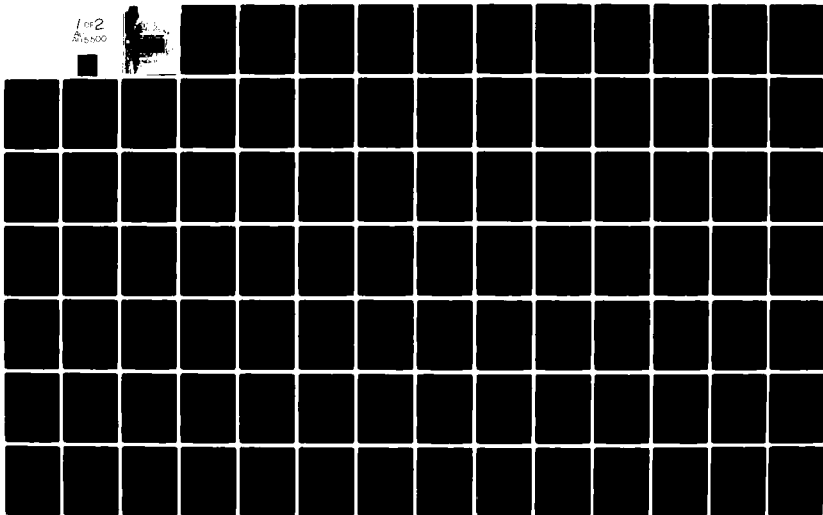
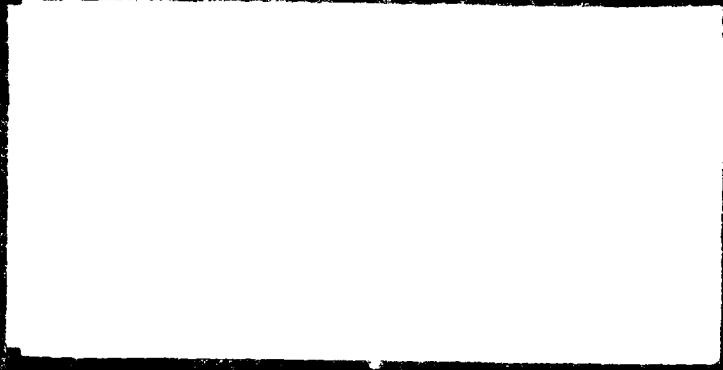


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A COMPARISON OF FINITE-DIFFERENCE METHODS  
FOR THE SOLUTION OF THE TRANSIENT HEAT  
CONDUCTION EQUATION IN INHOMOGENEOUS MEDIA

THESIS

AFIT/GNE/PH/82-4

Kenneth W. Blevins  
Lt USN

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A COMPARISON OF FINITE-DIFFERENCE METHODS  
FOR THE SOLUTION OF THE TRANSIENT HEAT  
CONDUCTION EQUATION IN INHOMOGENEOUS MEDIA

THESIS

Presented to the Faculty of the School of Engineering  
of the Air Force Institute of Technology  
Air University  
in Partial Fulfillment of the  
Requirements for the Degree of  
Master of Science

by  
Kenneth W. Blevins, B.S.  
Lt USN  
Graduate Nuclear Effects  
March 1982

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## Preface

This report is the result of my investigation of the Explicit, Pure Implicit, Crank-Nicolson and Douglas finite-Difference methods for solution of the one-dimensional transient heat-conduction equation in inhomogeneous material.

Initially, I sought to solve three variations of the basic problem for several values of the Fourier Modulus,  $\Delta t/(\Delta x)^2$ , and test two or three methods for handling the inherent discontinuity found in the problem. However, time and computer assets allowed for complete solution of only two variations of the problem for four values of the Fourier modulus, with one treatment of the discontinuity. Yet, the value of traditional finite-difference schemes over newer, more sophisticated schemes for engineering work was still substantiated.

I would like to express my appreciation to Dr. Bernard Kaplan of the Air Force Institute of Technology for his guidance, and to Dr. W. Kessler of the Air Force Materials Laboratory for sponsoring this research project. (Also, to Sharon Gabriel for doing such a magnificent and professional job with the typing that I can't miss getting a passing grade!)

Kenneth W. Blevins

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Abstract

The transient heat conduction equation is solved for inhomogeneous media using the Explicit, Pure-Implicit, Crank-Nicolson and Douglas finite-difference methods, and the numerical solutions are investigated with respect to accuracy and stability. The inherent discontinuity between the initial and boundary conditions is accounted for by mesh refinement. For the two versions of the problem for which the four numerical methods are investigated, all four methods are found to be of equivalent accuracy for small values of the Fourier Modulus,  $\Delta t / (\Delta x)^2$ . While the Pure-Implicit, Crank-Nicolson and Douglas methods are unconditionally stable, the Crank-Nicolson and Douglas methods are very inaccurate at large values of the Fourier Modulus due to oscillatory behavior.

A COMPARISON OF FINITE-DIFFERENCE METHODS  
FOR THE SOLUTION OF THE TRANSIENT HEAT  
CONDUCTION EQUATION IN INHOMOGENEOUS MEDIA

I. Introduction

General

Background. Very few practical engineering problems involving partial differential equations can be solved in closed form. The difficulty may be due to irregular or mixed geometry, or complicated boundary conditions. Further, closed form solutions that are obtainable usually contain infinite series, special functions, or transcendental equations for eigenvalues such that the numerical evaluation of an analytic solution itself may be a difficult task (Ref 16:3). Hence, numerical approximation methods are used which provide adequate numerical solutions simply and efficiently. Finite differences have been in use at least since 1768 (Ref 1:1), and are the most frequently used and universally applicable numerical approximation method for solving partial differential equations (Ref 20:4).

Various finite difference schemes of different degrees of sophistication are given in the literature for the numerical solution of the transient heat-transfer equation. For simplicity of presentation and to maintain generality, these schemes are usually presented for homogeneous materials.

Much work has been performed comparing the accuracy and efficiency of these different schemes in solving the homogeneous material transient heat-transfer problem. However, the solution of many important engineering heat transfer problems, such as those involving re-entry bodies and jet engine nozzles, requires handling non-homogeneous (composite) materials. Some of the finite-difference schemes available for use may be potentially more advantageous with respect to accuracy and computer time than those currently employed in engineering practice.

#### Finite Difference Formulation

When using the finite difference technique to solve a partial differential equation (PDE), a network of grid points must first be established throughout the region of interest. The grid lines are drawn parallel to the space and time axis and, for one-dimensional spatial coordinates, are separated by  $\Delta x$  and  $\Delta t$ . The intersections of the grid lines are the grid points or nodes and are identified by spatial and time coordinates. Let  $x$  and  $t$  be the independent variables of the PDE to be solved, and let the grid spacings be  $\Delta x$  for space and  $\Delta t$  for time. The spatial coordinate of an arbitrary node will be  $B$  and the spatial coordinates of the adjacent nodes,  $A$  and  $C$ . The value of  $U$  at a particular node will be specified, at time  $t$ , by a subscript and at time  $t+\Delta t$  by the same subscript and a prime superscript, as depicted in Figure 1.

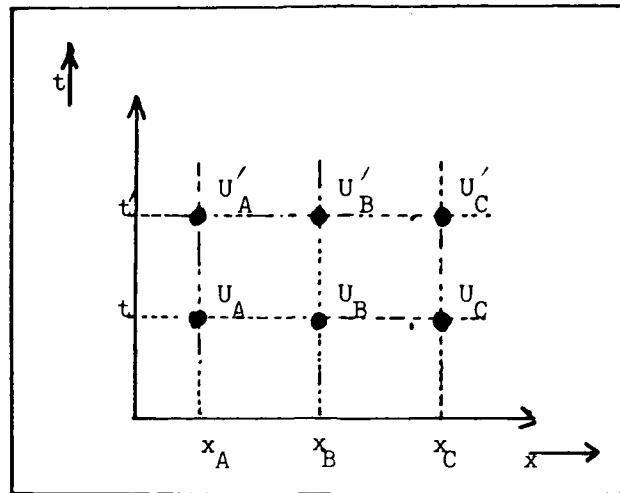


Figure 1. Grid Points and Notation

Assume the exact solution to the PDE is  $U_{A.S.} = U(x,t)$  and let the approximation to the exact solution be  $U_{F.D.S.}$ . Next, suitable finite difference expressions must be found which will approximate the partial derivatives of the original PDE. After substituting the finite difference expressions into the original PDE, the resulting finite-difference equation (FDE) is solved. However, the solution of the FDE is only an approximation to the actual solution of the original PDE because the derivatives have just been approximated by difference quotients over small intervals. As the size of the intervals approaches zero, the difference quotients approach the value of the derivatives they approximate.

The procedure used in this study for deriving the finite difference equations consists of approximating the derivatives

of the PDE by a truncated Taylor series. To do this, first refer to the grid points shown in Figure 1. For a node  $U_B$ , located halfway between nodes  $U_A$  and  $U_C$  such that  $\Delta x = x_B - x_A = x_C - x_B$  and  $\Delta t = t' - t$ , the Taylor series expansion about  $U_B$  along the  $x$  coordinate system gives

$$U_A = U_B - \Delta x \frac{dU_B}{dx} + \frac{1}{2} (\Delta x)^2 \frac{d^2U_B}{dx^2} \quad (1)$$

$$U_C = U_B + \Delta x \frac{dU_B}{dx} + \frac{1}{2} (\Delta x)^2 \frac{d^2U_B}{dx^2} \quad (2)$$

where terms of order 3,  $O(\Delta x^3)$ , have been neglected. Adding and subtracting the two equations and rearranging terms

$$\frac{dU_B}{dx} = \frac{U_C - U_A}{2(\Delta x)} \quad (3)$$

$$\frac{d^2U_B}{dx^2} = \frac{U_C - 2U_B + U_A}{(\Delta x)^2} \quad (4)$$

Equations (3) and (4) are respectively referred to as first and second central difference equations. Similarly, where  $U'(x,t) = U(x,t + \Delta t)$ , the first forward difference equation for the time variable is

$$\frac{dU_B}{dt} = \frac{U'_B - U_B}{\Delta t} \quad (5)$$

Approximating a PDE. The partial differential equation

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} \quad (6)$$

may be approximated by substituting (4) and (5) into (6) to get

$$\frac{U'_B - U_B}{\Delta t} = \frac{U_A - 2U_B + U_C}{(\Delta x)^2} \quad (7)$$

which is a formula for the unknown value  $U'_B$  in terms of the known values  $U_A$ ,  $U_B$ ,  $U_C$ . Referring to Figure 2a, solving for one unknown directly in terms of known values is called an explicit method (Ref 20:13), and (7) is the Euler or Explicit formula.

A different approximation to (6) is given by

$$\frac{U'_B - U_B}{\Delta t} = \frac{U'_A - 2U'_B + U'_C}{(\Delta x)^2} \quad (8)$$

which is generally known as the Pure-Implicit formula. Referring to Figure 2b,  $U'_A$ ,  $U'_B$ ,  $U'_C$  are unknown and must be solved for in terms of  $U_B$  which is known. This leads to a set of  $n - 1$  equations in  $n - 1$  unknowns where  $n + 1$  is the number of grid points and the solution is known at the boundaries. The equations may be solved by straightforward Gaussian-elimination. However, when the

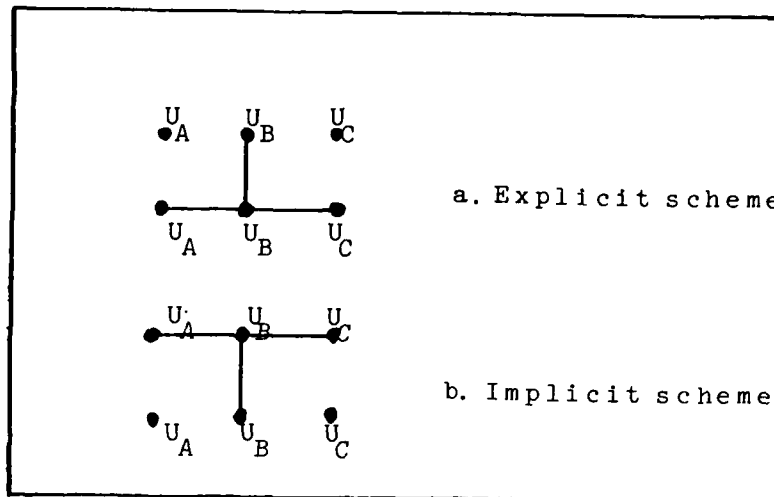


Figure 2. Schematic Representation of Explicit and Implicit Numerical Methods

matrix of the coefficients is written, the non-zero terms align themselves along the three main diagonals of the matrix, forming a tri-diagonal matrix, and a special adaptation of the Gaussian-elimination procedure, the Thomas method, may be used for the solution (Ref 18:199).

All forms of finite difference equations may be classified as explicit or implicit. Explicit formulae march forward in time as the solution at each present point is found in terms of preceding values, while implicit formulae involve the solution of simultaneous equations of present unknown values in terms of preceding known values (Ref 1:42).

General Finite Difference Equation. A general finite-difference form of Eq (6) has been given by Crandall (Ref 6: 318) as a weighted combination of the explicit and implicit relations pictured in Figure 2, and is given by

$$M(U'_B - U_B) = f(U'_A - 2U'_B + U'_C) + (1-f)(U_A - 2U_B + U_C) \quad (9)$$

where

$U$  = the approximate temperature at a specified grid point as shown in Figure 1

$M$  = the inverse Fourier Modulus, a dimensionless ratio  $(\Delta x)^2/(\Delta t)$

$f$  = weighting factor.

In general practice,  $0 \leq f \leq 1.0$ . A schematic for the general equation is given in Figure 3.

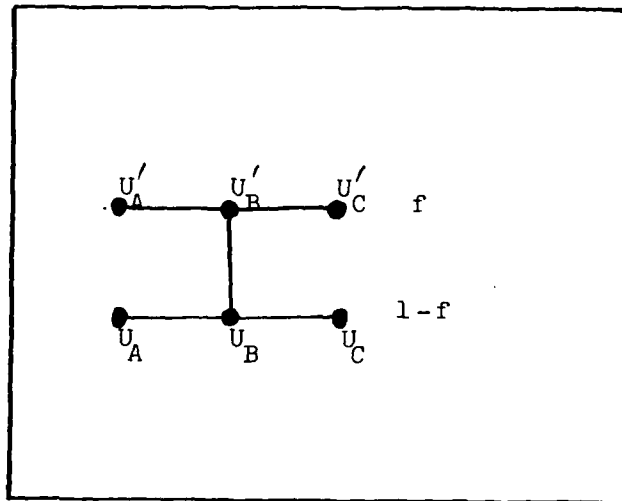


Figure 3. Schematic Representation of the General Finite-Difference Equation

Table 1 includes several values of  $f$  and common nomenclature for the finite-difference schemes thus determined.

Table 1	
<u>Finite Difference Schemes Determined by Values of the Weight Factor f</u>	
Value of f	Finite Difference Scheme
0	Explicit
1/2	Crank-Nicolson
1	Pure-Implicit
$\frac{1}{2}(1 - \frac{(\Delta x)^2}{6\alpha(x)\Delta t})$	Douglas

### Objective

The basic purpose of this thesis is to investigate the relative accuracy of the Explicit, Pure Implicit, Crank-Nicolson, and Douglas finite difference schemes used to represent the parabolic partial differential equation for transient heat conduction in non-homogeneous media, and to compare the methods for ease and efficiency of computation.

### Approach and Scope

A straightforward approach to investigating the accuracy of numerical methods is to solve a given problem analytically and numerically, and compare the errors of the methods used. This is the general approach used in this thesis. Although it would be ideal to apply these methods to a general two-

dimensional or three-dimensional time-dependent problem, and compare the solutions obtained to the analytic solution of the same problem, the analytic solution to such a problem is extremely difficult, if at all possible to obtain. Thus, this investigation was restricted to the study of a one-dimensional problem as found in Carslaw and Jaeger (Ref 4:312-313). Due to the limited usefulness and severe stability restrictions of the explicit form, as shown in Chapter II, the main thrust of my effort was to compare the Crank-Nicolson, Douglas and Pure Implicit forms of solution.

#### Computer Program

Investigation of the discussed numerical methods and numerical computation of the analytic solution was done with the use of computer programs written by the author in FORTRAN Version 5. The programs were executed on the Aeronautical Systems Division computer at Wright-Patterson Air Force Base, Ohio.

## II. Theory

### The Physical Problem

The heat transfer problem investigated is illustrated in Figure 4.

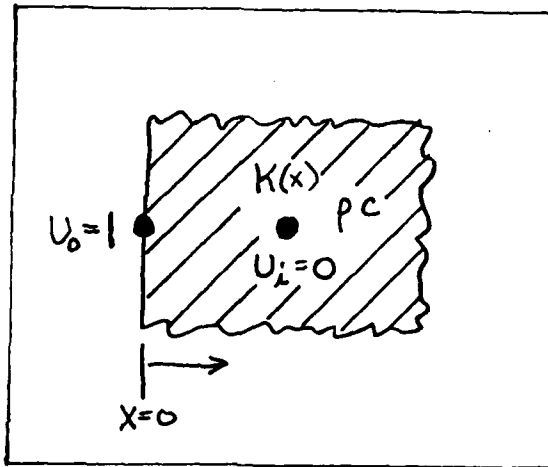


Figure 4. The Heat Transfer Problem

The problem consists of a solid which extends to infinity in the  $x$ -direction. The material contains no heat sources. The entire solid is initially cooled to  $0^\circ$ . Subsequently, the temperature at the surface of the solid at  $x$  equal to zero is immediately raised to and maintained at a temperature of one degree. The temperatures used have no significance other than to simplify the initial and boundary conditions. All other faces of the solid are insulated, thus heat is transferred only in the  $x$ -direction. The conductivity of the material is proportional to  $x$  to the  $n$ th power, where

n is greater than zero and less than unity, ( $0 < n < 1$ ). The material used has no bearing on the investigation, and the physical parameters of specific heat and density have been considered constant. The governing partial differential equation for this conduction problem is given by

$$\frac{\partial}{\partial x} \left( K \frac{\partial U}{\partial x} \right) - \rho c \frac{\partial U}{\partial t} = 0 \quad (10)$$

where

- U = the exact temperature at a specific node and time
- t = time
- x = node location
- $\rho$  = density
- c = specific heat
- K = conductivity at a specific node such that

$$K = K_0 x^n \quad 0 < n < 1$$

$$K_0 = \text{constant}$$

The initial and boundary conditions which must be satisfied are

$$U(x, 0) = 0$$

$$U(0, t) = 1$$

$$U(\infty, t) = 0$$

(11)

### Exact Solution

The exact solution to this problem is given by Carslaw and Jaeger (Ref 4:412-413) as

$$U(x,t) = \frac{1}{\Gamma(v)} \int_X^{\infty} e^{-\mu} \mu^{v-1} d\mu \quad (12)$$

where

$U$  = temperature at node  $x$  and time  $t$

$\mu$  = variable of integration

$v$  =  $(1 - n)/(2 - n)$   $0 < n < 1$

$\Gamma(v)$  = Gamma function evaluated at  $v$

$X$  =  $(x^2 - n)/((2 - n)^2 kt)$

$k$  =  $K_0/\rho c$  where  $K_0$ ,  $\rho$ ,  $c$  were defined for (10).

The integral in Eq (12) must be evaluated numerically. The approximation used for this computation was given by Gradshteyn and Ryzik (Ref 9:940-941) as

$$\int_X^{\infty} e^{-t} t^{\alpha-1} dt = \Gamma(\alpha) - \sum_{n=0}^{\infty} \frac{(-1)^n X^{(\alpha+n)}}{n! (\alpha+n)} \quad (13)$$

Figure 5 depicts the exact analytical solution for four variations of the problem where  $n = 0.0$ ,  $0.25$ ,  $0.5$ , and  $0.75$ , and Figure 6 depicts the temperature profile at several times for  $n = .25$ .

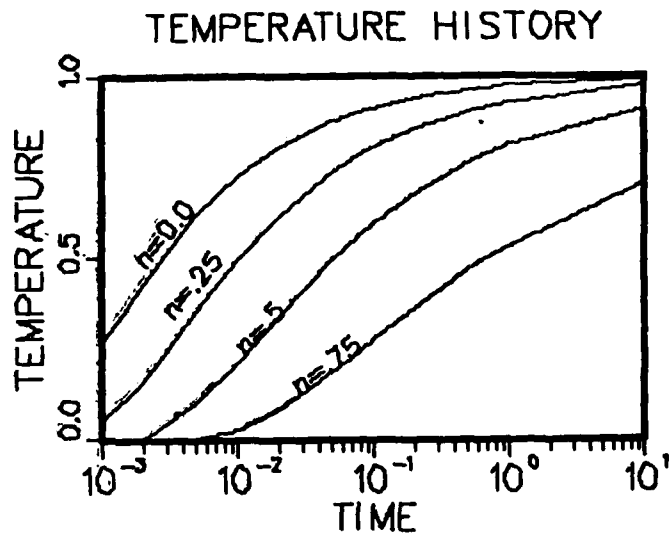


Figure 5. Exact Solution for  $n=0$ ,  
.25, .5, and .75 at  $x=.05$

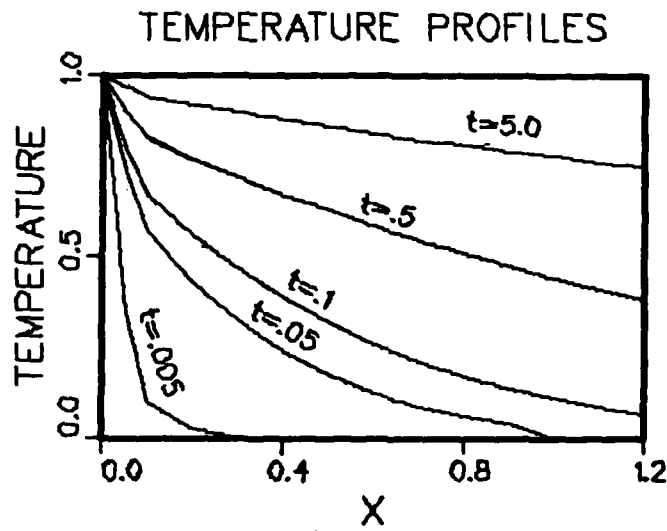


Figure 6. Temperature Profiles for  $n=.25$ .

### Numerical Solution

Equation (1) was solved numerically after dividing the material into ten internal sections of equal width  $\Delta x$  as shown in Figure 7 where the labeled nodes correspond to specific locations within the solid.

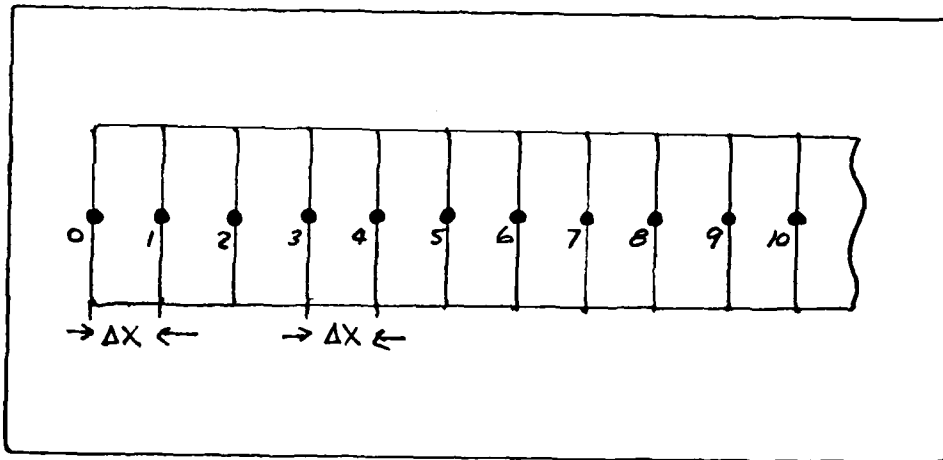


Figure 7. Node Location

Next, the finite-difference equations were derived in similar fashion as discussed on pages 2-4. Referring to Figure 8, the Taylor series expansion about  $U_B$  in region a may be found as was (1), and then rearranged as

$$\Delta x_a \left( \frac{\partial U_B}{\partial x} \right)_a = U_A - U_B - \frac{(\Delta x_a)^2}{2} \left( \frac{\partial^2 U_B}{\partial x^2} \right)_a \quad (14)$$

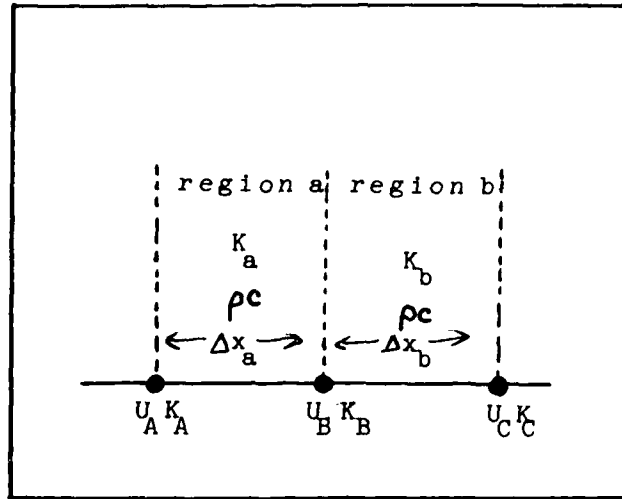


Figure 8. Node Arrangement for Deriving Finite Difference Equations

The time derivative in region a may be written as

$$\left( \frac{\partial U_B}{\partial t} \right)_a = \left( \frac{U'_B - U_B}{\Delta t} \right)_a \quad (15)$$

Evaluating (10) in medium a about node B

$$K_a \left( \frac{\partial^2 U_B}{\partial x^2} \right)_a = \rho c \left( \frac{\partial U_B}{\partial t} \right)_a \quad (16)$$

Substituting (15) and (16) into (14) and rearranging,

$$\Delta x_a \left( \frac{\partial U_B}{\partial x} \right)_a = U_A - U_B - \frac{(\Delta x_a)^2}{2} \left( \frac{\rho c}{K_a} \right) \left( \frac{U'_B - U_B}{\Delta t} \right)_a \quad (17)$$

and similarly for region b

$$\Delta x_b \left( \frac{\partial U_B}{\partial x} \right)_b = U_C - U_B - \frac{(\Delta x_b)^2}{2} \left( \frac{\rho c}{K_b} \right) \left( \frac{U'_B - U_B}{\Delta t} \right) \quad (18)$$

Since the heat flux between the two regions must be continuous at point B,

$$K_a \left( \frac{\partial U_B}{\partial x} \right)_a = K_b \left( \frac{\partial U_B}{\partial x} \right)_b \quad (19)$$

Substituting (17) and (19) into (19) and rearranging

$$\frac{K_a}{\Delta x_a} (U_A - U_B) - \frac{K_b}{\Delta x_b} (U_B - U_C) = \left( \frac{\Delta x_a + \Delta x_b}{2} \right) \left( \frac{\rho c}{\Delta t} \right) (U'_B - U_B) \quad (20)$$

which is the explicit formulation of the finite difference equation for (1) for unequal node spacing and variable conductivity. Similarly, the general finite difference explicit expression for variable conductivity and unequal node spacing may be written as

$$\begin{aligned} \left( \frac{\Delta x_a + \Delta x_b}{2} \right) \left( \frac{\rho c}{\Delta t} \right) (U'_B - U_B) = & f \left[ \frac{K_a}{\Delta x_a} (U'_A - U'_B) - \frac{K_b}{\Delta x_b} (U'_B - U'_C) \right] \\ & + (1-f) \left[ \frac{K_a}{\Delta x_a} (U_A - U_B) \right. \\ & \left. - \frac{K_b}{\Delta x_b} (U_B - U_C) \right] \quad (21) \end{aligned}$$

It remains to choose an approximation for  $K_a$  and  $K_b$ , the conductivities of region a and region b, respectively. Four recommended approximations are the arithmetic mean, the harmonic mean, the integral value, and the value at the midpoint of the interval. These four approximations to the value of  $K_a$  and  $K_b$  in (21) are included in Table 2.

Table 2			
<u>Approximation Formulae for Conductivity</u>			
Name	Formula		Ref
	$K_a$ (Region a)	$K_b$ (Region b)	
Arithmetic Mean	$\frac{K_A + K_B}{2}$	$\frac{K_B + K_C}{2}$	(15:297)
Harmonic Mean	$\frac{2K_A K_B}{K_A + K_B}$	$\frac{2K_B K_C}{K_B + K_C}$	(17:45)
Mid-Point	$K\left(\frac{A+B}{2}\right)$	$K\left(\frac{B+C}{2}\right)$	(12:25)
Integral Value	$(\Delta x_a) \left[ \int_A^B \frac{dx}{K(x)} \right]^{-1}$	$(\Delta x_b) \left[ \int_B^C \frac{dx}{K(x)} \right]^{-1}$	(12:24)

All expressions for conductivity equate when  $K_A = K_B = K_C$ , and (20) reduces to (7) as is required when the diffusivity  $K/\rho c$ , is equal to unity and the node spacing and conductivity are constant.

### Boundary Condition at Infinity

Fox (Ref 8:91-92) suggests that an effective treatment for the boundary condition at infinity, (11)  $U(\infty, t) = 0$ , is to ensure the last two nodes considered have zero values to the number of significant figures retained. This should accurately satisfy the boundary condition, and this method was used in this investigation.

### Discontinuity

The initial and boundary conditions

$$U(0, t) = 1$$

$$U(x, 0) = 0$$

give rise to a discontinuity at the origin because the limiting value of the initial temperature is unity as  $x$  tends to zero, whereas the limiting value of the boundary temperature is zero as  $t$  tends to zero. This discontinuity can give rise to a poor finite-difference solution near  $x$  equal zero for small values of time (Ref 20:58). A similar discontinuity, in an investigation by Martin (Ref 10:72), caused poor results when untreated. Martin eliminated the discontinuity by substituting the exact analytical solution after the initial time step (Ref 10:73) and reported a significant improvement in solution accuracy. Smith (Ref 20:58-59) suggests a method for handling this problem which involves a transformation of

the independent variables from  $(x,t)$  to  $(X,T)$  where

$$X = xt^{-\frac{1}{2}}$$

$$T = t^{\frac{1}{2}}$$

The result of this transformation is an expansion of the origin at  $x = t = 0$  onto the positive side of the new  $X$  axis, while the old  $x$  axis is concentrated at a point at infinity on the new  $X$  axis. This transforms the jump condition at  $x = t = 0$  into a continuous change defined over the positive side of the  $X$  axis. Another approach, suggested by Ames (Ref 1:224-225), is to use the mean initial value of the temperature at the origin for the first time step to reduce sensitivity of the finite difference approximation to the discontinuity. A fourth method discussed by Ames (Ref 1:228) and Ketter (Ref 10:335-339, 371-379), and used by Campbell, Kaplan, and Moore (Ref 2:325-326) is that of mesh refinement. In mesh refinement, the effect of the discontinuity is diminished by subdividing the space/time mesh near the discontinuity.

### Error Analysis

Background. Solutions of partial differential equations (PDE) by methods of finite difference equations (FDE) are subject to several types of errors referred to in this report as truncation error, round-off error, and discretization error.

Truncation error is the difference between the exact solution of the FDE and the analytic solution of the PDE. The truncation error is due to the use of finite increments in approximating the derivatives and is generated by the truncation of higher order terms in the approximation of the PDE. The order of the truncation error is approximated by the estimate of the magnitude of the first neglected term in the Taylor series expansion used to derive the FDE (Ref 1:24). Round-off error is due to the limitation on the number of significant figures carried by the computer in the solution of the problem. The magnitude of this error is a function of the number and type of calculations involved in the problem solution. If an infinite number of decimal places were carried in the computations, the round-off error would vanish (Ref 19:298). In this report, the algebraic sum of the truncation error and round-off error is called the discretization error. This error is the difference between the exact analytic solution and the computed finite difference solution.

General. The accuracy attainable with finite difference methods will generally depend upon the fineness of the grid spacing and the order of the finite difference approximation. Reducing the grid spacing increases the number of equations to be solved, increasing the required number of calculations and the problem of round-off error. Using higher order approximations yields greater accuracy for a fixed mesh size, but results in complicated finite-difference expressions (Ref 6:377).

Although it is the discretization error that is actually being evaluated, it is reasonable to assume this error roughly equal to the truncation error. Therefore, if the error is given by

$$e = g(\Delta x)^2$$

for a node spacing of  $\Delta x$ , then the result of decreasing the spacing to  $\Delta x/2$  can be expressed by

$$\frac{e_1}{e_{1/2}} = \frac{g_1(\Delta x)^2}{g_{1/2}(\Delta x/2)^2} = 4$$

Similarly, the effect of halving the node spacing when the error is given by

$$e = g(\Delta x)^4$$

is

$$\frac{e_1}{e_{1/2}} = \frac{g_1(\Delta x)^4}{g_{1/2}(\Delta x/2)^4} = 16$$

The value of the ratio of the errors due to a change in the node spacing by a factor of two is defined as the discretization error ratio in this investigation. Thus, a discretization error ratio of 4 indicates accuracy of order

$(\Delta x)^2$  ( $O(\Delta x)^2$ ) , and a ratio of 16 indicates  $O(\Delta x)^4$  accuracy. The truncation error associated with any particular finite difference scheme may usually be determined by a Taylor series expansion of the finite-differences about a particular point within the mesh. Using this method, Campbell (Ref 13:20-22) has shown that, for solutions to problems involving homogeneous materials, the Explicit, Pure-Implicit, and Crank-Nicolson F.D.M.s are second order accurate,  $O(\Delta x)^2$  , and the Douglas method is fourth order accurate,  $O(\Delta x)^4$  .

Mitchell (Ref 12:28) derives the truncation error for an implicit finite-difference scheme corresponding to the Crank-Nicolson formulation for variable conductivity and shows it to be  $O(\Delta x)^2$  . However, Smith (Ref 20:216), in treating irregular boundaries, suggests that unequal node spacing for problems involving constant conductivity increases the truncation error to  $O(\Delta x)$  . The author did not derive the theoretical truncation error for finite-differences involving variable conductivity and unequal node spacing, but suggests that it would be  $O(\Delta x)$  on the basis of the cited report by Smith.

Absolute Error Magnitude. The basic objective of this thesis was to compare the finite difference solutions obtained using the Explicit, Pure-Implicit, Crank-Nicolson and Douglas methods. For this analysis, absolute error magnitudes were used. That is,

$$\epsilon = U_{A.S.} - U_{F.D.S}$$

where

- $\epsilon$  = absolute error magnitude which is the absolute value of the discretization error
- $U_{A.S.}$  = exact value of  $U$  at node  $x$  at time  $t$  from the analytic solution
- $U_{F.D.S.}$  = finite difference approximation of  $U$  at node  $x$  at time  $t$

Thus, the results of this investigation, as discussed in Chapter IV and depicted graphically in Appendix C, are presented in terms of the absolute value of the discretization errors and the discretization error ratios for each finite-difference method evaluated.

### Stability Analysis

Instability. If the magnitude of the difference between the exact numerical solution and the finite-difference approximation grows exponentially as the calculation proceeds, then the numerical scheme is termed unstable.

Condition for Stability. For homogeneous materials where the conductivity is constant, the stability limits are shown in Table 3.

When conductivity varies only with the spatial variable, as in this investigation, Richtmyer and Morton (Ref 18:195) give the general condition for stability as

Table 3		
<u>Stability Criteria for Finite Difference</u>		
<u>Methods for Homogeneous Material</u>		
Scheme	f	Stability Criteria
Explicit	0	$\Delta t / (\Delta x)^2 \leq \frac{1}{2}$
Pure Implicit	1	Unconditional
Crank-Nicolson	$\frac{1}{2}$	Unconditional
Douglas	$\frac{1}{2} \left( 1 - \frac{(\Delta x)^2}{6\Delta t} \right)$	Unconditional
General Equation	$\frac{1}{2} \leq f \leq 1$	Unconditional
	$0 \leq f \leq \frac{1}{2}$	$2\Delta t / (\Delta x)^2 \leq 1 / (1 - 2f)$

$$2\alpha(x)\Delta t(1 - 2f) / (\Delta x)^2 < 1 \quad (22)$$

where

$$\alpha(x) = K/\rho c, \text{ thermal diffusivity}$$

and all other variables have previously been defined. Using Eq (22) stability criteria may be found for each method by appropriate substitution for the variable f as follows:

Explicit Method:

Substituting  $f = 0$  into (22)

$$2\alpha(x)\Delta t/(\Delta x)^2 < 1$$

and the stability condition is

$$\alpha(x)\Delta t/(\Delta x)^2 < \frac{1}{2} \quad (23)$$

Implicit Method:

Substituting  $f = 1$  into (22)

$$2\alpha(x)\Delta t(1-2)/(\Delta x)^2 < 1$$

Thus, the requirement for stability is

$$-2\alpha(x)\Delta t/(\Delta x)^2 < 1$$

which is always true as  $\alpha(x)$ ,  $\Delta t$  and  $(\Delta x)$  are always positive, thus the Implicit Method is unconditionally stable.

Crank-Nicolson Method:

Substituting  $f = \frac{1}{2}$  into (22)

$$2\alpha(x)\Delta t(1-1)/(\Delta x)^2 < 1$$

Thus the requirement for stability is

$$0 < 1$$

which is always true, and the Crank-Nicolson Method is unconditionally stable.

Douglas Method:

Substituting  $f = \frac{1}{2}(1 - \frac{(\Delta x)^2}{6\alpha(x)\Delta t})$  into (22)

$$2\alpha(x)\Delta t [1 - 2(\frac{1}{2}(1 - \frac{(\Delta x)^2}{6\alpha(x)\Delta t}))] / (\Delta x)^2 < 1$$

Rearranging

$$2\alpha(x)\Delta t [(\Delta x)^2 / 6\alpha(x)\Delta t] / (\Delta x)^2 < 1$$

and the requirement for stability is

$$\frac{1}{3} < 1$$

which is always true. Thus, the Douglas Method is unconditionally stable.

As was true for homogeneous material problems, only the Explicit FDE, for the methods investigated, presents a problem concerning stability. Substitute

$$\alpha(x) = K(x)/\rho c = K_0 x^n / \rho c$$

into (23) and let  $K_0/\rho c = 1.0$ . Then, Eq (23) becomes

$$x^n \Delta t / (\Delta x)^2 < \frac{1}{2} \tag{24}$$

which is the stability limit for the Explicit FDE as used in this investigation. For each value of  $n$ ,  $\Delta t$ , and  $\Delta x$ , a maximum value of  $x$  is calculated for which the

Explicit finite-difference solution is stable. The results of calculations for  $n = 0$  to  $n = .75$  are shown in Figure 9 and listed in Table 4 for  $n = .1$  to  $n = .75$ .

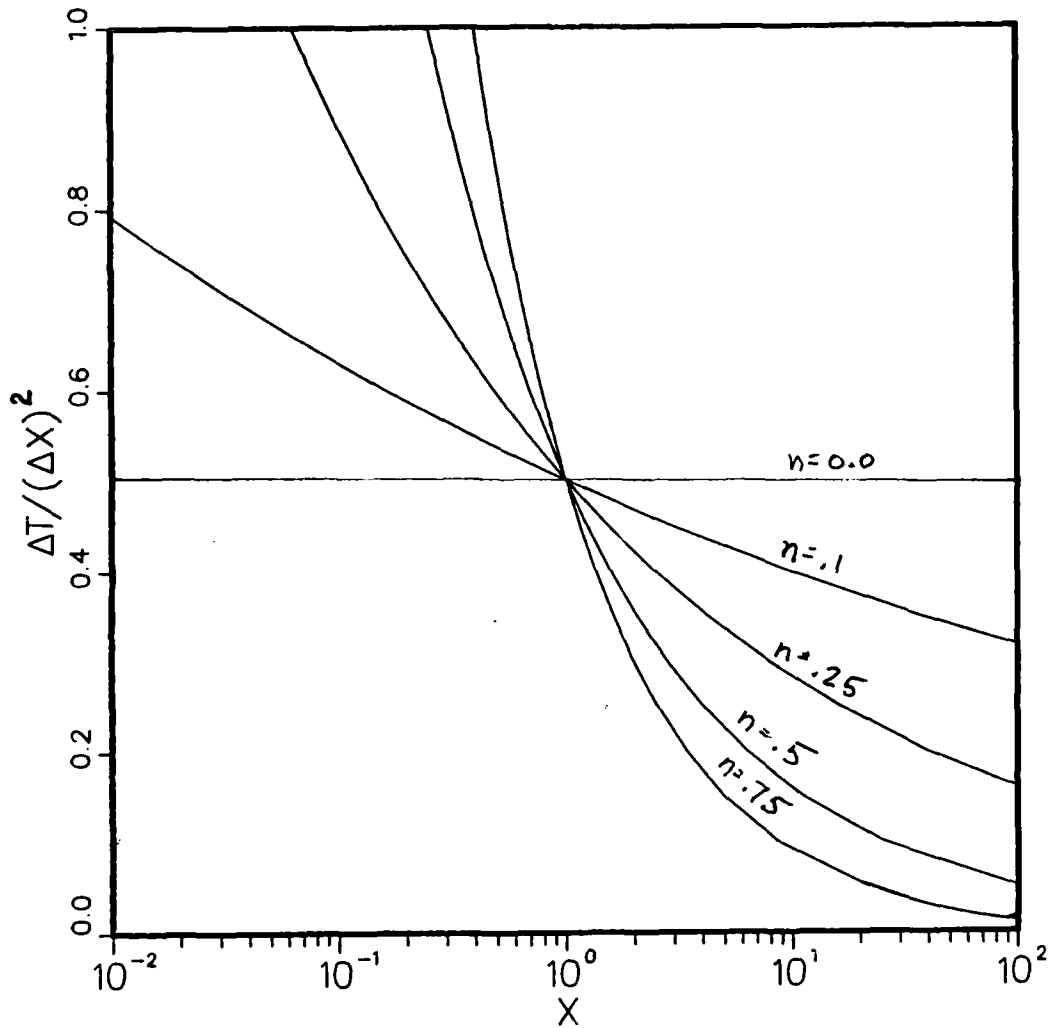


Figure 9. Stability Curves for Explicit Finite Difference Method for  $\eta=0, .1, .25, .5, \text{ and } .75$

Table 4  
 Maximum Value of x for Stability  
 of Explicit Finite Difference Method  
 where Criteria for Stability is  $x^n \Delta t / (\Delta x)^2 < \frac{1}{2}$

t/(x)	n = .1	n = .25	n = .5	n = .75
.050		10000.000	100.000	21.544
.100		625.000	25.000	8.550
.150	169350.878	123.457	11.111	4.979
.200	9536.743	39.063	6.250	3.393
.250	1024.000	16.000	4.000	2.520
.300	165.382	7.716	2.778	1.976
.350	35.401	4.165	2.041	1.609
.400	9.313	2.441	1.563	1.347
.450	2.868	1.524	1.235	1.151
.500	1.000	1.000	1.000	1.000
.550	.386	.683	.826	.881
.600	.162	.482	.694	.784
.650	.073	.350	.592	.705
.700	.035	.260	.510	.639
.750	.017	.198	.444	.582
.800	.009	.153	.391	.534
.850	.005	.120	.346	.493
.900	.003	.095	.309	.457
.950	.002	.077	.277	.425
1.000	.001	.062	.250	.397

### III. Procedure

#### General Approach

Initial Phase. Phase One of this investigation began with a study of conduction heat transfer and a literature search which included a search for one and two dimensional transient heat conduction problems involving variable conductivity with analytic solutions. Primary texts for the heat transfer study were Myers (Ref 15) and Patankar (Ref 16). No two-dimensional problems were found, but one of several one-dimensional problems found in Carslaw and Jaeger (Ref 4) was chosen for investigation and is presented in Chapter II.

Second Phase. This phase consisted of deriving the finite difference equations for non-homogeneous material and variable node spacing using engineering notation, applying the initial and boundary conditions of the problem, and developing the matrix equations for the numerical solution of the problem. The matrix equations are presented in Appendix A.

Third Phase. Phase Three began with development of a computer program to numerically evaluate the analytic solution to the problem discussed in Chapter II. Concurrently, the finite-difference equations were programmed for constant node spacing, and methods for analyzing and presenting data were evaluated. The method of error analysis used by

Campbell, Kaplan, and Moore (Ref 2) was chosen and is explained in Chapter IV. Thus, the results are presented as the absolute value of the pointwise discretization error (at  $x = .05$  and  $x = 0.1$ ) and the discretization error ratio at the same points for each numerical method for several choices of time and space increments as was discussed in Chapter II.

Fourth Phase. The fourth phase of the investigation began with a study of error and stability in the finite difference methods. Richtmyer and Morton (Ref 18) and Fox (Ref 8) were the primary texts used in the study. The stability limits as discussed in Chapter II were used to determine the time and space parameters for the computer runs. Also during this phase, a method for approximating the conductivity as discussed in Chapter II was chosen, and the computer codes written in Phase Three were validated.

Fifth Phase. The initial mesh of 10 nodes was subdivided into 20, 40, and then 80 nodes. Correspondingly,  $\Delta t$  was reduced by factors of four to keep the Fourier Modulus constant. This was done for  $n$  equal to .25 and .5. Table 5 shows the relationship of absolute time to incremental time for spatial subdivisions considered. Next, the first cell was subdivided into two equal segments to reduce the effect of the discontinuity at the origin at  $x = t = 0$ , as discussed in Chapter II. This was done for

Table 5			
<u>Relationship of Absolute Time</u>			
<u>to Incremental Time for Spatial Subdivisions Considered</u>			
<u>Subdivisions</u>	<u>Time Increment</u>		
	20	40	80
Real Time			
.01	1	4	16
.02	2	8	32
.05	5	20	80
.1	10	40	160
.2	20	80	320
.5	50	200	800

20, 40, and 80 nodes, for  $n = .25$  and  $.5$ . The resulting changes in degree of accuracy of each method was analyzed and compared against the previous results from equal grid spacing for all four finite-difference methods under investigation.

The most significant effect of the boundary-condition-at-infinity (11) is to fix the number of time steps a calculation can proceed, based on the size of the time increment,  $\Delta t$ , to avoid violating this boundary condition. In order to take larger time steps and keep the same number of nodes, it is necessary to increase the size of the spatial increment,  $\Delta x$ , by an amount adequate to ensure the temperature at the last two nodes remains equal to zero. Thus, the initial grid

size with 20 nodes was doubled, the first space increment subdivided into two equal segments, and then subsequent runs were made for  $n = .25$  and  $.5$  for 20, 40, and 80 nodes for the Pure-Implicit, Crank-Nicolson and Douglas methods for  $\Delta t/(\Delta x)^2$  equal to 1.0, 2.0 and 5.0. These results were also analyzed and compared, as were the previous results.

#### Computer System and Programs

Computer System. The computer system used for this project is one designed by the Control Data Corporation. It consists of input and output devices, peripheral processors, and two central processors. The central processors are a CDC 6613 and a CDC Cyber 74 which operate in parallel. Each has 131,000 60-bit words of central memory. Magnetic disc and drum storage were used as temporary storage devices.

Computer Programs. Four major programs were written during this investigation. There were also numerous other programs written for error analysis and plotting purposes. The language used for all programs was FORTRAN 5.

Although cost and computer run time are important in most computer work, the thrust of this investigation was in the direction of comparing the finite-difference methods investigated for accuracy and stability. The programs which were written were designed for generality and to make use of mass data storage and temporary files. Thus, no effort

was made to compare cost and run times for the various options used. However, with the exception of the Explicit finite-difference scheme, all the methods considered were implicit involving tri-diagonal matrices and thus should have been roughly comparable with respect to computation time. Also, the Douglas Method was the most complicated method to code as the weighting factor,  $f$ , had to be calculated for each node.

#### IV. Results

##### Exact Solution

As discussed in Chapter II, the analytic solution, Eq (12), contained an integral which had to be evaluated numerically. To validate the computer program for evaluating the analytic solution, the parameter  $n$  was set equal to zero. Since a zero value of  $n$  is equivalent to constant conductivity (since  $K = K_0 x^n$  in this investigation), the author sought and found another form of the solution for the investigated problem for constant conductivity:

$$U(x,t) = 1 - \operatorname{erf} \left( \frac{x}{\sqrt{2Kt}} \right)$$

where

$\operatorname{erf}$  = error function

$K$  = conductivity = constant

and  $x$  and  $t$  have been previously defined. An ASD library routine was then used to evaluate the error function. A comparison of the results for several values of  $x$  and one value of  $t$  is provided in Table 6 as an example of the results of this program validation.

##### Numerical Solutions

Conte and DeBoor (Ref 6) was the source for the Thomas Algorithm as programmed for the tri-diagonal matrix solutions

Table 6  
A Comparison Table for Validating  
the Computer Program for the Exact Analytical Solution  
(t = .00625)

x	Thesis Solution	Library Solution
.05	.65472084	.65472085
.1	.37109335	.37109337
.2	.07363830	.07363827
.4	.00034672	.00034662

for this investigation. After all programs were debugged and error-free, each was modified to solve an applicable heat transfer problem from Carnahan, et al (Ref 3) and the results were verified with the published textbook results to complete program validation.

Conductivity Approximation

The results of the error comparisons made using three common methods for approximating the conductivity are presented graphically in Appendix B for the Explicit, Pure-Implicit, Crank-Nicolson, and Douglas finite difference methods for a Fourier Modulus of  $\frac{1}{2}$  and with  $n = .25$  and  $n = .5$ .

For conductivity which varies linearly, the mid-point and arithmetic mean approximations are identical. For very

small intervals and slowly varying conductivity (non-linear variation), the mid-point and arithmetic mean approximations should be nearly equal. When the conductivity varies by relatively large amounts, the harmonic mean should provide the best approximation of the three methods examined.

While the arithmetic and harmonic mean approximations were generally more accurate than the mid-point approximation for both variations on the problem presented, ( $n = .25$  and  $n = .5$ ), there was no consistency as to whether the harmonic or arithmetic mean was the more accurate. Thus, the arithmetic mean was chosen for the rest of the investigation as it was the simpler method to program.

### Discontinuity

The discontinuity at  $x = t = 0$  as discussed in Chapter II was treated by mesh refinement as discussed in Chapter III. The order of accuracy improved by a factor of two over the unmodified solutions for all finite-difference methods with  $n$  equal to  $.25$  as shown in Figures 10, 11, 12, and 13. The improvement is not dramatic. In fact, for the variation where  $n$ , the exponent in the conductivity term was equal to  $0.5$ , the error improvement in the graded mesh compared to the equally spaced mesh disappeared after approximately ten time steps which is shown by comparing Figures 14 and 15, and 16 and 17. More improvement in error reduction could be made, perhaps with one of the other methods discussed in Chapter II.

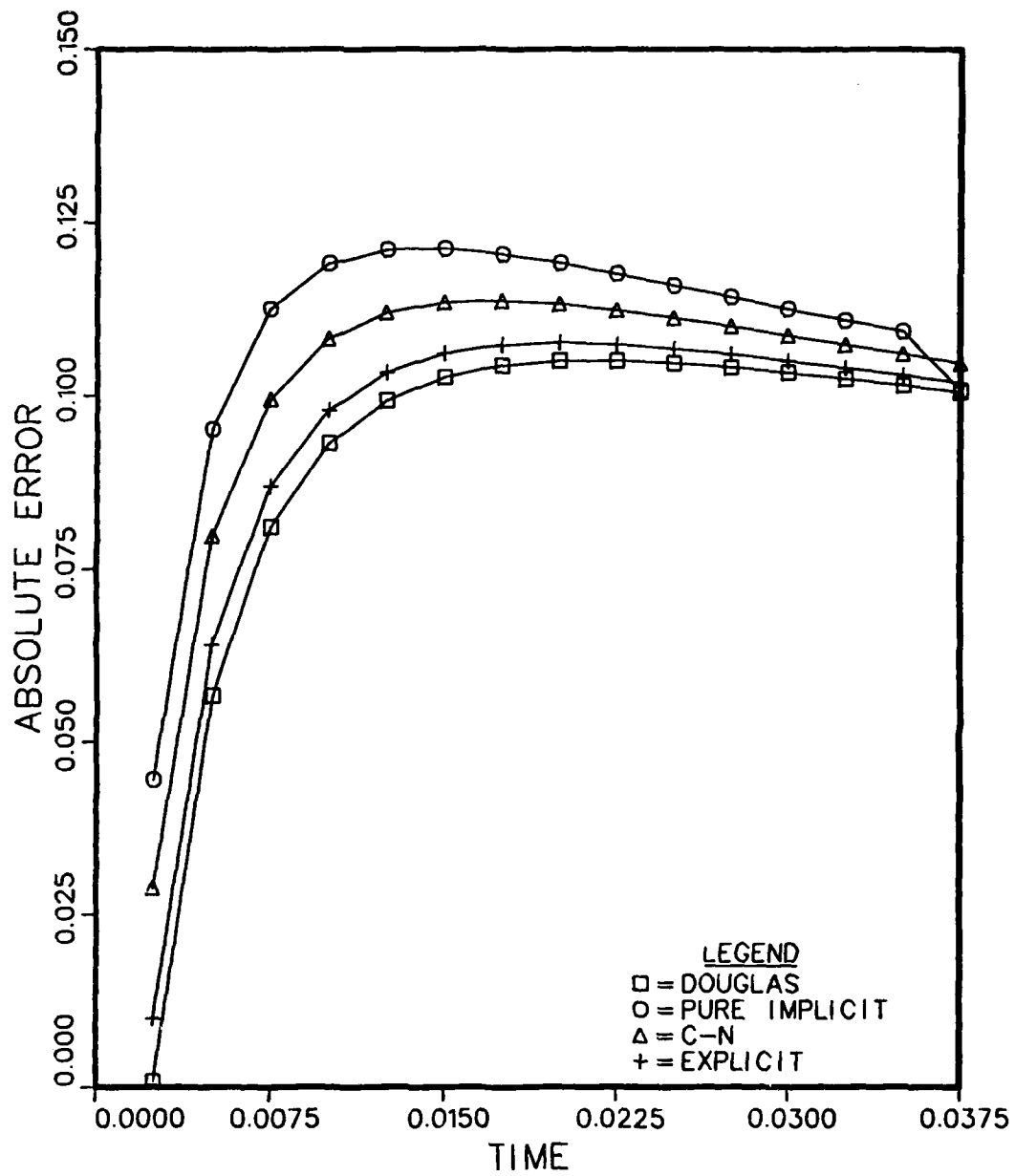


FIGURE 10. Absolute value of discretization error vs Time at  $x=0.05$ : Ungraded mesh  $n=25$

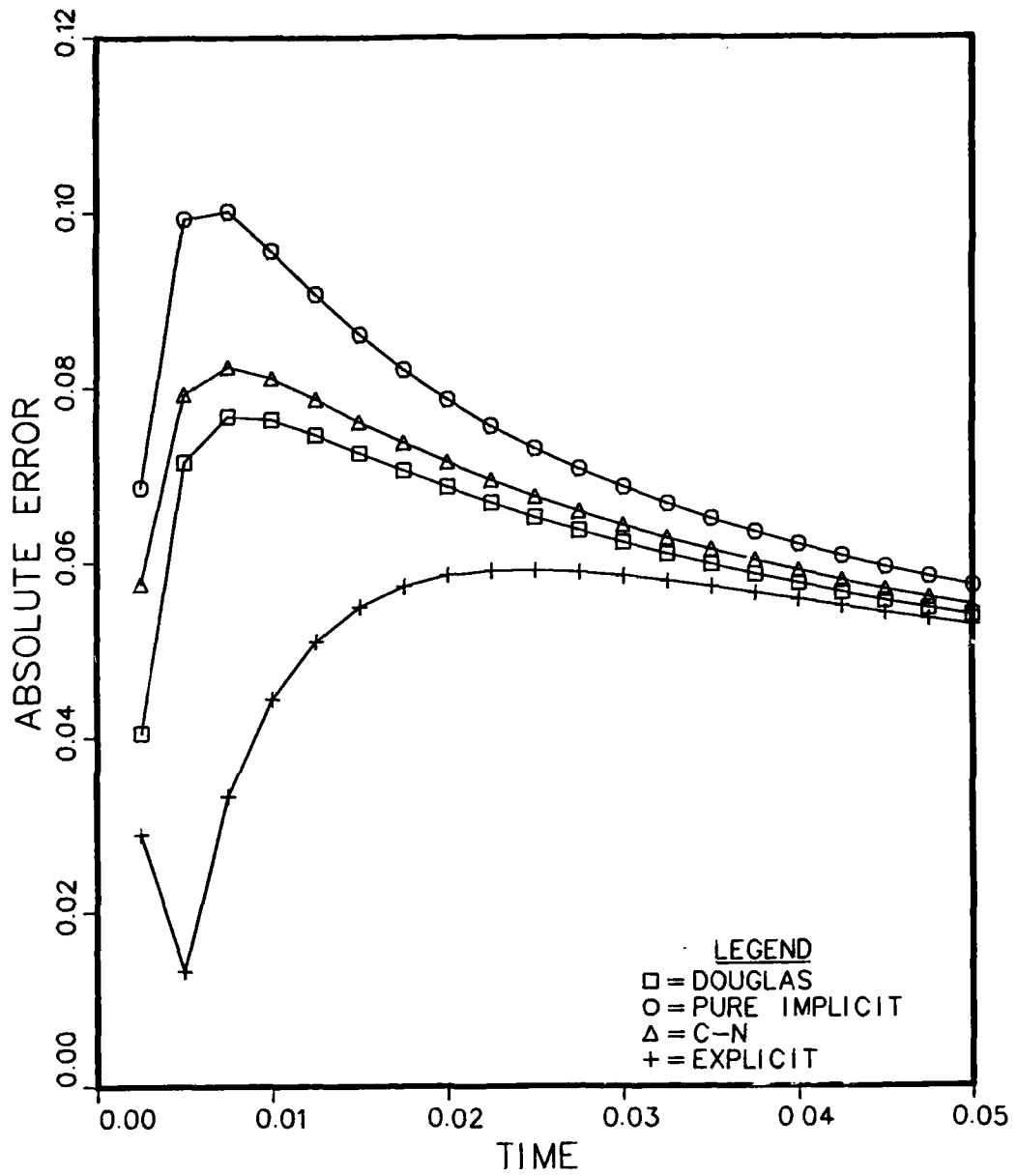


FIGURE 11. Absolute value of discretization error vs Time at  $x=0.5$ : Graded mesh  $n=25$

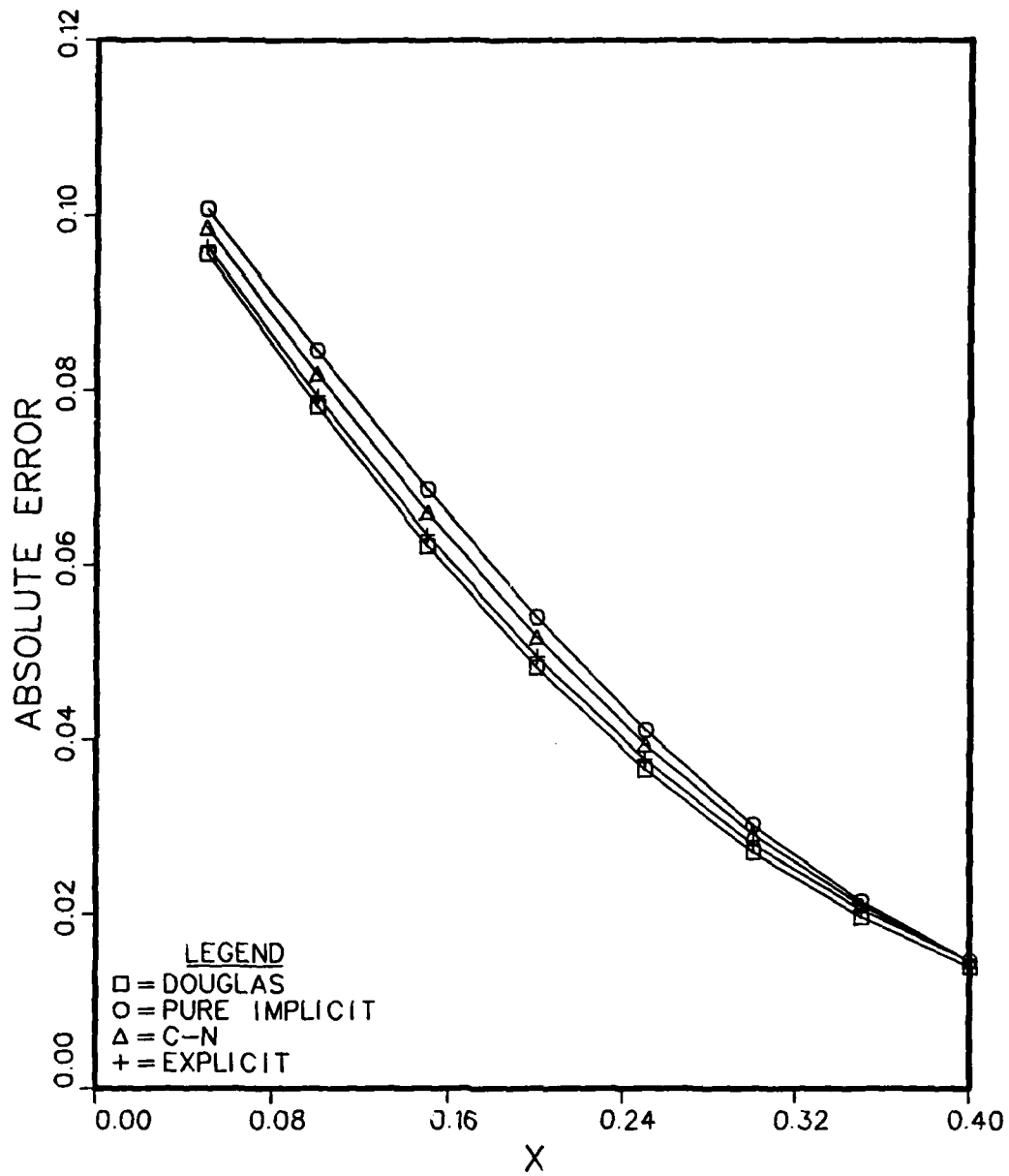


FIGURE 12. Absolute value of discretization error vs X at Time=.05: Ungraded mesh n=.25

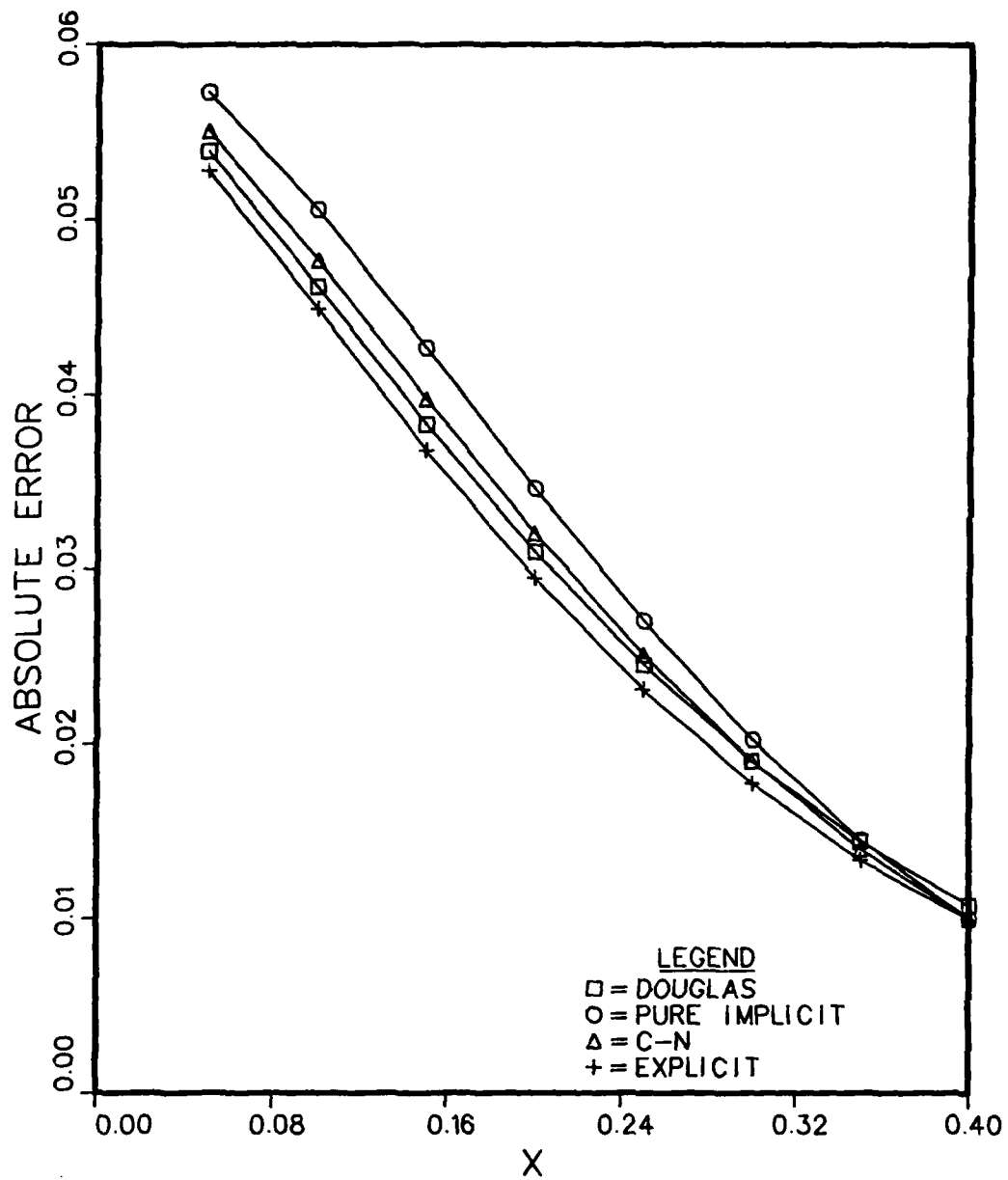


FIGURE 13. Absolute value of discretization error vs X at Time=.05: Graded mesh n=.25

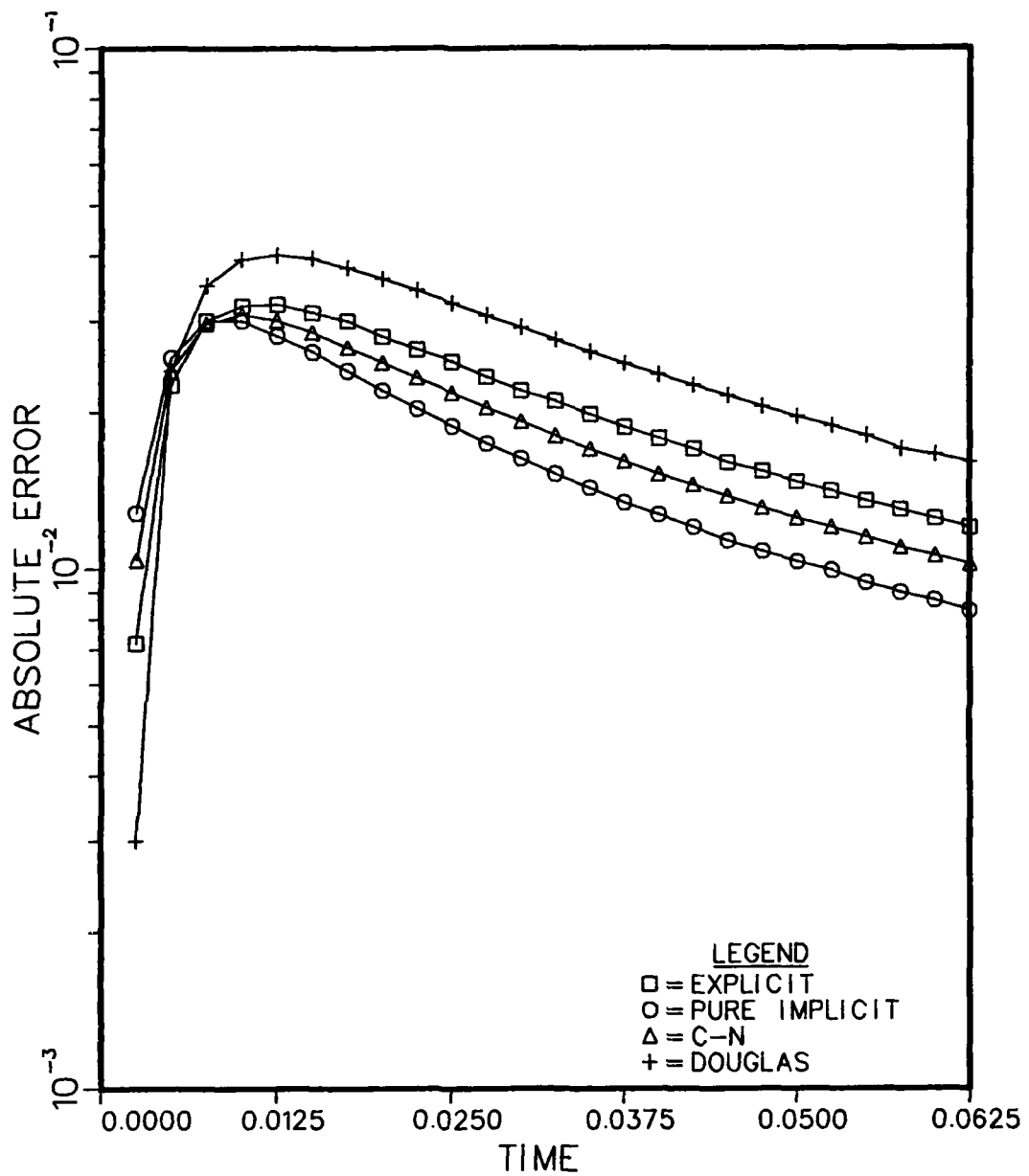


FIGURE 14. Absolute value of discretization error vs Time at  $x=1$ : Ungraded mesh  $n=5$

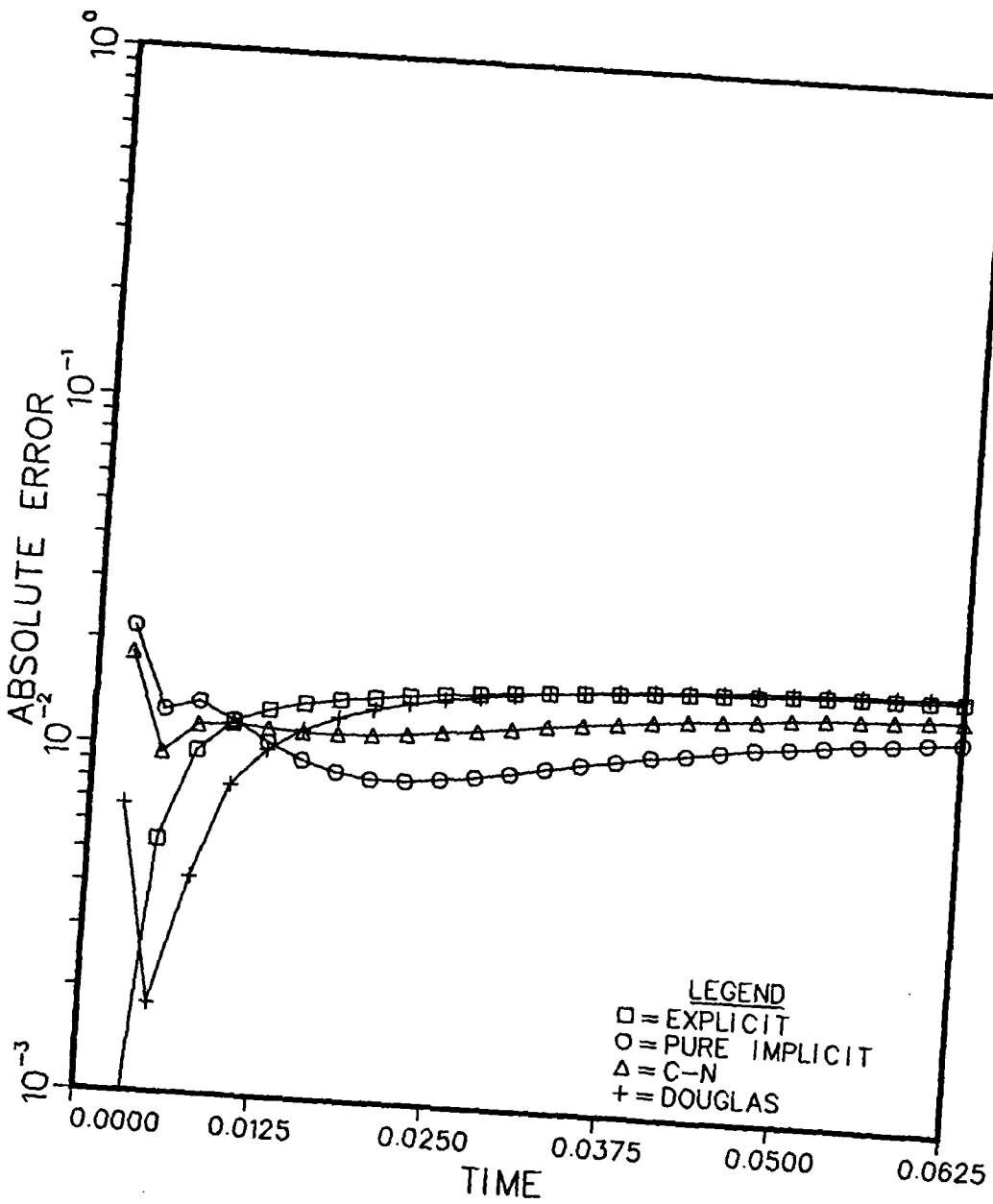


FIGURE 15. Absolute value of discretization error vs Time at  $x=1$ : Graded mesh  $n=5$

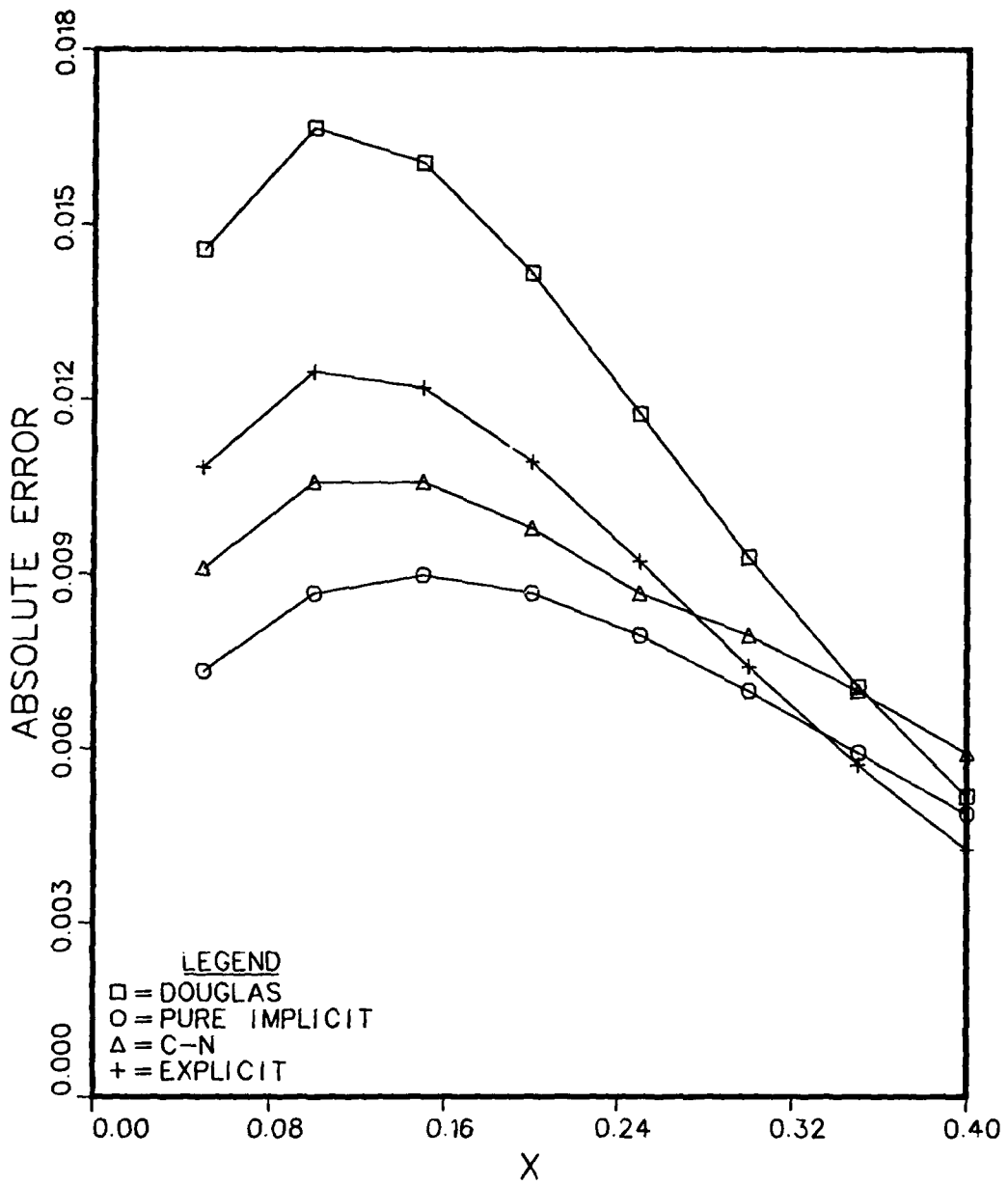


FIGURE 16. Absolute value of discretization error vs X at Time=.06: Ungraded mesh n=5

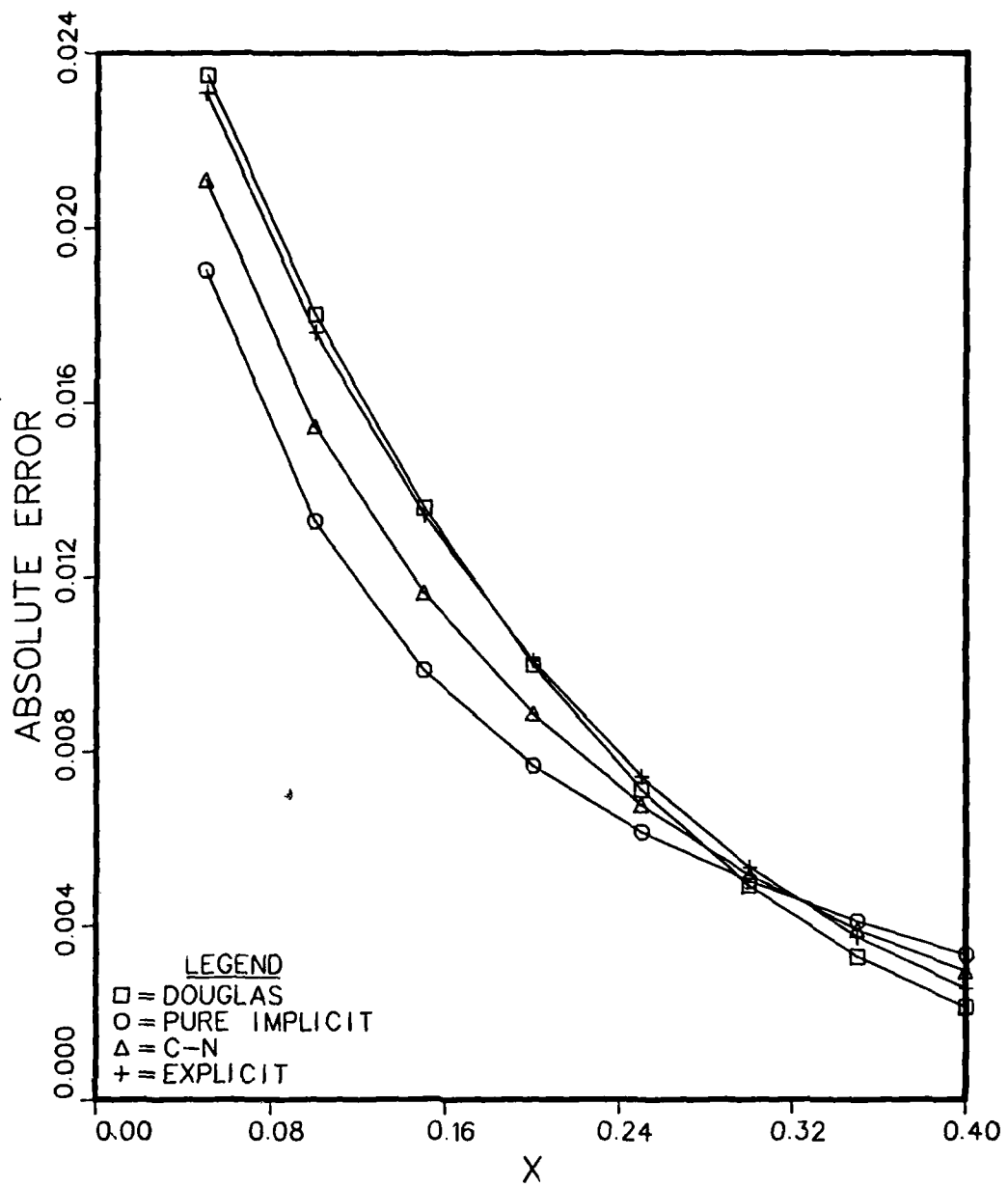


FIGURE 17. Absolute value of discretization error vs X at Time=.06: Graded mesh n=.5

### Stability

Although the Pure-Implicit, Crank-Nicolson, and Douglas Methods are unconditionally stable, the graphic results in Appendix C, Section II, show Crank-Nicolson and Douglas Methods are not unconditionally accurate. Patankar and Beliga (Ref 17:27-31) and Crandall (Ref 7:389) discuss conditions and limitations for oscillatory behavior of finite difference methods in detail. While Crandall's results do not directly apply to problems involving variable conductivity, the results of Appendix C imply that analogous oscillatory limits must exist. Patankar and Beliga offer two alternative finite-difference schemes which do apply to problems involving variable conductivity and each is unconditionally stable and has no oscillatory behavior. However, time and computer resources did not permit using these methods in this investigation. The author's results did verify that the Pure-Implicit scheme is free from oscillatory behavior as was shown by Patankar and Beliga (Ref 17:29).

### Error

With the exception of the results for  $n = .5$  for an ungraded mesh, the discretization error ratio ranged from 1.3 to 1.7 for all methods on all variations of the problem. This indicates  $O(\Delta x)$  accuracy as discussed in Chapter II. In all graphs in Appendix C, as well as Figures 10-17, it

is noted that the absolute value of the discretization error and also the discretization error ratios exhibit erratic behavior at very early times. This behavior with respect to time is characteristic of finite-difference solutions of parabolic equations, and all plots show, as Smith (Ref 20:58) indicates, a characteristic improvement in accuracy near  $x$  equal zero as the time increases.

While the graphic results are discussed in more detail in Appendix C, a general result was that for  $n$  equal to .25, the Douglas Method was usually the most accurate method and for  $n$  equal to .5, the Pure-Implicit Method was the most accurate. However, there was usually small difference in the relative accuracy of the methods with the exception of when the Crank-Nicolson and Douglas Method solutions exhibited oscillatory behavior. Then, the Pure-Implicit Method was significantly most accurate.

Error versus  $x$ . The discretization error ratio and absolute value of the discretization error were each plotted against  $x$  for each variation of the parameters  $n$  and  $\Delta t/(\Delta x)^2$ . Representative graphs are included in Appendix C. As at  $x$  equal to 0.05 and 0.1, the discretization error ratio improved with time to a range of 1.3 to 1.7 for all variations of the problem. All finite-difference methods were approximately equal in accuracy except when  $\Delta t/(\Delta x)^2$  was equal to 5. Then, the Pure-Implicit Method was significantly most accurate across the mesh. Also, the solution

at nodes where the temperature was very nearly zero behaved similarly to the solution near  $x = t = 0$ . That is, the solution improved with time at all points.

## V. Conclusions and Recommendations

### Conclusions

Although the Crank-Nicolson and Douglas finite-difference schemes are increasingly more sophisticated than the traditional Explicit and Pure-Implicit schemes, they did not prove any significant advantage in accuracy in this investigation. In all cases, for both variations of the problem ( $n = .25$ ,  $n = .5$ ) there was little difference in accuracy among the methods. Because of the oscillatory behavior of the Crank-Nicolson and Douglas schemes when the value of the Fourier Modulus was large, the Pure-Implicit scheme proved most advantageous.

Although not verified theoretically, all four finite difference methods appear to be first order accurate for the type of problem investigated, when the discontinuity at  $x = t = 0$  is treated by mesh refinement.

### Recommendations

Martin (Ref 11) achieved a significant improvement in the discretization error ratio when he treated a discontinuity similar to the one handled in this investigation by substituting the exact analytic solution after the first time step. The same should be done for this problem to see if similar improvements are achieved. However, this method of treating the discontinuity has no real significant

advantage since the analytic solution is rarely known for "real-world" engineering problems. Similarly, the boundary-condition-at-infinity may be treated by substitution of the exact solution for the last two nodes for all time steps. This would remove the limitation on the number of time steps a calculation may proceed as discussed in Chapter II.

The choice of the conductivity approximation was based on a comparison of absolute discretization error at  $x = 0.1$  for equal spaced nodes only. The majority of the results obtained were from calculations involving a graded network. As shown in Appendix C, the solutions of all four finite-difference methods investigated behaved differently, depending upon the value of  $n$ , the variable in the exponent in the conductivity term,  $K = K_0 x^n$ . Thus, comparisons of the finite-difference methods should be made using the harmonic mean for the conductivity approximation, at least for  $n = .5$ . The harmonic mean may provide a more satisfactory approximation to the exact solution than the arithmetic mean, since the conductivity varies more across a given interval for larger values of  $n$ .

An analytic expression for the truncation error should be derived and verified for finite-differences for variable conductivity and mesh size. These methods should also be tested on other problems involving variable conductivity where the conductivity expression is simpler (there are several suitable solved problems in Carslaw and Jaeger

(Ref 4:323-324), and the results compared with those of this investigation.

Although Crank-Nicolson and Douglas schemes have the advantage of unconditional stability, they both have oscillatory limits. An investigation should be made of the use of the exponential scheme or power-law scheme as discussed by Patankar and Beliga (Ref 17:27-32) for a problem involving variable conductivity, and the results included with those of this investigation.

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## APPENDIX A

### Development of Matrix Equations

The general form of the finite-difference equation, as discussed in Chapter II, is

$$\begin{aligned}
 & \left(\frac{\Delta x_a + \Delta x_b}{2}\right) \left(\frac{\rho c}{\Delta t}\right) (U'_B - U_B) \\
 & = f \left[ \frac{K_a}{\Delta x_a} (U'_A - U'_B) - \frac{K_b}{\Delta x_a} (U'_B - U'_C) \right] \\
 & + (1-f) \left[ \frac{K_a}{\Delta x_a} (U_A - U_B) - \frac{K_b}{\Delta x_b} (U_B - U_C) \right] \tag{A-1}
 \end{aligned}$$

which, for the Explicit method ( $f = 0$ ) may be written as

$$U'_B = 2pU_A + (1 - 2p - 2q) U_B + 2qU_C$$

where

$$p = \frac{\Delta t K_a}{\rho c \Delta x_a (\Delta x_a + \Delta x_b)}$$

and

$$q = \frac{\Delta t K_b}{\rho c \Delta x_b (\Delta x_a + \Delta x_b)}$$

Using the boundary condition  $U(0,t) = 1$ , the following matrix relation results (for four nodes):

$$\underline{U}' = \underline{AU} + \underline{C}$$

where

$$\underline{A} = \begin{bmatrix} 1-2p_1-2q_1 & 2q_1 & & \\ 2p_2 & 1-2p_2-2q_2 & 2q_2 & \\ & 2p_3 & 1-2p_3-2q_3 & 2q_3 \\ & & 2p_4 & 1-2p_4-2q_4 \end{bmatrix}$$

$$\underline{C} = \begin{bmatrix} 2p_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

For the Pure-Implicit method ( $f = 1$ ), Eq (A-1) may be written

$$-2pU'_A + (1+2p+2q)U'_B - 2qU'_C = U_B$$

where  $p$  and  $q$  are as previously defined. The matrix relation (for four nodes) is

$$\underline{B} \underline{U}' + \underline{C} = \underline{U}$$

where

$$\underline{B} = \begin{bmatrix} 1+2p_1+2q_1 & -2q_1 & & & \\ -2p_2 & 1+2p_2+2q_2 & -2q_2 & & \\ & -2p_3 & 1+2p_3+2q_3 & -2q_3 & \\ & & -2p_4 & 1+2p_4+2q_4 & \end{bmatrix}$$

$$\underline{C} = \begin{bmatrix} 2p_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

For the Crank-Nicolson method ( $f = \frac{1}{2}$ ), Eq (A-1) may be written as

$$-pU'_A + (1+p+q)U'_B - qU'_C = pU_A + (1-p-q)U_B + qU_C$$

with  $p$  and  $q$  as previously defined, and the matrix relation written as

$$\underline{A} \underline{U}' + \underline{C}' = \underline{B} \underline{U} + \underline{C}$$

where

$$\underline{A} = \begin{bmatrix} 1+p_1+q_1 & -q_1 & & & \\ & -p_2 & 1+p_2+q_2 & -q_2 & \\ & & -p_3 & 1+p_3+q_3 & -q_3 \\ & & & -p_4 & 1+p_4+q_4 \end{bmatrix}$$

$$\underline{B} = \begin{bmatrix} 1-p_1-q_1 & q_1 & & & \\ & p_2 & 1-p_2-q_2 & q_2 & \\ & & p_3 & 1-p_3-q_3 & q_3 \\ & & & p_4 & 1-p_4-q_4 \end{bmatrix}$$

$$\underline{C} = \begin{bmatrix} p_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\underline{C}' = \begin{bmatrix} -p_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

For the Douglas Method,  $f = \frac{1}{2} \left( 1 - \frac{(\Delta x)^2}{6\alpha(x)\Delta t} \right)$ , and the value of  $f$  at each node varies with variations in the conductivity and the grid spacing. Thus, Eq (A-1) is rewritten

$$\begin{aligned} -2pf_A U'_A + [1+2f_B(p+q)] U'_B - 2qf_C U'_C \\ = 2p(1-f_A)U_A + [(f_B-1)(p+q)] U_B + 2q(1-f_C)U_C \end{aligned} \quad (A-2)$$

where  $p$  and  $q$  have been previously defined and  $f_A$ ,  $f_B$ ,  $f_C$  denote the value of the weighting factor  $f$  at nodes  $A$ ,  $B$ , and  $C$ , respectively. Thus, (A-2) may be rewritten as

$$\begin{aligned} -2rU'_A + (1+2s)U'_B - 2tU'_C \\ = 2(p-r)U_A + (s-p-q)U_B + 2(q-r)U_C \end{aligned}$$

where

$$r = pf_A$$

$$t = qf_C$$

$$s = (p+q)f_B$$

and all other variables have been previously defined.

The matrix relation (for four nodes) is

$$\underline{A} \underline{U}' + \underline{C}' = \underline{B} \underline{U} + \underline{C}$$

where

$$\underline{A} = \begin{bmatrix} 1+s_1 & -2t_1 & & & \\ -2r_2 & 1+s_2 & -2t_2 & & \\ & -2r_3 & 1+s_3 & -2t_3 & \\ & & -2r_4 & 1+s_4 & \end{bmatrix}$$

$$\underline{B} = \begin{bmatrix} s_1-p_1-q_1 & 2(q_1-r_1) & & & \\ 2(p_2-r_2) & s_2-p_2-q_2 & 2(q_2-r_2) & & \\ & 2(p_3-r_3) & s_3-p_3-q_3 & 2(q_3-r_3) & \\ & & 2(p_4-r_4) & s_4-p_4-q_4 & \end{bmatrix}$$

$$\underline{C} = \begin{bmatrix} 2(p_1-r_1) \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\underline{C}' = \begin{bmatrix} -2r_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

## APPENDIX B

### Comparison of Conductivity Approximation Methods

This appendix contains the graphical results of the comparison of three conductivity approximation methods which were discussed in Chapter II. The results are plotted as the absolute value of the discretization error versus time at  $x = .1$  for the Explicit, Pure-Implicit, Crank-Nicolson and Douglas finite difference methods, for  $n = .25$  and  $n = .5$ . In all cases, the numerical solution was obtained using a mesh of 40 equally spaced nodes with  $\Delta t/(\Delta x)^2$ , the Fourier Modulus, equal to 0.5.

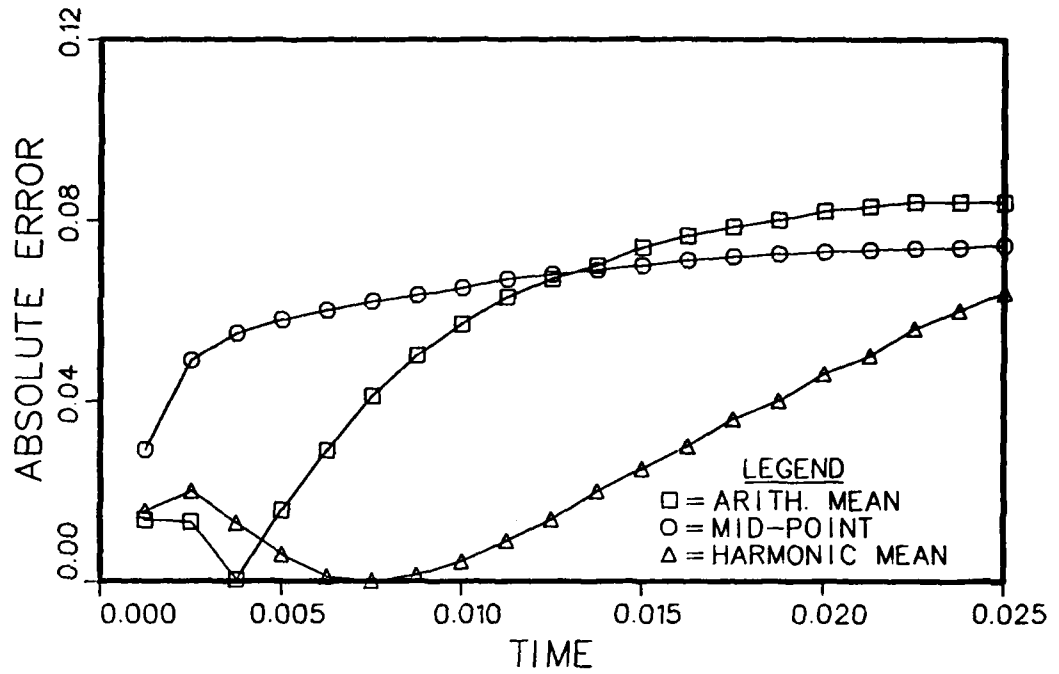


FIGURE 1  
 IMPLICIT F.D. Method: Error comparison at  $x=0.1$   
 (for  $n=25$ ) for conductivity approximation schemes

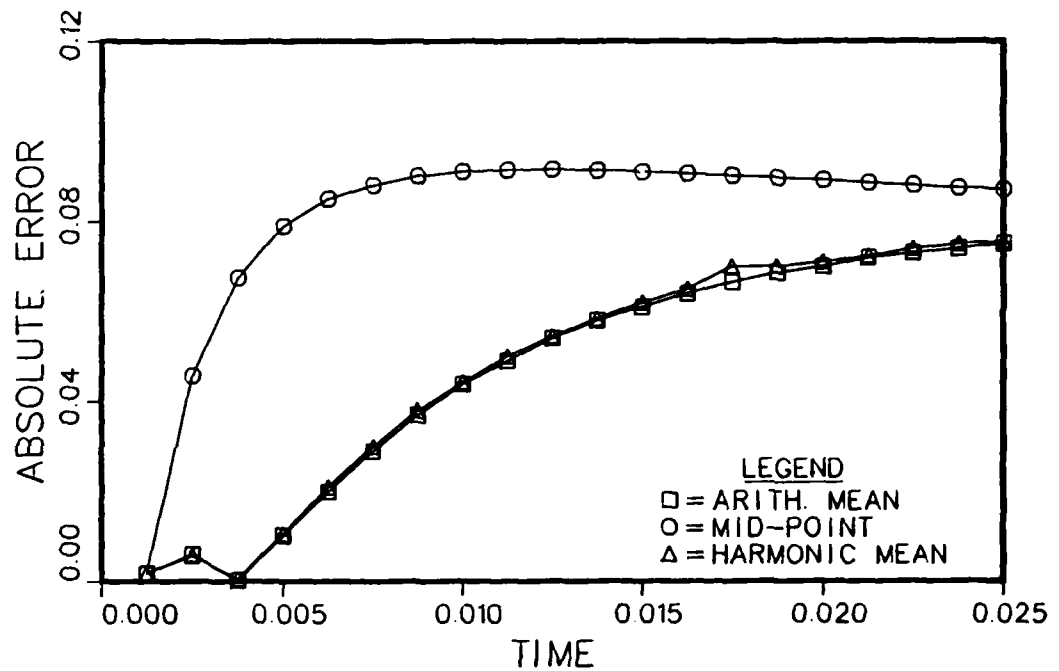


FIGURE 2  
 EXPLICIT F.D. Method: Error comparison at  $x=0.1$   
 (for  $n=25$ ) for conductivity approximation schemes

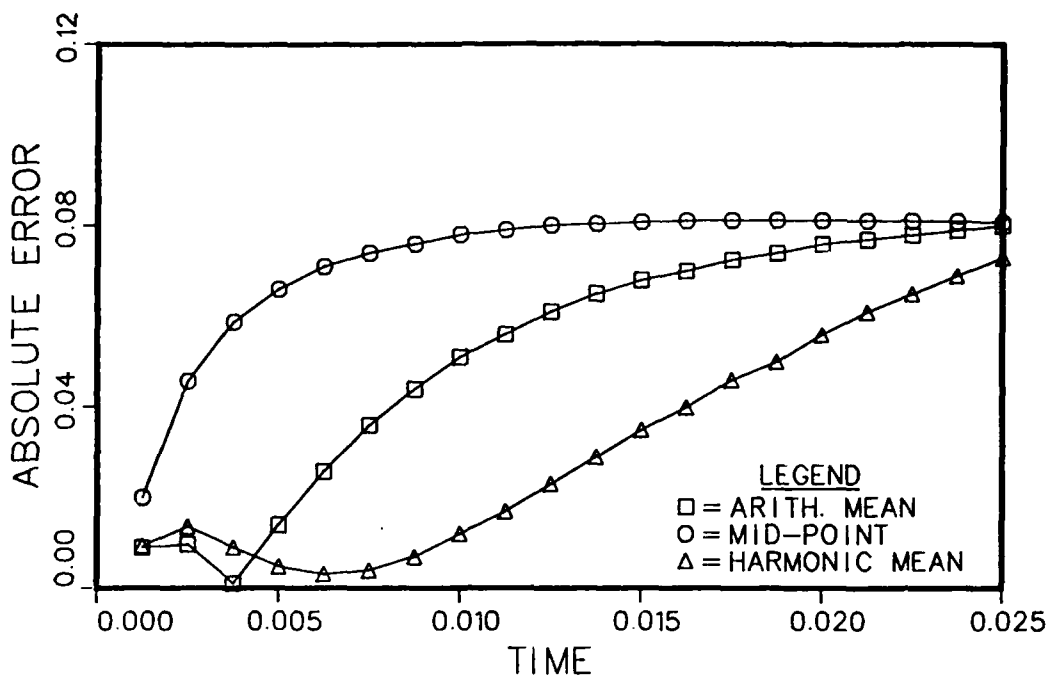


FIGURE 3  
 CRANK-NICOLSON F.D. Method: Error comparison at  $x=0.1$  (for  $n=25$ ) for conductivity approximation schemes

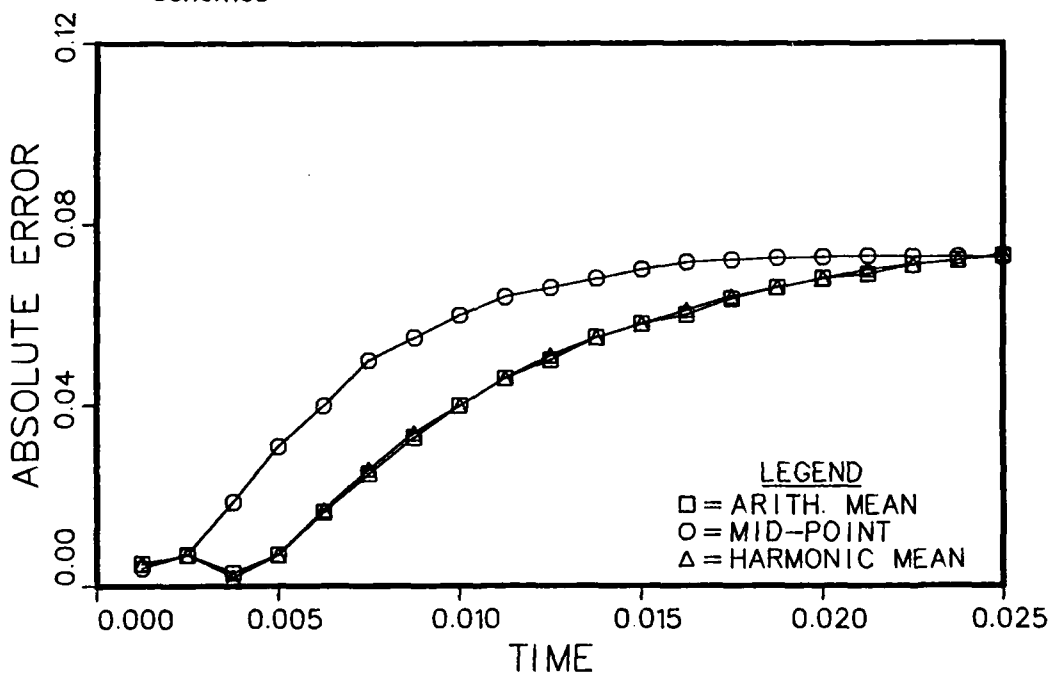


FIGURE 4  
 DOUGLAS F.D. Method: Error comparison at  $x=0.1$  (for  $n=25$ ) for conductivity approximation schemes

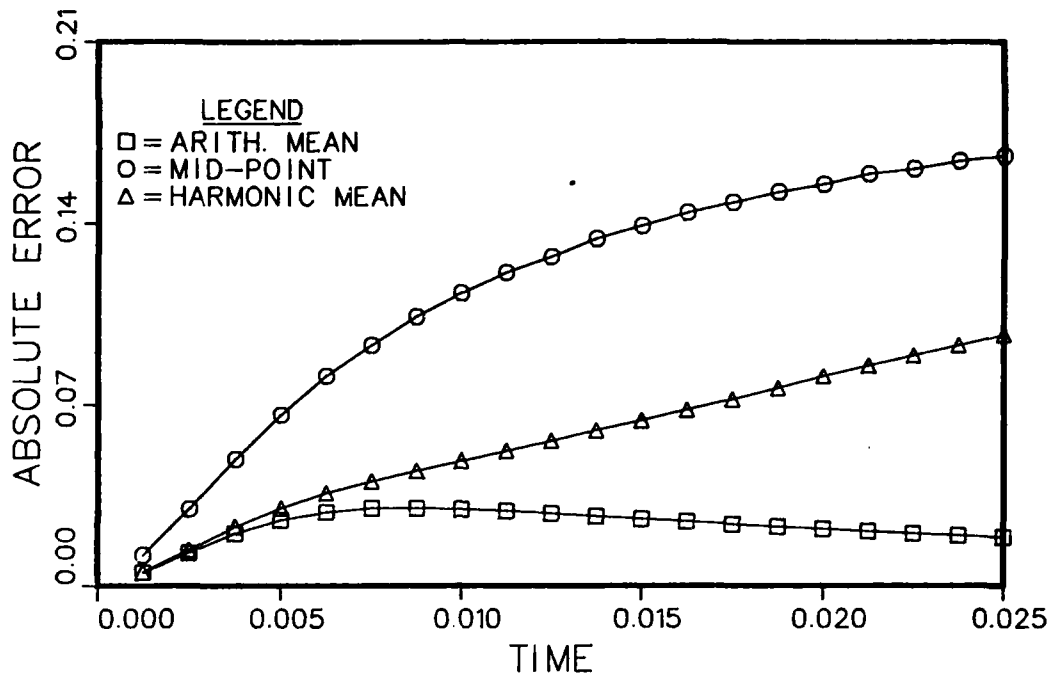


FIGURE 5  
 IMPLICIT F.D. Method: Error comparison at  $x=0.1$   
 (for  $n=50$ ) for conductivity approximation schemes

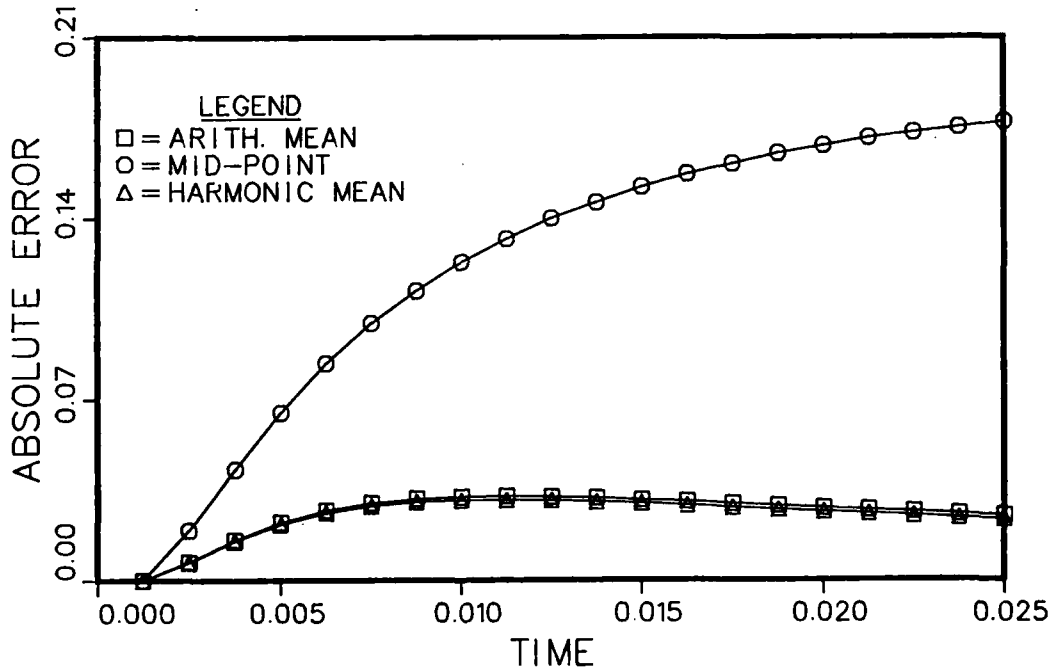


FIGURE 6  
 EXPLICIT F.D. Method: Error comparison at  $x=0.1$   
 (for  $n=50$ ) for conductivity approximation schemes

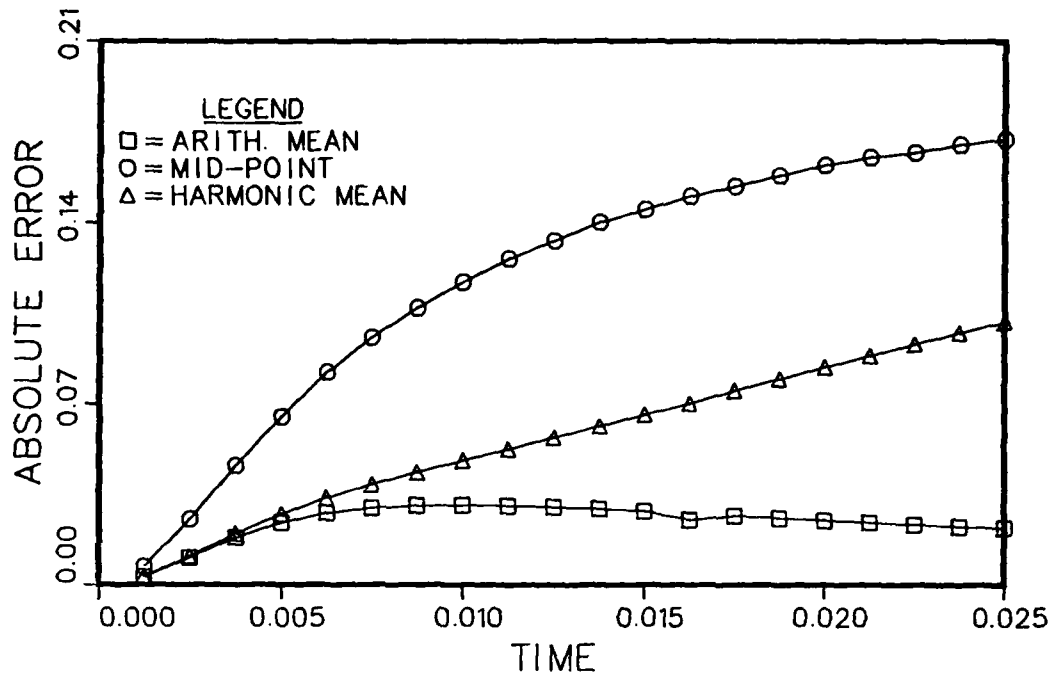


FIGURE 7  
 CRANK-NICOLSON F.D. Method: Error comparison at  $x=0.1$  (for  $n=50$ ) for conductivity approximation schemes

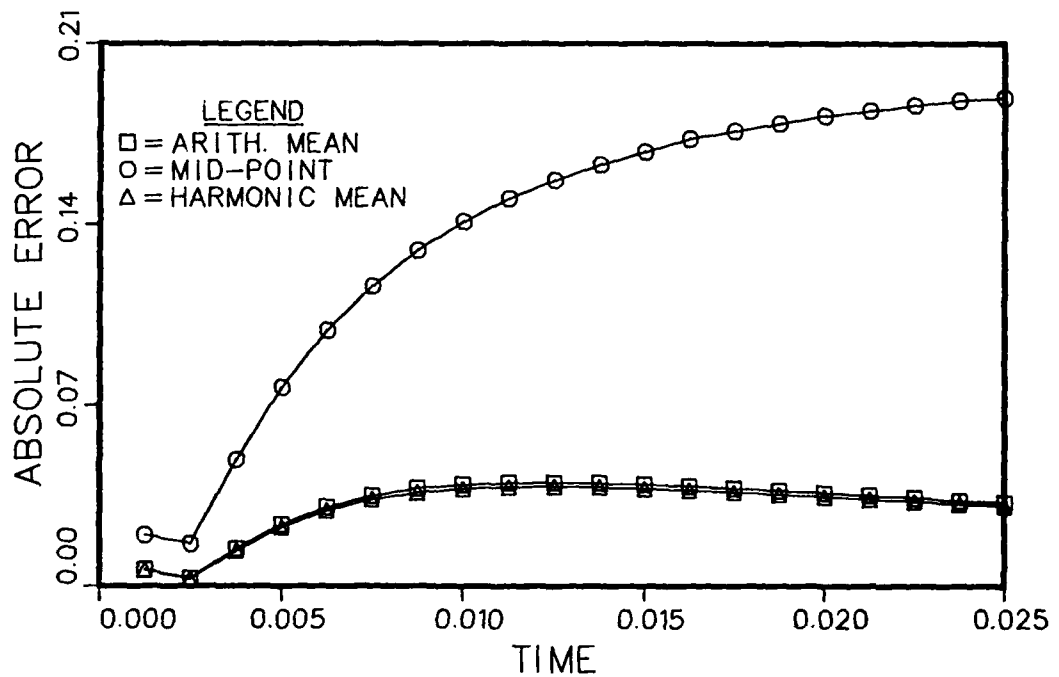


FIGURE 8  
 DOUGLAS F.D. Method: Error comparison at  $x=0.1$  (for  $n=50$ ) for conductivity approximation schemes

## APPENDIX C

### Computer Generated Plots of Results

This appendix contains a sample of the graphical results of this investigation presented as plots of the absolute value of the discretization error versus time and node location and the discretization error ratio versus time and node location for the Explicit, Pure-Implicit, Crank-Nicolson and Douglas finite-difference schemes. For all plots, the absolute value of the discretization error is labeled absolute error. Discretization error and discretization error ratio have been previously defined.

The plots are presented in two sections. Each section is prefaced with a short descriptive note. However, individual plots are not necessarily discussed. The sections are organized according to the value of the Fourier Modulus ( $\Delta t/(\Delta x)^2$ ) used in calculation. Section I includes the graphical results of the Explicit, Pure-Implicit, Crank-Nicolson and Douglas Methods with the Fourier Modulus equal to 0.5 and  $n$  equal to .25. Section II includes the graphical results of the Pure-Implicit, Crank-Nicolson and Douglas Methods with the Fourier Modulus equal to 5 and  $n = .25$ . The preface of each of the sections includes a key to the organization of the plots included in the section.

Although calculations were performed for 20, 40, and 80 nodes, the plots of absolute error versus time and

absolute error versus  $x$  for 20, 40, and 80 nodes were so similar that only those plots for 40 nodes are included. Exceptions are in Section II where the solution for 20 nodes behaved differently than that for 40 and 80 nodes. There, the graph for 20 nodes is also included.

As discussed in Chapter III, there was small difference in accuracy among the finite-difference methods compared except for the oscillatory behavior observed with the Fourier Modulus equal to 2 and 5. Thus, the plots included in this appendix are presented as representative of all of the data which was analyzed in this investigation as discussed in Chapter III.

## Section I

This section includes the graphical results of the Explicit, Pure-Implicit, Crank-Nicolson and Douglas Methods with the Fourier Modulus equal to  $\frac{1}{2}$  and  $n$  equal to .25. The following key shows which parameter options are included in this set of graphs.

Table C-I				
<u>Key to the Plots in Section I</u>				
Figure No.	Number of Nodes	x	Time	Error*
C-I-1	40	.05	.00125-.05	AE
C-I-2	40	.1	.00125-.0625	AE
C-I-3	20/40	.05	.00125-.05	DER
C-I-4	40/80	.05	.00125-.05	DER
C-I-5	20/40	.1	.00125-.0625	DER
C-I-6	40/80	.1	.00125-.0625	DER
C-I-7	40	.05-.4	.025	AE
C-I-8	40	.05-.4	.05	AE
C-I-9	20/40	.05-.4	.025	DER
C-I-10	40/80	.05-.4	.025	DER
C-I-11	20/40	.05-.4	.05	DER
C-I-12	40/80	.05-.4	.05	DER

\*AE: Absolute Error  
DER: Discretization Error Ratio

Although all methods exhibit approximately the same accuracy, the Douglas Method is generally most accurate, providing the least discretization error, and the Explicit, Crank-Nicolson, and Pure-Implicit follow in descending order. However, the order is reversed when comparing discretization error ratio, as the Pure-Implicit Method error is consistently most improved by halving  $\Delta x$ , and the Douglas Method error least improved. Similar results were attained for  $n$  equal to .5 except that the Pure-Implicit and Crank-Nicolson Methods were then most accurate and the Explicit and Douglas Methods provided the higher discretization error ratios. The graphs and discussion of results in this section are equally representative of those for a Fourier Modulus equal to 1.

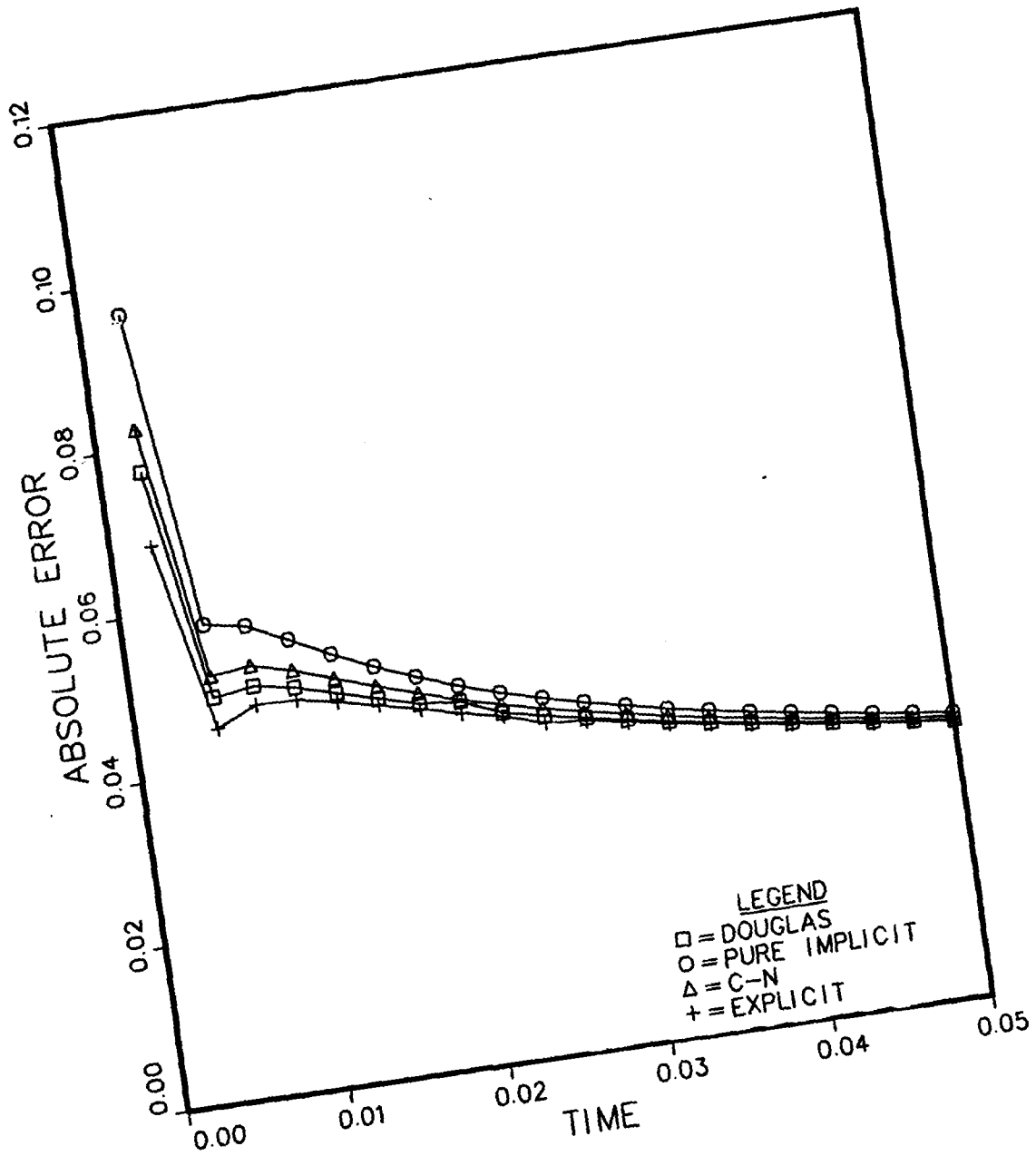


FIGURE C-1-1. Absolute value of discretization error vs Time at  $x=0.5$ :  $n=25$  40 nodes

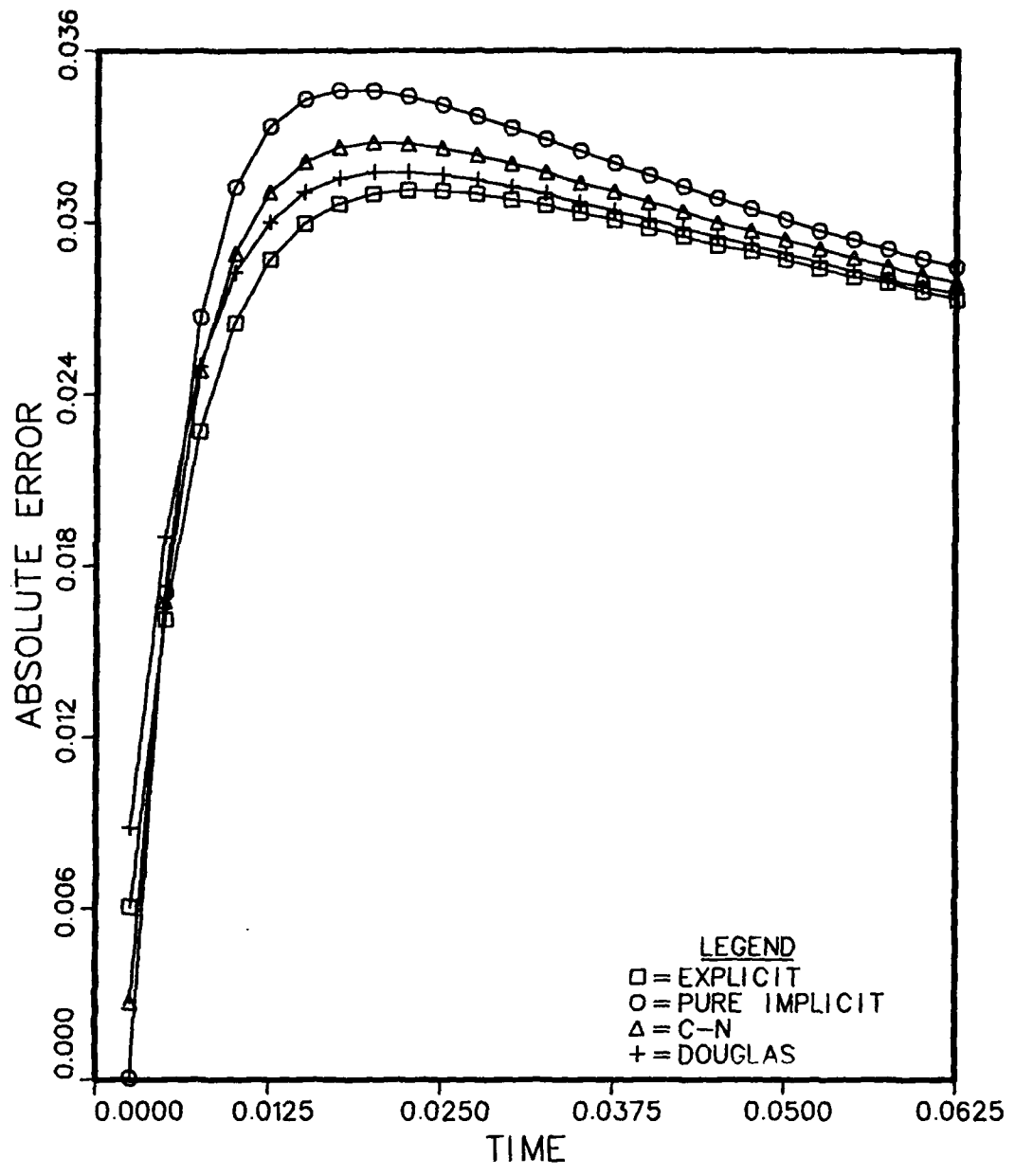


FIGURE C-1-2. Absolute value of discretization errors  
Time at x=1: n=25 40 nodes

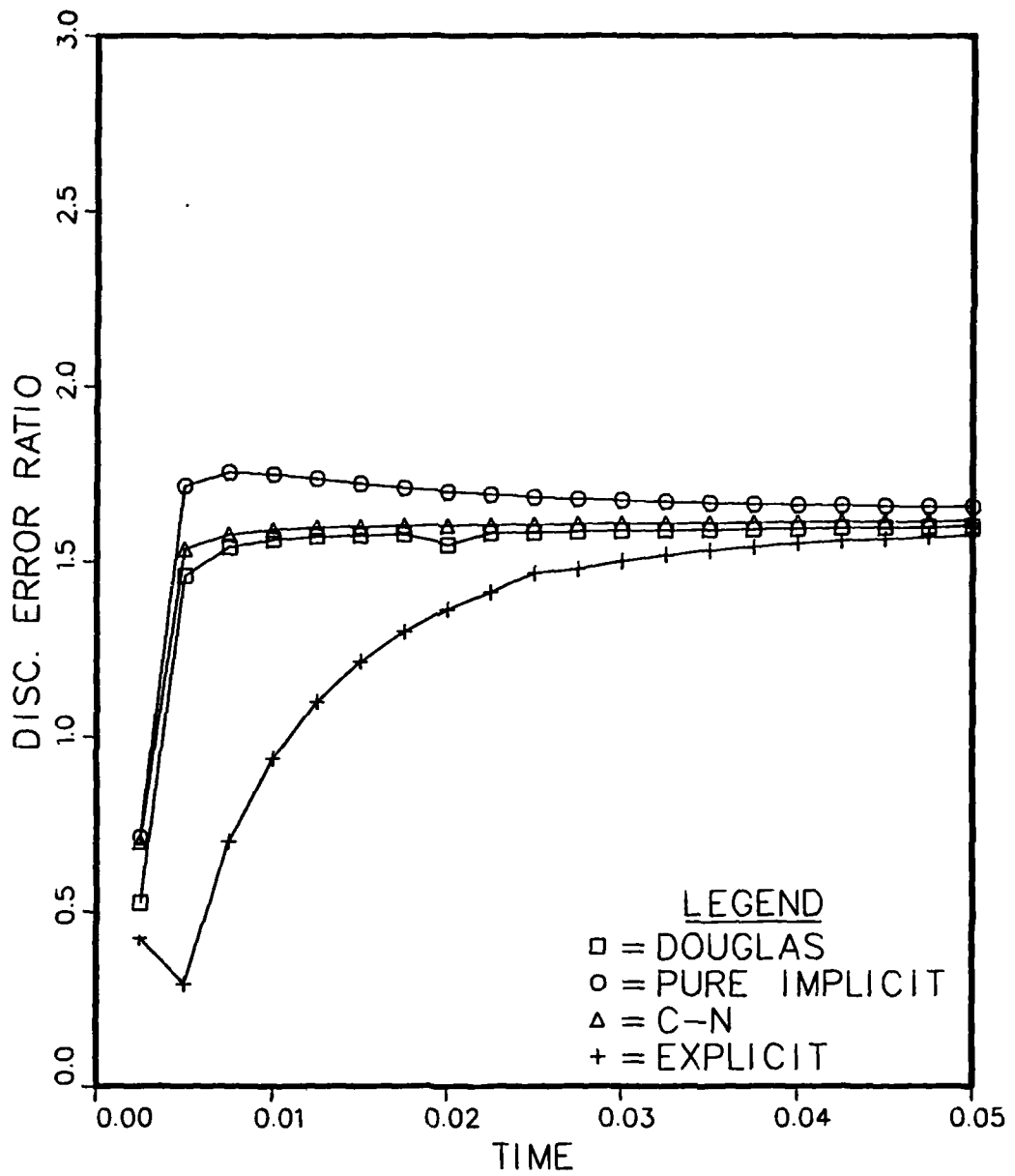


FIGURE C-1-3. Absolute value of discretization error ratio vs Time at  $x=0.5$  for 20/40 nodes:  $n=25$

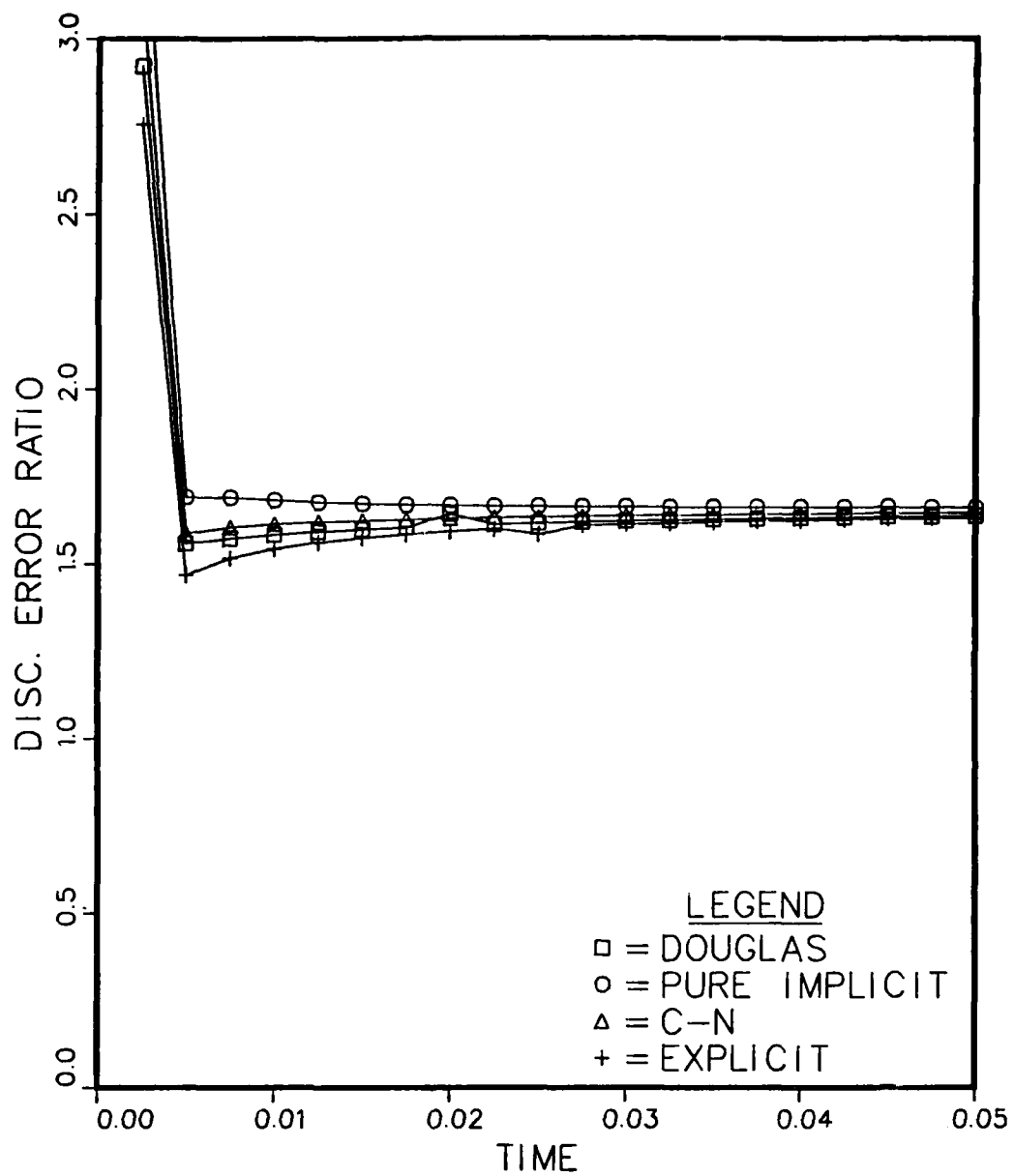


FIGURE C-1-4. Absolute value of discretization error ratio vs Time at  $x=0.5$  for 40/80 nodes:  $n=25$

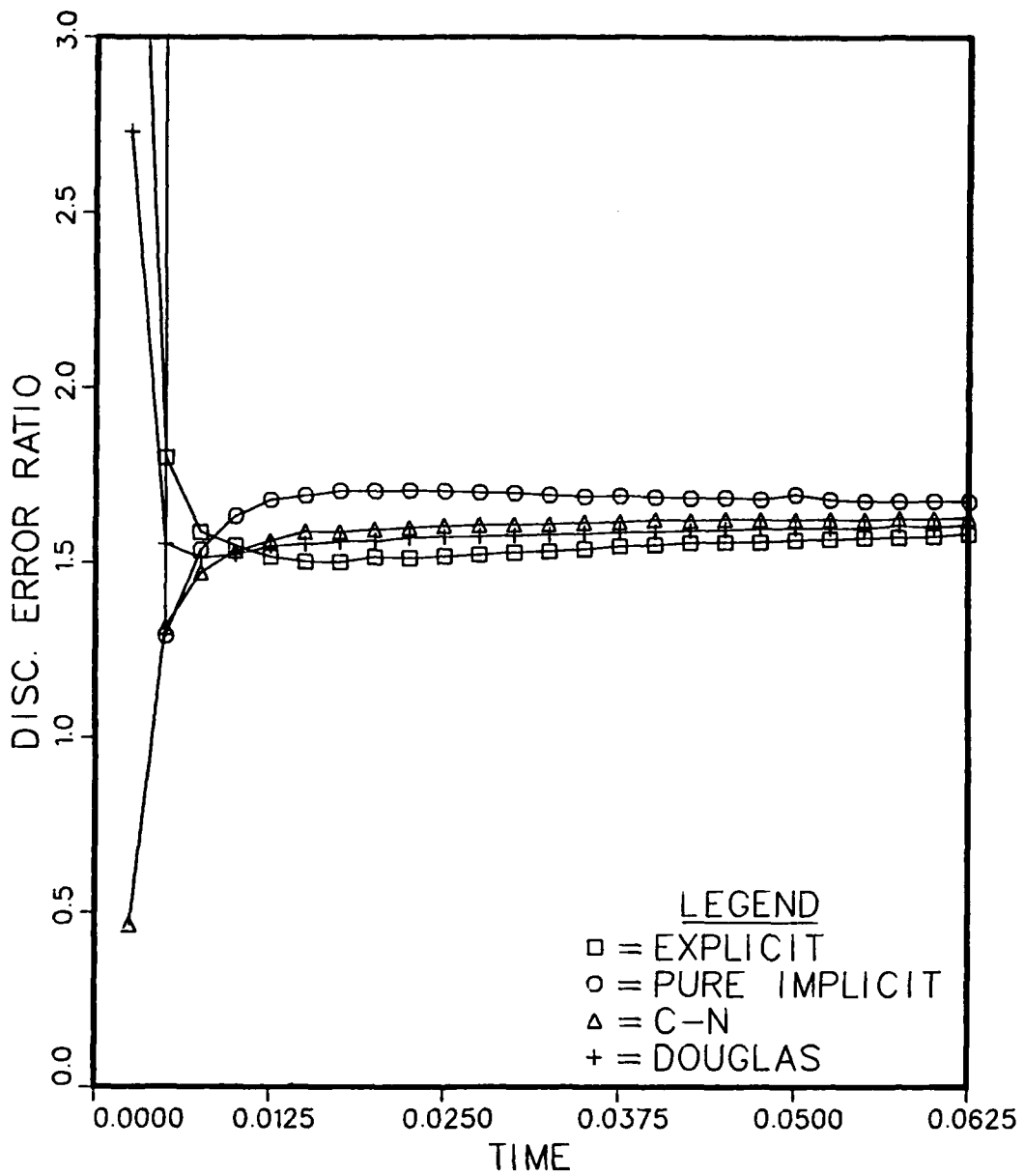


FIGURE C-1-5. Absolute value of discretization error ratio vs Time at  $x=1$  for 20/40 nodes:  $n=.25$

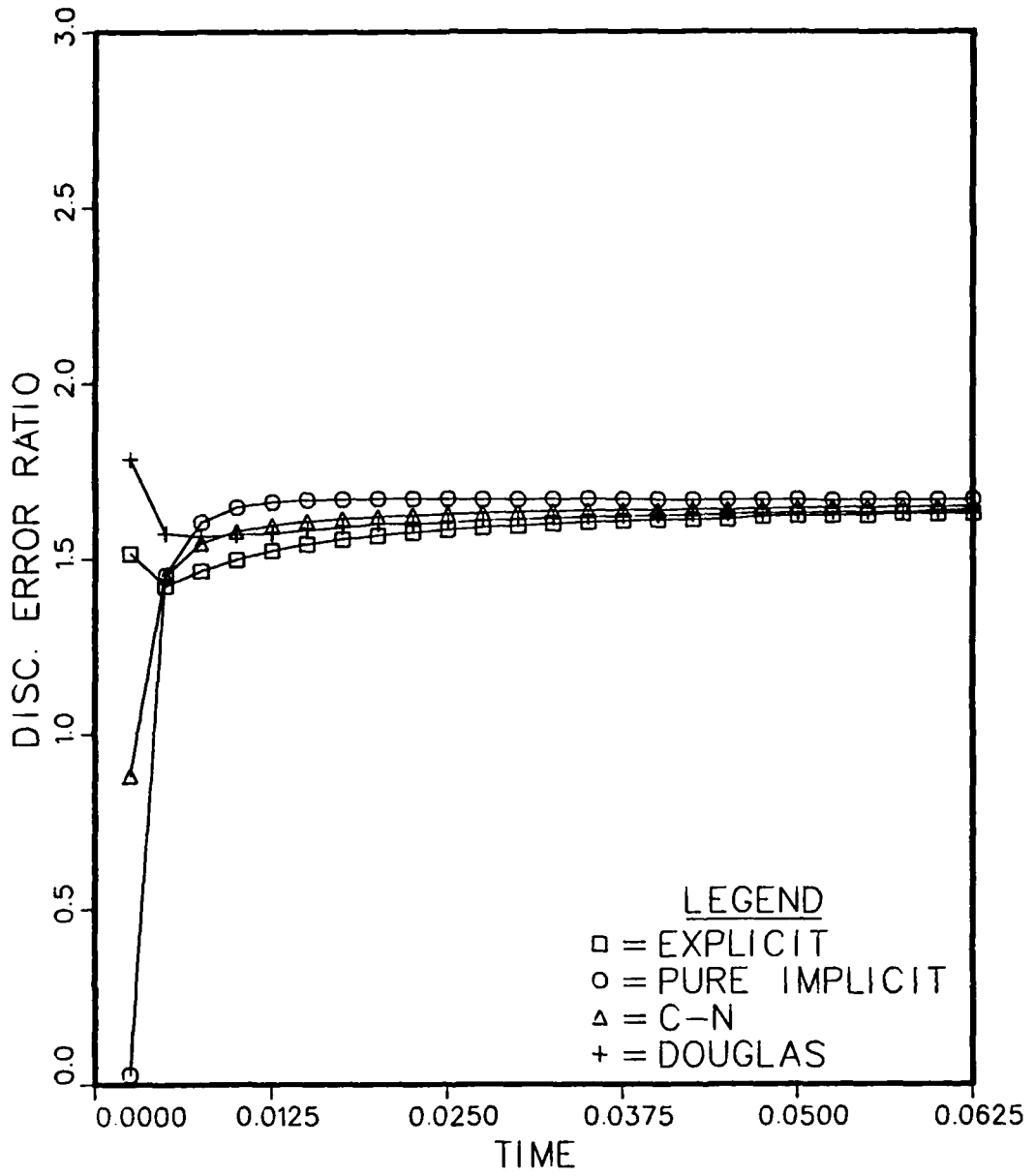


FIGURE C-1-6. Absolute value of discretization error ratio vs Time at  $x=1$  for 40/80 nodes:  $n=25$

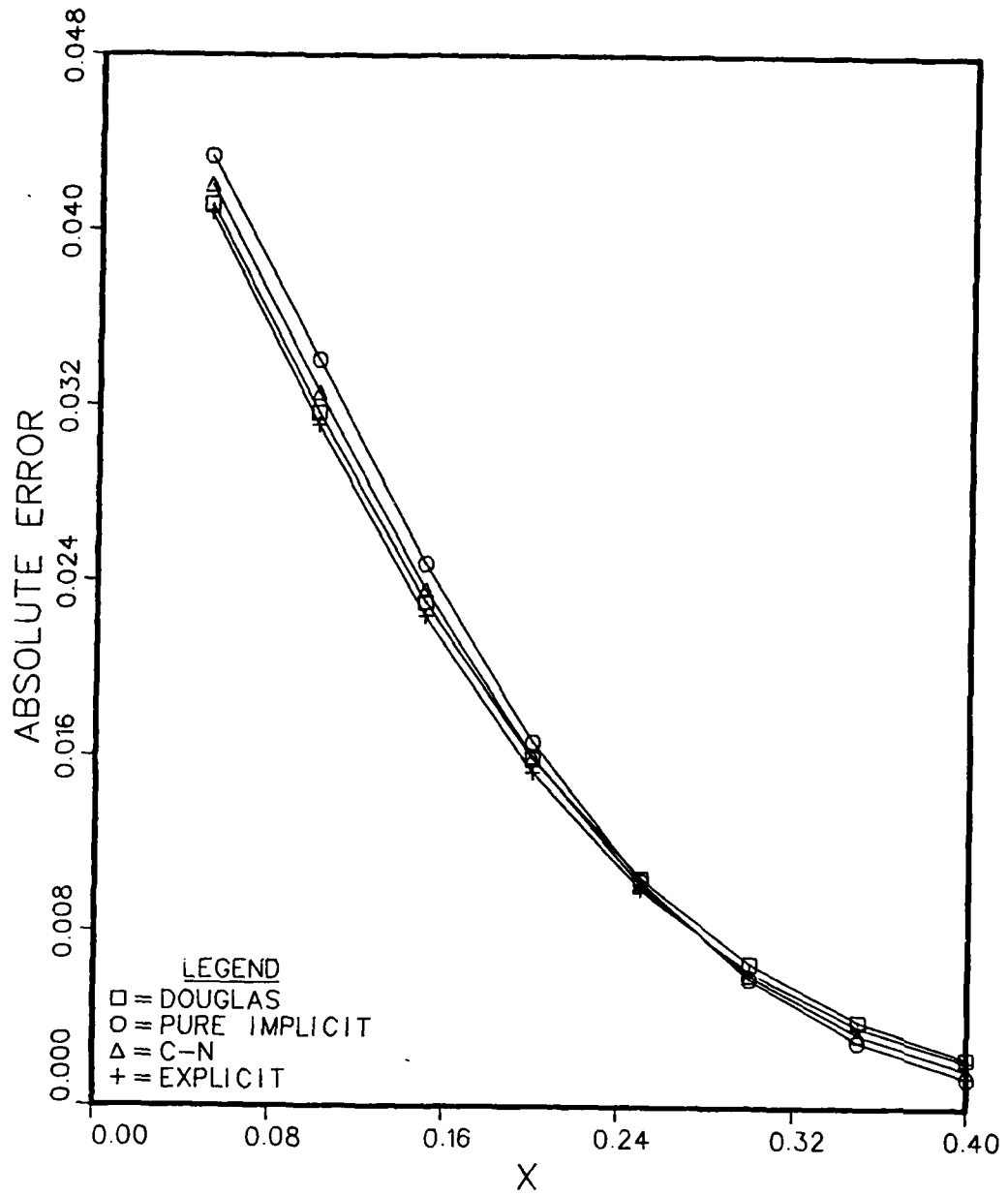


FIGURE C-1-7. Absolute value of discretization errors X at Time=.025: n=25 40 nodes

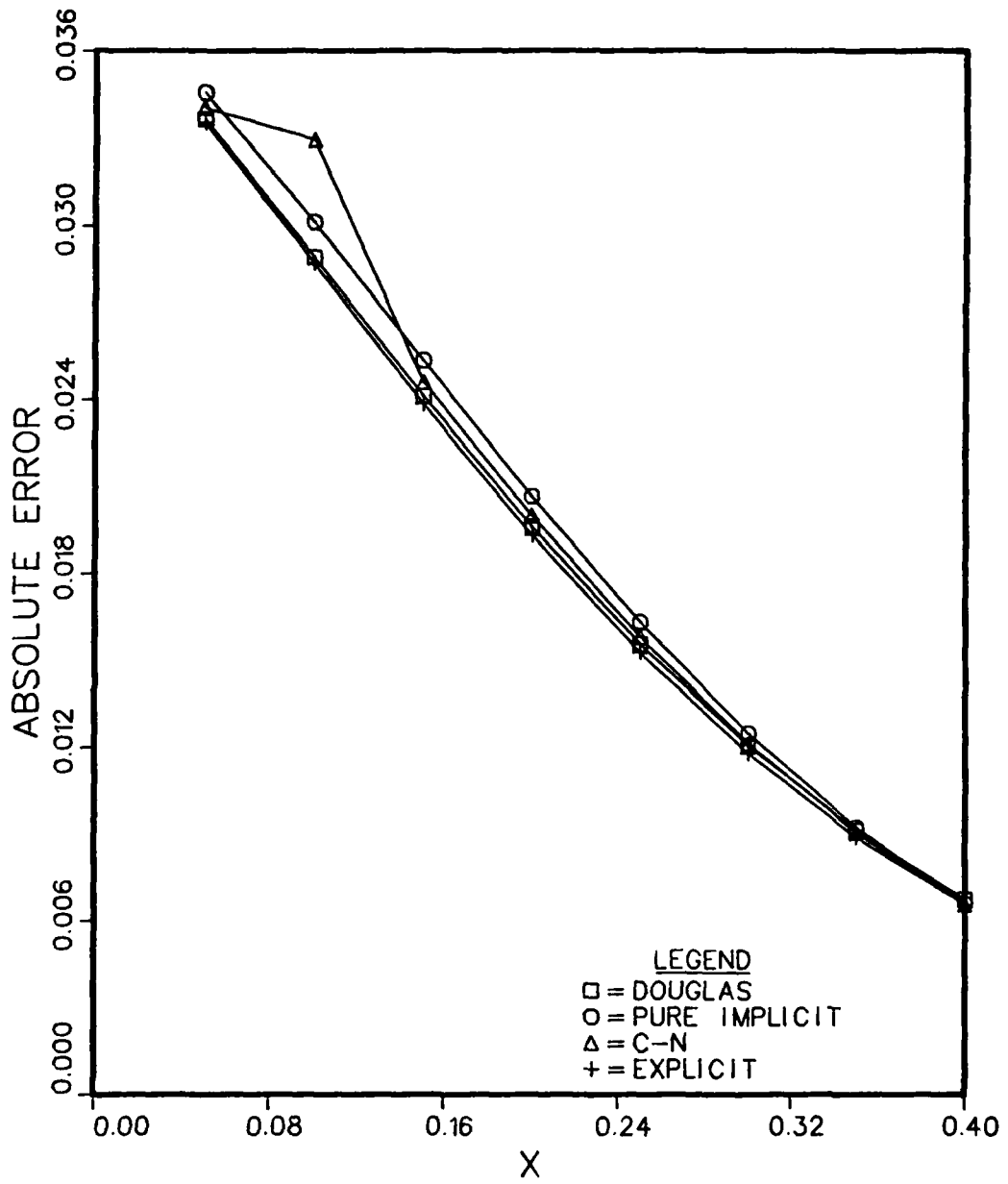


FIGURE C-1-8. Absolute value of discretization errors vs X at Time=.05: n=25 40 nodes

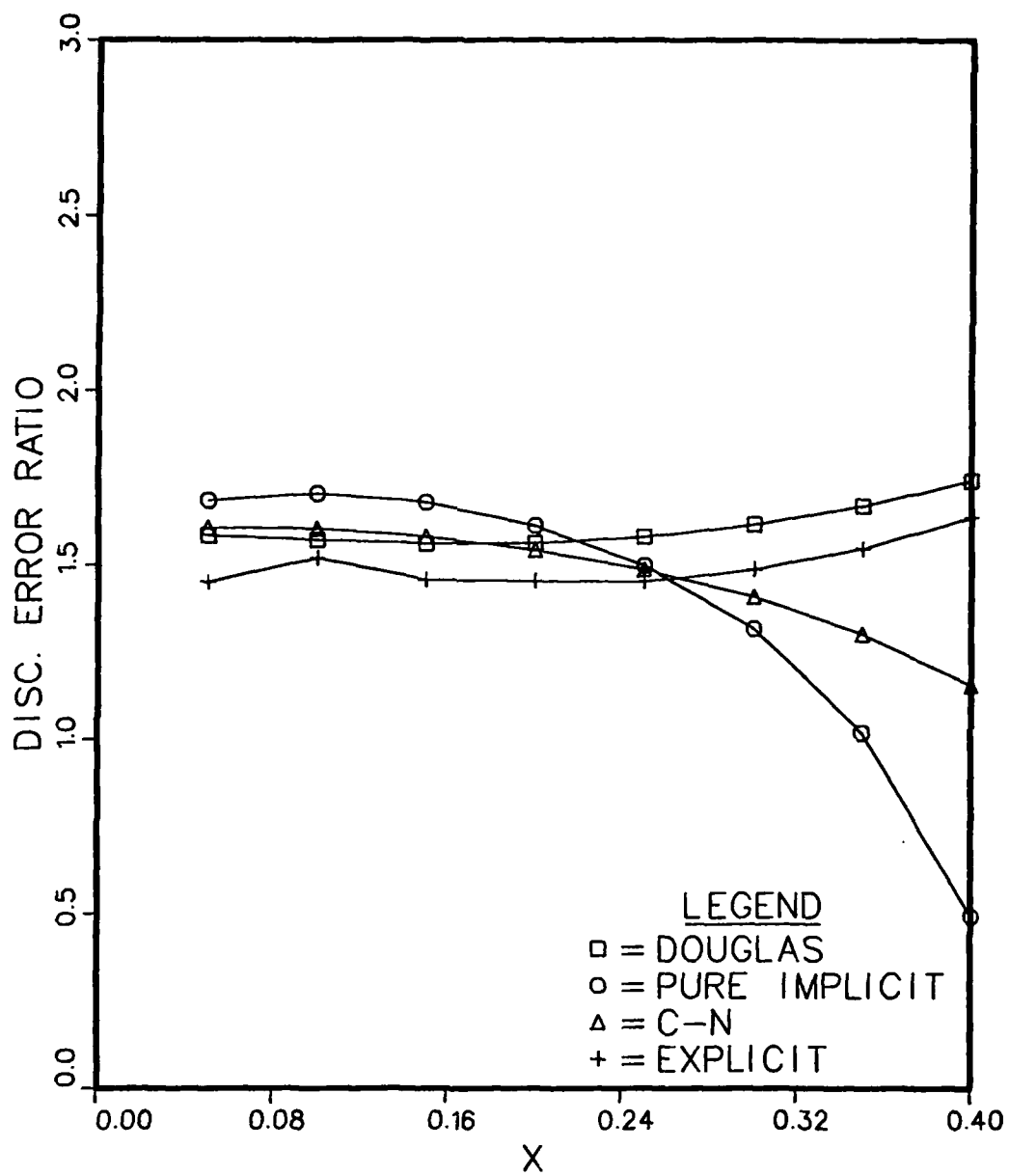


FIGURE C-1-9. Absolute value of discretization error ratio vs X at Time=.025 for 20/40 nodes: n=.25

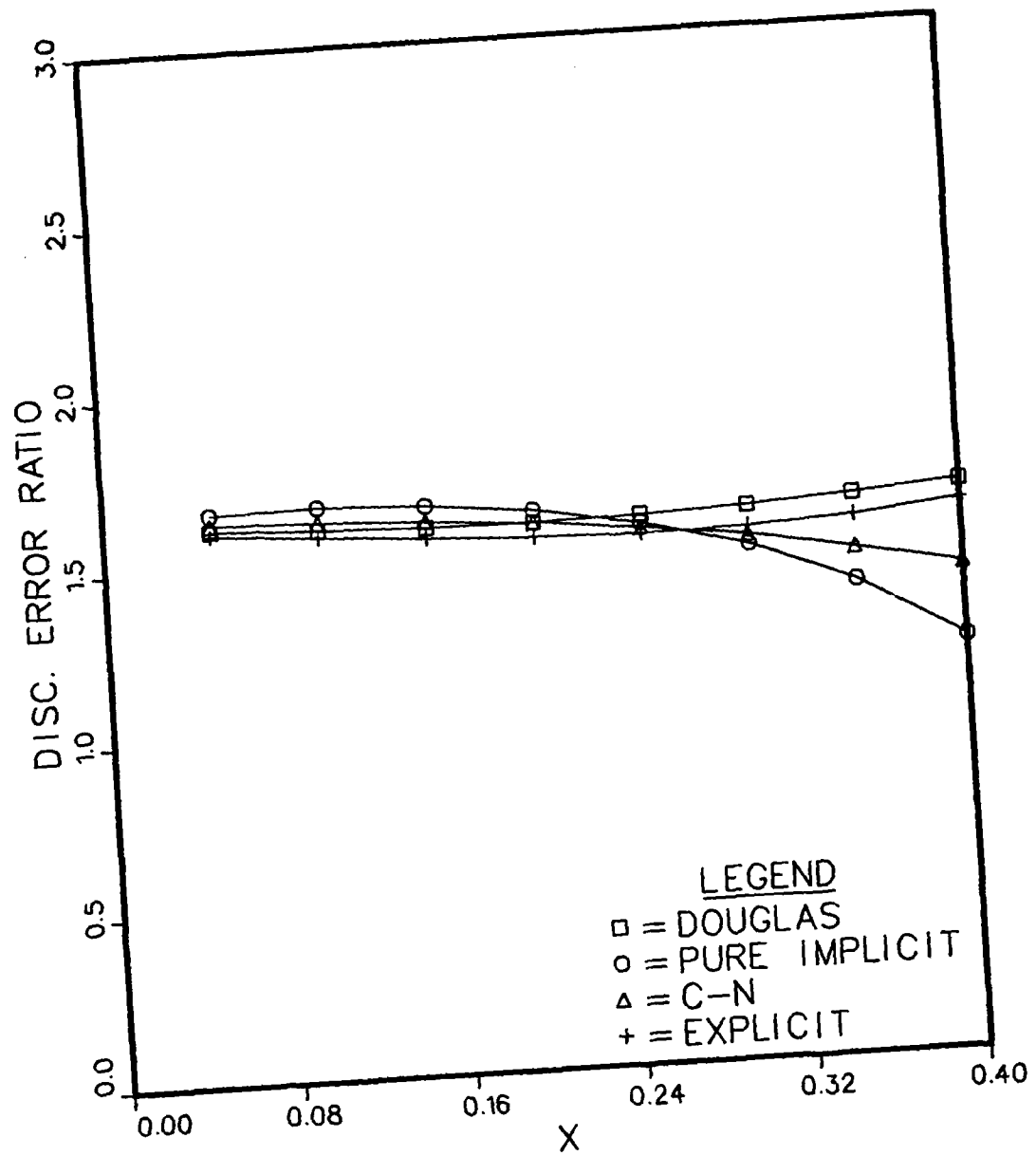


FIGURE C-1-10. Absolute value of discretization error ratio vs X at Time=.025 for 40/80 nodes: n=25

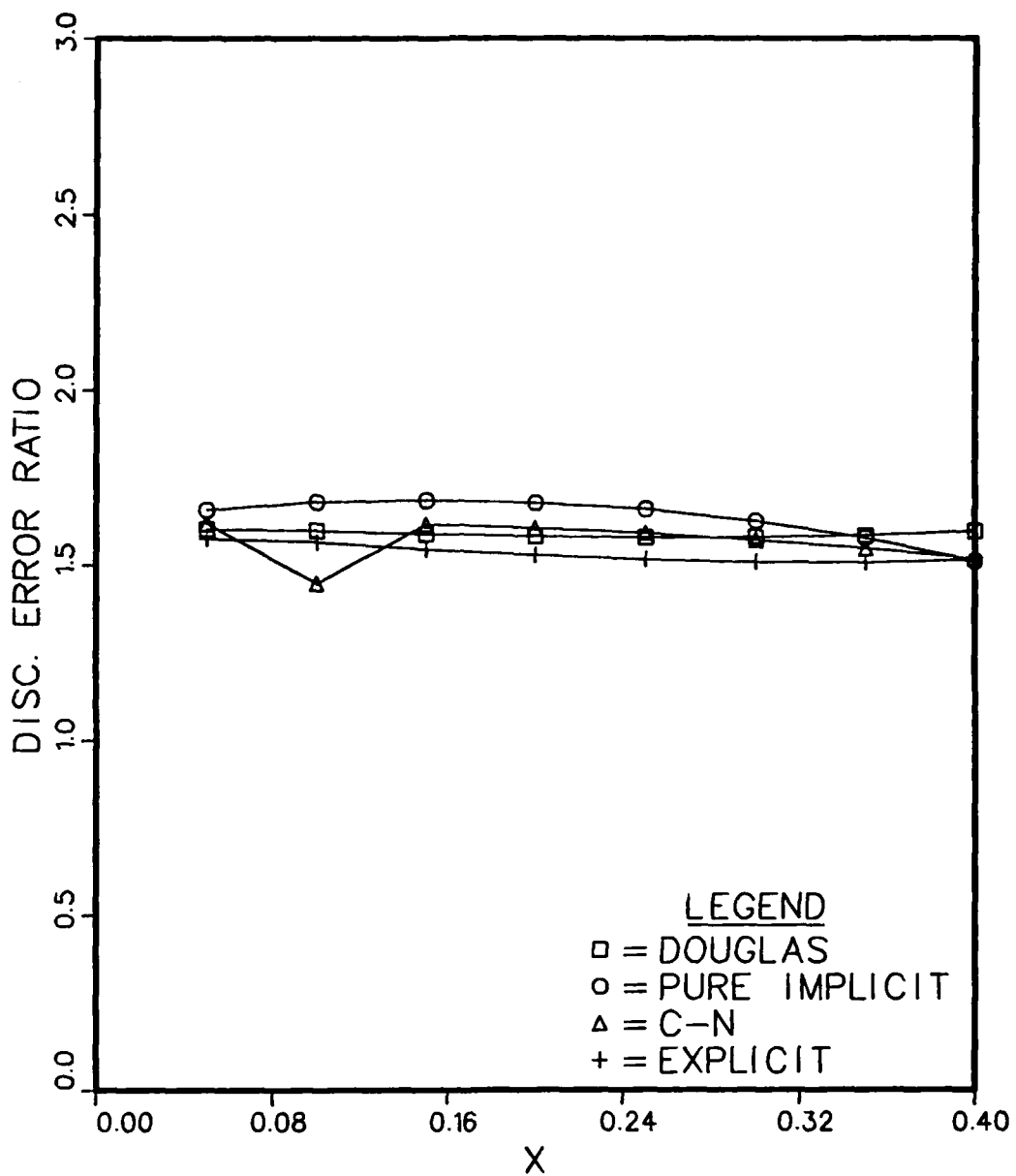


FIGURE C-1-11. Absolute value of discretization error ratio vs X at Time=.05 for 20/40 nodes: n=.25

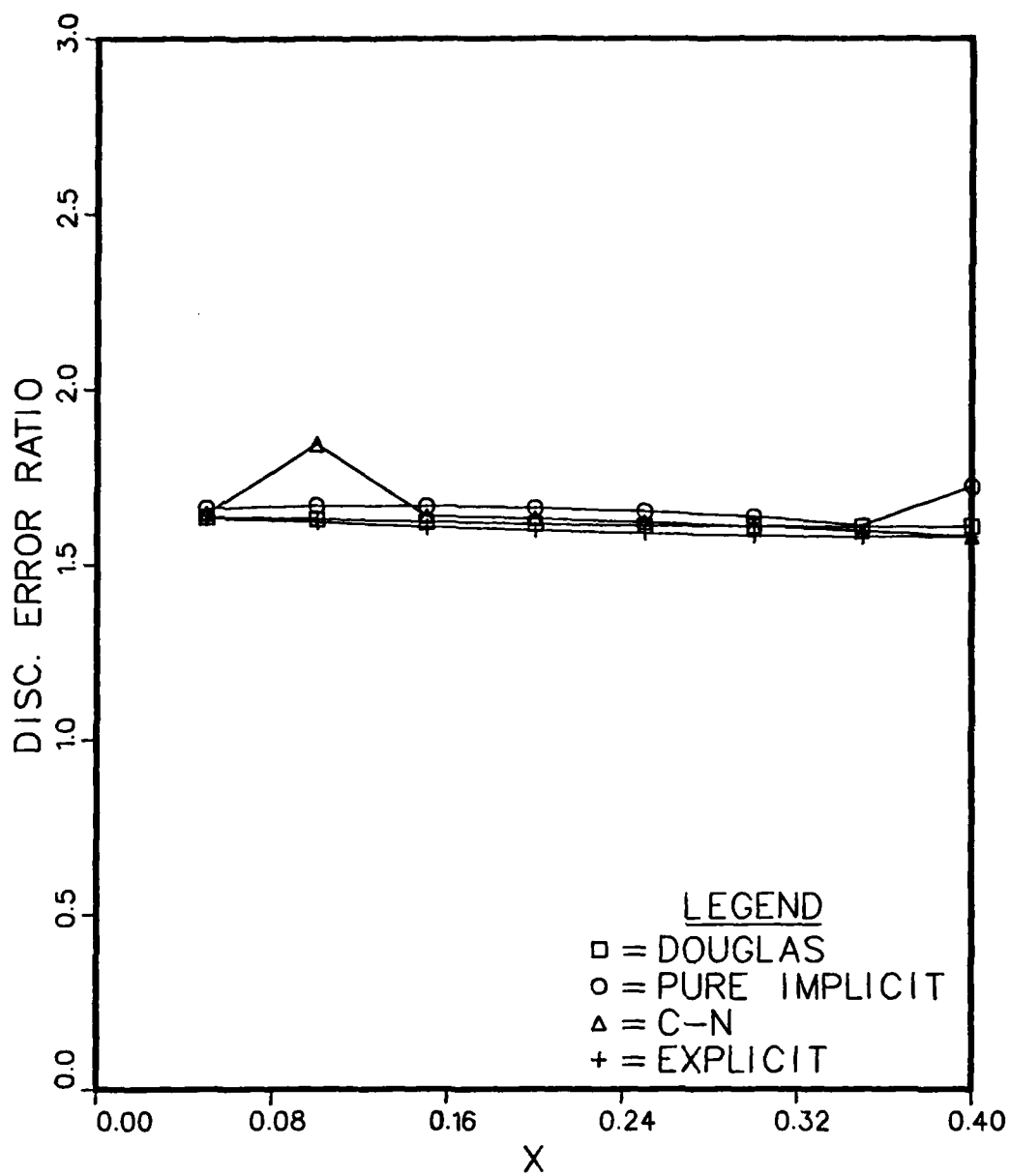


FIGURE C-1-12. Absolute value of discretization error ratio vs X at Time=.05 for 40/80 nodes: n=25

## Section II

This section includes the graphical results of the Pure-Implicit, Crank-Nicolson, and Douglas Methods with the Fourier Modulus equal to 5.0 and  $n$  equal to .25. The following key shows which parameter options are included in this set of graphs.

Figure No.	Number of Nodes	x	Time	Error*
C-II-1	20	.05	.05-1.0	AE
C-II-2	40	.05	.05-1.0	AE
C-II-3	20	.1	.05-1.0	AE
C-II-4	40	.1	.05-1.0	AE
C-II-5	20/40	.05	.05-1.0	DER
C-II-6	40/80	.05	.05-1.0	DER
C-II-7	20/40	.1	.05-1.0	DER
C-II-8	40/80	.1	.05-1.0	DER
C-II-9	20	.05-1.0	.25	AE
C-II-10	40	.05-1.0	.25	AE
C-II-11	20/40	.05-1.0	.25	DER
C-II-12	40/80	.05-1.0	.25	DER
C-II-13	20	.05-1.0	.5	AE
C-II-14	40	.05-1.0	.5	AE
C-II-15	20/40	.05-1.0	.5	DER
C-II-16	40/80	.05-1.0	.5	DER

\* AE: Absolute Error  
DER: Discretization Error Ratio

Both the Crank-Nicolson and Douglas Method solutions oscillate with time. The magnitude of the oscillation is greatest in the Douglas Method solution. Oscillations are observed only in the solutions obtained from calculations made with a mesh of 20 nodes. For meshes of 40 and 80 nodes, all methods were of the same accuracy; the Douglas Method most accurate across the mesh, the Pure-Implicit Method the least accurate. Similar results were observed with the value of the Fourier Modulus equal to 2; however, the observed oscillations damped sooner for the smaller value of the Fourier Modulus. Results of calculations performed with  $n$  equal to .5 paralleled those made with  $n$  equal to .25 except that for mesh sizes of 40 and 80 nodes, the Pure-Implicit Method was the most accurate and the Douglas Method the least accurate, similar to results discussed in Section I.

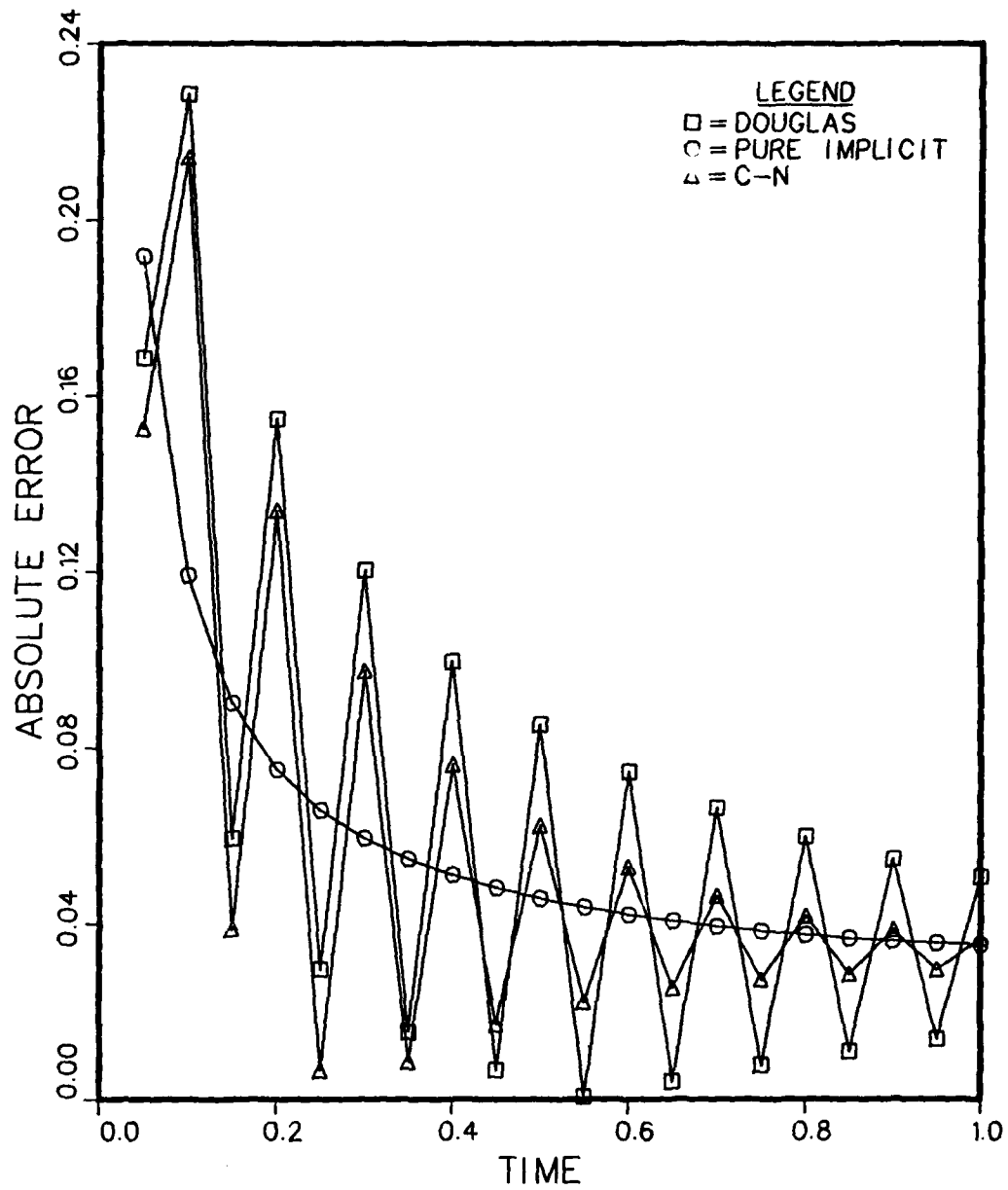


FIGURE C-II-1. Absolute value of discretization error vs Time at  $x=0.5$ :  $n=25$  20 nodes

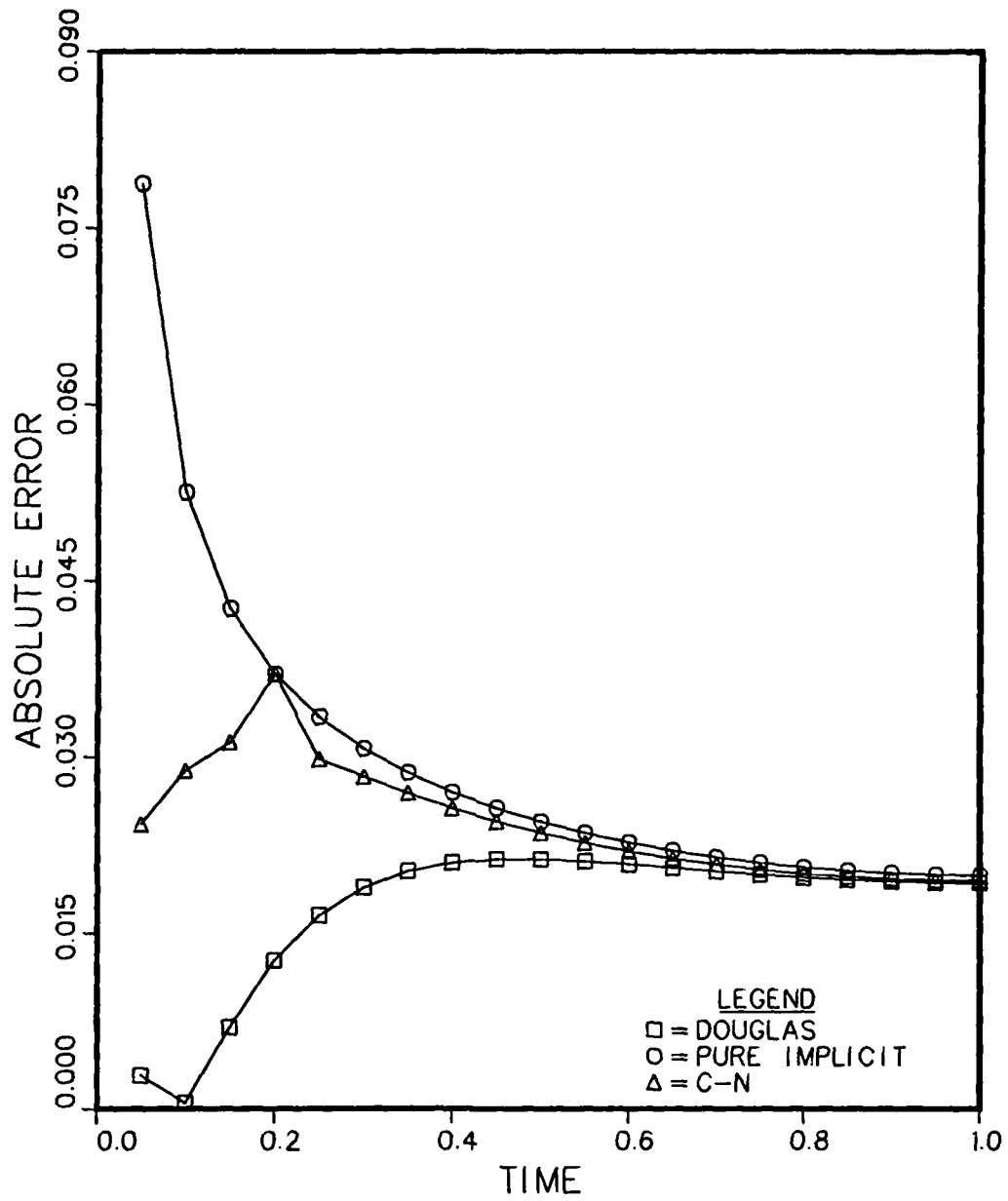


FIGURE C-II-2. Absolute value of discretization error vs Time at  $x=0.05$ ;  $n=25$  40 nodes

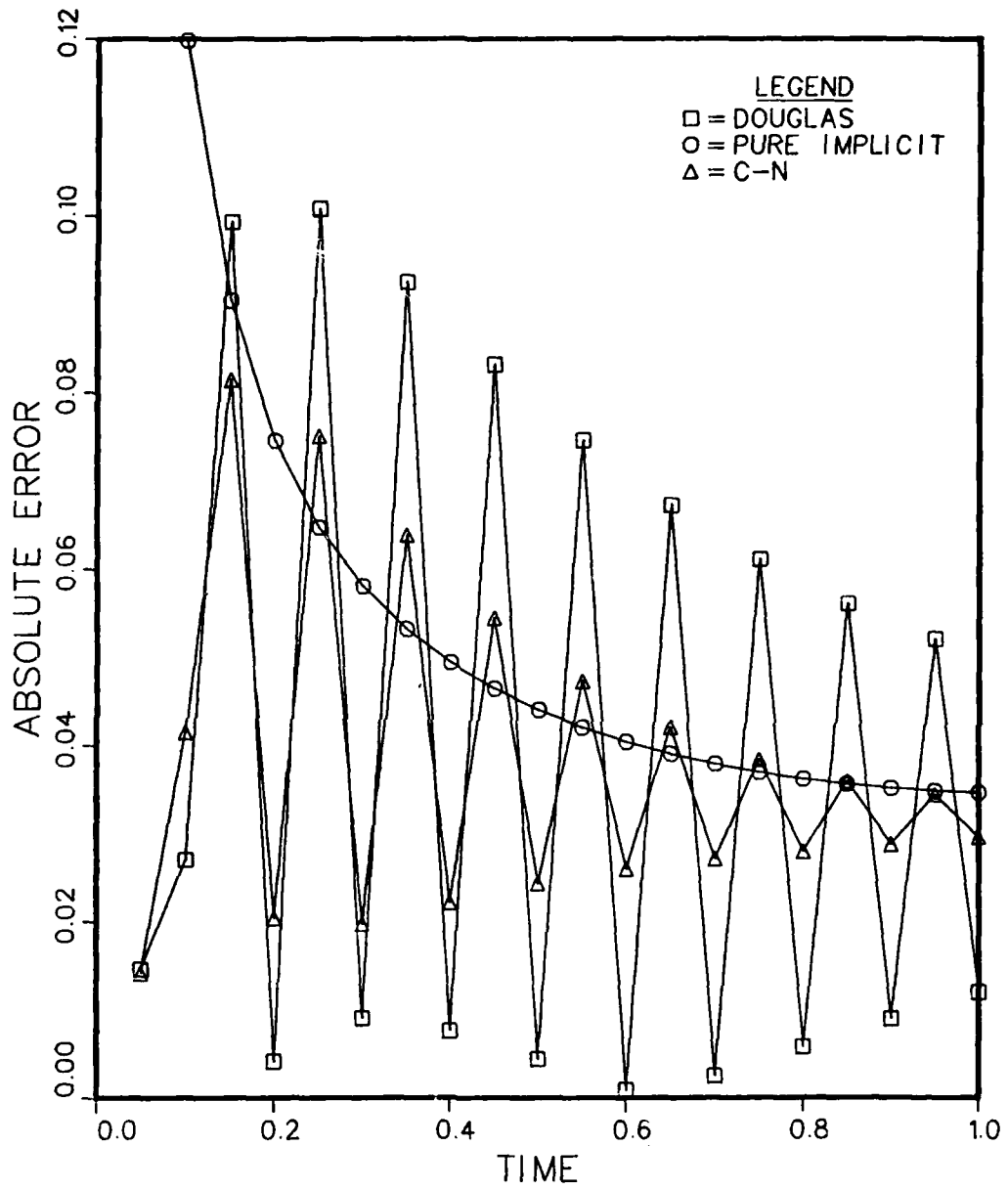


FIGURE C-II-3. Absolute value of discretization error vs Time at  $x=1$ :  $n=25$  20 nodes

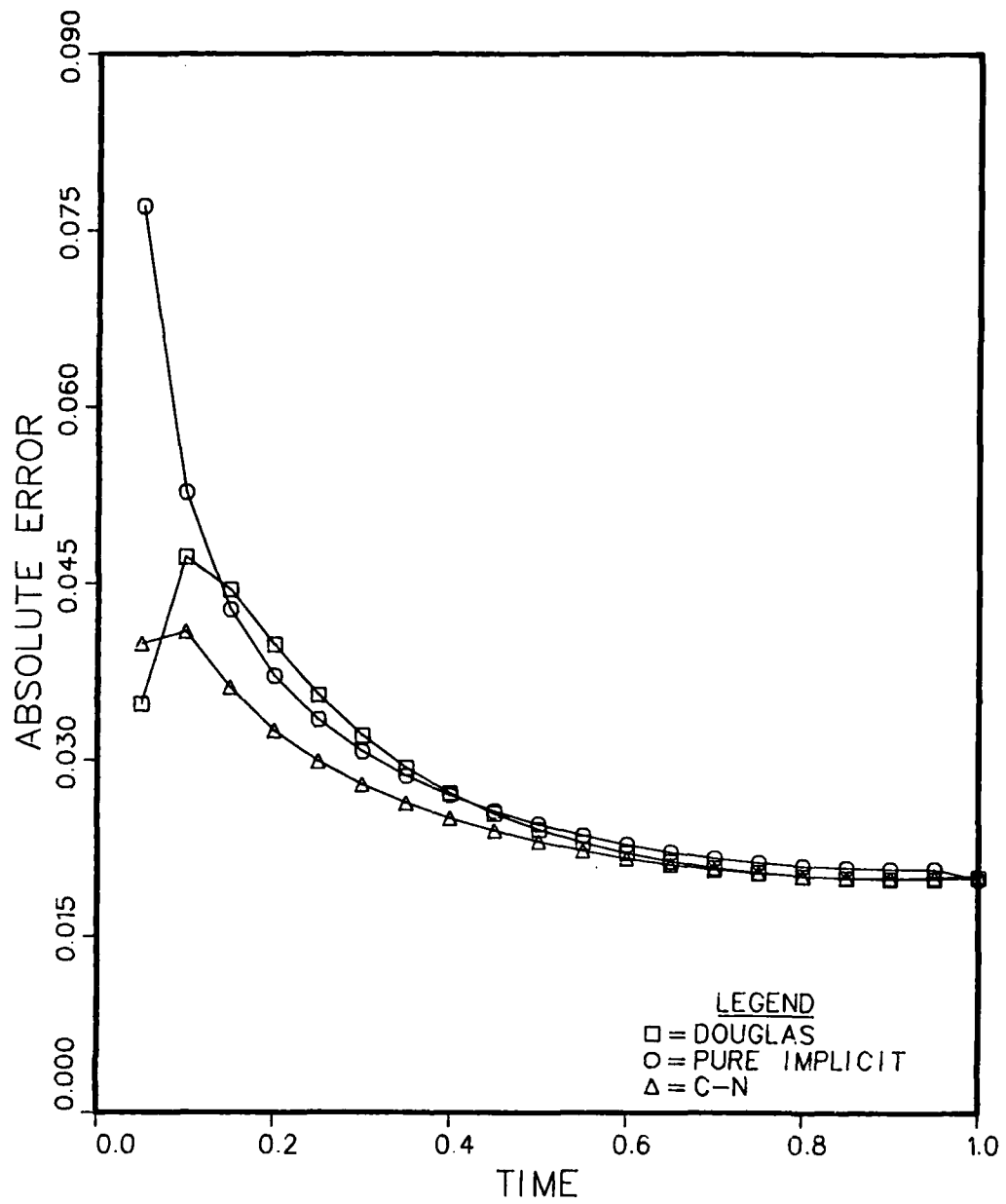


FIGURE C-II-4. Absolute value of discretization error vs Time at  $x=1$ ;  $n=25$  40 nodes

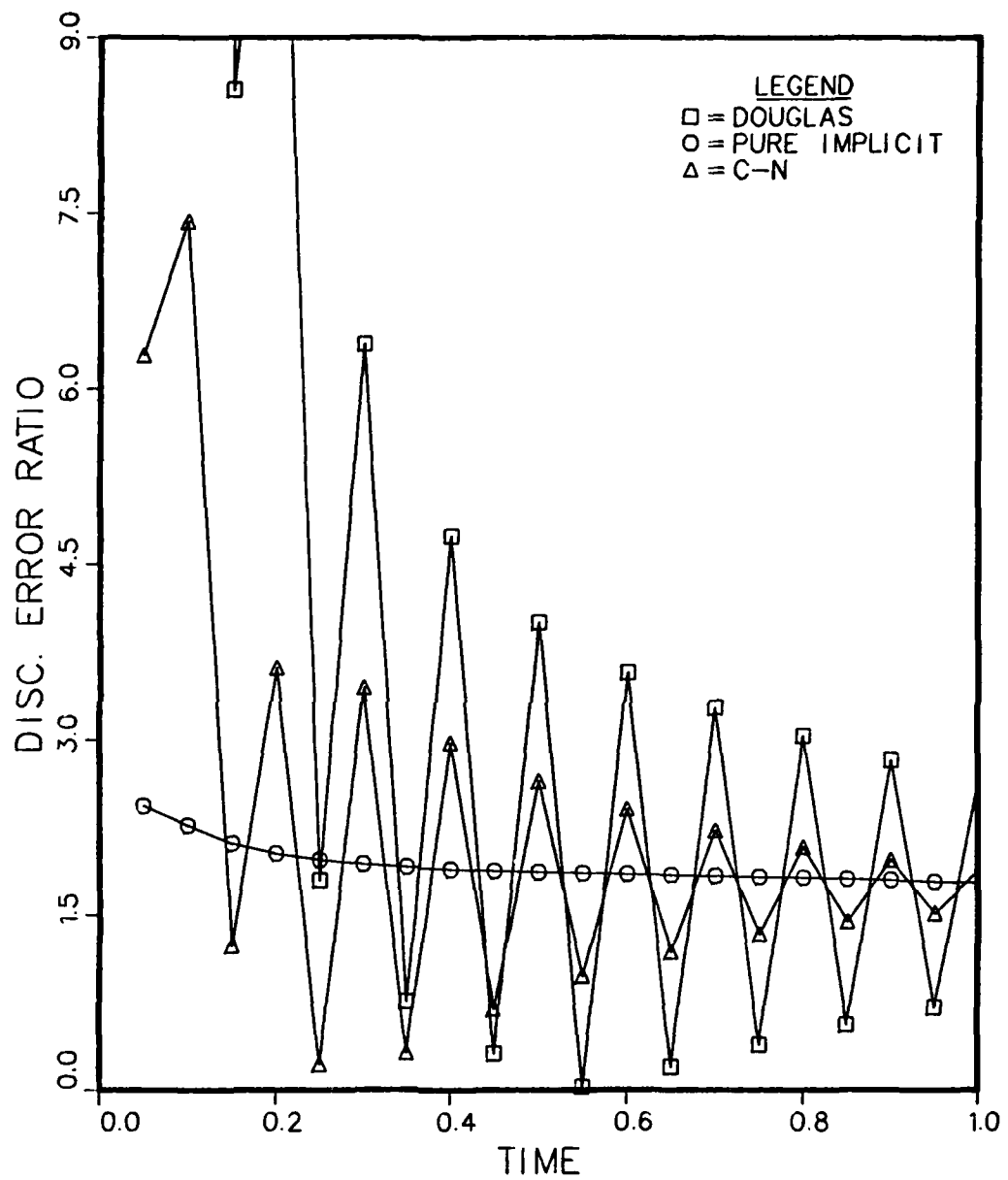


FIGURE C-II-5. Absolute value of discretization error ratio vs Time at  $x=0.5$  for 20/40 nodes:  $n=25$

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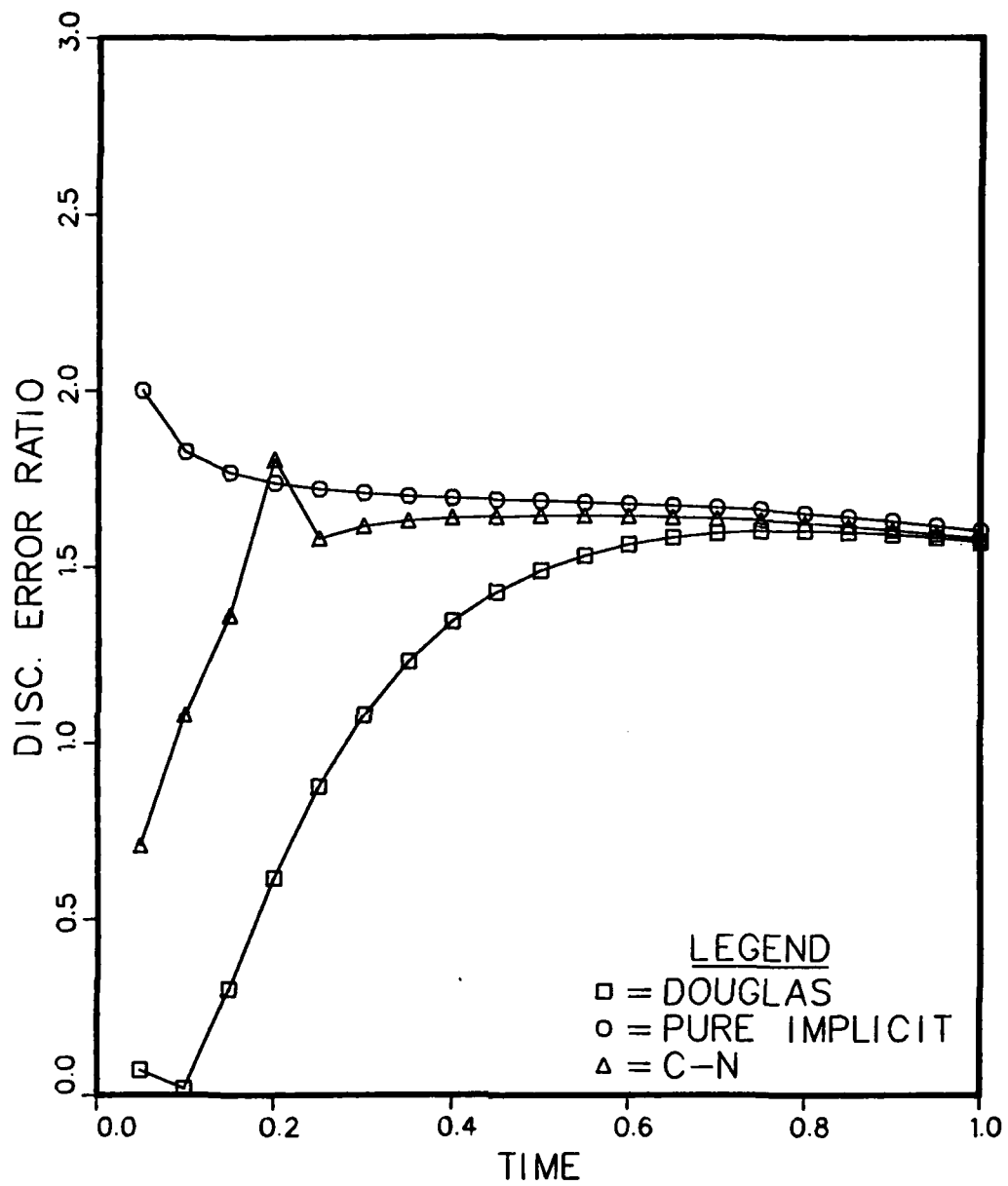


FIGURE C-II-6. Absolute value of discretization error ratio vs Time at  $x=0.5$  for 40/80 nodes:  $n=25$

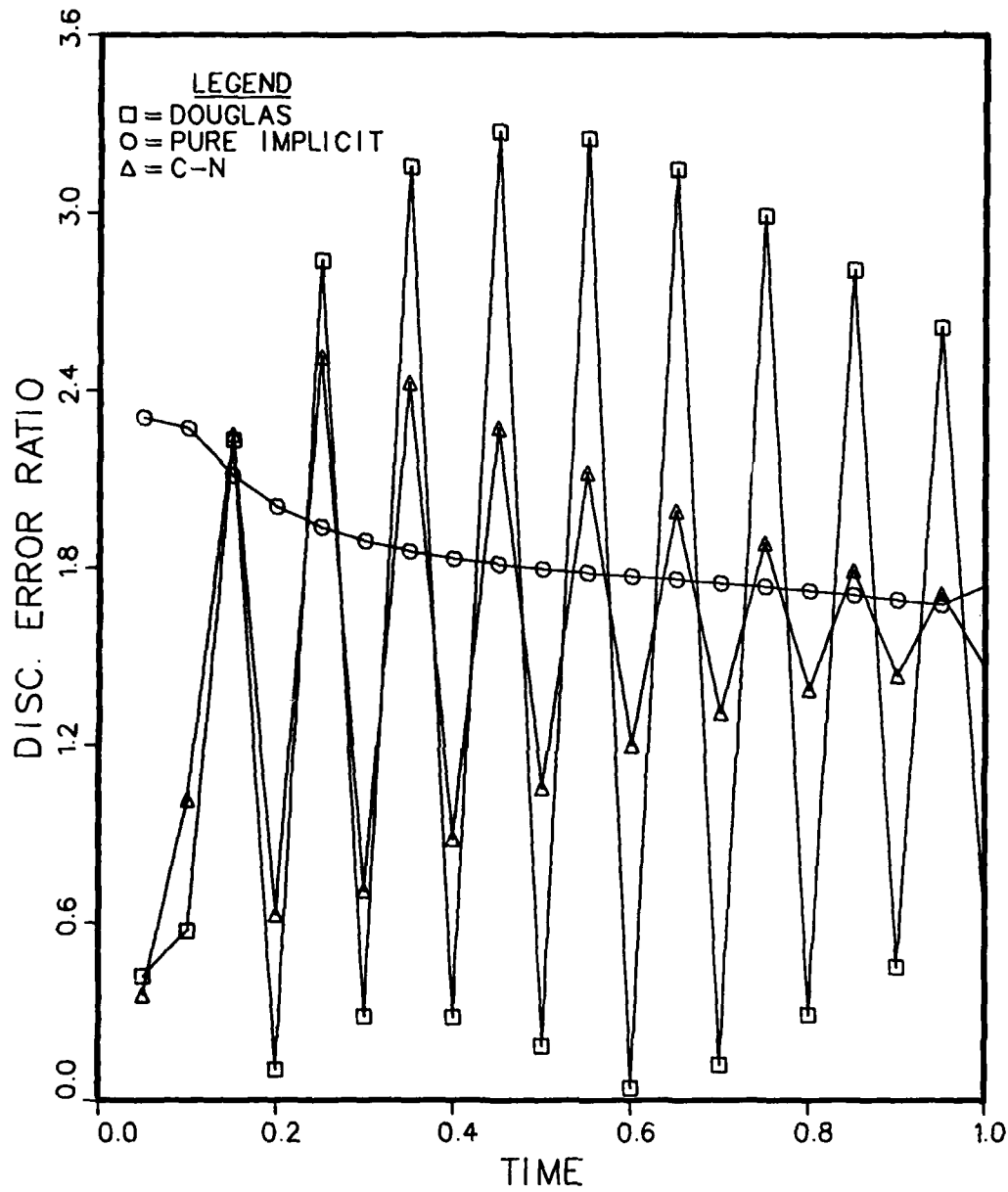


FIGURE C-II-7. Absolute value of discretization error ratio vs Time at  $x=1$  for 20/40 nodes:  $n=25$

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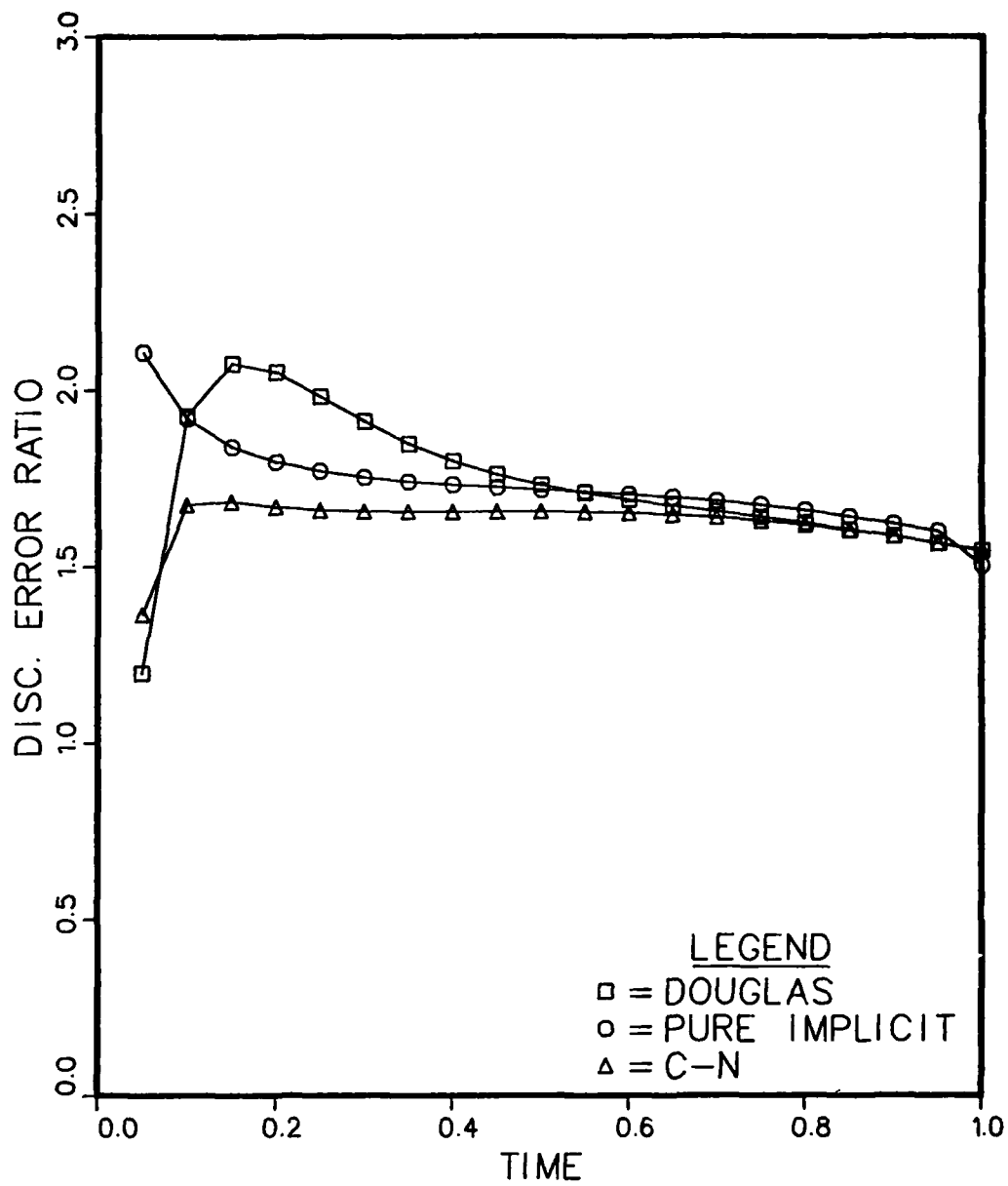


FIGURE C-II-8. Absolute value of discretization error ratio vs Time at  $x=1$  for 40/80 nodes:  $n=25$

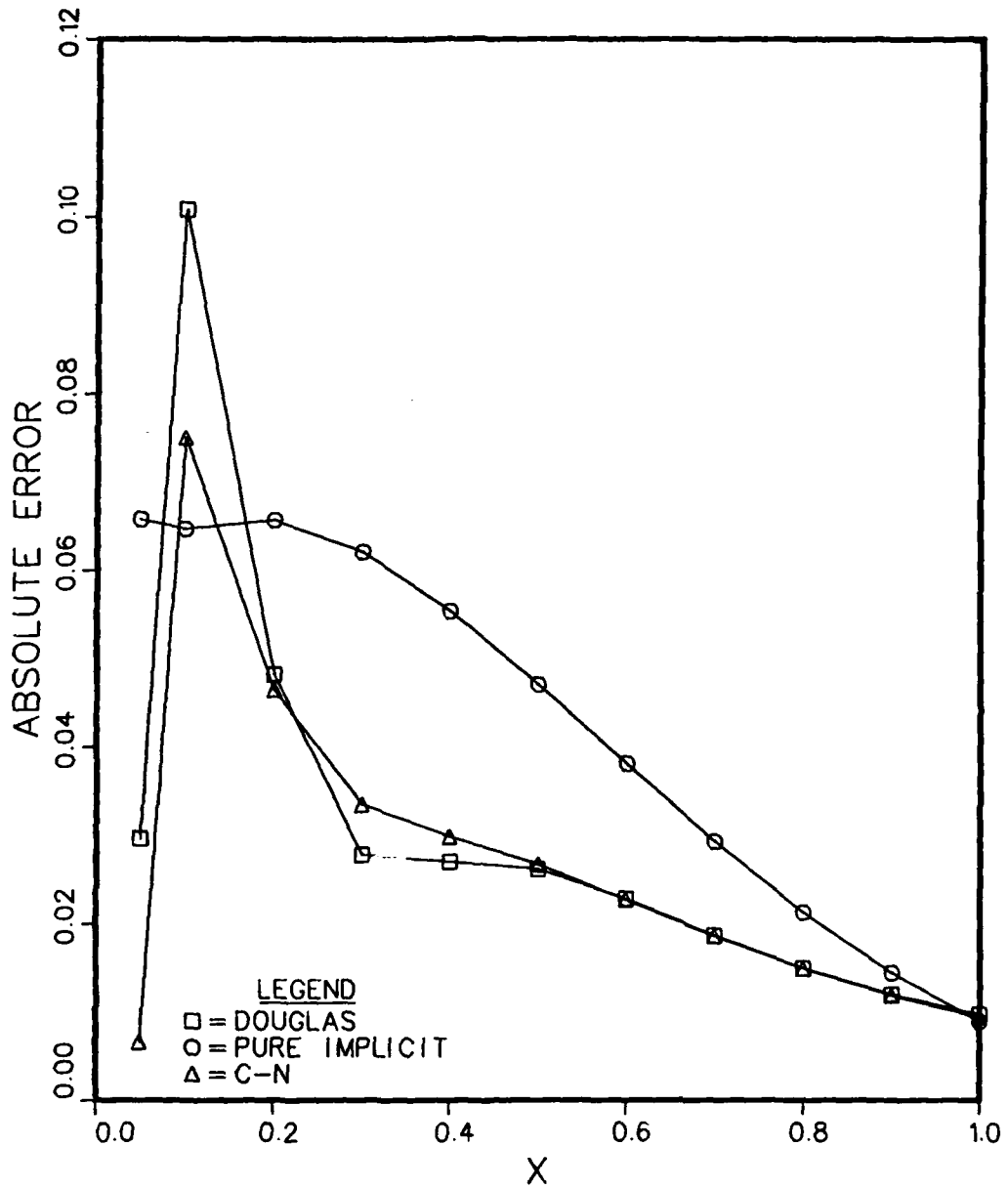


FIGURE C-II-9. Absolute value of discretization error vs X at Time=25: n=25 20 nodes

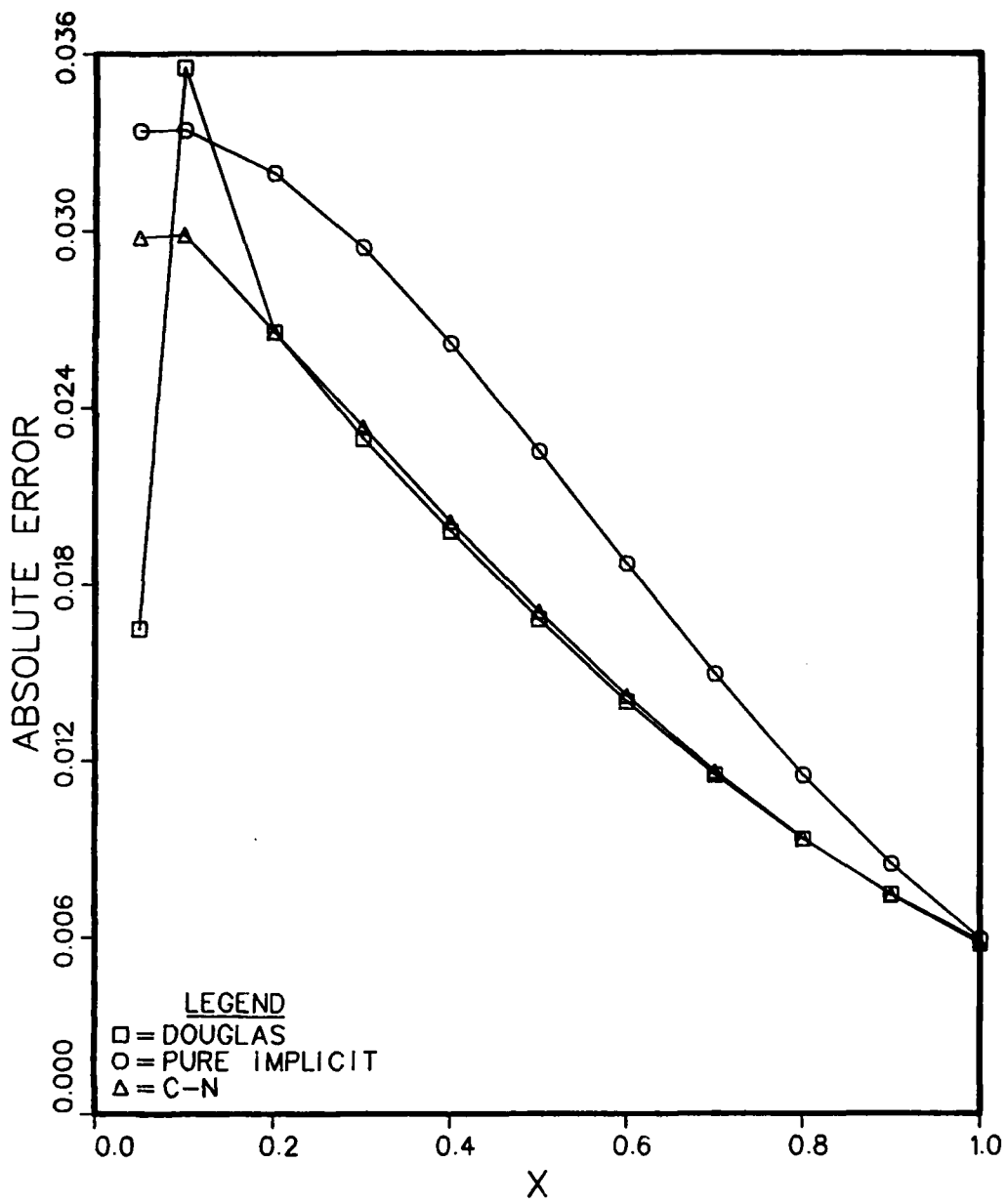


FIGURE C-II-10. Absolute value of discretization error vs X at Time=25: n=.25 40 nodes

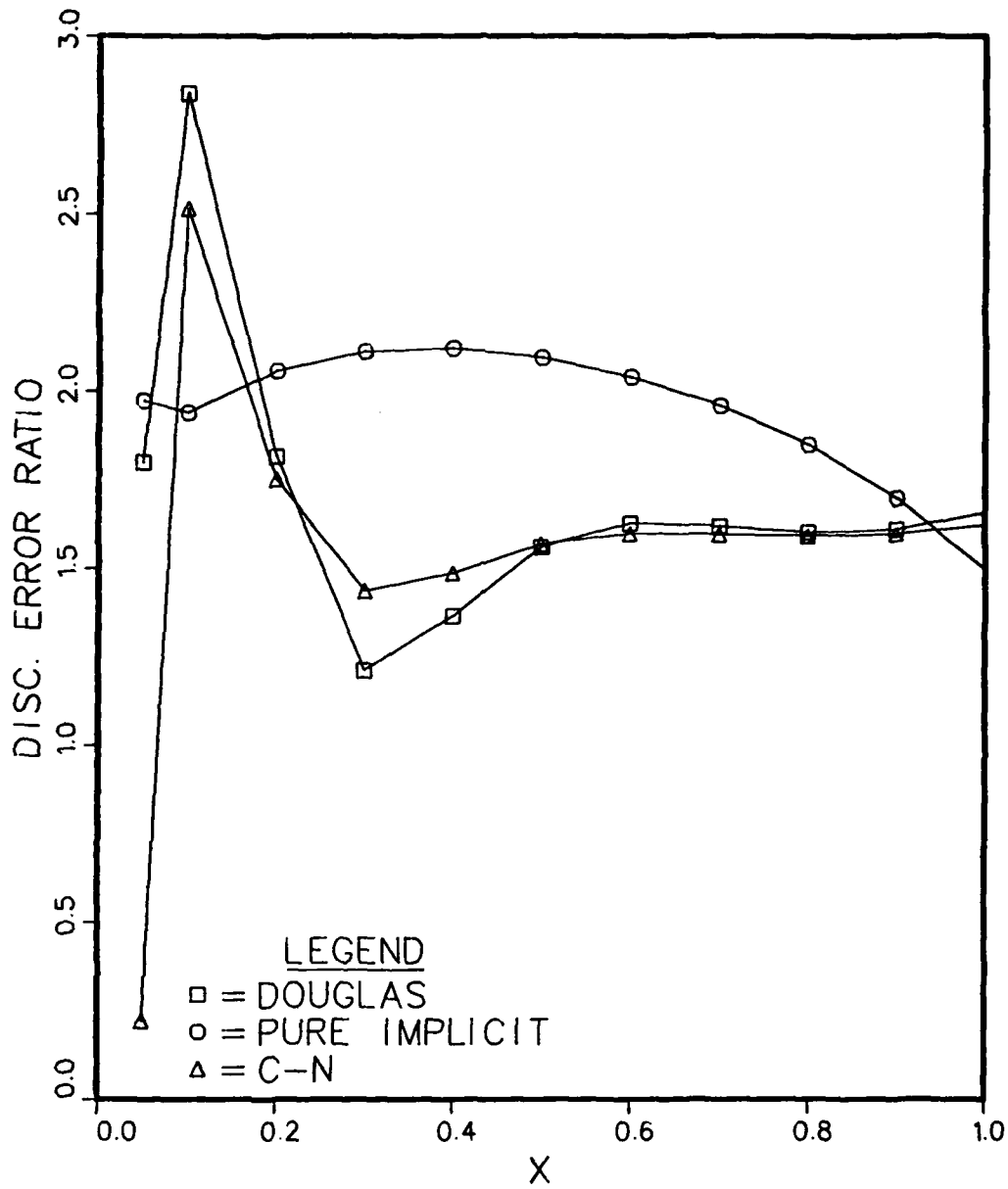


FIGURE C-II-11. Absolute value of discretization error ratio vs X at Time=.25 for 20/40 nodes; n=25

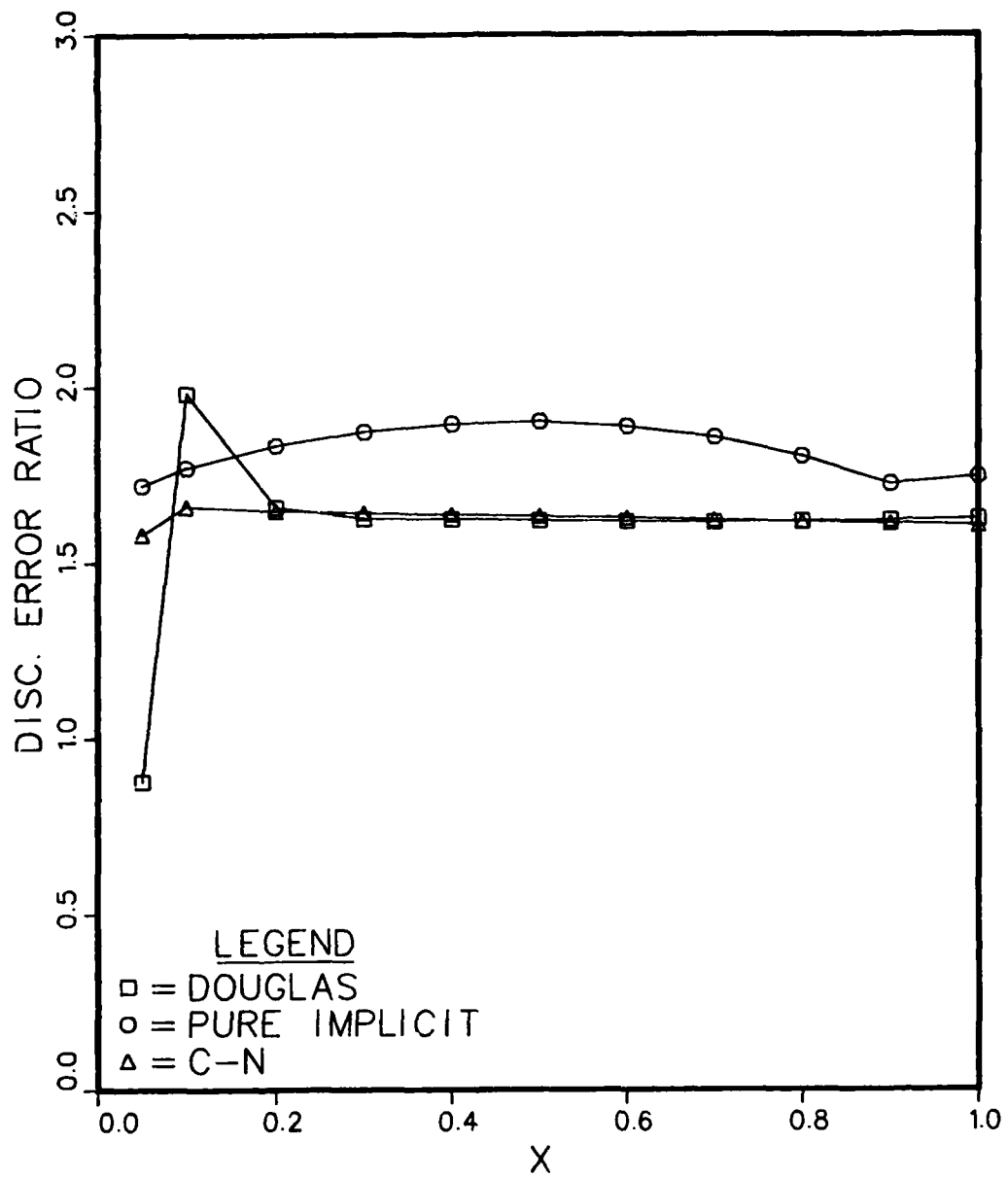


FIGURE C-II-12. Absolute value of discretization error ratio vs X at Time=.25 for 40/80 nodes: n=.25

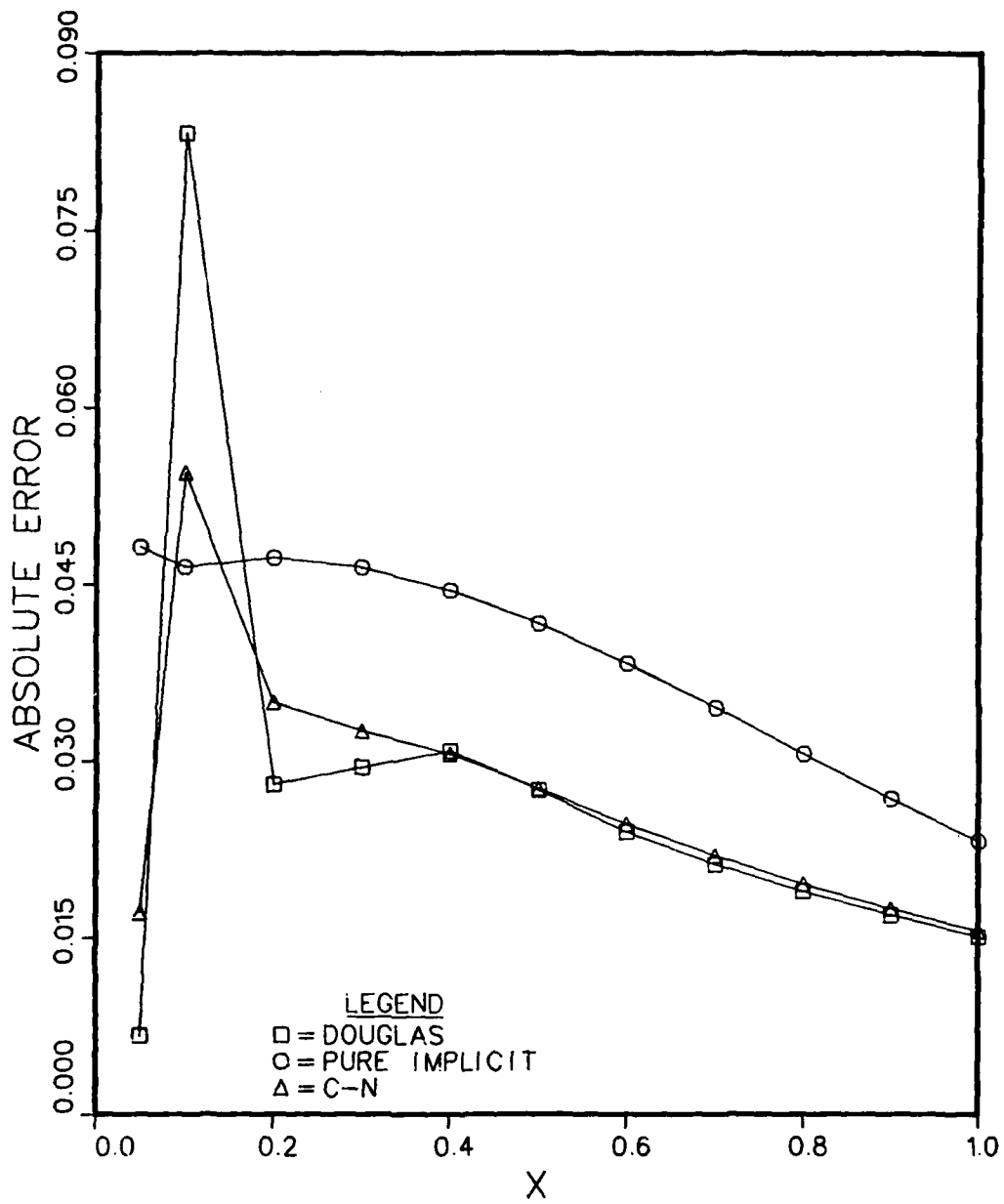


FIGURE C-II-13. Absolute value of discretization error vs X at Time=.5: n=.25 20 nodes

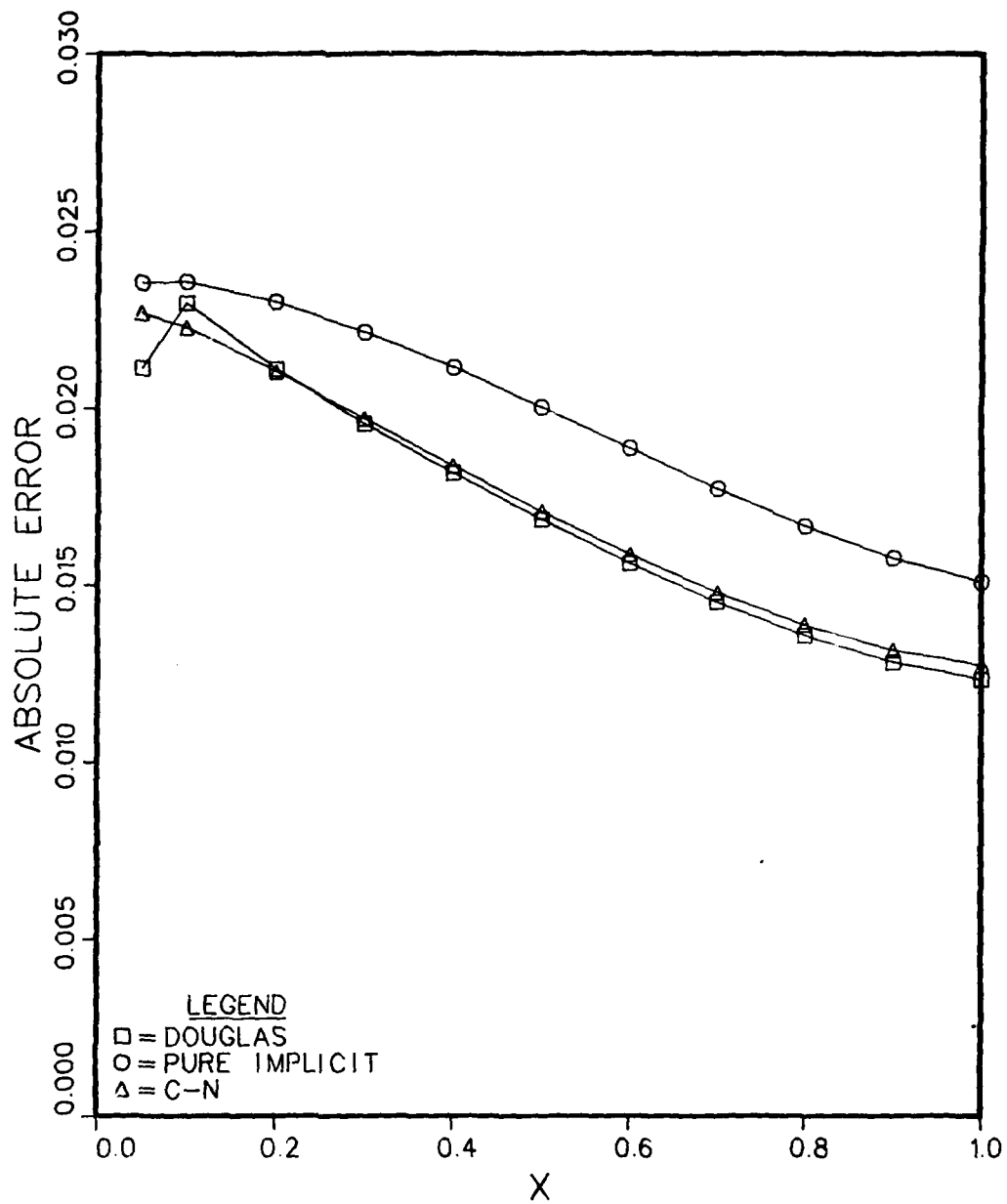


FIGURE C-II-14. Absolute value of discretization error vs X at Time=.5: n=25 40 nodes

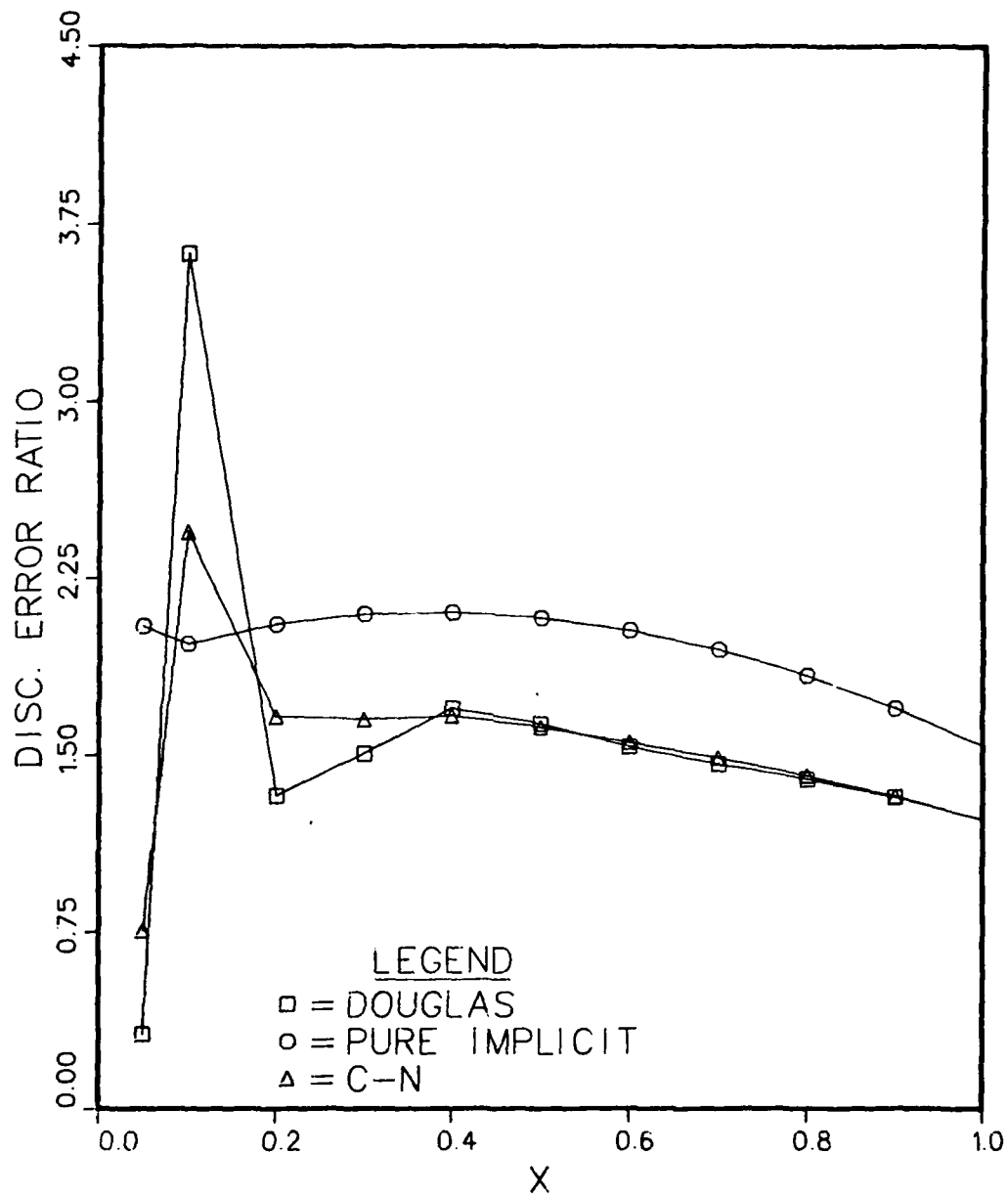


FIGURE C-II-15. Absolute value of discretization error ratio vs X at Time=5 for 20/40 nodes:  $n=20$

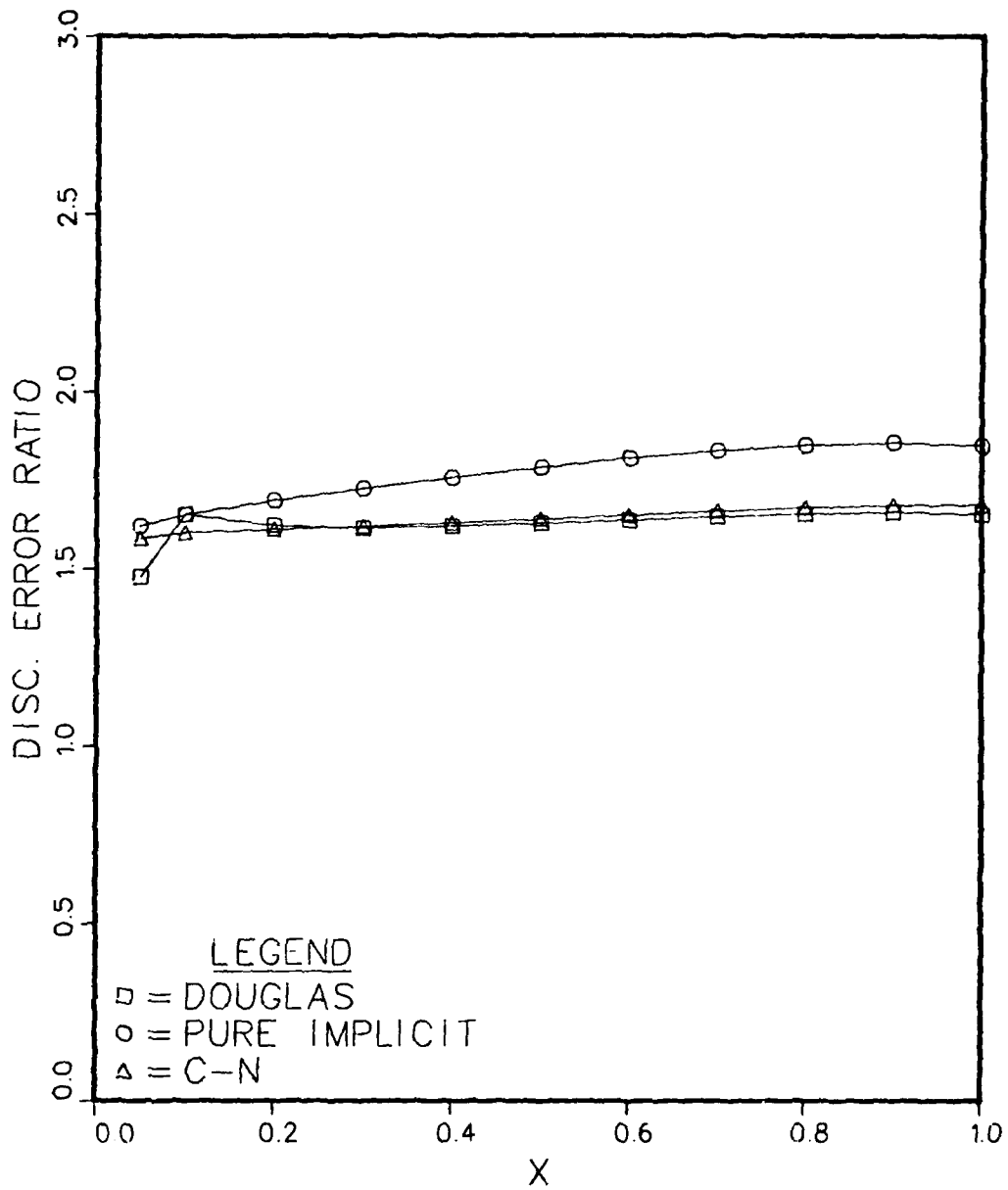


FIGURE C-II-16. Absolute value of discretization error ratio vs X at Time=.5 for 40/80 nodes: n=.25

### Vita

Kenneth William Blevins was born on 26 August 1948 in Tulsa, Oklahoma. After graduation from Derby Senior High School in Derby, Kansas, in 1966, he enrolled in Friends University, Wichita, Kansas. He left Friends University in 1968 to enlist in the United States Navy Reserve. He was selected for the Navy Enlisted Scientific Education Program (NESEP) in 1974. Lieutenant Blevins was commissioned an Ensign in the United States Navy upon graduation from North Carolina State University, Raleigh, North Carolina, in December 1976 with a degree of Bachelor of Science, Nuclear Engineering. After completion of Surface Warfare Officer's School in June 1977, Lt Blevins was assigned to the USS Josephus Daniels (CG-27), where he served initially as Missile Officer and later as Main Propulsion Assistant. He entered the Graduate Nuclear Effects curriculum at the Air Force Institute of Technology in August 1980.

Permanent Address: 4564 Meadowview  
Wichita KS 67216

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Transient Heat Conduction Equation      Variable Conductivity Diffusion Equation      Crank-Nicolson Method Finite-Difference Methods      Douglas Method		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The transient heat conduction equation is solved for inhomogeneous media using the Explicit, Pure-Implicit, Crank-Nicolson and Douglas finite-difference methods, and the numerical solutions are investigated with respect to accuracy and stability. The inherent discontinuity between the initial and boundary conditions is investigated for mesh refinement. For the various values of conduction coefficient and boundary conditions investigated, all four methods are found to be of equivalent accuracy for small values of $\Delta x$ . (Continued on reverse)		

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BLOCK 20: ABSTRACT (Cont')

the Fourier Modulus,  $\Delta t/(\Delta x)^2$ . While the Pure-Implicit, Crank-Nicolson and Douglas Methods are unconditionally stable, the Crank-Nicolson and Douglas Methods are very inaccurate at large values of the Fourier Modulus due to oscillatory behavior.

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