This is to certify that the

thesis entitled

EMPIRICAL TIME STEP EQUATIONS FOR THE RADIAL FIELD PROBLEMS

presented by

Wie Tjung Tan

has been accepted towards fulfillment
of the requirements for

M.S. degree in Agricultural Engineering

Larry Hogerlund
Major professor

Date 8-4-95

EMPIRICAL TIME STEP EQUATIONS FOR THE RADIAL FIELD PROBLEMS

By

Wie Tjung Tan

A THESIS

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

MASTER OF SCIENCE

Agricultural Engineering

Department of Agricultural Engineering

1995

ABSTRACT

EMPIRICAL TIME STEP EQUATIONS FOR THE RADIAL FIELD PROBLEM

By

Wie Tjung Tan

A variety of time-dependent problems in science and engineering are governed by a class of partial differential equations called parabolic. Applying a numerical procedure changes the space and time-dependent partial differential equation into a time-dependent system of ordinary differential equations. That can be solved using numerical integration methods in time. This process requires a time step value that produces an accurate result.

Empirical time step equations were developed for the radial field problem using numerical experimentation. The study was limited to radial problems consisting of a solid disk, solved using linear elements, a lumped formulation for the capacitance matrix and the single step integration methods in time.

The empirical time step equations developed in this study were

Forward difference method:

$$\Delta t = 3.91 \frac{N^{-2.13}}{\lambda_1}$$

Central difference method:

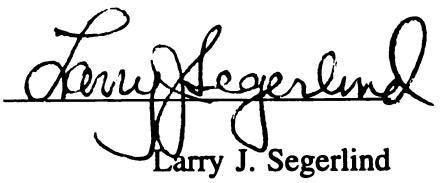
$$\Delta t = 5.28 \frac{N^{-1.66}}{\lambda_1}$$

Backward difference method:

$$\Delta t = 0.12\frac{N^{-1.81}}{\lambda_1}$$

The time step equations were validated using eight different problems involving a combination of materials and boundary conditions.

Approved:



Larry J. Segerlind
Major Professor

Robert von Bernuth
Chair Person

To my mom Jut Kioe

ACKNOWLEDGMENT

A very special thank to Dr. Segerlind for the time spent guiding and correcting my thesis. Everything that he has done to me, I greatly appreciated. Thank to Dr. Bralts and Dr. Martin as my committee members.

A great appreciation to all of my friends at Michigan State University and the Agricultural Engineering Department especially, that help me finish my work and study at Michigan State University.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER ONE

INTRODUCTION

A variety of time-dependent problems in science and engineering are governed by a class of partial differential equations called parabolic. These equations are also referred to as the diffusion equations. These equations have the general form

$$c \frac{\partial U}{\partial t} = k \nabla.(\nabla U) + Q \qquad (1\text{-}1)$$

where c and k are material coefficients and U is the unknown variable: temperature, moisture content, pressure head, and so forth. The diffusion equation governs several biosystem processes including the heating and cooling of food products, grain drying, water infiltration through the soil, and salt movement into and through the soil. The movement of odors from production and waste facilities through the air is also governed by the diffusion equation. The derivation of (1-1) is included in almost every engineering and mathematics book dealing with the solution of the diffusion equations. Powers (1987), Ozisik (1980), Pakantar (1980), and Churchill and Brown (1987) are a few examples.

Applying a numerical procedure such as the finite element or the finite difference method to (1-1), changes the space and time-dependent partial differential equation into a time-dependent system of ordinary differential equations. This conversion is discussed in books dealing with the numerical solution of partial differential equations (Narasimhan, 1978, Segerlind, 1984, and Smith, 1985). The system of ordinary differential equations has the general form

$$[C]\frac{\partial\{U\}}{\partial t} + [K]\{U\} - \{F\} = \{0\} \qquad (1\text{-}2)$$

where [C] is the global capacitance matrix, [K] is the global stiffness matrix, and {F} is the forcing function.

Finite element or finite difference methods can be used to solve (1-2) in the time domain. Although the finite element method has clear advantages over the finite difference method in the space domain, (1-1), this advantage does not extend to the time domain, Segerlind (1984). There are many schemes available for solving (1-2). Many criteria are used to test these schemes including stability, oscillation, and accuracy. Despite the fact that many authors have presented and discussed solution procedures for the system of ordinary differential equations in (1-2), there is a lot of art and experience involved in selecting the proper scheme and time step to obtain an accurate solution, particularly in two- and three-dimensional problems.

Mohtar (1994) has pioneered the development of empirical equations that can be used to estimate the time step required to solve (1-2) accurately when using any one of the three single step methods; Euler's forward difference method, the central difference method and the backward difference method. Mohtar developed equations that included the lowest eigenvalue as a parameter. Equations were developed for the one-dimensional form of (1-1) and the two-dimensional case when the grid was restricted to square elements. Each of the equations given by Mohtar had the general form

$$\lambda_1 \Delta t = C\, N^{b} \tag{1-3}$$

where λ_1 is the lowest eigenvalue for the problem being solved, N is the number of nodes in the region, C and b are empirically determined coefficients and Δt is the time step.

The general objective of this study was to extend the work started by Mohtar (1994) to the diffusion equation in radial coordinates

$$D_r \frac{\partial^2 U}{\partial r^2} + \frac{D_r}{r} \frac{\partial U}{\partial r} = D_t \frac{\partial U}{\partial t} \tag{1-4}$$

This study can be considered a preliminary step to a study of axisymmetric shapes.

CHAPTER TWO

REVIEW OF LITERATURE

A complete literature search of published work on the numerical solution of partial differential equations and their implementation is probably impossible. Among the extensive published resources on the subject, there are at least two questions that remain unanswered. These questions are: "How did the investigators who developed the methods come up with the time step value they used in their numerical solution?" and "Do the stability, and oscillation criteria for selecting a time step ensure an accurate solution?" Although the numerical solution of (1-1) and (1-2) are presented in numerous books and technical articles, Mohtar (1994) presented a review of literature that shows these two questions have not been answered. Mohtar's research was directed at answering these questions for specific applications of the diffusion equation. This research continues by considering the radial field problem. The review of literature given here discusses a few general publications related to solving (1-1) and (1-2) and the work done by Mohtar (1994).

The numerical solution of the system of ordinary differential equations have been discussed for several years, Zienkiewicz (1971) and Segerlind (1976). The finite element and finite difference methods for solving time-dependent field problems have been explained in finite element books or technical papers. Allaire (1985) discussed solving the one-dimensional problem using Euler's single step method. Euler's method was also used to solve a non-dimensional form of the one-dimensional diffusion equation by Smith

(1985). Three node linear triangular elements were used to solve heat transfer problems, Jaluria and Torrance (1986). Segerlind (1984) discusses using the four node quadrilateral elements. The error bounds for different orders of a finite element method solution are given by Shih (1984).

Some authors have used a mathematical approached to define the time step value (Gear, 1971, Stoer and Bulivsch, 1980, Myers, 1977 and Reddy, 1984), and/or computer programs (Pakantar, 1991). Ortega (1990), Rushton and Tomlinson (1971), and Henrici (1977) developed various types of error procedures which were associated with the time step values. Williams (1980) and Fried (1979) discussed stability requirements for the numerical solution of partial differential equations. Haghighi and Segerlind (1988) used Maadooliat's (1983) non-oscillation criteria to solve the coupled heat and mass transfer equations in finite element method. Irudayaraj (1991) and Irudayaraj et al., (1990) used a stability criteria for selecting the time step value in a coupled heat and mass transfer problem. Segerlind and Scott (1988) defined the time step estimate using a non-oscillation criteria. Maadoliat (1983) and Segerlind (1984) discussed numerical solutions for the physical reality and oscillations in finite element problems. In fluid flow, Peraire et al., (1988) defined a Courant stability criteria. Cleland and Earle (1984) solved food freezing problems using six different finite difference methods. They reduced the time step and resolved the problem until the calculated results did not change.

Mohtar (1994) was among the first researchers to define the time step values based on an experimental accuracy criteria. He investigated the one-dimensional problem and a two-dimensional grid with square elements. The general procedure developed by Mohtar was to (a) define a measure of the error, (b) solve a problem using several different

values of the time step (Δt) and several subdivisions of the problem in space, (c) plot the error value against the number of nodes and select the time step value, Δt, that produced a specified error, (d) empirically fit an equation to the time step data using the lowest eigenvalue as a basic parameter, and (e) checked the equations by solving a different set of problems.

In one-dimensional problems, Mohtar (1994) defined the accuracy ratio as:

$$e = \frac{\sum_{j=1}^{n}\sum_{i=1}^{m} |NODE_{ij} - APDE_{ij}|}{\sum_{j=1}^{n}\sum_{i=1}^{m} |AODE_{ij} - APDE_{ij}|} \tag{2-1}$$

where NODE is the numerical solution for the system of ordinary differential equations, APDE is the analytical solution for the partial differential equation, AODE is the analytical solution for the system of ordinary differential equations, and n and m are the number of sampling points in the space and time domain. The dynamic time step equations developed by Mohtar for three single step methods are

Forward Difference:

$$\Delta t = 0.27\frac{N^{-1.6}}{\lambda_1} \tag{2-2}$$

Central Difference:

$$\Delta t = 1.13\frac{N^{-1.18}}{\lambda_1} \tag{2-3}$$

Backward Difference:

$$\Delta t = 30.6\frac{N^{-3.91}}{\lambda_1} \tag{2-4}$$

In each equation, Δt is the time step value, N is the number of free nodes and λ_1 is the lowest eigenvalue for the system. The time step estimates were validated using four different problems; a sine wave variation and a linear variation with the boundary temperatures known and two problems with derivative boundary conditions. The problems were solved using fractions or multiples of the calculated time step. Time step values of one-half, two, and three times Δt were used along with the ratio

$$e = \frac{\sum_{i=1}^{m} NODE_i}{\sum_{i=1}^{m} APDE_i} \tag{2-5}$$

The accuracy ratio for $\Delta t/2$ and Δt were equivalent. The results for multiples of two and greater were less accurate than the results for Δt.

In two dimensional problems, Mohtar (1994) defined the accuracy ratio as:

$$e = \frac{\sum_{j=1}^{n}\sum_{i=1}^{m} \frac{|NODE_{ij}-APDE_{ij}|}{NODE_{ij}}}{mn} \tag{2-6}$$

where NODE is the numerical solution for the system of ordinary differential equations, APDE is the analytical solution for the partial differential equation, m is the number of sampling points in the space domain, and n is the number of sampling points in the time domain. The sampling points in the time domain were at 9.5, 19, 28.6, 38.1, 47.6, 57.1,

66.7, 76.2, 85.7 and 95.2 percent of the time to steady state.

The accuracy ratio used with the two-dimensional problem was different from the accuracy ratio, (2-1), used with one-dimensional problems because the analytical solution of the system of ordinary differential equations, AODE, became too difficult to evaluate. Mohtar (1994) restricted the two-dimensional study to square elements and square grids because he wanted to compare the finite element and finite difference formulations in space. Using (2-5) and a five percent error in the calculated values when compared to the analytical solution of the partial differential equation, Mohtar developed the empirical time step estimates for a two-dimensional square grid given below. Equations (2-7) through (2-9) are for the finite difference formulation in space while the next three are for the finite element method in space.

Forward Finite Difference:

$$\Delta t = 1.19 \frac{N^{-1.01}}{\lambda_1} \tag{2-7}$$

Central Finite Difference:

$$\Delta t = 1.6 \frac{N^{-0.55}}{\lambda_1} \tag{2-8}$$

Backward Finite Difference:

$$\Delta t = 0.05 \frac{N^{-0.1}}{\lambda_1} \tag{2-9}$$

Galerkin Forward Difference:

$$\Delta t = 1.8\frac{N^{-1.04}}{\lambda_1} \tag{2-10}$$

Galerkin Central Difference:

$$\Delta t = 1.6\frac{N^{-0.55}}{\lambda_1} \tag{2-11}$$

Galerkin Backward Difference:

$$\Delta t = 0.05\frac{N^{-0.1}}{\lambda_1} \tag{2-12}$$

The equations are valid when the number of nodes used with the finite difference formulation in space is equal to or greater than nine. The equations are valid for the finite element method in space, when the number of nodes is equal to or greater than twenty five.

CHAPTER THREE

OBJECTIVES

The general objective of this study was to developed empirical equations for calculating the time step required to numerical solve the system of ordinary differential equations related to the time-dependent radial field problem. The specific objectives in this study were to develop an empirical time step estimate for the three single step integration methods that satisfy an accuracy criteria and the stability requirements and validate the time step equations by solving a different set of problems.

This study was limited to

-the linear radial element

-three single step integration methods: forward difference, central difference, and backward difference

-using the finite element method in space

-use a lumped formulation for the capacitance matrix.

The time step equations were placed in the same form as used by Mohtar (1994)

$$\Delta t = \frac{C}{\lambda_1 N^a} \tag{3-1}$$

where Δt is the time step value, λ_1 is the smallest eigenvalue of the system, N is the number of nodes used to solve the problem, and a and C are parameters to be determined.

CHAPTER FOUR

THE RADIAL FIELD EQUATION

The one-dimensional time dependent field equation for radial coordinates is

$$D_r \frac{\partial^2 U}{\partial r^2} + \frac{D_r}{r}\frac{\partial U}{\partial r} = D_t \frac{\partial U}{\partial t} \tag{4-1}$$

where U is the pressure in flow problems, temperature in heat conduction problems, and concentration in solute transport problems, D_r and D_t are material properties, and r is the radial distance. The analytical solution of the left side of (4-1) is an infinite series solution involving Bessel functions (Myers, 1971, Boyce and Diprima, 1986, Ozisik, 1980, Kreyszig, 1988, and Zill, 1993). The general form of the steady state differential equation in radial coordinates is

$$\frac{d^2 u}{dr^2} + \frac{1}{r}\frac{du}{dr} + u = 0 \tag{4-2}$$

and a series solution is obtained by assuming

$$u(r) = a_0 + a_1 r + a_2 r^2 + \ldots = \sum_{n=0}^{\infty} a_n r^n \tag{4-3}$$

Using the method of Frobenius gives

$$u(r) = r^s \sum_{n=0}^{\infty} a_n r^n \tag{4-4}$$

where s is a parameter to be determined. The first and the second derivatives of (4-4) are

$$\frac{du}{dr} = \sum_{n=0}^{\infty} (n + s)a_n r^{n+s-1} \tag{4-5}$$

and

$$\frac{d^2u}{dr^2} = \sum_{n=0}^{\infty} (n + s)(n + s - 1)a_n r^{n+s-2} \tag{4-6}$$

Substituting (4-4), (4-5), and (4-6) into (4-2) gives

$$\sum_{n=0}^{\infty} (n+s)(n+s-1)a_n r^{n+s-1} + \sum_{n=0}^{\infty} (n+s)a_n r^{n+s-1} + \sum_{n=0}^{\infty} a_n r^{n+s+1} = 0 \tag{4-7}$$

Equation (4-7) combines to give a Bessel function of first kind of order zero (Myers, 1971)

$$J_0(r) = \sum_{n=0}^{\infty} \frac{(-1)^n r^{2n}}{2^{2n}(n!)^2} = 1 - \frac{r^2}{2^2.1} + \frac{r^4}{2^4(2!)^2} - \ldots \tag{4-8}$$

and a Bessel function of second kind of order zero

$$Y_0(r) = \frac{2}{\pi}\left[J_0(r)\left(\ln\frac{r}{2}+\gamma\right) + \sum_{n=1}^{\infty} \frac{(-1)^{n-1}h_n}{2^{2n}(n!)^2} r^{2n}\right] \tag{4-9}$$

where h = 0, 1, 2, ... and γ = 0.57722 is called the Euler-Mascheroni constant. The solution of (4-2) is a linear combination of (4-8) and (4-9) giving

$$u = AJ_0(r) + BY_0(r) \tag{4-10}$$

where A and B are parameters to be determinate using the boundary conditions.

Bessel functions of integer order can also be developed for the first and the second kinds of order k

$$J_k(r) = \sum_{n=0}^{\infty} \frac{(-1)^n r^{2n+k}}{2^{2n+k} n!(n+k)!} \tag{4-11}$$

$$Y_k(r) = \frac{2}{\pi} J_k(r)\left(\ln \frac{r}{2} + \gamma\right) + \frac{r^k}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^{n-1}(h_n + h_{n+k})}{2^{2n+k} n!(n+k)!} r^{2n}$$

$$- \frac{r^{-k}}{\pi} \sum_{n=0}^{k-1} \frac{(k-n-1)!}{2^{2n-k} n!} r^{2n} \tag{1-12}$$

where k is an integer. The general solution in integer order gives

$$u = AJ_k(r) + BY_k(r) \tag{4-13}$$

The solution of equation (4-2) can also be written using the general Bessel equation

$$U = AJ_0(\lambda r) + BY_0(\lambda r) \tag{4-14}$$

where λ is a positive number.

The solution of (4-1) that includes the transient term is more involved than discussed above. The solution has eigenvalues as well as the Bessel functions. Since the Bessel functions are defined by infinite series, the analytical solution to (4-1) is really a numerical solution because of the need to evaluate the Bessel functions and the summation of an infinite series.

4.1 THE STEP CHANGE PROBLEM

The step change problem in radial coordinates contains all the frequency components and has the shortest time to steady state. The boundary and initial conditions for the step change problem are $U(r_0,t) = U_0$, and $U(r,0) = U_i$, Figure 4.1. Equation (4-1) is usually written as

$$\frac{\partial^2 U}{\partial r^2} + \frac{1}{r}\frac{\partial U}{\partial r} = \frac{1}{\alpha}\frac{\partial U}{\partial t} \tag{4-15}$$

where α = Dr/Dt. The boundary conditions in Figure 4.1 are not homogeneous, therefore, a new variable $T = U - U_0$ can be defined and (4-15) becomes

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{4-16}$$

The boundary and initial condition change to $T(0,t) < \infty$, $T(r_0,t) = 0$, and $T(r,0) = U_i - U_0$. The analytical solution to (4-15) for the step change problem, Myers (1971), is

$$\frac{U(r,t)-U_0}{U_i-U_0} = 2\sum_{m=1}^{\infty} \frac{J_0(\lambda_m r)e^{-(\lambda_m r_0)^2(\alpha t/r_0^2)}}{(\lambda_m r_0)J_1(\lambda_m r_0)} \tag{4-17}$$

where U_i is the initial temperature, U_0 is outside surface temperature, α is the thermal diffusivity for thermal problems, t is time, and the $(\lambda_m r_0)$ satisfy $J_0(\lambda_m r_0) = 0$.

4.2 NUMERICAL SOLUTION IN SPACE

Equation (4-1) can be solved in space using the finite element or finite difference methods to produce a system of ordinary differential equations in time

$$[C]\frac{\partial\{U\}}{\partial t} + [K]\{U\} - \{F\} = \{0\} \tag{4-18}$$

where [C] is the global capacitance matrix, [K] is the global stiffness matrix, and {F} is the forcing function (Segerlind, 1984). The finite element procedure was used in this study for two reasons. First, the global matrix [K] remains symmetric. Second, the singularity that occurs at r = 0 for the finite difference method does not occur for the

finite element method.

The finite element matrices for one-dimensional radial element are

-Lumped capacitance matrix:

$$[C^{(e)}] = \frac{2\pi L D_t}{6}\begin{bmatrix} R_i+2\bar{r} & 0 \\ 0 & R_j+2\bar{r} \end{bmatrix} \tag{4-19}$$

-Stiffness matrix:

$$[K^{(e)}] = \frac{2\pi \bar{r} D_r}{L}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{4-20}$$

where L is the element length, R_i is the radial distance of the left node of the element, R_j is the radial distance to the right node, and $2\bar{r} = R_i + R_j$

The general form of the solution of the system of ordinary differential equations for the single step methods is

$$([C]+\theta\Delta t[K])\{U\}_2 = ([C]-(1-\theta)\Delta t[K])\{U\}_1 + \Delta t(\theta\{F\}_1+(1-\theta)\{F\}_1) \tag{4-21}$$

where $\theta = 0$ gives the Euler's forward difference method, $\theta = 0.5$ gives the central difference method, and $\theta = 1$ gives the backward difference method, Segerlind (1984).

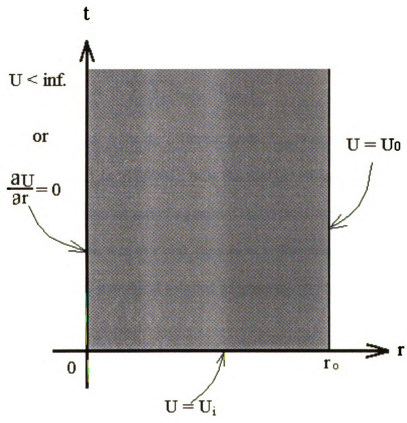


Figure 4.1. Mathematical description for the step change problem

CHAPTER FIVE

METHODOLOGY AND EMPIRICAL EQUATIONS

Accurate solutions were the main goal in this study. The differences between two solutions was evaluated using the L_1 norm

$$e = \sum_{j=1}^{n} \sum_{i=1}^{m} \left| T_{Cal_{ij}} - T_{Ref_{ij}} \right| \tag{5-1}$$

where T_{Cal} are the solution values from the different grids, T_{Ref} is a reference solution for a fine grid (41 nodes) and small Δt (0.00004), m is the number of sampling points in the space domain, and n is the number of sampling points in the time domain. The only node investigated in the space domain was at r = 0, thus m = 1. The time step and reference values were developed using the numerical solution of equation (4-21). The time to steady state was approximated as:

$$t_{ss} = \frac{4}{\lambda_1} \tag{5-2}$$

where λ_1 is the lowest eigenvalue of the system. The lowest eigenvalue can be evaluated using the forward iteration method once [C] and [K] are known, Bathe and Wilson (1976). The calculated value can also be obtained from the analytical solution. For the radial step change problem, λ_1 is 5.76. Equation (5-2) is obtained from the first term of the analytical solution which is $e^{-\lambda t}$. As t increases the value of e will be close to zero or when $\lambda_1 t = 4$, $e^{-4} = 0.018$ and approximately 98 percent of the transient has been completed.

Numerical experiments were conducted to develop the time step estimate for the radial element problems. Each experiment included the numerical solution of the system of ordinary differential equations, using a lumped finite element formulation. The unit step change problem on a solid disk was used to generate the data. The disk had a radius of one and D_r and D_t were also taken as unity. The time to steady state was divided into 12 intervals which were placed at 10, 15, 20, 25, 30, 35, 40, 45, 55, 65, 75, and 85 percent of the time to steady state. The experiment was repeated four times using four different uniform grids. The grids had 6, 11, 16, and 21 nodes, respectively. The calculated values, T_{Cal}, were obtained using Δt values of 0.00004, 0.00005, 0.00008, ..., 0.04 seconds in each grid. The reference values (T_{Ref}) were developed using the smallest Δt and a grid with 41 nodes. The reference values are given in Table 5.1. The L_1 norm was considered accuracy, when the error level was set at five percent or less of the L_1 norm for the 41 grid region. The L_1 norm for each grid are shown in Figures 5.1, 5.2, and 5.3 for the three different integration methods. Tables 5.2, 5.3, and 5.4 contain the calculated time step values for each integration method.

The L_1 norm as related to the number of nodes is presented in Figures 5.1 through 5.3. The time step prediction equations were developed by fitting the L_1 norm of each grid to the regression equation as:

$$\lambda_1 \Delta t = C N^a \tag{5-3}$$

where Δt is 1.05 times the L_1 norm value of the smallest time step of each grid, N is the number node of the element, C and a are the parameters to be determined and constants, and λ_1 is the smallest eigenvalue in radial element, which is 5.76. Table 5.5 shows the

Table 5.1. The reference values for the step change problem

t, seconds	u(0,t)
0.04	0.9961568
0.08	0.9176823
0.12	0.7731668
0.16	0.6272756
0.20	0.5018747
0.24	0.3994882
0.28	0.3173846
0.36	0.1999947
0.44	0.1259605
0.52	7.932691E-2
0.60	4.995764E-2
0.68	3.146178E-2

Time to steady state is 0.80 seconds

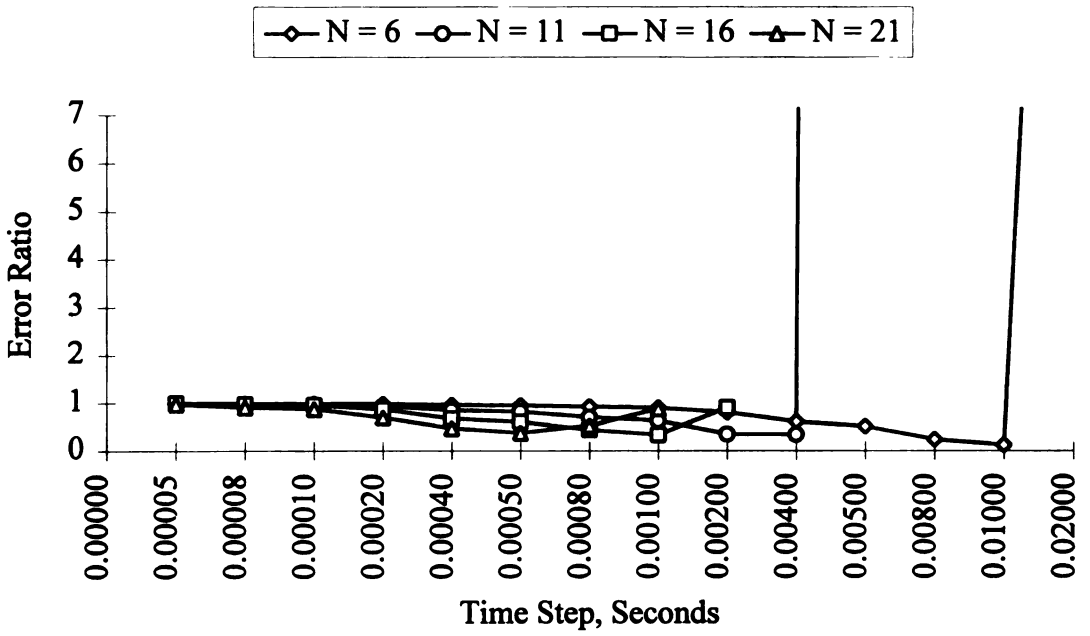


Figure 5.1. The error ratio for the forward difference method

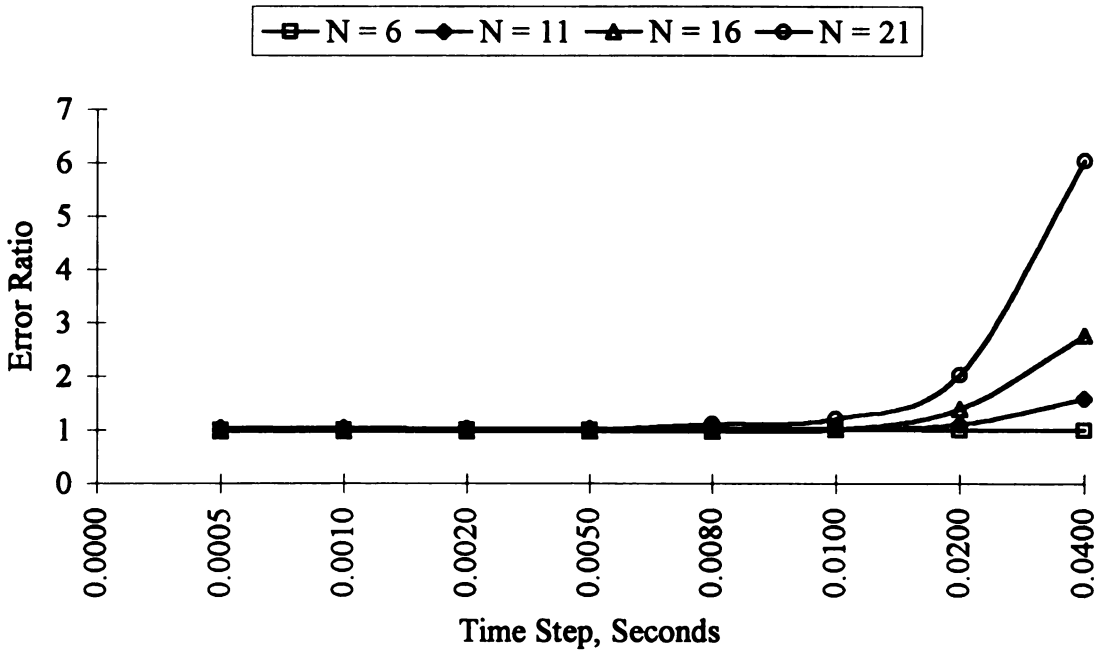


Figure 5.2. The error ratio for the central difference method

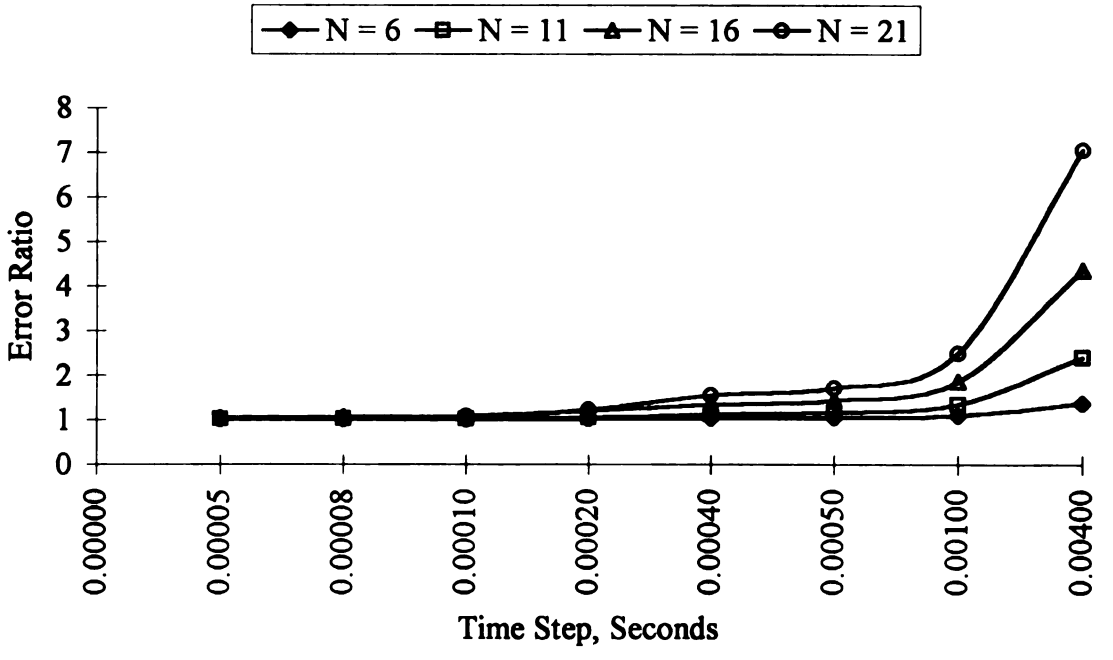


Figure 5.3. The error ratio for the backward difference method

Table 5.2. Calculated time step values for the forward difference method

Δt, sec	0.000040	0.000100	0.000500	0.001000	0.002000	0.004000	0.005000	0.010000	0.020000
6 Nodes	0.988475	0.988529	0.988966	0.989510	0.990619	0.992900	0.994068	1.000000	1.000000
	0.906691	0.906723	0.907249	0.907897	0.909238	0.912081	0.913589	0.922136	1.000000
	0.774136	0.774072	0.774120	0.774147	0.774207	0.774299	0.774327	0.774207	0.884644
	0.637097	0.636961	0.636644	0.636205	0.635322	0.633485	0.632528	0.627331	0.763880
	0.515829	0.515662	0.515173	0.514518	0.513205	0.510520	0.509148	0.501990	0.663309
	0.414725	0.414550	0.414008	0.413289	0.411851	0.408939	0.407463	0.399898	0.586315
	0.332437	0.332267	0.331732	0.331025	0.329615	0.326772	0.325337	0.318054	0.530984
	0.212937	0.212792	0.212339	0.211740	0.210548	0.208155	0.206955	0.200911	0.473959
	0.136239	0.136125	0.135769	0.135299	0.134364	0.132492	0.131555	0.126863	0.472806
	8.71E-02	8.71E-02	8.68E-02	8.64E-02	8.57E-02	8.43E-02	8.36E-02	8.01E-02	0.515365
	5.57E-02	5.57E-02	5.55E-02	5.52E-02	5.47E-02	5.37E-02	5.31E-02	5.06E-02	0.595822
	3.57E-02	3.56E-02	3.55E-02	3.53E-02	3.49E-02	3.42E-02	3.38E-02	3.19E-02	0.713079
11 Nodes	0.994330	0.994385	0.994850	0.995435	0.996614	0.998892	1.000000	Unstable	Unstable
	0.915615	0.915684	0.916312	0.917115	0.918768	0.922259	0.893775		
	0.774550	0.774519	0.774498	0.774473	0.774405	0.774199	0.693771		
	0.630701	0.630609	0.630189	0.629665	0.628595	0.626369	0.474094		
	0.506060	0.505945	0.505369	0.504652	0.503203	0.500249	0.237749		
	0.403772	0.403653	0.403045	0.402289	0.400769	0.397693	-4.32E-02		
	0.321462	0.321349	0.320764	0.320038	0.318580	0.315644	-0.41934		
	0.203355	0.203262	0.202777	0.202177	0.200974	0.198560	-1.83506		
	0.128561	0.128489	0.128114	0.127649	0.126719	0.124858	-5.49919		
	8.13E-02	8.12E-02	8.09E-02	8.06E-02	7.99E-02	7.85E-02	-15.4773		
	5.14E-02	5.13E-02	5.11E-02	5.09E-02	5.04E-02	4.94E-02	-42.9804		
	3.25E-02	0.032447	3.23E-02	3.21E-02	3.18E-02	3.10E-02	-118.999		

Table 5.2. Calculated time step values for the forward difference method (continued)

Δt, sec	0.000040	0.000100	0.000500	0.001000	0.002000	0.004000	0.005000	0.010000	0.020000
16 Nodes	0.995428	0.995513	0.995991	0.996588	0.997841	1.000323	Blank regions indicate		
	0.917002	0.917124	0.917776	0.918602	0.920311	31850.94	unstable results.		
	0.773915	0.773942	0.773911	0.773864	0.773757	8.68E+09			
	0.628808	0.628776	0.628347	0.627801	0.626693	4.60E+14			
	0.503669	0.503614	0.503034	0.502303	0.500832	1.50E+19			
	0.401287	0.401226	0.400618	0.399854	0.398321	3.98E+23			
	0.319076	0.319016	0.318433	0.317702	0.316238	9.66E+27			
	0.201367	0.201317	0.200836	0.200234	0.199031	5.05E+36			
	0.127013	0.126974	0.126602	0.126138	0.125210				
	0.080107	8.01E-02	7.98E-02	7.95E-02	7.88E-02				
	5.05E-02	5.05E-02	5.03E-02	5.00E-02	4.95E-02				
	3.19E-02	3.18E-02	3.17E-02	0.031526	3.12E-02				
21 Nodes	0.995838	0.995907	0.996391	0.996996	1.445693				
	0.917455	0.917544	0.918204	0.919039	-3.6E+10				
	0.773629	0.773610	0.773577	0.773525	-2.5E+18				
	0.628097	0.628017	0.627586	0.627037	-6.8E+25				
	0.502806	0.502703	0.502123	0.501392	-1.4E+33				
	0.400409	0.400302	0.399696	0.398932					
	0.318243	0.318141	0.317561	0.316831					
	0.200685	0.200600	0.200123	0.199522					
	0.126487	0.126421	0.126052	0.125590					
	7.97E-02	7.97E-02	0.079392	7.90E-02					
	5.02E-02	5.02E-02	5.00E-02	4.98E-02					
	3.17E-02	3.16E-02	3.15E-02	0.031315					

Table 5.3. Calculated time step values for the central difference method

Δt, sec	0.000040	0.000500	0.001000	0.004000	0.005000	0.008000	0.010000	0.020000	0.040000
6 Nodes	0.988442	0.988422	0.988422	0.988392	0.988375	0.988294	0.988212	0.987352	0.984410
	0.906621	0.906605	0.906614	0.906709	0.906769	0.907025	0.907263	0.909302	0.915081
	0.774088	0.774081	0.774089	0.774160	0.774207	0.774403	0.774586	0.776169	0.784957
	0.637065	0.637065	0.637071	0.637095	0.637113	0.637184	0.637250	0.637808	0.640029
	0.515806	0.515811	0.515815	0.515812	0.515813	0.515811	0.515811	0.515796	0.515430
	0.414703	0.414711	0.414715	0.414699	0.414693	0.414660	0.414630	0.414374	0.413328
	0.332416	0.332425	0.332429	0.332409	0.332401	0.332357	0.332317	0.331982	0.330541
	0.212917	0.212927	0.212930	0.212911	0.212903	0.212860	0.212822	0.212498	0.211181
	0.136222	0.136231	0.136234	0.136219	0.136212	0.136178	0.136147	0.135887	0.134842
	8.71E-02	8.71E-02	8.71E-02	8.71E-02	8.71E-02	0.087102	8.71E-02	8.69E-02	8.61E-02
	5.57E-02	5.57E-02	5.57E-02	5.57E-02	0.055730	5.57E-02	5.57E-02	5.55E-02	5.50E-02
	3.56E-02	3.57E-02	3.57E-02	3.56E-02	3.56E-02	0.035632	3.56E-02	3.55E-02	3.51E-02
11 Nodes	0.994200	0.994267	0.994260	0.989768	0.994113	0.993857	0.993617	0.991892	0.987881
	0.915404	0.915529	0.915533	0.909735	0.915755	0.916119	0.916463	0.919499	0.924552
	0.774372	0.774522	0.774523	0.774537	0.774662	0.774887	0.775097	0.776850	0.789779
	0.630553	0.630709	0.630707	0.634611	0.630746	0.630807	0.630864	0.631335	0.632640
	0.505930	0.506084	0.506080	0.511606	0.506072	0.506058	0.506045	0.505926	0.504347
	0.403655	0.403800	0.403796	0.409711	0.403771	0.403729	0.403691	0.403362	0.402611
	0.321358	0.321490	0.321487	0.327217	0.321457	0.321409	0.321364	0.320984	0.319087
	0.203272	0.203379	0.203376	0.208153	0.203349	0.203305	0.203265	0.202925	0.201582
	0.128498	0.128580	0.128578	0.132292	0.128557	0.128522	0.128491	0.128224	0.127214
	8.12E-02	8.13E-02	8.13E-02	8.41E-02	8.13E-02	8.12E-02	8.12E-02	8.10E-02	8.02E-02
	5.13E-02	5.14E-02	5.14E-02	0.053418	5.14E-02	0.051352	5.13E-02	0.051189	5.06E-02
	3.25E-02	3.25E-02	3.25E-02	3.39E-02	0.032473	3.25E-02	3.24E-02	3.23E-02	3.19E-02

Table 5.3. Calculated time step values for the central difference method (continued)

Δt, sec	0.000040	0.000500	0.001000	0.004000	0.005000	0.008000	0.010000	0.020000	0.040000
16 Nodes	0.995424	0.995394	0.995390	0.995275	0.995204	0.994888	0.994599	0.992687	0.988478
	0.917017	0.916967	0.916975	0.917122	0.917211	0.917606	0.917978	0.921360	0.926203
	0.774016	0.773953	0.773956	0.774042	0.774093	0.774321	0.774533	0.776234	0.790237
	0.628954	0.628885	0.628885	0.628906	0.628918	0.628976	0.629029	0.629480	0.630366
	0.503829	0.503760	0.503758	0.503750	0.503746	0.503729	0.503713	0.503578	0.501698
	0.401444	0.401379	0.401377	0.401359	0.401348	0.401305	0.401265	0.400922	0.400363
	0.319223	0.319163	0.319160	0.319140	0.319128	0.319078	0.319032	0.318644	0.316573
	0.201487	0.201438	0.201436	0.201418	0.201407	0.201363	0.201322	0.200980	0.199647
	0.127105	0.127067	0.127065	0.127051	0.127043	0.127008	0.126976	0.126710	0.125741
	8.02E-02	8.01E-02	8.01E-02	8.01E-02	8.01E-02	8.01E-02	8.01E-02	7.99E-02	7.91E-02
	5.06E-02	5.06E-02	5.06E-02	5.05E-02	5.05E-02	5.05E-02	5.05E-02	5.04E-02	4.98E-02
	3.19E-02	3.19E-02	3.19E-02	3.19E-02	3.19E-02	3.19E-02	3.19E-02	3.17E-02	0.031322
21 Nodes	0.995791	0.995788	0.995782	0.995660	0.995584	0.995242	0.994934	0.992953	0.988676
	0.917382	0.917388	0.917397	0.917549	0.917642	0.918047	0.918429	0.921955	0.926730
	0.773617	0.773625	0.773631	0.773717	0.773770	0.773998	0.774209	0.775878	0.790279
	0.628121	0.628129	0.628133	0.628153	0.628166	0.628223	0.628274	0.628718	0.629420
	0.502843	0.502852	0.502854	0.502846	0.502841	0.502823	0.502806	0.502667	0.500682
	0.400448	0.400457	0.400459	0.400441	0.400430	0.400386	0.400345	0.399998	0.399519
	0.318281	0.318289	0.318290	0.318270	0.318258	0.318208	0.318161	0.317770	0.315624
	0.200716	0.200723	0.200724	0.200706	0.200695	0.200650	0.200609	0.200266	0.198937
	0.126510	0.126516	0.126516	0.126502	0.126494	0.126459	0.126427	0.126160	0.125213
	7.97E-02	7.97E-02	7.97E-02	7.97E-02	0.079721	0.079695	7.97E-02	0.079472	7.87E-02
	5.03E-02	5.03E-02	5.03E-02	5.02E-02	5.02E-02	0.050223	5.02E-02	5.01E-02	4.95E-02
	3.17E-02	3.17E-02	3.17E-02	3.17E-02	3.17E-02	3.17E-02	3.16E-02	3.15E-02	0.031106

Table 5.4. Calculated time step values for the backward difference method

Δt, sec	0.000040	0.000050	0.000080	0.000100	0.000200	0.000400	0.000500	0.001000	0.004000
6 Nodes	0.988397	0.988371	0.988320	0.988305	0.988219	0.987992	0.987887	0.987357	0.984293
	0.906593	0.906555	0.906467	0.906456	0.906375	0.906099	0.905977	0.905361	0.901878
	0.774132	0.774099	0.774025	0.774043	0.774096	0.774050	0.774046	0.774010	0.773768
	0.637161	0.637135	0.637077	0.637117	0.637267	0.637402	0.637488	0.637907	0.640303
	0.515928	0.515906	0.515856	0.515906	0.516101	0.516323	0.516453	0.517091	0.520808
	0.414831	0.414813	0.414769	0.414821	0.415027	0.415277	0.415421	0.416127	0.420285
	0.332540	0.332525	0.332485	0.332535	0.332735	0.332984	0.333126	0.333823	0.337954
	0.213024	0.213013	0.212979	0.213021	0.213190	0.213402	0.213523	0.214117	0.217655
	0.136307	0.136299	0.136272	0.136306	0.136438	0.136605	0.136700	0.137168	0.139963
	8.72E-02	8.72E-02	0.087174	8.72E-02	8.73E-02	8.74E-02	8.75E-02	8.79E-02	9.00E-02
	5.58E-02	5.58E-02	5.58E-02	5.58E-02	5.59E-02	5.59E-02	0.056003	5.63E-02	5.78E-02
	3.57E-02	3.57E-02	3.57E-02	3.57E-02	3.57E-02	3.58E-02	3.58E-02	3.60E-02	3.72E-02
11 Nodes	0.994245	0.994245	0.994189	0.994146	0.994031	0.993801	0.993687	0.993114	0.989768
	0.915503	0.915513	0.915421	0.915363	0.915209	0.914900	0.914750	0.913993	0.909735
	0.774565	0.774600	0.774543	0.774516	0.774520	0.774525	0.774532	0.774544	0.774537
	0.630792	0.630843	0.630809	0.630804	0.630907	0.631108	0.631216	0.631719	0.634611
	0.506181	0.506236	0.506214	0.506219	0.506361	0.506641	0.506788	0.507489	0.511606
	0.403897	0.403951	0.403935	0.403945	0.404095	0.404391	0.404547	0.405293	0.409711
	0.321582	0.321633	0.321620	0.321631	0.321776	0.322061	0.322211	0.322931	0.327217
	0.203453	0.203494	0.203485	0.203496	0.203616	0.203852	0.203976	0.204574	0.208153
	0.128637	0.128669	0.128662	0.128671	0.128764	0.128947	0.129043	0.129507	0.132292
	8.13E-02	8.13E-02	8.13E-02	8.14E-02	8.14E-02	8.16E-02	0.081630	8.20E-02	8.41E-02
	5.14E-02	5.14E-02	5.14E-02	5.14E-02	5.15E-02	5.16E-02	0.051636	5.19E-02	0.053418
	3.25E-02	3.25E-02	0.032514	3.25E-02	3.26E-02	3.26E-02	3.27E-02	3.28E-02	3.39E-02

Table 5.4. Calculated time step values for the backward difference method (continued)

Δt, sec	0.000040	0.000050	0.000080	0.000100	0.000200	0.000400	0.000500	0.001000	0.004000
16 Nodes	0.995331	0.995339	0.995295	0.995272	0.995155	0.994923	0.994806	0.994218	0.990798
	0.916862	0.916892	0.916824	0.916795	0.916638	0.916325	0.916169	0.915385	0.910985
	0.773903	0.773967	0.773940	0.773948	0.773957	0.773976	0.773985	0.774012	0.774093
	0.628871	0.628952	0.628951	0.628980	0.629089	0.629306	0.629414	0.629935	0.632932
	0.503760	0.503846	0.503857	0.503894	0.504040	0.504333	0.504479	0.505192	0.509379
	0.401385	0.401469	0.401483	0.401521	0.401674	0.401981	0.402135	0.402887	0.407344
	0.319169	0.319248	0.319262	0.319299	0.319446	0.319740	0.319888	0.320611	0.324917
	0.201444	0.201509	0.201521	0.201551	0.201672	0.201915	0.202037	0.202635	0.206214
	0.127072	0.127122	0.127131	0.127154	0.127248	0.127436	0.127530	0.127993	0.130770
	0.080151	8.02E-02	8.02E-02	8.02E-02	8.03E-02	8.04E-02	8.05E-02	8.08E-02	8.29E-02
	5.06E-02	5.06E-02	5.06E-02	5.06E-02	5.07E-02	5.08E-02	5.08E-02	5.11E-02	5.26E-02
	3.19E-02	3.19E-02	3.19E-02	3.19E-02	3.20E-02	3.20E-02	3.21E-02	3.22E-02	3.33E-02
21 Nodes	0.995735	0.995726	0.995694	0.995664	0.995544	0.995312	0.995195	0.994602	0.991151
	0.917324	0.917301	0.917252	0.917215	0.917051	0.916739	0.916584	0.915792	0.911351
	0.773640	0.773626	0.773625	0.773625	0.773630	0.773655	0.773669	0.773701	0.773821
	0.628191	0.628181	0.628209	0.628231	0.628334	0.628557	0.628670	0.629196	0.632235
	0.502931	0.502924	0.502961	0.502992	0.503132	0.503429	0.503581	0.504295	0.508510
	0.400541	0.400533	0.400572	0.400605	0.400752	0.401062	0.401221	0.401973	0.406446
	0.318370	0.318362	0.318400	0.318431	0.318572	0.318869	0.319021	0.319743	0.324058
	0.200790	0.200783	0.200813	0.200840	0.200957	0.201201	0.201326	0.201922	0.205503
	0.126568	0.126562	0.126586	0.126607	0.126696	0.126885	0.126982	0.127442	0.130219
	7.98E-02	7.98E-02	7.98E-02	7.98E-02	7.99E-02	8.00E-02	0.080085	8.04E-02	8.25E-02
	5.03E-02	5.03E-02	0.050292	0.050304	5.04E-02	5.05E-02	5.05E-02	5.08E-02	5.23E-02
	0.031693	0.031691	3.17E-02	3.17E-02	3.17E-02	3.18E-02	0.031853	3.20E-02	3.31E-02

Δt values used in the best fit equation (5-3) for each integration method.

Table 5.5. The time step values used in the best fit equation for each integration method

Number of Nodes	Forward Difference		Central Difference		Backward Difference	
	Δt	$\Delta t * \lambda_1$	Δt	$\Delta t * \lambda_1$	Δt	$\Delta t * \lambda_1$
6	0.015	0.08640	0.050	0.2880	0.00100	0.005760
11	0.004	0.02304	0.015	0.0864	0.00020	0.001152
16	0.002	0.01152	0.010	0.0576	0.00015	0.000864
21	0.001	0.00576	0.006	0.0346	0.00010	0.000576

The empirical equation for each integration method can be calculated using the linear programming tool-solver function included in Microsoft Excel for Windows, Version 5.0, or a scientific calculator. The results are given below as equations (5-4) through (5-6) for the three integration methods. These equations can be used to predicted an appropriate time step value to accurately integrate a system of ordinary differential equations.

-Forward difference method:

$$\Delta t = 3.91 \frac{N^{-2.13}}{\lambda_1} \qquad (5\text{-}4)$$

-Central difference method:

$$\Delta t = 5.28\frac{N^{-1.66}}{\lambda_1} \tag{5-5}$$

-Backward difference method:

$$\Delta t = 0.12\frac{N^{-1.81}}{\lambda_1} \tag{5-6}$$

A plot of the time step estimates is presented in Figure 5.4. This figure shows that the central difference method has the largest time step while the backward difference method has the lowest time step value for the particular grid.

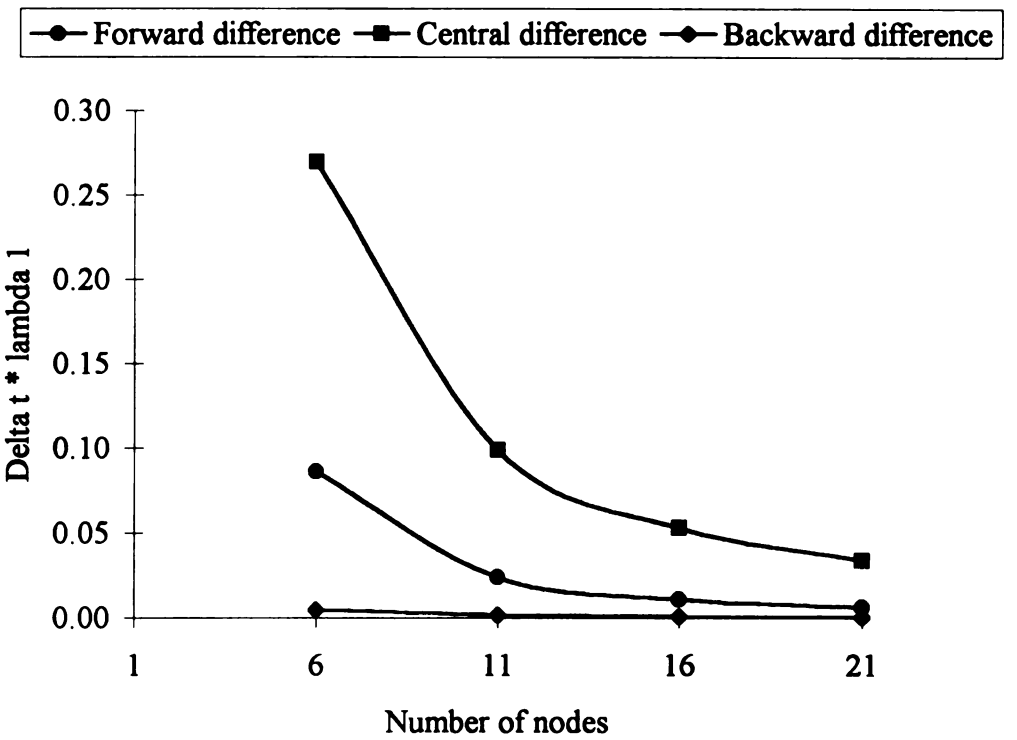


Figure 5.4. Time step estimates for the three different integration methods

CHAPTER SIX

EVALUATION OF THE TIME STEP ESTIMATES

The time step estimates presented in the previous chapter were developed using the step change problem on a solid disk of radius one and assuming $D_r = D_t = 1$. The ability of these equations to predict the time step for other problems was evaluated using different materials and other boundary conditions.

The comparison problems consisted of two different materials, steel and copper, individually and in combination using grids of 11 and 21 nodes, respectively. Eight different material combinations were used. The combinations were steel, copper, half steel and half copper, and half copper and half steel, each with prescribed temperatures at the boundary. Half steel and half copper with a derivative boundary condition of M equal to 10, half copper and half steel with M = 10, half steel and half copper with M = 50, and half copper and half steel with M = 50. The eight combinations are summarized in Table 6.1. The value of M corresponds to the product of a convection coefficient and surface area. The fluid temperature was taken as zero.

The procedure for evaluating the time step equations was as follows.

1. The smallest and largest eigenvalues were calculated and were used to estimate the time step for integrating the system of ordinary differential equations. These time step values are summarized in Table 6.1.
2. Time steps corresponding to $\Delta t/2$, $2\Delta t$, and $4\Delta t$ were determined.
3. Each of the eight comparison problems were solved using $\Delta t/2$, Δt, $2\Delta t$, and $4\Delta t$

Table 6.1. Time step values for the three different integration methods

Materials	Nodes	M	λ_{min}	λ_{max}	Δt, sec		
					F D	C D	B D
Steel	11	-	0.401*	27.30	0.0732	0.2465	0.00391
(1/α=14.29)	21	-	0.404*	108.57	0.0184	0.0843	0.00121
Copper	11	-	6.666*	453.57	0.0044	0.0147	0.00023
(1/α=0.86)	21	-	6.709*	1804.01	0.0011	0.0050	0.00007
Steel &	11	-	0.565	421.68	0.0047	0.1730	0.00274
Copper	21	-	0.566	1802.06	0.0011	0.0591	0.00085
Copper	11	-	0.844	477.30	0.0042	0.1160	0.00184
& Steel	21	-	0.853	1764.90	0.0011	0.0397	0.00057
Steel &	11	10	0.333	463.87	0.0043	0.2961	0.00470
Copper	21	10	0.333	1853.15	0.0011	1.1012	0.00146
Copper	11	10	0.228	476.83	0.0042	0.4325	0.00686
& Steel	21	10	0.228	1756.87	0.0011	0.1478	0.00213
Steel &	11	50	0.498	533.72	0.0037	0.1980	0.00314
Copper	21	50	0.499	1934.00	0.0010	0.0676	0.00097
Copper	11	50	0.570	476.81	0.0042	0.1729	0.00274
& Steel	21	50	0.573	1756.78	0.0011	0.0589	0.00085

* The λ_{min} was used to calculated the time step values for the forward difference method (FD) otherwise λ_{max} governed the time step. CD is the central difference method and BD is the backward difference method. λ_{min} was used to calculate the time step for the central and backward difference methods

for each of the three integration schemes.

4. The solution values for $\Delta t/2$, $2\Delta t$, and $4\Delta t$ were compared with the solution values for Δt at six different points. The specific comparison points in time varied with the size of the time step and the integration method. The comparison points in time were at 4, 8, 12, 16, 20, and 24 Δt. The six values obtained using each integration method for each comparison problem are summarized in Tables 6.2 and 6.3.

5. The solution values at $\Delta t/2$, $2\Delta t$, and $4\Delta t$ were compared to the solution values for Δt using regression equations. The regression information is summarized in Table 6.4. The data from the eight comparison problems were lumped together for the central and backward difference methods. The regression analysis for the forward difference method were divided into two groups; one for when λ_{min} controlled the time step and one for when λ_{max} controlled the selection. The forward difference method was unstable for $2\Delta t$ and $4\Delta t$, thus, the only comparison was for Δt and $\Delta t/2$.

Table 6.2. Time step values for different materials, 11 node grid

Materials	Forward difference				Central difference				Backward difference			
	Δt (with λ_{min})	$\Delta t/2$	Δt (with λ_{max})	$\Delta t/2$	Δt	$\Delta t/2$	$2\Delta t$	$4\Delta t$	Δt	$\Delta t/2$	$2\Delta t$	$4\Delta t$
Copper	1	1	1	1	0.95014	0.94871	0.95104	0.94761	1	1	1	1
	1	0.99929	1	0.99678	0.71381	0.71298	0.71820	0.75140	1	1	1	1
	0.99302	0.98914	0.95812	0.96965	0.49162	0.49174	0.49138	0.48834	1	1	1	1
	0.96478	0.96020	0.85915	0.91375	0.33330	0.33358	0.33211	0.32109	1	1	1	1
	0.91782	0.91440	0.71711	0.84141	0.22531	0.22556	0.22421	0.22436	1	1	1	1
	0.85996	0.85819	0.53530	0.76373	0.15222	0.15243	0.15135	0.14581	1	1	1	0.99999
Steel	1	1	1	1	0.94866	0.94714	0.94973	0.94647	1	1	1	1
	1	0.99920	1	0.99675	0.70922	0.70841	0.71348	0.74718	1	1	1	1
	0.99225	0.98825	0.95756	0.96950	0.48644	0.48657	0.48617	0.48244	1	1	1	1
	0.96235	0.95774	0.85675	0.91344	0.32855	0.32883	0.32734	0.31629	1	1	1	1
	0.91353	0.91019	0.71090	0.84095	0.22128	0.22155	0.22018	0.22037	1	1	1	1
	0.85406	0.85243	0.52203	0.76317	0.14896	0.14918	0.14808	0.14242	1	1	1	1

Table 6.2. Time step values for the different materials, 11 node grid (continued)

Materials	Forward difference		Central difference				Backward difference			
	Δt	Δt/2	Δt	Δt/2	2Δt	4Δt	Δt	Δt/2	2Δt	4Δt
Half	1	1	0.90691	0.90417	0.91438	0.91938	1	1	1	1
copper	1	1	0.64319	0.64296	0.64285	0.67337	1	0.99999	1	1
and half	1	0.99999	0.43674	0.43699	0.43595	0.41999	1	0.99999	1	1
steel	0.99999	0.99999	0.29527	0.29554	0.29428	0.29012	1	0.99999	1	0.99999
	0.99997	0.99996	0.19953	0.19977	0.19860	0.19729	0.99999	0.99999	0.99999	0.99999
	0.99989	0.99986	0.13483	0.13502	0.13406	0.12842	0.99999	0.99999	0.99999	0.99999
Half	1	1	0.87136	0.86849	0.88392	0.8969	1	1	1	1
steel	1	1	0.60148	0.60155	0.59864	0.62064	1	1	1	1
and half	1	1	0.40712	0.40739	0.40577	0.38563	1	1	1	0.99999
copper	0.99999	0.99999	0.27524	0.27549	0.27439	0.27640	0.99999	1	0.99999	0.99999
	0.99999	0.99998	0.18606	0.18628	0.18530	0.18054	0.99999	0.99999	0.99999	0.99999
	0.99995	0.99993	0.12578	0.12596	0.12510	0.12104	0.99999	0.99999	0.99999	0.99998
Half	1	1	0.87849	0.87667	0.85060	0.87621	0.99999	1	0.99999	0.99998
copper	1	1	0.87282	0.87367	0.87876	0.84186	0.99998	0.99999	0.99995	0.99986
and half	1	0.99999	0.87367	0.87364	0.87944	0.90329	0.99988	0.99992	0.99979	0.99957
steel	0.99999	0.99999	0.87372	0.87364	0.87608	0.85361	0.99958	0.99966	0.99939	0.99898
with	0.99997	0.99996	0.87367	0.87364	0.87380	0.88433	0.99892	0.99907	0.99861	0.99799
M = 10	0.99991	0.99988	0.87364	0.87364	0.87288	0.87005	0.99779	0.99800	0.99735	0.99656

Table 6.2. Time step values for different materials, 11 node grid (continued)

Materials	Forward difference		Central difference				Backward difference			
	Δt	Δt/2	Δt	Δt/2	2Δt	4Δt	Δt	Δt/2	2Δt	4Δt
Half	1	1	0.98119	0.98186	0.98038	0.98504	1	1	1	1
steel	1	1	0.98034	0.98033	0.98156	0.97439	1	1	0.99999	0.99999
and half	1	1	0.98030	0.98029	0.98041	0.98335	0.99999	0.99999	0.99999	0.99999
copper	0.99999	0.99999	0.98029	0.98029	0.98009	0.97961	0.99999	0.99999	0.99999	0.99998
with	0.99999	0.99999	0.98029	0.98029	0.98013	0.97966	0.99998	0.99998	0.99997	0.99995
M =10	0.99999	0.99998	0.98030	0.98029	0.98022	0.98145	0.99995	0.99996	0.99994	0.99989
Half	1	1	0.92110	0.92182	0.92905	0.94551	1	1	1	1
copper	1	1	0.88133	0.88168	0.87975	0.86381	1	1	1	0.99999
and half	1	0.99999	0.87488	0.87497	0.87346	0.86929	1	1	0.99999	0.99999
steel	0.99999	0.99999	0.87384	0.73862	0.87351	0.88091	0.99999	0.99999	0.99999	0.99999
with	0.99997	0.99996	0.87368	0.87368	0.87373	0.86775	0.99999	0.99999	0.99999	0.99997
M = 50	0.99991	0.99988	0.87365	0.87365	0.87374	0.87727	0.99998	0.99998	0.99996	0.99993
Half	1	1	0.98543	0.98569	0.98679	0.99002	1	1	1	1
steel	1	1	0.98071	0.98076	0.98058	0.97677	1	1	1	1
and half	1	1	0.98032	0.98033	0.98007	0.98002	1	1	1	0.99999
copper	1	1	0.98029	0.98029	0.98022	0.98164	1	1	0.99999	0.99999
with	0.99999	0.99999	0.98029	0.98029	0.98030	0.97902	0.99999	1	0.99999	0.99999
M = 50	0.99999	0.99999	0.98029	0.98029	0.98031	0.98115	0.99999	0.99999	0.99999	0.99998

Table 6.3. Time step values for different materials, 21 node grid

Materials	Forward difference				Central difference				Backward difference			
	Δt (with λ_{min})	$\Delta t/2$	Δt (with λ_{max})	$\Delta t/2$	Δt	$\Delta t/2$	$2\Delta t$	$4\Delta t$	Δt	$\Delta t/2$	$2\Delta t$	$4\Delta t$
Copper	1	1	1	1	0.99979	0.99988	0.99948	0.99850	1	1	1	1
	1	1	1	0.99677	0.99031	0.99042	0.98966	0.98722	1	1	1	1
	1	1	1	0.96965	0.94730	0.94708	0.94825	0.95027	1	1	1	1
	1	1	1	0.91375	0.87405	0.87381	0.87505	0.88037	1	1	1	1
	1	0.99999	0.99997	0.84141	0.78790	0.78774	0.78856	0.79144	1	1	1	1
	0.99998	0.99992	0.99956	0.76373	0.70081	0.70073	0.70115	0.70226	1	1	1	1
Steel	1	1	1	1	0.99977	0.99987	0.99944	0.99841	1	1	1	1
	1	1	1	1	0.98959	0.98970	0.98897	0.98651	1	1	1	1
	1	1	1	1	0.94460	0.94436	0.94560	0.94790	1	1	1	1
	1	1	1.00000	0.99999	0.86922	0.86897	0.87023	0.87568	1	1	1	1
	1	1	0.99998	0.99992	0.78146	0.78130	0.78210	0.78491	1	1	1	1
	0.99998	1	0.99949	0.99951	0.69333	0.69325	0.69366	0.69471	1	1	1	1

Table 6.3. Time step values for different materials, 21 node grid (continued)

Materials	Forward difference		Central difference				Backward difference			
	Δt	Δt/2	Δt	Δt/2	2Δt	4Δt	Δt	Δt/2	2Δt	4Δt
Half	1	1	0.99899	0.99924	0.99827	0.99645	1	1	1	1
copper	1	1	0.97465	0.97450	0.97495	0.97369	1	1	1	1
and half	1	1	0.90425	0.90391	0.90571	0.91199	1	1	1	1
steel	1	1	0.81180	0.81161	0.81259	0.81734	1	1	1	1
	1	1	0.71767	0.71759	0.71799	0.71856	1	1	1	1
	1	1	0.63014	0.63012	0.63020	0.63046	1	1	1	1
Half	1	1	0.99638	0.99672	0.99523	0.99262	1	1	1	1
steel	1	1	0.94840	0.94800	0.95027	0.95310	1	1	1	1
and half	1	1	0.85813	0.85788	0.85906	0.86663	1	1	1	1
copper	1	1	0.76020	0.76011	0.76058	0.76138	1	1	1	1
	1	1	0.66814	0.66812	0.66822	0.66806	1	1	1	1
	1	1	0.58547	0.58549	0.58542	0.58563	1	1	1	1
Half	1	1	0.96652	0.96634	0.97131	0.97762	1	1	1	1
copper	1	1	0.94190	0.94213	0.94016	0.93631	1	1	1	1
and half	1	1	0.93699	0.93705	0.93614	0.93164	1	1	1	1
steel	1	1	0.93599	0.93601	0.93599	0.94008	1	1	1	1
with	1	1	0.93579	0.93579	0.93594	0.93305	1	1	1	0.99999
M = 10	1	1	0.93575	0.93575	0.93583	0.93685	1	1	1	0.99999

Table 6.3. Time step values for different materials, 21 node grid (continued)

Materials	Forward difference		Central difference				Backward difference			
	Δt	Δt/2	Δt	Δt/2	2Δt	4Δt	Δt	Δt/2	2Δt	4Δt
Half	1	1	0.99761	0.99746	0.99790	0.99813	1	1	1	1
steel	1	1	0.99236	0.99239	0.99214	0.99293	1	1	1	1
and half	1	1	0.99063	0.99064	0.99060	0.98953	1	1	1	1
copper	1	1	0.99015	0.99016	0.99014	0.99017	1	1	1	1
with	1	1	0.99003	0.99003	0.99002	0.99013	1	1	1	1
M = 10	1	1	0.98999	0.98999	0.98999	0.98980	1	1	1	1
Half	1	1	0.99714	0.99714	0.99691	0.99633	1	1	1	1
copper	1	1	0.97678	0.97667	0.97765	0.98094	1	1	1	1
and half	1	1	0.95845	0.95848	0.95822	0.95846	1	1	1	1
steel	1	1	0.94791	0.94796	0.94772	0.94565	1	1	1	1
with	1	1	0.94223	0.94227	0.94211	0.94213	1	1	1	1
M= 50	1	1	0.93920	0.93922	0.93912	0.93878	1	1	1	1
Half	1	1	0.99932	0.99931	0.99930	0.99922	1	1	1	1
steel	1	1	0.99534	0.99532	0.99547	0.99616	1	1	1	1
and half	1	1	0.99237	0.99238	0.99232	0.99219	1	1	1	1
copper	1	1	0.99099	0.99100	0.99095	0.99053	1	1	1	1
with	1	1	0.99040	0.99041	0.99038	0.99042	1	1	1	1
M= 50	1	1	0.99015	0.99016	0.99014	0.99008	1	1	1	1

Table 6.4. Regression results between Δt and $\Delta t/2$, $2\Delta t$, and $4\Delta t$.

		$\Delta t/2$	$2\Delta t$	$4\Delta t$
Combination λ_{min} and λ_{max} for Forward Difference Method	X Coefficient	1.02343	Unstable	Unstable
	Std Err of Coef	0.00353	Unstable	Unstable
	R Squared	0.99888	Unstable	Unstable
Forward Difference Method (λ_{max})	X Coefficient	0.50525	Unstable	Unstable
	Std Err of Coef	0.03871	Unstable	Unstable
	R Squared	0.64445	Unstable	Unstable
Central Difference Method (λ_{min})	X Coefficient	0.99961	1.00149	1.00637
	Std Err of Coef	0.00021	0.00143	0.00408
	R Squared	1.00000	0.99981	0.99846
Backward Difference Method (λ_{min})	X Coefficient	0.88975	1.21677	1.62889
	Std Err of Coef	0.00270	0.00628	0.02132
	R Squared	0.99914	0.99750	0.98415

CHAPTER SEVEN

DISCUSSION AND CONCLUSION

The empirical equations for calculating the time step required to solve the system of ordinary differential equations for radial field problems have been successfully obtained. Based on an accuracy criteria or the stability requirements (Table 6.4), these equations define a usable time step.

The forward difference method is conditionally stable, therefore, both λ_1 and λ_{max} must be evaluated. The time step value should be the lowest of the two possible values. The R squared value in Table 6.4 indicates that the integration is accurate when the procedure is used. Solutions in time using a time step based only on the stability criteria are not accurate. The R squared value is 0.64 in this case.

The time step equation for the central difference method appears to be conservative since the R squared value for $4\Delta t$ is still 0.998. Time step value for the backward difference method gives accurate results at $2\Delta t$ with greater error at $4\Delta t$.

Time step value calculated for the forward difference method should be rounded down because of the stability criteria. The time step values for the central and backward difference methods can be rounded up or down to a convenient value for displaying the results.

7.1 FUTURE STUDY

Determine empirical time step equations for a solid ring, and spherical elements. Continue the research into two- and three-dimensional problems.

BIBLIOGRAPHY

Allaire, P. E. 1985. Basics of the Finite Element Method: Solid Mechanics, Heat Transfer, and Fluid Mechanics. W. C. Brown Publishers. Dubuque, Iowa.

Bathe, K. and E. L. Wilson. 1976. Numerical Methods in Finite Element Analysis. Prentice-Hall, Englewood Cliffs. New Jersey.

Boyce, E. W. and R. C. Diprima. 1986. Elementary Differential Equations. Fourth Edition. John Wiley & Sons, Inc. New York.

Churchill, R. V. and J. W. Brown. 1987. Fourier Series and Boundary Value Problem. Fourth Edition. McGraw-Hill Book Company, New York.

Cleland, A. C. and R. L. Earle. 1984. Assessment of Freezing Time Prediction Method. Journal of Food Science. Vol. 49(4): 1034-1042. Chicago, Illinois.

Fried, I. 1979. Numerical Solution of Differential Equations. Academic Press, New York.

Gear, G. W. 1971. Numerical Initial Value Problems in Ordinary Differential Equations. Printice-Hall, Englewood Cliffs, New Jersey.

Haghighi, K. and L. J. Segerlind. 1988. Modeling Simultaneous Heat and Mass Transfer in an Isotropic Sphere-A Finite Element Approach. Transactions of the American Society of Agricultural Engineers. Vol. 31(2):629-637.

Henrici, P. 1977. Error Propagation for Difference Methods. Krieger Pub. Co. Huntington, New York.

Irudayaraj, J. 1991. Moving Evaporative Front Prediction Using the Finite Element Method. Paper Presented at the 1991 International Winter Meeting of the American Society of Agricultural Engineers, St. Joseph, MI.

Irudayaraj, J., K. Haghighi, and R. L. Stroshine. 1990. Nonlinear Finite Element Analysis of Coupled Heat and Mass Transfer Problems with an Application to Timber Drying. Drying Technology Vol. 8(4):731-749. New York.

Jaluria, Y. and K. Torrance. 1986. Computational Heat Transfer. Hemisphere Pub. Co. New York.

Kreyszig, E. 1988. Advanced Engineering Mathematics. Sixth Edition. John Wiley & Sons, Inc. New York.

Maadooliat, R. 1983. Element and Time Step Criteria for Solving Time Dependent Field

Problems Using the Finite Element Method. Ph.D. Dissertation, Michigan State University.

Mohtar, R. H. 1994. Dynamic Time Step Estimates for Transient Field Problems. Ph.D. Dissertation, Michigan State University.

Mohtar, R. H. and L. J. Segerlind. 1992. Time Step Criteria for Solving Unsteady Engineering Field Problems. Paper Presented at the 1992 International Winter Meeting of the American Society of Agricultural Engineers (No. 91-7551). St. Joseph, MI.

Myers, G. E. 1971. Analytical Methods in Conduction Heat Transfer. McGraw-Hill, Inc. New York.

Myers, G. E. 1977. The Critical Time Step for Finite Element Solutions to Two Dimensional Heat-Conduction Transients. ASME Paper (No. 77-WA/HT-14). American Society of Mechanical Engineers, New York.

Narasimhan, T. N. 1978. A Perspective on Numerical Analysis of the Diffusion Equation. Advances in Water Resources. Vol. 1(3):147-155.

Ortega, J. M. 1990. Numerical Analysis: A Second Course. Reprinted by the Society for Industrial and Applied Mathematics Part of the Classics in Applied Mathematics Series (No. 3).

Ozisik, N. M. 1980. Heat Conduction. John Wiley & Sons, New York.

Pakantar, S. V. 1980 Numerical Heat Transfer and Fluid Flow. Hemisphere Publishers Company, New York.

Patankar, S. V. 1991. Computation of Conduction and Duct Flow Heat Transfer. A Textbook featuring the computer program CONDUCT. Innovative Research, Inc. Maple Grove, Minnesota.

Peraire, J., J. Peiro, L. Formaggia, K. Morgan, and O. C. Zienkiewicz. 1988. Finite Element Euler Computations in Three Dimensions. International Journal for Numerical Methods in Engineering Vol. 26:2135-2159.

Power D. 1987. Boundary Value Problems. Third Edition. Harcourt Brace Javanavich, Pub. Academic Press.

Reddy, J. N. 1984. An Introduction to the Finite Element Method. McGraw-Hill Book Co. New York.

Rushton, K. R. and L. M. Tomlinson. 1971. Digital Computer Solutions of Ground Water Flow. Journal of Hydrology Vol. 12:339-362.

Segerlind, L. J. 1976. Applied Finite Element Analysis. John Wiley & Sons, New York.

Segerlind, L. J. 1984. Applied Finite Element Analysis. Second Edition. John Wiley & Sons, Inc. New York.

Segerlind, L. J. 1994-1995. Personal Communications.

Segerlind, L. J. And E. P. Scott, 1988. Selecting a Time Step Value for Numerical Solution Involving Food Materials. Paper Presented at the 1988 International Summer Meeting of the American Society of Agricultural Engineers (No. 88-6011). St. Joseph, MI.

Shih, T. M. 1984. Numerical Heat Transfer. Hemisphere Pub. Co., New York.

Smith, G. D. 1985. Numerical Solution of Partial Differential Equations: Finite Difference Methods. Third Edition. Oxford Applied Mathematics and Computing Science Series. Clarendon Press, Oxford.

Stoer, J. and Bulivsch. 1980. Introduction to Numerical Analysis. Springer-Verlag, New York.

Williams, W. E. 1980. Partial Differential Equations. Oxford Applied Mathematics and Computing Science Series. Clarendon Press, Oxford.

Zienkiewicz, O. C. 1971. The Finite Element Method in Engineering Science. McGraw-Hill Book Co. London.

Zill, D. G. 1993. A first Course in Differential Equations. Fifth Edition. PWS-Kent Publishing Company. Boston, Massachusetts.