlinear terms are important and cannot be neglected, and the effects from these nonlinear terms have been efficiently dealt with by the adopted linearisation schemes.

From the results of these convergence test cases, it is believed that, by using the linearisation schemes adopted herein, solution of the linearised differential system converges to the true solution of the original nonlinear system.

### 3.2 The LTDRM Formulations

Having succeeded in establishing a linearisation of the governing equation, we now derive LTDRM formulations applied to the two-dimensional diffusion equations with nonlinear source terms.

If the direct iteration scheme is utilised, Equation (3.5) is then Laplace transformed with respect to \( t \) into

\[
\nabla^2 U = \{ap - \beta \hat{g}(\hat{u})\} U - au_0,
\]

which is subject to the boundary conditions

\[
U = \frac{\hat{u}}{p}, \quad \text{on } \Gamma_1,
\]

\[
Q = \frac{\partial U}{\partial n} = \frac{\hat{q}}{p}, \quad \text{on } \Gamma_2,
\]

where \( p \) is the Laplace parameter, and \( U \) and \( Q \) are the Laplace transforms of \( u \) and \( q \) respectively.

Following the procedure described in Chapter 2, after the DRM is applied to Equation (3.24), we have the final matrix equation of the form

\[
HU - GQ = S \left[ \{ap - \beta \hat{g}(\hat{u})\} U - au_0 \right],
\]
where the subscript $i$ denotes nodal value and all the matrices have already been defined in the previous chapter. By defining a diagonal matrix $T$ by

$$T_{i,i} = [ap - \beta \tilde{g}(\tilde{u})]_i,$$  \hspace{1cm} (3.28)

and a vector $d$ by

$$d_i = [au_0]_i,$$  \hspace{1cm} (3.29)

Equation (3.27) can be written in the form

$$(H - ST)U = GQ - Sd.$$  \hspace{1cm} (3.30)

On the other hand, if the Taylor series expansion scheme is employed, upon performing the Laplace transformation with respect to $t$, Equation (3.9) becomes

$$\nabla^2 U = \{ap - \beta g_2(\tilde{u})\}U - \left\{ au_0 + \frac{\beta}{p} g_1(\tilde{u}) \right\}.$$  \hspace{1cm} (3.31)

Then, after applying the DRM in the Laplace-transformed space, the matrix equation

$$HU - GQ = S \left[\{ap - \beta g_2(\tilde{u})\}U - \left\{ au_0 + \frac{\beta}{p} g_1(\tilde{u}) \right\}\right]_i,$$  \hspace{1cm} (3.32)

is obtained, and the final matrix equation thus takes the same form as that in Equation (3.30), i.e.,

$$(H - ST)U = GQ - Sd,$$  \hspace{1cm} (3.33)

with diagonal entries of $T$ now being the nodal values of $ap - \beta g_2(\tilde{u})$ and entries of $d$ being the nodal values of $au_0 + \frac{\beta}{p} g_1(\tilde{u})$.

The linear systems of equations (3.30) and (3.33) can now be solved subject to the imposed boundary conditions and the numerical solution in the time domain is obtained via the Stehfest’s algorithm.

For brevity, the formulation based on the direct iteration scheme will be called \textbf{LTDRM-D} hereafter and the formulation based on the Taylor series expansion approach will be referred to as \textbf{LTDRM-T}.
3.3 Numerical Examples and Discussions

In all of our numerical experiments, the iteration was performed in such a way that whenever a new solution \( u \) was obtained, a stopping criteria

\[
\frac{\bar{u} - u}{\bar{u} + u} < \varepsilon,
\]

with which the accuracy of the final solution is controlled by a pre-set small number \( \varepsilon \), was checked at all nodes. If Equation (3.34) was not satisfied, the value of \( \bar{u} \) at every node was replaced by the corresponding new value of \( u \). The iterative process then proceeded until Equation (3.34) was satisfied. With an appropriate initial guess for the iteration to start with (the initial conditions were usually selected), the iteration converged very quickly.

One should notice that iterations needed in the solution procedure are quite efficient in the sense that the systems in Equations (3.30) and (3.33) are linear and most importantly, the matrix \( T \) is the only one that needs to be updated after each iteration is completed. With this excellent property, not only can the storage space be reduced (mainly due to the DRM in the Laplace-transformed space), but also a large amount of computational time, which would otherwise be required to update other matrices, can be saved.

To illustrate the LTDRM described in the previous section and demonstrate its accuracy and efficiency, we shall, in this section, present several numerical examples of nonlinear transient heat conduction problems including the microwave heating of a square slab and the spontaneous ignition of a unit circular cylinder. Two steady-state problems, whose analytical solutions are available, shall also be examined.

3.3.1 Microwave heating of a square slab

As the first example, we adopt a problem studied by Zhu et al. [107], i.e., the heating of a square slab using microwave energy. Microwave heating can be
modelled by the forced heat equation
\[ \nabla^2 u = \frac{\partial u}{\partial t} - \eta(u)|E|^2, \] (3.35)
which governs the absorption and diffusion of heat, and Maxwell’s equations, which govern the propagation and decay of the microwave radiation through the material. In Equation (3.35), \( \eta(u) \) is the thermal absorptivity, \( |E| \) is the amplitude of the electric field, and a constant thermal diffusivity has been assumed and normalised to unity. In general, Equation (3.35) and Maxwell’s equations are nonlinearly coupled due to the temperature dependence of material properties such as the electric conductivity, magnetic permeability, and electric permeability. However, if these material properties are assumed constant [43, 53], the amplitude of the electric field is exponentially dependent on the spatial variables, say,
\[ |E| = e^{-\frac{x}{\gamma}}, \] (3.36)
for a decay from an incident boundary at \( x = 0 \), where \( \gamma \) is the decay constant, and thus Equation (3.35) is uncoupled from Maxwell’s equations, leading to a simplified model equation
\[ \nabla^2 u = \frac{\partial u}{\partial t} - \eta(u)e^{-\gamma x}. \] (3.37)

Since many materials used in industry have the rate at which the microwave energy is absorbed, i.e., the thermal absorptivity, increasing with temperature by the power law [42], Equation (3.37) becomes
\[ \nabla^2 u = \frac{\partial u}{\partial t} - \beta e^{-\gamma x}u^n, \] (3.38)
which was used as a model equation describing the microwave heating of a square slab by Zhu et al. [107]. The boundary and initial conditions in [107] were given respectively as
\[ u = 1, \quad \text{on } x = 0, 1 \text{ and } y = 0, 1, \] (3.39)
\[ u = 1, \quad \text{at } t = 0. \] (3.40)
Herein we shall consider nonlinear cases, especially when \( n = 2 \) and 3, for which Zhu et al. [107] used the coupled DRM and a finite difference scheme in the time domain to obtain their numerical solutions. We ran our model with the same power \( n \) and compared our results with theirs.

To implement the LTDRM, we first need to linearise Equation (3.38) and obtain

\[
\nabla^2 u = \frac{\partial u}{\partial t} - \beta \gamma e^{-\gamma \tau} \tilde{u}^{n-1} u,
\]

(3.41)

and

\[
\nabla^2 u = \frac{\partial u}{\partial t} - \beta \gamma (1 - n) \tilde{u}^n - n \beta \gamma e^{-\gamma \tau} \tilde{u}^{n-1} u,
\]

(3.42)

to which the LTDRM-D and LTDRM-T can now be applied, respectively.

The discretisation adopted here is similar to that used in [107]; 40 constant elements were placed on the boundary and 36 internal nodes were uniformly placed inside of the slab. Linear boundary elements were also employed. However, no noticeable difference in the results was found and therefore we shall only present the results obtained with constant elements here. The tolerance for stopping the iterations, \( \varepsilon \), was chosen to be \( 1.0 \times 10^{-3} \), and the initial condition was always

---

Table 3.1: Absolute differences between LTDRM and DRM solutions for temperature on the slab for the case \( n = 2 \): (a) \( \beta = 4.7, \gamma = 0 \) and \( t = 1.7 \); (b) \( \beta = 11, \gamma = 2 \) and \( t = 1.6 \); (c) \( \beta = 21, \gamma = 4 \) and \( t = 2.1 \)

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>LTDRM-D</th>
<th>LTDRM-T</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>a</td>
<td>b</td>
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<tr>
<td>0.1428</td>
<td>0.8571</td>
<td>0.000</td>
<td>0.002</td>
</tr>
<tr>
<td>0.2857</td>
<td>0.7142</td>
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<tr>
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<td>0.8571</td>
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<tr>
<td>0.4285</td>
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</table>
used as the first iteration. Numerical solutions of the temperature distribution in the slab were calculated using the LTDRM-D and LTDRM-T for three different sets of values of $\beta$, $\gamma$ and $t$. For comparison purposes, the absolute differences between the LTDRM solutions and the corresponding values obtained by the method coupling the DRM with a finite difference scheme in the time domain [107], at some selected points on the slab, are tabulated in Tables 3.1 and 3.2, for the cases $n = 2$ and $n = 3$, respectively.

It is evident from these tables that the agreement between the solutions obtained from LTDRM and DRM are remarkable. Additionally, the results from both LTDRM-D and LTDRM-T are found to be almost exactly the same, but results from the LTDRM-D seem to be in a better agreement with those from the DRM. However, while the number of iterations needed to find converged solutions using the LTDRM-D is of an average of 16 steps for the cases shown in Tables 3.1 and 3.2, convergent solutions for the LTDRM-T were attained within an average of 5 iterations, thus showing the higher efficiency of the LTDRM-T over the LTDRM-D.

Furthermore, results shown in Tables 3.1 and 3.2 are very encouraging as they
Table 3.3: Estimates of the critical values $\beta_c$ for the case $n = 2$

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>F-K</th>
<th>DRM</th>
<th>LTDRM-D</th>
<th>LTDRM-T</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.9</td>
<td>4.7</td>
<td>4.79</td>
<td>4.78</td>
</tr>
<tr>
<td>2</td>
<td>11.4</td>
<td>11</td>
<td>11.28</td>
<td>11.27</td>
</tr>
<tr>
<td>4</td>
<td>20.1</td>
<td>21</td>
<td>21.11</td>
<td>21.09</td>
</tr>
</tbody>
</table>

show that the proposed iteration schemes work with the problems containing weak as well as strong nonlinearities. It should be noted that if there is no nonlinear source term, the Equation (3.38) reduces to the well-known heat equation and the solution is simply $u = 1$ subject to the boundary and initial conditions described in Equations (3.39) – (3.40). It is because of the source term that a temperature higher than 1 can be obtained, as can be seen in Figures 3.3(a–c). Undoubtedly, the nonlinear source term plays an important role, which cannot be ignored.

Another interesting aspect of studying this microwave heating problem is due to the occurrence of the so-called “hotspots”, which are the localised areas of high temperature that develop as the material is being irradiated [107]. Hotspots can be used to quicken a process such as smelting or can damage samples in heating processes such as sintering ceramics. Therefore, a correct prediction of hotspot occurrence is important in any industrial process in which a microwave heating process is involved. The occurrence of hotspots is dependent on the critical value of $\beta$, above which hotspots occur and below which a steady state is obtained. It is therefore quite interesting to examine whether or not the LTDRM can be used to correctly predict critical $\beta$ values as was done in [107].

The critical value $\beta_c$ is defined as the largest $\beta$ such that the steady state of Equation (3.38) can be obtained. To calculate the critical $\beta$ values, a simple loop was added to our program used to calculate the solution at any observation time. Numerically, the steady state of Equation (3.38) is deemed to be reached if the difference of the temperature at two different time levels is less than a small number, say $1.0 \times 10^{-4}$, at every collocation point. Our results for the critical
values $\beta_c$ using the LTDRM-D and LTDRM-T, are tabulated in Table 3.3 and 3.4 for the cases $n = 2$ and 3, respectively. The $\beta_c$ values obtained by Zhu et al. [107] and by using the Frank-Kamenetskii’s approximation method [107, 37] are also listed in these tables. It can be seen that our results agree well with those obtained by Zhu et al. using their numerical model and by using the Frank-Kamenetskii’s approximation method.

After the critical value $\beta_c$ is determined, we shall now observe the pattern of the temperature distribution which depends on the values of parameters $\beta$ and $\gamma$. The steady-state temperature profiles for several different values of $\beta$ and $\gamma$ are graphically presented in Figure 3.3(a–c). Since an exponential decay of the electric-field in the $x$-direction is assumed, the problem is thus symmetric about the cross section $y = 0.5$ where the highest temperature also occurs. Therefore, we choose to present the steady-state temperature profiles, obtained from using the LTDRM-T, along this cross section in Figures 3.3(a–c) for the case $n = 2$. From these figures, one can see a general pattern of the temperature distribution. With a fixed $\gamma$, the steady-state temperature at every spatial point increases monotonically with the increasing value of $\beta$; the highest steady-state temperature is reached when $\beta = \beta_c$ ($\beta_c = 4.78$, 11.27 and 21.09 in Figures 3.3(a–c), respectively). Once $\beta > \beta_c$, hotspots occur eventually. One can also notice that, as $\gamma$ is increased, the point of the maximum temperature moves from the centre of the slab toward the left boundary where the heat absorption is the strongest, and thus the gradient of the temperature field becomes larger and larger in the neighbourhood of this edge. Consequently, the material will be damaged first at
Figure 3.3: (a) Steady-state temperature profiles along x-axis at \( y = 0.5 \) for the case \( \gamma = 0 \).
Figure 3.3: (b) Steady-state temperature profiles along x-axis at $y = 0.5$ for the case $\gamma = 2$. 

\[ \beta = 11.27 \]

\[ \beta = 9 \]

\[ \beta = 5 \]
Figure 3.3: (c) Steady-state temperature profiles along x-axis at \( y = 0.5 \) for the case \( \gamma = 4 \).
this edge as one would naturally expect. A similar pattern was also observed for the case $n = 3$.

As far as the numerical efficiency of the LTDRM is concerned, the excellent efficiency has been clearly demonstrated in Chapter 2, especially when the solution at a large observation time is calculated. The numerical efficiency of the LTDRM is even further enhanced when nonlinear iterations are involved, since iterations are only performed for a single timestep. In contrast, the total number of iterations in a time-domain method [107] is equal to a double summation over the number of iterations at each timestep and the number of timesteps. Moreover, when only the solution at a specific time is needed, all the intermediate solutions and the associated iterations as well as the computer storage are eventually discarded and thus wasted; this becomes worse if the desired solution is at a large time. This can be better illustrated by an example.

For the case $n = 2$ and $\beta = 21$, Zhu et al. [107] had to go through 73 iterations altogether before a convergent solution at $t = 2.1$ was obtained. With the same level of accuracy, we obtained our results with only 18 iterations using the LTDRM-D. However, the number of iterations should be multiplied by the number of solutions needed in the Laplace-transformed space (6 as described in Chapter 2), resulting in solving Equation (3.30) a total number of 108 times. In comparison, the LTDRM-T needed only 6 iterations which required solving Equation (3.33) 36 times. At the first glance our LTDRM-D does not seem to be economical at all compared to a time-domain method. However, the number of iterations associated with a time-domain method will increase at least linearly, as the observation time is increased, whereas the number of iterations required by the LTDRM virtually remains the same.

In addition, it was found later, for this particular problem, that we were able to improve the convergence rate of the direct iteration scheme if the relaxation technique was incorporated. That is after Equation (3.30) is solved and the value of $u$ is found, the value of $\tilde{u}$ is updated by relaxation as

$$\tilde{u} = u + \sigma (u - \tilde{u}), \quad (3.43)$$

with $\sigma$ being the relaxation parameter ranging between 0 and 1. The iteration then proceeds until convergence is obtained. With the relaxation being adopted, the number of iterations required by the LTDRM-D can be reduced from 18 to 7 with the relaxation parameter taken to be 0.5.

Furthermore, a higher efficiency of the LTDRM than time-domain methods is even more evident when determining the critical value $\beta_c$. Generally speaking, when the parameter to be determined is near its critical value, the steady state is approached very slowly. This creates a considerable difficulty in terms of the computational time involved, when one tries to find the critical value with a reasonable accuracy, using any finite-difference time-stepping method. Take the current microwave heating problem as an example. When $\beta$ values are in the vicinity of $\beta_c$, the efficiency of the time-domain method used in [107] worsens dramatically as the steady state of Equation (3.38) is slowly reached. It is therefore very costly to calculate the critical value $\beta_c$ since quite a large number of solutions at intermediate timesteps needs to be calculated. On the other hand, no such problems exist for the LTDRM. As mentioned before, the LTDRM is very effective especially when solving for a solution at a large observation time. Thus, for a fixed value of $\beta$, one can always decide whether $\beta$ is greater or less than $\beta_c$ from the success or failure in obtaining a solution at a sufficiently large timestep. Consequently, a do-loop incorporated with the bisection method can be easily designed to calculate $\beta_c$. It should be noted that the number of iterations involved virtually remains the same, regardless of the size of the observation time level. This allows one to choose a timestep as large as one wishes so that reaching the steady-state solution is guaranteed even if $\beta$ is only slightly less than $\beta_c$. Clearly, the number of iterations in the LTDRM depends virtually on the values of $\beta$ (it varied from 2 iterations for small $\beta$ values to a maximum of 7 iterations for the critical values $\beta_c$ using the LTDRM-T, and 5 to 20 iterations using the LTDRM-D, in all of our numerical experiments for this problem); the advantage of using the LTDRM to determine $\beta_c$ is therefore obvious.
3.3.2 Steady-state solutions

Though the results of the LTDRM have been compared with some numerical results in the previous example, it is desirable that a more systematic test of our nonlinear iteration schemes against an analytical solution be carried out, as the numerical solutions given by Zhu et al. [107] may themselves involve certain degree of numerical errors. Due to the difficulty in finding analytical transient solutions for Equation (3.38), a steady-state problem was studied instead with the geometry being altered to a unit circle and an essential boundary condition with the value of \( u = 1 \) being prescribed on the boundary. The steady state of the temperature distribution is governed by

\[
ur_\tau + \frac{1}{r} ur + \beta u^2 = 0, \tag{3.44}
\]

if \( n \) and \( \gamma \) in Equation (3.38) are chosen to be 2 and 0, respectively. Note that not only can an analytical solution of Equation (3.44) be found (see Equation (3.52) below), it can also be regarded as the steady-state solution of the equation

\[
u_{r\tau} + \frac{1}{r} u_r + \beta u^2 = u_t. \tag{3.45}
\]

Hence, it is ideal to use Equation (3.45) as the governing equation for our next test example. In fact, since theoretically an infinitely long timestep is needed now to reach the steady state, it is a quite "severe test" for our LTDRM.

In order to find the analytical solution of Equation (3.44), we assume that, for \( \beta < \beta_c, u(0), u'(0), u''(0), \ldots \) are all finite so that a Taylor series expansion of \( u \) about the centre is obtained as

\[
u(r) = u(0) + ru'(0) + \frac{r^2}{2!} u''(0) + \cdots. \tag{3.46}
\]

If we now rewrite Equation (3.44) as

\[
r u_{r\tau} + u_r + \beta ru^2 = 0, \tag{3.47}
\]

and letting \( r \to 0 \), we have

\[
u'(0) = u_r(0) = 0. \tag{3.48}
\]
Differentiating Equation (3.47) \( n \) times and letting \( r \to 0 \), one can show that, for \( n \) even,

\[
u''(0) = u^{(8)}(0) = \cdots = u^{(n+1)}(0) = \cdots = 0, \tag{3.49}
\]

and, for \( n \) odd,

\[
(n + 1)u^{(n+1)}(0) = -\beta n \left\{ u(0)u^{(n-1)}(0) + (n - 1)u'(0)u^{(n-2)}(0) + \right.
\]

\[\left. (n - 1)(n - 2)u''(0)u^{(n-3)}(0) + \cdots \right\}. \tag{3.50}
\]

Finally, we have

\[
u(r) = u(0) + \frac{r^2}{2!}u''(0) + \frac{r^4}{4!}u^{(4)}(0) + \cdots, \tag{3.51}
\]
or

\[
u(r) = u(0) - \frac{r^2}{2!}\beta u^2(0) + \frac{r^4}{4!}\left\{ \frac{3}{4}\beta^2 u^3(0) \right\} - \cdots, \tag{3.52}
\]

which converges rapidly provided that the temperature at the centre is known.

The value of \( u(0) \) is determined from imposing the boundary condition such that

\[
1 = u(0) - \frac{1}{2!}\beta u^2(0) + \frac{1}{4!}\left\{ \frac{3}{4}\beta^2 u^3(0) \right\} - \cdots. \tag{3.53}
\]

With the temperature at the centre being known from Equation (3.53), the steady-state temperature at other points inside the unit circle can then be computed according to Equation (3.52).

To implement the LTDRM in solving this problem, 32 constant elements were placed on the boundary and 41 internal nodes were placed inside the circle, as shown in Figure 3.4. Again, when linear elements were used, no significant difference in the results was observed. A linearisation of Equation (3.45) was first carried out and then solved by the LTDRM subject to the initial condition being set as unity. The numerical results of the temperature at a large time, representing the steady-state solution, were obtained after 4 iterations using LTDRM-T (7 iterations using LTDRM-D). These results on the circles of 0.1 unit apart from the centre are tabulated in Table 3.5 together with the exact values for the case \( \beta = 1.2 \). One can obviously see a good agreement between the numerical and exact solutions as shown in terms of percentage errors, all of which are less
Figure 3.4: Boundary and internal nodes used for the circular disk.
than 2.3%. Once again, one also notices that the solutions obtained from both LTDRM-D and LTDRM-T are almost exactly the same.

### 3.3.3 Spontaneous ignition of a unit circular cylinder

Having now demonstrated, through the previous two examples, that the LTDRM-T is more efficient than the LTDRM-D while rendering results of the same level of accuracy, it has to be pointed out that there is a problem associated with the LTDRM based on a direct iteration scheme. Our numerical experiments showed that the iteration scheme used in the LTDRM-D usually gave poor results when we tried to apply it to problems containing higher nonlinearity than the power-law form, such as that in a spontaneous ignition problem in which the source term varies exponentially with the unknown function. Therefore, only the LTDRM-T is employed in this section to study the spontaneous ignition of a unit circular cylinder. This problem was also studied by Partridge and Wrobel [71] using the DRM with a finite-difference time-marching scheme.

---

**Table 3.5: Temperature on the circular disk for the case $\beta = 1.2$**

<table>
<thead>
<tr>
<th>$r$</th>
<th>Analytical</th>
<th>LTDRM-D</th>
<th>Error (%)</th>
<th>LTDRM-T</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.655</td>
<td>1.618</td>
<td>2.2</td>
<td>1.620</td>
<td>2.2</td>
</tr>
<tr>
<td>0.1</td>
<td>1.647</td>
<td>1.610</td>
<td>2.2</td>
<td>1.612</td>
<td>2.2</td>
</tr>
<tr>
<td>0.2</td>
<td>1.622</td>
<td>1.587</td>
<td>2.2</td>
<td>1.589</td>
<td>2.2</td>
</tr>
<tr>
<td>0.3</td>
<td>1.583</td>
<td>1.549</td>
<td>2.1</td>
<td>1.551</td>
<td>2.1</td>
</tr>
<tr>
<td>0.4</td>
<td>1.528</td>
<td>1.498</td>
<td>2.0</td>
<td>1.499</td>
<td>2.0</td>
</tr>
<tr>
<td>0.5</td>
<td>1.462</td>
<td>1.434</td>
<td>1.9</td>
<td>1.436</td>
<td>1.9</td>
</tr>
<tr>
<td>0.6</td>
<td>1.383</td>
<td>1.360</td>
<td>1.7</td>
<td>1.362</td>
<td>1.7</td>
</tr>
<tr>
<td>0.7</td>
<td>1.296</td>
<td>1.278</td>
<td>1.4</td>
<td>1.279</td>
<td>1.4</td>
</tr>
<tr>
<td>0.8</td>
<td>1.202</td>
<td>1.188</td>
<td>1.2</td>
<td>1.189</td>
<td>1.2</td>
</tr>
<tr>
<td>0.9</td>
<td>1.102</td>
<td>1.093</td>
<td>0.8</td>
<td>1.094</td>
<td>0.8</td>
</tr>
</tbody>
</table>
Chapter 3: Diffusion problems with nonlinear source terms

The nonlinear transient heat conduction problem of the spontaneous ignition of a reactive solid is known to be governed by the transient diffusion equation with a nonlinear reaction-heating term, due to a single first-order rate process, as [108]

\[
K \nabla^2 T + \rho Q z e^{-E/RT} = \rho c \frac{\partial T}{\partial t},
\]

(3.54)

for isotropic materials, where \( \rho, c, K \) are density, specific heat and thermal conductivity, respectively; \( Q \) is the heat of decomposition of the solid; \( z \) is the collision number; \( E \) is the Arrhenius activation energy; and \( R \) is the universal gas constant.

The problem can be described as finding the temperature distribution in a solid reactive material immersed in a bath at ambient temperature \( T_a > T_0 \), where \( T_0 \) is the initial temperature of the solid. In the absence of the reaction-heating term, the governing equation reduces to the well-known heat equation; thus, at a certain time the temperature distribution within the solid will reach a steady state where its value is equal to \( T_a \) everywhere. The significance of the presence of the reaction-heating term is to increase the temperature in the solid above the ambient value \( T_a \). For each kind of reactive material, a temperature \( T_m \) can be determined above which a spontaneous ignition will occur.

By introducing a new variable [10]

\[
u = E \frac{(T - T_a)}{RT_a^2},
\]

(3.55)

and employing the Frank-Kamenetskii approximation [2]

\[
e^{-E/RT} = e^{-E/RT_a} e^u,
\]

(3.56)

Equation (3.54) becomes

\[
\nabla^2 u + \gamma e^u = a \frac{\partial u}{\partial t},
\]

(3.57)

where \( a = 1/k \), with \( k \) being the thermal diffusivity (\( = K/\rho c \)) and

\[
\gamma = \frac{\rho Q E z}{K RT_a^2} e^{-E/RT_a}.
\]

(3.58)

It is common to define the dimensionless Frank-Kamenetskii parameter as \( \delta = l^2 \gamma \), where \( l \) is a characteristic length of the problem being considered.
For a given geometrical shape of the solid, it has been shown in [37] that whether the temperature within the solid eventually reaches the steady state or the value $T_m$, depends entirely on the sole parameter $\delta$. The critical value $\delta_c$ which separates these two completely different final states can be evaluated from Equation (3.57) with the temporal derivative term being set to zero [2, 71]. For the cases $\delta < \delta_c$, a thermal equilibrium can be attained with the steady-state temperature in the solid being larger than $T_a$ everywhere but less than $T_m$. On the other hand, if $\delta$ is greater than $\delta_c$, a steady state cannot be reached; the temperature in the solid eventually reaches $T_m$ at a certain time interval, called the induction time [108], and consequently spontaneous ignition occurs. Therefore, the value of $\delta_c$ is important in modelling the spontaneous ignition process and can also be determined from Equation (3.57) by the LTDRM, using a similar technique to that described in the microwave heating problem in finding $\beta_c$. Several values of $\delta_c$ for common two-dimensional geometrical shapes can be found, for example, in References [2, 17, 71]. It is worth noting that although the two problems, i.e., microwave heating and spontaneous ignition problems, are mathematically the same in essence, the source term in the latter is of a much higher nonlinearity than that in the former. It is therefore desirable to see if the LTDRM based on the linearisation scheme using Taylor series expansion can be applied to such a highly nonlinear problem.

To demonstrate the application of the LTDRM to a diffusion equation with a highly nonlinear source term, the spontaneous ignition of a long circular cylinder of unit radius taken from Reference [71] is considered. Initially, the cylinder is of uniform temperature $T_0 = 298$ K and is abruptly submerged at time $t = 0$ sec in a bath of temperature $T_a = 400$ K. The cylinder is of a uniform isotropic reactive material, with ignition temperature $T_m = 425$ K. The problem is subject to an essential boundary condition where $T = T_a$ is imposed at all boundary nodes. The other numerical values of the physical parameters are $a = 1285.71$ sec/cm$^2$, $E = 47500$ kcal/M and $R = 1.987$ cal/(MK).

Time-domain methods in conjunction with the FEM and DRM have been
adopted to solve the spontaneous ignition problems by Anderson and Zienkiewicz [2] and Partridge and Wrobel [71], respectively. They all pointed out that at the earlier timesteps, when the heat generated by the reaction is obvious, a large $\Delta t$ may be used but it must be reduced quickly as $t$ gets closer to the ignition time. Therefore, a variable timestep was employed due to some varying stability characteristics of the spontaneous-ignition process. The value of $\Delta t$ was altered such that at each timestep the average temperature change at all interior nodes is maintained between 5 K and 20 K [2, 71].

To implement the LTDRM, the boundary of the cylinder was discretised with 16 linear elements and 19 internal nodes were placed at an interval of 0.1 m along a diagonal (the $y$–axis). This discretisation is the same as that adopted in [71]. The LTDRM was then applied to the linearised equation of Equation (3.57), i.e.,

\[
\nabla^2 u = a \frac{\partial u}{\partial t} - \gamma e^\delta u - \gamma e^\delta (1 - \bar{u}).
\]  

(3.59)

Once the unknown $u$ has been obtained, the temperature $T$ can be calculated from Equation (3.55). The critical value $\delta_c$ was numerically estimated by the LTDRM to be 2.08 which agrees very well with the analytical value of 2.00 given in [71].

After the value of $\delta_c$ has been found, the main interest is now to find the ignition time for the cases where $\delta > \delta_c$. It is however necessary to incorporate the multistep and bisection techniques into the LTDRM. In the multistep algorithm, the result from the previous step is used as an initial condition for the next step which is similar to a finite-difference time-stepping process. However, the timestep size in multistep-LTDRM can be much larger than that of a time-marching scheme. When either the iteration fails or the temperature is over the ignition temperature for at least one point inside the cylinder, the bisection is then used to halve the timestep before the calculation at that step is repeated. The starting timestep was set to be 100 sec in all the cases presented below.

Results shown in Figure 3.5(a) are temperature profiles for the case $\delta = 1$. The temperatures at time $t = 130$ sec and 670 sec were calculated separately from the multistep-bisection algorithm in order to be able to compare the results with those
shown in [71]. Then the multistep-bisection algorithm was used and the procedure converged to a steady-state solution $T_s$ with $T_a < T_s < T_m$ at all internal points at time $t = 2400$ sec, as $\delta$ was less than $\delta_c$ in this case. The results obtained from the LTDRM and DRM agree well with each other. One should however notice that the time taken for the temperature to reach the thermal equilibrium is different in both methods. This can be explained as follows. The incremental time used in the DRM is doubled if the average temperature change at all interior nodes is less than 5 K before the procedure proceeds to the next timestep. Since the change in temperature becomes very small when the temperature is above the ambient value or the steady-state solution is near, the incremental time is always doubled thus resulting in a large time increment and also a large observation time. In contrast, there is no requirement for the minimum temperature change when using the LTDRM; therefore, the steady-state temperature is attained at a smaller observation time. It should also be noted here that such a large difference in time, at which the steady-state solution is declared to be reached, is expected when using different numerical models or even the same model with different runs when $\delta < \delta_c$, and when the approach to the steady state is very slow. On the other hand, it is absolutely necessary for any numerical model to be able to accurately predict the ignition time when $\delta > \delta_c$, as will be shown below.

Temperature profiles for the case $\delta = 4$ are depicted in Figure 3.5(b). In this case the temperatures at time $t = 130$ sec and 670 sec were again calculated separately. Then the LTDRM with the multistep-bisection algorithm was used to find the ignition time. The process was completed at time $t = 1142$ sec. Since $\delta$ is now greater than $\delta_c$, the ignition is expected to occur. As we can see from Figure 3.5(b), the ignition temperature is first reached at the centre of the cylinder and then the ignition occurred. The results obtained here once again agree well with those found in [71].

Temperature profiles for the case $\delta = 50$ are shown in Figure 3.5(c) illustrating a good agreement between the results obtained from the LTDRM and DRM. In this case the ignition temperature is first reached at the points with a distance
Figure 3.5: (a) Temperature distribution in the cylinder for the case $\delta = 1$. 
Figure 3.5: (b) Temperature distribution in the cylinder for the case $\delta = 4$. 
Figure 3.5: (c) Temperature distribution in the cylinder for the case $\delta = 50$. 
Table 3.6: Ignition time and first-ignition points for different $\delta$ values

<table>
<thead>
<tr>
<th>$\delta$</th>
<th>Ignition time (s)</th>
<th>Ignition points</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DRM</td>
<td>LTDRM</td>
</tr>
<tr>
<td>1.0</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>1.9</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>2.1</td>
<td>5884</td>
<td>5938</td>
</tr>
<tr>
<td>4.0</td>
<td>1145</td>
<td>1142</td>
</tr>
<tr>
<td>10.0</td>
<td>723</td>
<td>717</td>
</tr>
<tr>
<td>20.0</td>
<td>555</td>
<td>547</td>
</tr>
<tr>
<td>50.0</td>
<td>351</td>
<td>349</td>
</tr>
<tr>
<td>200.0</td>
<td>129</td>
<td>124</td>
</tr>
</tbody>
</table>

Note: starred-values are maximum temperature of 0.8 m away from the centre (i.e., $r = 0.8$). It should be noted that since the problem is axially symmetric, all the points with the same distance from the centre will ignite at the same time.

The results for ignition times and points for several values of $\delta$ are summarised in Table 3.6, showing the ignition points moving from the centre towards the outer surface of the cylinder as $\delta$ increases. As mentioned in [71], this trend of movement of the ignition points agrees with that found from a theoretical study.

In this spontaneous ignition problem, the significance of the nonlinear source term has been clearly demonstrated in Figures 3.5(a–c). Had there been no source term, the temperature distribution within the solid could have only reached the ambient temperature, the steady state of a uniform temperature distribution. It is because of the existence of the source term that a temperature higher than the ambient temperature can be eventually reached and an ignition will initiate when the value of the Frank-Kamenetskii parameter is greater than the critical value $\delta_c$. The accuracy of the LTDRM was illustrated via the good comparison between the results from the LTDRM and the time-domain method used in [71]. As for
the efficiency, the LTDRM is still more efficient than time-domain methods if the solution at a particular time needs to be sought. The reduction of the efficiency of the LTDRM is due to the ignition time being sought. Nevertheless, the timestep size used in the multistep-bisection-LTDRM algorithm can still be much larger than that used in a finite-difference time integration; the efficiency of the LTDRM is by no means undermined.

3.3.4 The Liouville equation

The Liouville equation:

\[ \nabla^2 u = \frac{\lambda^2}{8} e^{-u}, \quad (3.60) \]

is an important equation appearing as the governing equation in many different areas of mathematical physics, applied science and engineering [32, 36]. Since it has a well-known special analytical solution [96], i.e.,

\[ u(x, y) = 2 \ln\left[ \frac{\lambda}{4\sqrt{1 - \epsilon^2}} (\cosh x + \epsilon \cos y) \right], \quad (3.61) \]

for \( \lambda > 0 \) and \( 0 \leq \epsilon^2 < 1 \), and can be regarded as the steady state of the equation

\[ \nabla^2 u = \frac{\partial u}{\partial t} + \frac{\lambda^2}{8} e^{-u}, \quad (3.62) \]

it is ideal for use as our last test example. We have often mentioned that the LTDRM is very efficient for the calculation of solutions at large time. Since theoretically an infinitely long timestep is now required to reach the steady state, this example can therefore be used to support such efficiency of our LTDRM.

Equation (3.62) was linearised by the Taylor series expansion as

\[ \nabla^2 u = \frac{\partial u}{\partial t} - \frac{\lambda^2}{8} e^{-\tilde{u}} u + \frac{\lambda^2}{8} e^{-\tilde{u}} (1 - \tilde{u}), \quad (3.63) \]

and the problem was solved by the LTDRM on a unit square subject to the essential boundary condition with the value of \( u \) in Equation (3.61) being prescribed on the boundary, and the initial condition with the value of \( u \) at \( t = 0 \) being set to unity. The discretisation was done with 40 equal constant elements being placed on the boundary and two different sets of uniformly distributed internal nodes.
being employed: (a) 9 nodes and (b) 36 nodes. Convergent numerical results were normally obtained within 4 iterations with the tolerance being set to $1.0 \times 10^{-3}$. Various solutions at a large time, with $\epsilon$ and $\lambda$ being taken for many different values within the ranges given in Equation (3.61), were found numerically and they all compared very favorably with the analytical solution. However, only the results with $\epsilon$ and $\lambda$ being $-0.9$ and $7$, respectively are presented here. In Figures 3.6(a-b), the point-wise absolute errors between the LTDRM and analytical solutions are displayed with the maximum errors being about (a) $9.63 \times 10^{-3}$ and (b) $3.84 \times 10^{-3}$. The corresponding maximum relative errors are found to be (a) $16.23\%$ and (b) $1.64\%$, respectively. One can clearly see that the error is reduced considerably as the number of internal nodes is increased; a roughly 4-fold of increase of the internal nodes resulted in a more than 8-fold of increase in accuracy. Considering the high nonlinearity associated with the nonhomogeneous term, such a convergence rate is undoubtedly acceptable.

If on the other hand, we switched back to a time-domain method with the nonlinear term linearised locally at each timestep, the maximum absolute errors between numerical and exact solutions were found to be $1.63 \times 10^{-1}$ and $8.17 \times 10^{-2}$ and the corresponding maximum relative errors were about $161\%$ and $57\%$ with a timestep of 0.1 being adopted and 9 and 36 internal nodes being uniformly distributed, respectively. If the number of internal nodes was further increased to 100, the maximum absolute and relative errors were reduced to $3.82 \times 10^{-2}$ and $22\%$, respectively. However, compared to the maximum absolute and relative errors associated with the LTDRM, i.e., $3.84 \times 10^{-3}$ and $1.64\%$, respectively, with only 36 internal nodes being used, the LTDRM seems to have performed much better than the time-domain method.

Once again, to demonstrate the importance of the nonlinear term, we also solved the same problem without the source term but with the same boundary conditions. The point-wise absolute errors are shown in Figure 3.6(c) with the maximum absolute error being about $4.29 \times 10^{-1}$ which is of two-order-of-magnitude higher than those associated with solving Equation (3.63). The cor-
Figure 3.6: (a) Error distributions from using 9 nodes.
Figure 3.6: (b) Error distributions from using 36 nodes.
Figure 3.6: (c) Error distributions without source term.
responding maximum relative error was found to be 1976%. Furthermore, the difference between results obtained from using two different sets of internal nodes was found to be negligible; the possible argument that such a large difference in terms of numerical error is associated with a particular distribution of the internal collocation nodes is therefore ruled out. Although such a huge relative error mainly resulted from a division by a very small number in the exact solution, the average error is still very high confirming that the nonlinear term has significant impact towards the solution of the problem.

For the sake of a better visualisation, the numerical values of $u$ along $x$-axis at the cross section $y = 0.25$ obtained from solving Equation (3.63) and the one without the nonlinear source term are plotted in Figure 3.7, together with the exact values from Equation (3.61). The large difference between the exact $u$ values and those obtained from solving the problem without the nonlinear source term is clearly visible whereas there is virtually no difference between the exact $u$ values and those obtained from solving Equation (3.63). Therefore, we are certainly convinced that the nonlinear term, having played a very important role which cannot be ignored, has been correctly accounted for by the LTDRM based on the Taylor series expansion scheme.

### 3.4 Conclusions

The LTDRM is extended to the solution of nonlinear transient diffusion problems. In particular, two sets of problems governed by a diffusion equation with a nonlinear source term in the power-law or exponential form are used as test examples. The successful performance of the extended LTDRM on the nonlinear problems, especially when the nonlinear source term is highly nonlinear, relies mainly on the linearisation of the nonlinear source term. In this chapter, two linearisation schemes are adopted; one based on a direct iteration scheme and another on the first-order Taylor series expansion. The accuracy and efficiency of the LTDRM are clearly demonstrated through our numerical examples. It is
Figure 3.7: The $u$ values along the cross section at $y = 0.25$. 
shown that the LTDRM based on the a Taylor series expansion is more efficient than the LTDRM used in conjunction with a direct iteration scheme. However, it is found that the convergence rate of the direct iteration can be improved if a relaxation technique is incorporated, and this convergence rate is comparable to that of the Taylor series expansion. On the other hand, in some other types of nonlinear diffusion equations, the relaxation technique used here may not be necessary and the direct iteration scheme can be more effective than the Taylor series expansion scheme, as will be seen in the next chapter.

Particularly, an emphasis should be given on the significance of successfully solving the Liouville equation in which the source term is highly nonlinear. It is exciting to have observed that the numerical solution obtained from solving the corresponding time-dependent equation by the LTDRM agreed so excellently, at a large time, with the exact solution of the Liouville equation. Because of this last example we believe that the LTDRM is a highly efficient and robust method to be used for solving diffusion equations with a nonlinear source term, especially when only the solution at a large observation time or the steady state solution is needed.

Although only equations with nonlinear source terms are discussed in this chapter, the way that the iteration schemes are constructed has also shed some light on designing similar nonlinear iterative procedures for the LTDRM to be used to solve other types of diffusion equations, which will be presented in the next chapter.
Chapter 4

Diffusion Problems with Nonlinear Material Properties and Nonlinear Boundary Conditions

The Laplace Transform Dual Reciprocity Method (LTDRM) has been developed for linear transient diffusion equations and its efficiency and accuracy have been demonstrated in Chapter 1. However, problems encountered in engineering practice and applied science and governed by diffusion equations are usually nonlinear. In Chapter 2, we have shown the successful application of the LTDRM to diffusion problems with nonlinear source terms. Two other most important nonlinear features that appear in those problems are the temperature-dependent material properties and nonlinear boundary conditions due to heat radiations. The study of these problems is of great importance and has several applications such as, among many others, nonlinear heat transfer in nuclear reactor components [86], chemical reactor analysis and combustion [37]. In this chapter, the LTDRM is thus further extended to these types of nonlinear transient diffusion problems.

When a problem involves temperature-dependent thermal conductivity, the nonlinear governing equation, in steady-state cases, can always be reduced to
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a linear one through the Kirchhoff transformation [15, 64]. The problem then becomes linear provided that only Dirichlet and Neumann boundary conditions are imposed. If convective and radiative boundary conditions are present, the problem will still be nonlinear in the transformed space and an iterative procedure is required for a numerical solution. Examples of the steady-state problems solved with the Boundary Element Method (BEM) can be found, for example, in the works of Bialecki and Nowak [9], Khader and Hanna [47], and Azevedo and Wrobel [6].

For transient cases, on the other hand, the Kirchhoff transform can be used only to simplify the governing equation; the transformed equation is generally still nonlinear since it contains a temperature-dependent thermal diffusivity. However, this transformed equation can be linearised by using a mean value of the thermal diffusivity [82, 85]. In a more general approach, Wrobel and Brebbia [101] used a further change of variable, by introducing a modified time variable as an integral of diffusivity coefficient, to obtain a linear equation in terms of the new variable. The problem was then solved by the Dual Reciprocity Method (DRM) to avoid the domain integration which would have otherwise arisen if the BEM had been used. But, since the new variable is now a function of position, an iterative process had to be adopted.

As an alternative to the Kirchhoff transformation in the BEM analysis, a straightforward approach, in which a DRM formulation can be derived directly from the original equation, was proposed by Partridge [65] for steady-state problems. Despite the fact that an iterative procedure is always necessary in this approach, the heat source term, if exists, can be taken into account easily.

In the case of time-dependent problems, a finite-difference time-marching scheme is usually adopted in the solution procedure. However, any time-marching scheme suffers from a common drawback; the timestep size is restricted by either a stability criterion and/or the truncation errors involved in approximating the time derivative with a finite difference. Thus, usually very small timesteps must be taken and a large amount of computer time is required in order to obtain the
solution at a specific time, especially for solutions at large time. Furthermore, all the intermediate results would be wasted if all one needs is the solution at the last time step. Such a deficiency becomes even worse in nonlinear cases, because iterations are now required at each timestep.

On the other hand, it has been shown in Chapters 2 and 3 that the LTDRM can be used to obtain a solution at any specific time without step-by-step calculation in the time domain and computation of domain integrals. Thus, the memory size as well as the total number of operations are greatly reduced, leading to a significant saving of computational cost. The LTDRM has also been shown to possess good convergence properties and efficiency in obtaining accurate solutions for nonlinear problems.

In extending the LTDRM to nonlinear problems with temperature-dependent material properties and nonlinear boundary conditions, a linearisation of both the governing equation and the boundary conditions needs to be carried out first. In Chapter 3, it was shown that a Taylor series expansion scheme was better than a direct iteration scheme. For the particular problems considered in this chapter, a Taylor series expansion scheme has resulted in a much more complicated nonhomogeneous term. However, there has not been a great deal of improvement in the numerical accuracy to compensate for this extra complication. Therefore, only a direct iteration scheme is adopted here.

Once the linearisation has been carried out, the LTDRM can be applied and two integral formulations are obtained. Due to the presence of spatial derivatives in these formulations, another set of interpolation functions, which is different from that used to cast the domain integral into the boundary integrals, is employed to approximate these derivatives. A third integral formulation is also presented, based on the use of the Kirchhoff transform to firstly simplify the governing differential system, followed by a linearisation and the LTDRM procedure. These three integral formulations are then applied to solve various examples of heat conduction problems in different regular and irregular domains. Their advantages and disadvantages are also discussed.
4.1 The LTDRM Formulations

A transient diffusion equation for two-dimensional problems without heat source terms can generally be written as

$$\frac{\partial}{\partial x} \left( K \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( K \frac{\partial u}{\partial y} \right) = \rho C \frac{\partial u}{\partial t},$$

(4.1)
in which the thermal conductivity $K$, density $\rho$ and specific heat $c$ are considered to be known functions of temperature $u$. The problem is usually subject to either one or a combination of the following types of boundary conditions:

i) Dirichlet boundary condition

$$u = \bar{u}, \quad \text{on } \Gamma_1,$$

(4.2)

ii) Neumann boundary condition

$$q = K \frac{\partial u}{\partial n} = \bar{q}, \quad \text{on } \Gamma_2,$$

(4.3)

iii) Convective boundary condition

$$q = h(u_f - u), \quad \text{on } \Gamma_3,$$

(4.4)

iv) Radiative boundary condition

$$q = c_0 R(u_s^4 - u^4), \quad \text{on } \Gamma_4,$$

(4.5)

where $q$ represents heat flux; $h$ is a heat transfer coefficient; $u_f$ is the temperature of a surrounding medium; $c_0$ is the Stefan-Boltzmann constant, $c_0 = 5.667 \times 10^{-8}$ $W/(m^2 K^4)$; $R$ is the radiation interchange factor between surface $\Gamma_4$ and the environment having a temperature $u_s$; and $n$ denotes the unit outward normal on the boundary $\Gamma(= \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4)$ of a computational domain. In addition to these boundary conditions, an initial condition for the unknown function must also be prescribed at the time level $t_0 = 0$. 
It can be seen that Equation (4.1) and the boundary conditions (4.2)-(4.5) constitute a nonlinear problem for which no general theory with regard to its solution has yet been available. However, if the material properties are constants, the problem becomes linear provided that the radiation condition is not imposed. For the case of the thermal conductivity being temperature-dependent, Equation (4.1) can be simplified to a standard diffusion equation by the Kirchhoff transformation. But the transformed equation is generally still nonlinear as are boundary conditions (4.4) and (4.5), and a linearisation is needed before the LTDRM can be applied. Another method is to linearise directly the original differential system and then apply the LTDRM. These two types of methods are described in the following sections.

4.1.1 Direct formulations

Since various formulations can be derived if $K$ is known explicitly, we shall only consider, for simplicity, a linear variation of conductivity with temperature, i.e.,

$$K = K_0(1 + \beta u),$$

where $K_0$ and $\beta$ are material-dependent constants.

By substituting Equation (4.6) into Equation (4.1), the governing equation can be recast into a Poisson's type equation. The right-hand side of the new governing equation may be of different forms [65], two of which, for instance, are

$$\nabla^2 u = \frac{1}{k(u)} \frac{\partial u}{\partial t} - \frac{\beta}{1 + \beta u} \left( \frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial u}{\partial y} \right) = b,$$

or

$$\nabla^2 u = \frac{C(u)}{K_0 \beta u} \frac{\partial u}{\partial t} - \frac{1}{\beta u} \nabla^2 u - \frac{1}{u} \left( \frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial u}{\partial y} \right) = b,$$

where $k(u) = K/\rho c$ is the thermal diffusivity and $C(u) = \rho c$ is the heat capacity. It should be noticed that while the nonhomogeneous term $b$ on the right-hand side of Equation (4.7) involves only first-order spatial derivatives, $b$ in Equation (4.8) involves spatial derivatives up to the second order.
To prevent the presentation from becoming too diverse, we shall only use Equations (4.7) and (4.8) as our governing equations in this chapter. Accordingly, the LTDRM formulations corresponding to Equations (4.7) and (4.8) are presented below, and are designated LTDRM-1 and LTDRM-2, respectively, for convenience of later references.

A formulation involving first-order spatial derivatives: LTDRM-1

As usual, before the LTDRM can be applied, Equation (4.7) needs to be linearised. As suggested in Chapter 3 for a direct iteration scheme, we can rewrite Equation (4.7) into an iterative format when the solution at a specific time $t_1$ is being sought, as

$$
\nabla^2 u = \frac{1}{k(\tilde{u})} \frac{\partial u}{\partial t} - \frac{\beta}{1 + \beta \tilde{u}} \left( \frac{\partial \tilde{u}}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial \tilde{u}}{\partial y} \frac{\partial u}{\partial y} \right),
$$

where $\tilde{u}$ is the solution of the previous iteration. It should be noted that a linearisation scheme based on Taylor series expansion was not employed here since we found that for this particular problem it resulted in a much more complicated nonhomogeneous term and the extra complication was not significantly compensated for by improved numerical accuracy.

Taking the Laplace transform with respect to $t$ of Equation (4.9) yields

$$
\nabla^2 U = \frac{pU - u_0}{k(\tilde{u})} - \frac{\beta}{1 + \beta \tilde{u}} \left\{ \frac{\partial \tilde{u}}{\partial x} \frac{\partial U}{\partial x} + \frac{\partial \tilde{u}}{\partial y} \frac{\partial U}{\partial y} \right\},
$$

where $p$ is the Laplace parameter and $U$ is the Laplace transform variable of $u$. Now, if the same procedure of the DRM described in Chapter 2 is followed, a matrix equation after the DRM is applied to Equation (4.10) can be obtained as

$$
H U - G \left( \frac{\partial U}{\partial n} \right) = S b,
$$

where $b$ is a vector containing nodal values of the right-hand-side terms in Equation (4.10) and matrices $H$, $G$ and $S$ have been defined in Chapter 2. However, in order that Equation (4.11) can be solved, the spatial derivative terms included in $b$ require approximations which relate their values to those of $U$.

The DRM approximation to a derivative with respect to a spatial coordinate, say $x$, starts by approximating $U$ with a finite sum of interpolation functions,
similar to that done for the nonhomogeneous terms in the governing equation so that domain integrals can be transformed to equivalent boundary integrals, which can be written in a matrix form as \[ U = \tilde{F} \gamma. \] (4.12)

It should be noted that the choice of interpolation functions \( f \) with the corresponding matrix \( \tilde{F} \) in the equation above may differ from that of interpolation functions \( f \) used to convert domain integrals into boundary ones and will be discussed in details later.

Differentiation of Equation (4.12) gives
\[
\frac{\partial U}{\partial x} = \frac{\partial \tilde{F}}{\partial x} \gamma, \quad (4.13)
\]
but
\[
\gamma = \tilde{F}^{-1} U, \quad (4.14)
\]
hence
\[
\frac{\partial U}{\partial x} = \frac{\partial \tilde{F}}{\partial x} \tilde{F}^{-1} U. \quad (4.15)
\]

We shall now define a diagonal matrix \( T_x \) with its diagonal elements being defined as
\[
T_x(i,i) = \left[ \frac{\beta}{1 + \beta u} \frac{\partial \tilde{u}}{\partial x} \right]_i, \quad (4.16)
\]
with the subscript on the right-hand side denoting the term inside of the bracket be evaluated at the \( i \)th node. Similarly, a diagonal matrix \( T_y \) can be constructed. Upon further defining a matrix \( C \) as
\[
C = \left( T_x \frac{\partial \tilde{F}}{\partial x} + T_y \frac{\partial \tilde{F}}{\partial y} \right) \tilde{F}^{-1}, \quad (4.17)
\]
b can be written as
\[
b = (pK - C)U - Ku_0, \quad (4.18)
\]
where \( K \) is a diagonal matrix containing nodal values of \( 1/k(\tilde{u}) \). The final matrix equation is thus
\[
(H - pSK + SC)U = G \left( \frac{\partial U}{\partial n} \right) - SKu_0. \quad (4.19)
\]
A formulation involving second-order spatial derivatives: LTDRM-2

For Equation (4.8), an iterative scheme similar to Equation (4.9) can be designed as

$$\nabla^2 u = \frac{C(\bar{u})}{K_0 \beta \bar{u}} \frac{\partial u}{\partial t} - \frac{1}{\beta \bar{u}} \nabla^2 u - \frac{1}{\bar{u}} \left( \frac{\partial \bar{u}}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial \bar{u}}{\partial y} \frac{\partial u}{\partial y} \right).$$

(4.20)

Application of the Laplace transform yields

$$\nabla^2 U = \frac{C(\bar{u})}{K_0 \beta \bar{u}} (pU - u_0) - \frac{1}{\beta \bar{u}} \nabla^2 U - \frac{1}{\bar{u}} \left( \frac{\partial \bar{u}}{\partial x} \frac{\partial U}{\partial x} + \frac{\partial \bar{u}}{\partial y} \frac{\partial U}{\partial y} \right),$$

(4.21)

so that after an implementation of the DRM, we have a matrix equation similar to that in Equation (4.11), but $b$ is now a vector containing nodal values of the right-hand-side terms in Equation (4.21).

The DRM approximation to a second-order derivative with respect to a spatial coordinate, say $x$, is obtained by differentiating Equation (4.13) [65], i.e.,

$$\frac{\partial^2 U}{\partial x^2} = \frac{\partial^2 \bar{F}}{\partial x^2} \gamma,$$

(4.22)

and by using expression of $\gamma$ in Equation (4.14), we eventually have

$$\frac{\partial^2 U}{\partial x^2} = \frac{\partial^2 \bar{F}}{\partial x^2} \bar{F}^{-1} U.$$

(4.23)

Defining a diagonal matrix $U_x$ such that

$$U_x(i, i) = \left[ \frac{1}{\bar{u}} \frac{\partial \bar{u}}{\partial x} \right],$$

(4.24)

and a similar matrix $U_y$ and incorporating the expression for second-order derivatives described in Equation (4.23), we define a matrix $D$ as

$$D = \tilde{U} \left( \frac{\partial^2 \bar{F}}{\partial x^2} + \frac{\partial^2 \bar{F}}{\partial y^2} \right) \bar{F}^{-1} + \left( U_x \frac{\partial \bar{F}}{\partial x} + U_y \frac{\partial \bar{F}}{\partial y} \right) \bar{F}^{-1},$$

(4.25)

where $\tilde{U}$ is a diagonal matrix containing nodal values of $1/\beta \bar{u}$. Then $b$ becomes

$$b = (p\tilde{K} - D)U - \tilde{K}u_0,$$

(4.26)

where $\tilde{K}$ is a diagonal matrix containing nodal values of $C(\bar{u})/K_0 \beta \bar{u}$, and thus the final matrix equation is of the form

$$(H - pS\tilde{K} + SD)U = G \left( \frac{\partial U}{\partial n} \right) - S\tilde{K}u_0.$$

(4.27)
Boundary conditions

Before solving the system of equations (4.19) or (4.27), one needs to rearrange the terms in these equations as some boundary values, either $U$ or $\partial U/\partial n$, are known from the given boundary conditions. Except for the Dirichlet boundary condition which is linear, a linearisation of the boundary conditions is necessary.

After taking the Laplace transform, all the boundary conditions become

\[ U \mid_{\Gamma} = \frac{\bar{u}}{p}, \]  
(4.28)

\[ \frac{\partial U}{\partial n} \mid_{\Gamma} = \frac{-\bar{q}}{pK(\bar{u})}, \]  
(4.29)

\[ \frac{\partial U}{\partial n} \mid_{\Gamma} = h_c(\bar{u}) \left( \frac{u_f}{p} - U \right), \]  
(4.30)

\[ \frac{\partial U}{\partial n} \mid_{\Gamma} = h_r(\bar{u}) \left( \frac{u_s}{p} - U \right), \]  
(4.31)

where $h_c(u) = h/K(u)$ and $h_r(u) = [c_0 R/K(u)](u_f^2 + u^2)(u_s + u)$.

If only Dirichlet and Neumann boundary conditions are imposed, the problem can be readily solved with Equation (4.28) and/or Equation (4.29) being linked to the system of Equation (4.19) or Equation (4.27). However, if a convective boundary condition is also prescribed on part of the boundary $\Gamma$, Equation (4.19) now becomes

\[ (H - pSK + SC + GE)U = \frac{1}{p}Ge - SKu_0, \]  
(4.32)

and Equation (4.27) becomes

\[ (H - pS\bar{K} + SD + GE)U = \frac{1}{p}Ge - S\bar{K}u_0, \]  
(4.33)

where $e$ is a vector containing nodal values of $h_c(\bar{u})u_f$ and $E$ is a diagonal matrix containing nodal values of $h_c(\bar{u})$. When the radiation condition is present, entries in the vector $e$ become the nodal values of $h_r(\bar{u})u_s$ and diagonal elements of matrix $E$ become the nodal values of $h_r(\bar{u})$.

Choice of interpolation function

Various kinds of interpolation functions were proposed in the past for the dual reciprocity method [70]. However, best results were usually obtained with simple
expansions; the most widely adopted one was \( f = 1 + r \), where \( r \) is the distance between a field and a source point [69]. These interpolation functions have also been used to obtain accurate solutions throughout Chapters 2 and 3. Recently, Yamada et al. [104] showed that \( f = 1 + r \) is a radial basis function and illustrated its convergence properties which are the same as those described in the theory of radial basis function approximation by Powell [73].

When the nonhomogeneous term in a DRM analysis involves spatial derivatives, Partridge and Brebbia [69] showed that accurate results were obtained by using \( \tilde{f} = 1 + r \), the same as \( f \), for the approximation of derivative terms. However, apart from the fact that it is not valid for second-order derivatives, Zhang and Zhu [105] pointed out that the \( \tilde{f} \) in fact introduces singularities at the collocation points for first-order derivative approximations. To avoid this problem, they took \( f = \tilde{f} \) and proposed two forms of interpolation functions. The proposed interpolation functions \( 1 + r^2 + r^3 \) and \( 1 + r^3 \) led to more accurate results.

In the literature, \( \tilde{f} \) is usually taken to be of the same form as \( f \). However, Partridge [66] demonstrated that \( f \) and \( \tilde{f} \) can be different. Schclar and Partridge [79] also used the mixed interpolation functions when the approximation of second-order spatial derivatives were involved. Details on different types of interpolation functions and combination of these functions can be found in Reference [67]. In this chapter, we choose \( f = 1 + r \) for the transformation of the domain integrals into boundary ones and \( \tilde{f} = 1 + r^2 + r^3 \) for the approximation of the spatial derivatives of both first and second orders. The results obtained from this combination of interpolation functions were found to be most satisfactory as will be demonstrated in Section 4.2.

### 4.1.2 The Kirchhoff transform

When the thermal conductivity is temperature-dependent, a change of dependent variable by means of the Kirchhoff transformation will enable us to rewrite
Equation (4.1) into a simpler form. By constructing a new variable \( v = v(u) \) as

\[
v = T(u) = \int_{u^*}^{u} K(u) \, du,
\]

(4.34)

where \( u^* \) is an arbitrary reference value, Equation (4.1) can be transformed into the standard diffusion equation \([15, 64, 101]\)

\[
\nabla^2 v = \frac{1}{k(u)} \frac{\partial v}{\partial t}.
\]

(4.35)

In the Kirchhoff-transformed space, boundary conditions are also transformed as

- **Dirichlet condition:**
  \[
  v = T(u),
  \]
  (4.36)

- **Neumann condition:**
  \[
  \frac{\partial v}{\partial n} = -k \frac{\partial u}{\partial n} = \bar{q},
  \]
  (4.37)

- **Convection condition:**
  \[
  \frac{\partial v}{\partial n} = h[u_f - T^{-1}(v)],
  \]
  (4.38)

- **Radiation condition:**
  \[
  \frac{\partial v}{\partial n} = c_o R [u_s^4 - (T^{-1}(v))^4],
  \]
  (4.39)

where \( T^{-1} \) indicates the inverse transform of \( T \). Similarly, initial conditions can be transformed accordingly.

From the form of the thermal conductivity given in Equation (4.6), if we take \( u^* = 0 \), then the Kirchhoff transform (4.34) becomes

\[
v = T(u) = K_0 (u + \frac{\beta}{2} u^2),
\]

(4.40)

with the corresponding inverse transform

\[
u = T^{-1}(v) = \frac{1}{\beta} [\sqrt{1 + 2\beta v} - 1].
\]

(4.41)

Notice that for steady-state problems, the right-hand-side term of Equation (4.35) vanishes and thus the transformed differential system becomes linear provided that only Dirichlet and Neumann boundary conditions are prescribed. Otherwise, Equation (4.35) is generally still nonlinear since the thermal diffusivity \( k \) is a function of temperature. Nonlinearities also arise from the convection and radiation conditions due to the inverse Kirchhoff transformation shown in Equation (4.41).
To solve this transformed differential system by the LTDRM, a linearisation procedure similar to that in obtaining Equations (4.9) and (4.20) is first carried out. This leads to

\[ \nabla^2 v = \frac{1}{k(\tilde{u})} \frac{\partial v}{\partial t}, \]  

(4.42)

with the convective and radiative boundary conditions linearised as

\[ \frac{\partial v}{\partial n} = h[u_f - T^{-1}(\tilde{v})], \]  

(4.43)

\[ \frac{\partial v}{\partial n} = c_0 R[u_s^4 - \{T^{-1}(\tilde{v})\}^4], \]  

(4.44)

where \( \tilde{u} \) and \( \tilde{v} \) are the solutions of the previous iteration in the original and transformed problems respectively. After taking the Laplace transform with respect to \( t \), Equation (4.42) becomes

\[ \nabla^2 V = \frac{1}{k(\tilde{u})} \left(pV - v_0\right), \]  

(4.45)

with boundary conditions

- **Dirichlet condition:** \( V = \frac{T(\tilde{u})}{p}, \)

(4.46)

- **Neumann condition:** \( \frac{\partial V}{\partial n} = \frac{\tilde{q}}{p}, \)

(4.47)

- **Convection condition:** \( \frac{\partial V}{\partial n} = \frac{h}{p}(u_f - \tilde{u}), \)

(4.48)

- **Radiation condition:** \( \frac{\partial V}{\partial n} = \frac{c_0 R}{p}(u_s^4 - \tilde{u}^4), \)

(4.49)

where \( V \) is the Laplace transform variable of \( v \) and \( \tilde{u} = T^{-1}(\tilde{v}) \). An application of the DRM yields the final system of equations, which can be written in matrix form as

\[ (H - pSK)V = G \left( \frac{\partial V}{\partial n} \right) - SKv_0, \]

(4.50)

where all the matrices are the same as those which have already been defined earlier. After imposing boundary conditions, the linear system (4.50) can be solved iteratively until the convergent solution of a satisfactory accuracy is obtained.

For brevity, the LTDRM formulation using the Kirchhoff transform is designated as **LTDRM-K**.
4.2 Numerical Examples and Discussions

In this section, six examples with different nonlinear material properties, nonlinear boundary conditions and boundary shapes are provided in order to illustrate the versatility and robustness of the LTDRM. To demonstrate the accuracy of each of the LTDRM variations, numerical results obtained from adopting LTDRM-1, LTDRM-2 and LTDRM-K are compared with analytical solutions or other published numerical solutions. To compare with an analytical steady-state solution, an LTDRM solution is regarded as the corresponding LTDRM steady-state solution when time is sufficiently large.

In all the examples, the number of collocation nodes used in the LTDRM analysis is the minimum possible, as decreasing the number of nodes below this minimum number resulted in an intolerable numerical error. It has been shown in the previous chapters that for this type of problems results obtained using constant boundary elements have little difference to those obtained with higher-order elements such as linear elements. Hence, only the results obtained with constant boundary elements are presented here.

In each iteration, all the values of the unknowns obtained in the Laplace-transformed space were numerically converted to yield results in the time domain via the Stehfest’s algorithm [87]. For all the calculations presented below, the initial condition was always selected as the initial guess for the iterations. The convergence is said to be achieved if at every nodal point

\[
\frac{|\dot{u} - u|}{\dot{u} + u} < \varepsilon,
\]

where \( \varepsilon \) is a pre-set tolerance. With \( \varepsilon \) being taken as \( 1.0 \times 10^{-3} \), convergent solutions presented here were usually obtained within 5 iterations.

4.2.1 Heat conduction in a rectangular plate

In the first example, a heat conduction problem defined on a rectangular plate with length 2 cm and width 1 cm is studied. The two lateral surfaces, \( y = 0 \)
and \( y = 1 \), are kept insulated, while the other two boundaries, \( x = 0 \) and \( x = 2 \), are subject to the prescribed constant temperature, \( u = 100^\circ C \) and \( u = 10^\circ C \), respectively. The plate is initially at \( 30^\circ C \). The thermal conductivity is chosen as \( K = 2(1 + \beta u) \, W/(cm \, ^\circ C) \) and heat capacity \( C = 10(1 + \beta u) \, J/(cm^3 \, ^\circ C) \), where \( \beta = 0.1 \). With such a combination of parameters and boundary conditions, an exact solution can be obtained.

The discretisation for this problem consists of 36 equal constant elements placed on the boundary (see Figure 4.1) and 72 internal nodes placed uniformly inside the computational domain. A comparison between the LTDRM and the exact solutions for the temperature distribution along a cross-section at \( y = 0.5 \) is shown in Figure 4.2, from which we can see an excellent agreement among them. As the thermal conductivity and heat capacity have been chosen so that the thermal diffusivity is a constant, the problem thus becomes linear in the Kirchhoff-transformed space and no iteration is required for the LTDRM-K. Consequently, it is not surprising to observe that the LTDRM-K solutions are more accurate than the other two LTDRM solutions. Although iterations are needed for LTDRM-1 and LTDRM-2, results obtained from these formulations are still quite accurate with a maximum error of around 4%.

It should be noted that the good agreement shown in Figure 4.2 is not caused by weak nonlinearities. In order to demonstrate this, differences between two exact solutions with \( \beta = 0.1 \) and \( \beta = 0 \) are given in Figure 4.3. Although the difference at \( t = 1 \) is about 15%, it increases to a maximum of more than 50% as the time is increased to \( t = 5 \), when the steady state is approached. This suggests that nonlinearity in this problem is strong and that the LTDRM deals with highly nonlinear problems quite well.

### 4.2.2 The inclusion of convective boundary condition

The second example considered has the same configuration as that of the first one, but now a convective boundary condition is included. The plate is initially at \( 50^\circ C \), in contact with a medium whose ambient temperature is abruptly raised.
Figure 4.1: A sketch of the computational domain, boundary conditions and discretisation of the boundary in example 1.
Figure 4.2: A comparison between LTDRM and exact solutions for temperature distribution along a cross-section at $y = 0.5$. 
Figure 4.3: An illustration of the effect of nonlinearities: differences between the solutions of nonlinear and linear equations.
to 200°C. Heat is then exchanged with the surrounding medium by convection across the boundary $x = 2$ with the heat transfer coefficient $h = 3 \text{ W/(cm}^2 \text{ °C)}$. Other material properties are chosen to be $K = 0.5(1 + 0.2u) \text{ W/(cm °C)}$ and $\rho c = 1 + 0.5u \text{ J/(cm}^3 \text{ °C)}$.

This example was analysed by using 30 equal constant boundary elements and 32 evenly-spaced internal nodes. Figure 4.4 shows good agreement between the results obtained from the three LTDRM variants at two transient states. Unlike the previous example, only the exact steady-state solution can be found for this particular problem. Hence, the LTDRM solutions at large time are compared with this exact steady-state solution in Figure 4.5. Once again, an excellent agreement is observed.

For this example, since $K$ is not a constant, the convective boundary condition is nonlinear as well. Therefore, nonlinearities not only occur in the governing equation but also arise in the boundary condition. To investigate the nonlinear effects from both thermal conductivity and convective boundary condition, the difference between two exact solutions at the steady state with $K = 0.5(1 + 0.2u)$ and $K = 0.5$ was calculated. It was found that the maximum difference between these two solutions was more than 30% which illustrates that the nonlinearities in this case are still quite strong.

### 4.2.3 The inclusion of nonlinear boundary conditions

In this example, we examine a problem discussed by Bialecki and Nowak [9]. As they only discussed the steady-state solution of this two-dimensional heat conduction problem, and we are at present primarily interested in examining different variations of the LTDRM in dealing with transient problems, particularly at large time limit, it is ideal for us to modify Bialecki and Nowak's problem to a transient problem. The solution to our problem should approach their steady-state solution at large time. Through this example, we aim at testing the capability of the LTDRM in dealing with the nonlinearity arising from a strong radiative boundary condition.
Figure 4.4: A comparison among LTDRM solutions for temperature distribution along a cross-section at $y = 0.5$. 
Figure 4.5: A comparison between LTDRM and exact steady-state solutions for temperature distribution along a cross-section at $y = 0.5$. 
Chapter 4: Nonlinear diffusion problems

Heat conduction occurs on a square of length 1 m. Referring to Figure 4.6, the boundaries AB and DA are kept insulated while the boundary CD is subject to a prescribed Dirichlet boundary condition with the temperature maintained at 300 K. On the boundary BC heat is exchanged with the surrounding by both convection with an ambient temperature $u_f = 500$ K and radiation with a surface temperature $u_s = 500$ K. The heat transfer coefficient and the radiation interchange factor are assumed to be $h = 10$ W/(m$^2$ K) and $R = 1$, respectively. The thermal conductivity is taken as a constant, $K = 1$ W/(m K), while the heat capacity is chosen to be $C = \rho c = 1 + 0.5u$ J/(m$^3$ K). The initial temperature is assumed to be 210 K.

Forty equally-spaced constant boundary elements were used to discretise the boundary with twenty five internal nodes being uniformly distributed inside the square. As $K$ is taken to be a constant, the Kirchhoff transformation becomes unnecessary and the LTDRM-2 is not usable, thus only the LTDRM-1 is applied in this example. In Figure 4.7, the LTDRM-1 solution at large time is compared to that published in [9], and a very good agreement is observed. According to Bialecki and Nowak, the nonlinearity arising from the radiation condition in this problem is so strong that direct iteration schemes often fail to converge; they had to use an incremental method in order to get a convergent solution. However, using the LTDRM-1, convergence was obtained within 3 to 6 iterations!

In addition, to obtain a solution at the steady state, it took only one timestep for the LTDRM-1, whereas it would require a number of timesteps for a time-domain method (e.g., a method used in conjunction with a finite-difference time-marching scheme). Moreover, if all one wants is a solution at a large time, all the intermediate results obtained from using a time-domain method would be wasted. Clearly, the LTDRM-1 has certain advantages over a time-domain method.
Figure 4.6: A sketch of the computational domain, boundary conditions and discretisation of the boundary in example 3.
Figure 4.7: Temperature along the perimeter: a comparison between LTDRM-1 solution (dots) and that of Bialecki and Nowak (solid line).
4.2.4 Nonlinear material properties and nonlinear boundary conditions

A two-dimensional heat conduction problem similar to Example 3 is considered again in this example. In order to ensure that all the LTDRM formulations be employed and a comparison among transient solutions obtained from these formulations can be made, the thermal conductivity $K$ is now assumed to be a linear function of $u$, i.e., $K = 1 + 0.25u$, instead of being a constant as was adopted in the previous example. Boundaries AB and DA are now subject to a Dirichlet boundary condition, $u = 320$ K, whilst boundary CD is thermally insulated. Along boundary BC heat is still exchanged with the environment by both convection and radiation. However, parameters for the radiation condition are altered to $u_a = 1000$ K and $R = 0.7$. The heat transfer coefficient is also changed to $h = 40$ W/(m$^2$ K). The heat capacity is taken to be $C = 100(1 + 0.5u)$ J/(m$^3$ K) and the initial condition is assumed to be $u = 300$ K. All the remaining parameters and discretisation are the same as those described in the previous example.

The transient and steady-state LTDRM solutions are compared to each other in Figures 4.8 (a–c); good agreements between the LTDRM solutions can be clearly seen. To observe the effect of nonlinearity due to the thermal conductivity, the LTDRM-1 results with $K = 1$ and $K = 1 + 0.25u$ are provided in Figure 4.9. We can easily see that the maximum temperature at the boundary BC where heat exchanged with the surrounding with the presence of both convection and radiation is almost 900 K in the case of a constant $K$, while it is only about 500 K for the other case. Also, in the case of $K = 1$, we can see a temperature jump near the joint of the surface BC and the surface AB. As a sharp contrast, the temperature increases smoothly for $K = 1 + 0.25u$ case. Thus, the results shown in Figures 4.8(a–c) and 4.9 suggest that the nonlinearity due to the temperature dependence of the thermal conductivity is strong and has been properly accounted for by the LTDRM.
Figure 4.8: (a) Temperature along the perimeter: a comparison among LTDRM solutions at $t = 10$. 
Figure 4.8: (b) Temperature along the perimeter: a comparison among LTDRM solutions at $t = 50$. 
Figure 4.8: (c) Temperature along the perimeter: a comparison among LTDRM solutions at steady-state.
Figure 4.9: An illustration of the nonlinear effect of the thermal conductivity.
4.2.5 Heat conduction of an industrial furnace

The fifth example studies heat conduction on part of a cross-section of an industrial furnace as shown in Figure 4.10. A Dirichlet boundary condition $u = 320$ K is prescribed on boundaries AB and FA and a no-heat-flux boundary condition is imposed on surfaces BC and EF. Surface CDE is convecting heat from an environment having temperature $u_f = 500$ K. Additionally, heat is also exchanged by radiation on surface CDE with the surrounding having temperature $u_a = 1000$ K. The convective coefficient and radiation interchange factor are taken to be $h = 40$ W/(m² K) and $R = 0.7$, respectively. The thermal conductivity of the furnace is assumed to be linearly dependent on the temperature as $K = 1 + 0.25u$ W/(m K).

This problem was also studied by Bialecki and Nowak [9] for the steady-state case. However, to be consistent with the present interest in applying all the LTDRM formulations to transient problems, we have altered the steady-state problem to a transient one. The heat capacity is assumed to be $\rho c = 100(1 + 0.5u)$ J/(m³ K) and the initial condition is $u = 300$ K.

To analyse this problem, 28 constant boundary elements and 7 internal nodes were used in our discretisation as shown in Figure 4.10. Transient and steady-state solutions obtained from different LTDRM formulations are given in Figures 4.11(a–b), respectively. Obviously, the LTDRM solutions are in very good agreement for both cases. The effect of the nonlinearity from the thermal conductivity is also demonstrated in Figure 4.12 where a solution with $K = 1$ is depicted against that with $K = 1 + 0.25u$. As in the previous example with a simpler geometry but similar boundary conditions, we can see a big difference between these two solutions. To verify the accuracy of the present methods, it would be ideal if we could have compared the LTDRM solutions at steady state with those reported in [9]. However, we quickly realised that the results in Figure 4.6 of [9] were incorrectly published since they were obtained with $K$ being taken to be 1 rather than $1 + 0.25u$, as reported by the authors. Therefore, we compared these results with our LTDRM-1’s and they were found to be in good agreement, as shown in Figure 4.13.
Figure 4.10: A sketch of the computational domain, boundary conditions and discretisation of the boundary in example 5.
Figure 4.11: (a) Temperature along the perimeter: a comparison among LTDRM solutions at $t = 50$. 
Figure 4.11: (b) Temperature along the perimeter: a comparison among LTDRM solutions at steady-state.
Figure 4.12: An illustration of the nonlinear effect of the thermal conductivity.
Figure 4.13: Temperature along the perimeter: a comparison between LTDRM-1 solution (dots) and that of Bialecki and Nowak (solid line).
4.2.6 Heat conduction in an irregular-shaped plate

The final example is taken from Khader and Hanna [47], who investigated a very general case of two-dimensional steady heat conduction in an irregular-shaped plate, the boundary of which consists of straight and curved lines as shown in Figure 4.14. Again, as the interest of the current study lies in transient problems, this problem was modified to include the transient effect. However, the solution published in [47] can still be used to verify the accuracy of the LTDRM solutions at large time.

Heat conduction occurs on a plate having a thermal conductivity $K = 60(1 + 0.1u)$ W/(m K) and a heat capacity $\rho c = 100(1 + 0.1u)$ J/(m$^3$ K). The plate is initially at 100 K. The boundary of the plate is subject to all the four types of boundary conditions outlined in Section 4.1. In addition, one part of the boundary is also subject to mixed boundary conditions of both convection and radiation. Eighty eight constant elements were used to discretise the boundary and twenty two internal nodes were placed inside the plate. In accordance with the node requirement in the DRM analysis, the middle point of each element was chosen as a boundary node and numbered, as shown in Figure 4.14. The boundary condition imposed on each of these elements can be tabulated in Table 1, with the first column showing the number of the elements and the second column showing the corresponding boundary condition.

Although the thermal diffusivity is a constant in this case, unlike the first example, iterations are required for the LTDRM-K because of the simultaneous presence of both convection and radiation conditions. Figures 4.15 (a–b) show the comparisons of transient solutions obtained from all variations of the LTDRM. From these figures, we can see that all LTDRM results match well with each other. As a demonstration of the accuracy of the present methods, the LTDRM-1 solutions at large time with $K = 60$ are compared to those published in [47], as shown in Figures 4.16 (a–b). Good agreements can be observed in these figures. These results indicate that the present LTDRM is accurate and capable of solving nonlinear transient diffusion problems not only for those with nonlinear
Figure 4.14: A sketch of the computational domain and discretisation of the boundary in example 6.
### Table 4.1: Boundary conditions for irregular-shaped plate problem

<table>
<thead>
<tr>
<th>Element</th>
<th>Boundary Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1–4</td>
<td>$T = 300 \text{ K}$</td>
</tr>
<tr>
<td>5–22</td>
<td>Radiation, $u_s = 500 \text{ K}, R = 0.8$</td>
</tr>
<tr>
<td>23–26</td>
<td>$q = 1000 \text{ W}$</td>
</tr>
<tr>
<td>27–33</td>
<td>$q = 0$</td>
</tr>
<tr>
<td>34–36</td>
<td>Convection, $h = 30, u_f = 300 \text{ K}$</td>
</tr>
<tr>
<td>37–48</td>
<td>Convection + radiation, $h = 20, u_f = u_s = 500 \text{ K}, R = 0.9$</td>
</tr>
<tr>
<td>49–51</td>
<td>Radiation, $u_s = 600 \text{ K}, R = 0.75$</td>
</tr>
<tr>
<td>52–59</td>
<td>$T = 600 \text{ K}$</td>
</tr>
<tr>
<td>60–68</td>
<td>$q = 0$</td>
</tr>
<tr>
<td>69–70</td>
<td>$q = 100 \text{ W}$</td>
</tr>
<tr>
<td>71</td>
<td>$q = 200 \text{ W}$</td>
</tr>
<tr>
<td>72</td>
<td>$q = 300 \text{ W}$</td>
</tr>
<tr>
<td>73–75</td>
<td>$q = 400 \text{ W}$</td>
</tr>
<tr>
<td>76–88</td>
<td>Convection, $h = 40, u_f = 350 \text{ K}$</td>
</tr>
</tbody>
</table>
Figure 4.15: (a) A comparison among LTDRM solutions for the temperature distribution along the perimeter at time $t = 100$. 
Figure 4.15: (b) A comparison among LTDRM solutions for the temperature distribution along a cross-section at $y = 0.5$ at time $t = 100$. 
Figure 4.16: (a) A comparison between LTDRM-1 solution and that of Khader and Hanna for the temperature distribution at steady state along the perimeter.
Figure 4.16: (b) A comparison between LTDRM-1 solution and that of Khader and Hanna for the temperature distribution at steady state along a cross-section at $y = 0.5$. 

LTDRM-1 solution; _____ Khader and Hanna's solution
material properties and nonlinear boundary conditions, but also for those defined on irregular domains as well.

4.3 Conclusions

In this chapter, the LTDRM is extended to cover nonlinear transient diffusion problems with temperature-dependent material properties, nonlinear boundary conditions, and regular and irregular boundary shapes. Two approaches, with and without using the Kirchhoff transformation, are used to formulate time-free and boundary-only integral equations. The absence of domain integration and time marching in the solution procedure permits the present method to be used to obtain the solution at any desired observation time with a lesser computational cost compared with time-domain methods, especially when a solution at large time is required. In addition, it is shown that all the LTDRM formulations possess good convergence properties in obtaining accurate numerical results.

Through various examples, the LTDRM is shown to handle well a variety of boundary conditions and geometries. Although the thermal conductivity used in the present study is only of a linear variation with temperature, a more complex variation can be modelled by a piecewise linear representation for the conductivity curve as described in References [6, 51], allowing the present method to be modified to account for any kind of the thermal conductivity.

Among different LTDRM formulations presented, it is shown that numerical results obtained from the direct formulation are similar to those obtained from the Kirchhoff transformation. The direct formulation has advantages over the Kirchhoff transformation in the sense that the terms giving rise to domain integrals, e.g., heat-source terms, if they exist, can be taken care of easily using the technique given in Chapter 3. However, in some special cases with the internal heat source term being a constant or a harmonic function of spatial variables, the Kirchhoff transformation is still applicable (see the Appendix in Reference [47]). The Kirchhoff transformation also remains beneficial in some other cases.
such as when the thermal diffusivity is constant and only Dirichlet and Neumann boundary conditions are prescribed; iterations are not necessary for the Kirchhoff-transform formulation in these cases, whereas they are always required for a direct formulation.
Chapter 5

Concluding Remarks

In this thesis, a Laplace Transform Dual Reciprocity Method (LTDRM) is proposed and applied to find solutions of transient diffusion equations. A time-free and boundary-only integral formulation is the result of the dual reciprocity method being used in conjunction with the Laplace transform. Consequently, the dimension of the problem under consideration is virtually reduced by two. More precisely, a solution at any specific time can be attained without a step-by-step calculation in the time domain and computation of domain integrals.

Several examples of linear transient diffusion problems are presented and numerical solutions obtained show a very good agreement with the corresponding analytical solutions for small as well as large observation time with the same efficiency and accuracy.

A study concerning the efficiency of the numerical inversion scheme for the Laplace transform, reveals that accurate results in the time domain are obtained via the Stehfest’s algorithm with only six terms of solutions needed in the Laplace-transformed space. This makes the inversion process thrice faster than the one originally suggested by Stehfest.

An application of the LTDRM is then extended to nonlinear transient diffusion problems. Due to nonlinearities, a linearisation of the governing equation is therefore necessary. If boundary conditions are nonlinear, a linearisation is also required.
Two selected iteration schemes, i.e. direct iteration and Taylor series expansion schemes, are investigated in the analyses of transient diffusion problems with nonlinear source terms. The convergence rate associated with the Taylor series expansion scheme is found to be faster than that associated with the direct iteration scheme. However, if the direct iteration scheme is used under relaxation, the convergence rate is comparable to that of the Taylor series expansion scheme. On the other hand, unlike the Taylor series expansion approach, the direct iteration scheme has difficulty when the source terms are of strong nonlinearity. Although the Taylor series expansion scheme is shown to be better than the direct iteration scheme for diffusion equations with nonlinear source terms, the direct iteration scheme is still useful for some other cases such as diffusion equations with nonlinear material properties.

Four examples are provided as test examples, including a microwave heating problem with a nonlinear source term being a power function of temperature, and a spontaneous ignition problem where a reaction-heating term varies exponentially with temperature. The LTDRM is also used to solve a time-dependent version of the Liouville equation. All the numerical results obtained compared very well with the corresponding analytical and other published numerical results.

The LTDRM is further extended to the solution of nonlinear diffusion problems with temperature-dependent material properties and nonlinear boundary conditions. Due to a special form of nonlinearity, the Kirchhoff transform can be used to simplify a governing equation into a standard diffusion equation before a linearisation of this equation is carried out and the LTDRM is applied. Another approach is to apply the LTDRM directly to the linearised governing equation. Two integral formulations are obtained from this approach; one involves an approximation of first-order spatial derivatives only while the other involves an approximation of both first- and second-order spatial derivatives.

All three formulations are used to analyse six examples with different nonlinear material properties, nonlinear boundary conditions and boundary shapes. It is found that results obtained from these three formulations are similar. How-
ever, there are advantages and disadvantages associated with each formulation.

The direct approach will always require iterations, which are not needed for the Kirchhoff-transform approach in the case that the thermal diffusivity is constant and only Dirichlet and Neumann boundary conditions are prescribed. However, if the terms that give rise to the domain integrals, e.g., heat source terms, appear in the governing equation, they can be taken care of easily by the direct approach. On the other hand, the Kirchhoff transformation is only applicable for some special cases with the internal heat source term being a constant or a harmonic function of spatial variables.

From all the numerical results presented in this thesis, the LTDRM is shown to produce accurate results for linear diffusion problems and it is believed that the LTDRM possesses good convergence properties in obtaining accurate results for nonlinear problems. In addition, steady-state and transient solutions can be obtained with the same formulation. Moreover, solutions at large and small time can also be obtained with the same efficiency and accuracy. Thus, the LTDRM can be used as a powerful and fast algorithm for the solution of diffusion problems.

For future work, we may extend the LTDRM formulation to transient problems governed by convection-diffusion equations with a constant or variable velocity field. In addition, we may try to investigate the feasibility of applying the LTDRM to transient scalar wave propagation problems or hyperbolic heat conduction problems.

From the mathematical point of view, more theoretical studies are required in order to support numerical studies related to the convergence of the solution of a linearised system to the true solution of the original nonlinear differential system. However, this could be quite involved but well rewarding.
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Publications of the author


