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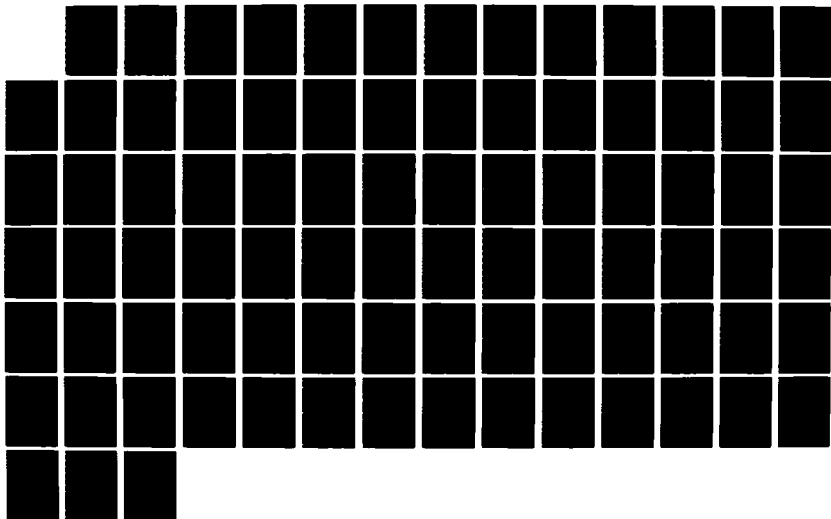
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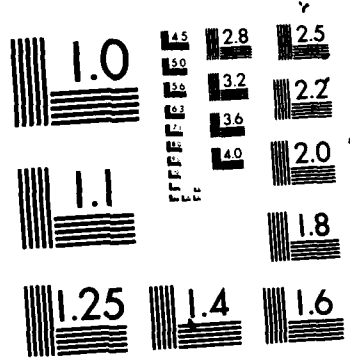
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OSCILLATORY BEHAVIOR OF FINITE
 DIFFERENCE METHODS FOR THE SOLUTION
 OF THE TWO DIMENSIONAL TRANSIENT
 HEAT (DIFFUSION) EQUATION

THESIS

Joseph E. Cuthrell
 Captain, USAF

AFIT/GNE/ENP/86M-2

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OSCILLATORY BEHAVIOR OF FINITE DIFFERENCE METHODS FOR
THE SOLUTION OF THE TWO DIMENSIONAL TRANSIENT
HEAT (DIFFUSION) EQUATION

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

Joseph E. Cuthrell, B.S.

Captain, USAF

March 1986

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Preface

This study began with the investigation of oscillatory solutions in the Peaceman-Rachford alternating direction implicit method as demonstrated in a previous thesis (6). After confirming these results, other finite difference methods were then considered for oscillatory analysis, including the relatively new exponential (power law) scheme of Patankar and Baliga.

I would like to thank Dr. Bernard Kaplan of the Air Force Institute of Technology who provided the guidance and assistance essential to the completion of this study. I would also like to express my thanks to Dr. N. Pagano of AFWAL/MLBC for sponsoring this thesis. Deep gratitude is also expressed to Mr. Joel Rice of AFIT/ADOC for his timely support and assistance.

Finally, I wish to acknowledge my gratitude to my wife, Jacqueline, for her great patience and understanding.

— Joseph E. Cuthrell



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Nomenclature

$\Delta x = \Delta y = H$ = spacial increment between nodal points

t = time (seconds)

Δt = time step

α = thermal diffusivity

$R = \alpha \Delta t / H^2$

$T(i, j, n)$ = Temperature at the i th, j th, node at time n ,
= $T(i\Delta x, j\Delta y, n\Delta t) = T(x, y, t)$

\underline{A} = notation for matrix A

\bar{b} = notation for column matrix b

DF = Dufort-Frankel difference method

SV = Saul'ev difference method

EXP = Exponential difference method

Abstract

The two dimensional transient heat (diffusion) equation with Dirichlet boundary conditions was solved using the Dufort-Frankel, Saul'ev, and, Exponential (Power-law) finite difference schemes. All methods were investigated for oscillatory behavior and comparisons of accuracy made.

To predict the time step at which oscillatory behavior would occur, the coefficient, matrix, and probabilistic methods of stability analysis were utilized. At time steps greater than the square of the mesh divided by the thermal diffusivity, oscillatory solutions were apparent in both the Dufort-Frankel and Saul'ev schemes. The exponential method, as predicted, did not oscillate for any size time step.

Although the exponential scheme was the most accurate at large time steps, the solution still contained enough error to be unusable in many engineering applications. At small time steps, all methods were more accurate than the fully implicit formulation.

The exponential method was found to be the slowest computationally. The Saul'ev scheme proved to be the fastest while still achieving the required degree of accuracy.

OSCILLATORY BEHAVIOR OF FINITE DIFFERENCE METHODS
FOR THE SOLUTION OF THE TWO DIMENSIONAL
TRANSIENT HEAT (DIFFUSION) EQUATION

I. Introduction

Background

Because only the simplest of boundary value problems can be solved by exact analytical methods, the engineer must rely on finite difference methods in solving "real world" problems with complicated and irregular geometries. Finite difference approximations allow a differential equation, together with its associated boundary and initial conditions, to be transformed into a set of algebraic equations readily solved utilizing a high speed digital computer.

Clearly, for finite difference approximations to be of practical use, a high degree of accuracy must be demanded. It is well known that difference approximations for derivatives contain "truncation" errors arising from the neglect of the higher order terms in its Taylor series representation. "Round-off" errors are also introduced since only a finite number of digits can be stored in computer memory.

A finite difference scheme is said to be "stable" if, as time progresses, these errors decay rather than grow in an unbounded fashion (2:98). "The inexperienced user is often surprised when stable methods produce physically unrealistic solutions that oscillate with time" (9:27). Although in stable methods, these oscillations decrease with time, they may produce sufficient inaccuracies to destroy the solution (9:27). Therefore, a thorough understanding as well as a means of predicting oscillatory behavior is essential in employing a finite difference method with any degree of confidence.

The Two Dimensional Transient Heat (Diffusion) Equation

Of particular interest to the nuclear engineer are boundary value problems involving the transient heat (diffusion) equation. The equation in two dimensional form is:

$$\frac{\partial T(x,y,t)}{\partial t} = \alpha \left[\frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2} \right]$$

where α is thermal diffusivity and T is temperature.

Problem Statement

The objective of this thesis is to determine if numerical oscillations exist in the following finite

difference approximations to the two dimensional transient heat (diffusion) equation:

1. Dufort-Frankel
2. Exponential
3. Saul'ev

In addition to the above methods, solutions found by the pure implicit method are computed for purposes of accuracy comparison.

Scope

The boundary value problems investigated are limited to the two dimensional transient heat equation applied on a unit square. Dirichlet boundary conditions and a thermal diffusivity of one are assumed. The unit square is partitioned into a grid of 81 interior nodes with $\Delta x = \Delta y$. The analysis of oscillatory behavior is conducted by following the temperatures of two interior nodes. All nodes will be included in the error analysis.

Approach

A previous thesis by Kropf demonstrated that stable oscillations existed in the Alternating Direction Implicit Method of Peaceman and Rachford when applied to a unit square (6:56). After confirming these results, a literature search was conducted to find other difference methods that could be subject to oscillatory behavior. The Dufort-Frankel, exponential, and Saul'ev finite difference schemes

were selected and tested for oscillations using the coefficient, probabilistic, and matrix methods. Two boundary value problems were then numerically solved using the above finite difference methods and investigated for the oscillations predicted.

Sequence of Presentation

General algebraic formulas for the finite difference methods considered are presented in Chapter II. The coefficient, probabilistic, and matrix methods of predicting oscillations are introduced in Chapter III.

Chapter IV presents numerical solutions for the two problems as well as accuracy comparisons for all methods. Finally, conclusions and recommendations are offered in Chapter V.

II. Difference Approximations to the Transient Heat (Diffusion) Equation

The Dufort-Frankel, Saul'ev, and exponential finite difference approximations will be investigated for oscillatory behavior and solution accuracy. The Dufort-Frankel and Saul'ev difference schemes are explicit methods that are known to be unconditionally stable in two dimensions (7:237). A relatively new implicit method, the exponential scheme of Patankar and Baliga, is also considered. In the one dimensional case, this method has been shown to be free of numerical oscillations and possess superior accuracy for any size time step (9:35). Here, the analysis is extended to two dimensions.

Standard difference notation is used in presenting all methods. Namely, $T(x,y,t) = T(i\Delta x, j\Delta y, n\Delta t) = T(i, j, n)$. Further, the following nomenclature is adopted:

$$H = \Delta x = \Delta y$$

and

$$R = \alpha\Delta t/H^2 = \Delta t/H^2$$

Dufort-Frankel Explicit Approximation

The Dufort-Frankel approximation was developed to circumvent the inherent instability of Richardson's three level explicit method (7:238). The formula, for two dimensions, is (App A):

$$\begin{aligned}
T(i,j,n+1) (1+4R) &= 2R [T(i+1,j,n) + T(i-1,j,n) \\
&+ T(i,j+1,n) + T(i,j-1,n)] \quad (1) \\
&+ (1-4R) T(i,j,n-1)
\end{aligned}$$

The method is effectively explicit if temperatures at both the (n-1) and (n) time steps are known or in the computationally limiting case of R equal to 1/4 (7:239). Given, as an initial condition, the temperatures at the (n-1) time level, an alternate method is needed to advance to time level (n) (7:239).

Saul'ev Explicit Approximation

The Saul'ev scheme, like the Dufort-Frankel, is explicit under certain conditions. However, the Saul'ev scheme employs alternate formulas for each successive time step. To advance to the (n+1) time level the equations are (7:237):

$$\begin{aligned}
T(i,j,n+1) (1+2R) &= R [T(i,j+1,n) + T(i+1,j,n) \\
&+ T(i-1,j,n+1) + T(i,j-1,n+1)] \quad (2a) \\
&+ (1-2R) T(i,j,n)
\end{aligned}$$

To proceed from the (n+1) to the (n+2) time step, the equations are (7:238):

$$\begin{aligned}
T(i,j,n+2) (1+2R) &= R [T(i+1,j,n+2) + T(i,j+1,n+2) \\
&+ T(i-1,j,n+1) + T(i,j-1,n+1)] \quad (2b) \\
&+ (1-2R) T(i,j,n+1)
\end{aligned}$$

Equation (2a) becomes explicit when $T(i-1, j, n+1)$ and $T(i, j-1, n+1)$ are known. If using rectangular geometry, this is accomplished by initiating the calculations in the lower left corner and proceeding up the grid from left to right (7:195). Similarly, Equation (2b) can be "made" explicit by starting in the upper right corner and proceeding down the grid from right to left (7:195).

Exponential Approximation

The exponential method of Patankar and Baliga was shown to be non-oscillatory in the one dimensional case (9:37). A thorough development of the method can be found in reference 9. The difference formula in two dimensions is

$$\begin{aligned}
 T(i, j, n+1) (1+4Rf) - Rf\{T(i+1, j, n+1) + T(i-1, j, n+1) \\
 + T(i, j+1, n+1) + T(i, j-1, n+1)\} \\
 = R(1-f)\{T(i+1, j, n) + T(i-1, j, n) (3) \\
 + T(i, j+1, n) + T(i, j-1, n)\} \\
 + [1-4R(1-f)] T(i, j, n)
 \end{aligned}$$

where

$$f = (1 / [1 - \exp(-4R)]) - (1 / (4R))$$

To achieve a computationally faster algorithm, the authors replaced the exponential term with the following power law approximation (9:32):

$$\text{For } 0 < 4R < 10 \quad f = 1 - [1 / (4R)] [1 - (1 - 0.1(4R))^5]$$

$$\text{For } 4R \geq 10 \quad f = 1 - [1 / (4R)]$$

This difference scheme, unlike the others, results in a system of equations to be solved simultaneously.

Methods of Solution

The Dufort-Frankel and Saul'ev explicit methods are solved in a straightforward manner with one equation for each unknown. However, both methods are explicit under certain conditions.

To "bootstrap" the three-level Dufort-Frankel scheme through the first two time steps, another finite difference method is needed. The "pure implicit" method was chosen because of its characteristic non-oscillatory behavior. With the first two time steps known, the method subsequently became explicit.

For an explicit Saul'ev scheme to be realized, the order in which the nodal points are calculated is important. For each odd time step, equation (2a) is used, starting in the lower left corner and proceeding up the grid from left to right. Alternatively, Equation (2b) is used for each even time step starting in the upper right corner and moving down the grid from right to left.

The exponential method resulted in a series of equations to be solved simultaneously. These were of the form

$$\underline{A} \bar{x} = \bar{b}$$

where \bar{x} is a column matrix of temperatures at time (n+1) and \bar{b} is a column matrix of the associated boundary conditions and temperatures at time (n). For N interior nodes, a real, symmetric, N x N matrix results for \underline{A} . The most computationally efficient method of solving this matrix equation is direct Gaussian elimination (13:105).

III. Oscillatory Behavior and Accuracy of Methods

Unfortunately, the stability of a finite difference method does not guarantee solution accuracy or even physical realism (9:27). Stability merely insures that numerically induced errors will not grow in successive levels of computation (2:98). For computational efficiency, the largest time step, which produces the required level of accuracy, should be utilized. If too large a time increment is used, numerical oscillations may result, destroying solution accuracy (9:27). Attention is now turned to three methods of stability analysis that are of use in predicting oscillatory behavior.

Coefficient Method

The method presented here was proposed in a previous paper (6:10). It is a direct extension of the one dimensional case offered by Myers (8:282). By applying Equations (1), (2), and (3) to a one nodal point grid with homogeneous boundary conditions, the following ratios are obtained:

Dufort-Frankel

$$T(i,j,n+1)/T(i,j,n-1) = (1-4R)/(1+4R)$$

Saul'ev

$$T(i,j,n+1)/T(i,j,n) = (1-2R)/(1+2R)$$

Exponential

$$T(i,j,n+1)/T(i,j,n) = \exp(-4R)$$

The value of this ratio (ρ) will reveal the behavior of the corresponding finite difference scheme (8:282):

For $0 < \rho < 1$ No oscillations, stable solution
For $-1 < \rho < 0$ Stable oscillations, stable solution
For $\rho < -1$ Unstable oscillations, unstable solution

It is readily apparent that all ratios lie between -1 and 1, and therefore, all methods are unconditionally stable. However, a region of stable oscillations is predicted for both the Dufort-Frankel and Saul'ev schemes (see Figure 1).

For the Dufort-Frankel method, oscillatory behavior is predicted when

$$R > 1/4$$

This value of R causes the ratio to become negative and stable oscillations should be observed.

Similarly, the Saul'ev scheme is predicted to oscillate when

$$R > 1/2$$

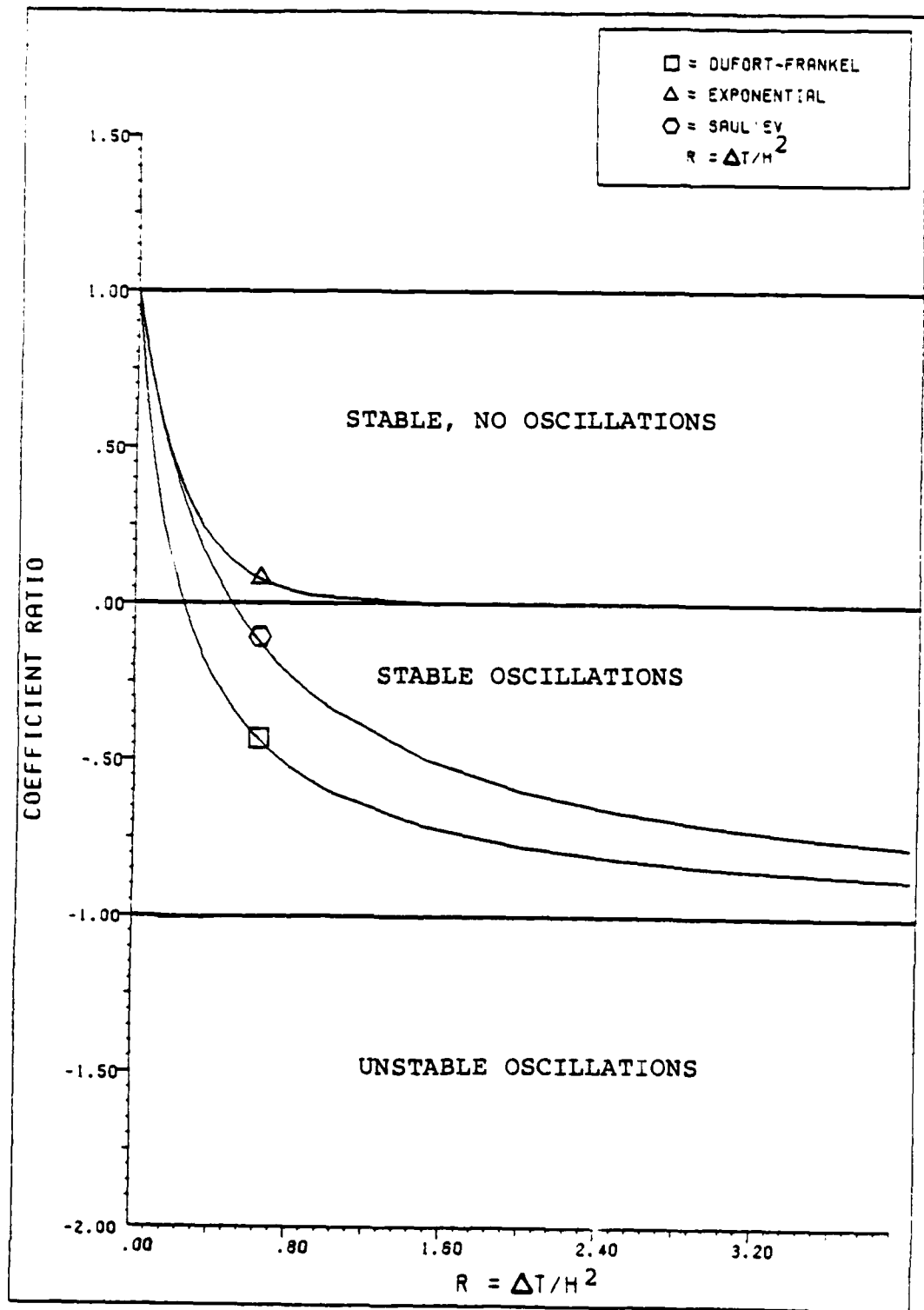


FIG 1. COEFFICIENT RATIO VS R

Note the method predicts only smooth, stable behavior for the exponential scheme since the ratio is always positive and less than unity.

It is important to remember that since no more than one node and homogeneous boundary conditions were assumed, the coefficient method can only approximate the values of R that cause numerical oscillations (8:289).

Matrix Method

Unlike the coefficient method, the matrix approach deals with the more general case in which there is more than one node. Myers presents this approach employing a two node grid (8:286). The method here will be extended to four nodes.

Consider a system of N finite difference equations that can be expressed as

$$\bar{u}^{(n+1)} = \underline{A} \bar{u}^{(n)}$$

where $\bar{u}^{(n+1)}$ and $\bar{u}^{(n)}$ are column matrices comprised of temperatures at times (n+1) and (n) respectively. The spectral radius of \underline{A} then determines the stability of the system (11:84). Namely, if the eigenvalue of largest modulus is less than or equal to unity, the system will be stable.

For example, when the exponential scheme is written in the above form and a four node grid is assumed, the

eigenvalues of \underline{A} are found to be (App B):

$$\lambda_1 = \lambda_2 = \exp(-4R)$$

$$\lambda_3 = 1 - (6R / (1 + 6Rf))$$

$$\lambda_4 = 1 - (2R / (1 + 2Rf))$$

It is easily verified that λ_4 is the dominant eigenvalue and lies between 0 and 1. Using the two node model of the Euler method, Myers finds the value of R which would make the dominant eigenvalue negative, and states that this is the "limit for stable oscillations" (8:286). In applying this reasoning to the exponential case, one concludes that for any value of R the dominant eigenvalue is always positive and less than unity. Thus, the matrix approach predicts only steady, stable numerical behavior in agreement with the coefficient method.

It is easy to see that this method becomes prohibitively laborious when large systems of equations (nodes) are considered (8:286).

Probabilistic Method

A probabilistic method of stability analysis is suggested by Kaplan (5:459). If the coefficients of an explicit finite difference scheme are given probabilistic interpretations, it has been shown that the stability limit can be derived (5:459). This concept can be taken a step further by utilizing the method to determine

oscillatory behavior in explicit methods. The method will be applied to the Dufort-Frankel scheme since it has not been demonstrated to be of use in implicit methods.

By giving the coefficients found in the Dufort-Frankel scheme a probabilistic interpretation, Equation (1) can be rewritten

$$\begin{aligned}
 T(i,j,n+1) = & P_x^- T(i+1,j,n) + P_x^+ T(i-1,j,n) \\
 & + P_y^- T(i,j+1,n) + P_y^+ T(i,j-1,n) \\
 & + P_o T(i,j,n-1)
 \end{aligned}$$

where

$$P_x^- = P_x^+ = P_y^- = P_y^+ = (2R)/(1+4R)$$

$$P_o = (1-4R)/(1+4R)$$

These coefficients are now given the following interpretations (5:459):

P_x^- : probability that a particle at $(i+1,j,n)$ can be found at $(i,j,n+1)$ or moving a step to the left in one time increment

P_x^+ : probability that a particle at $(i-1,j,n)$ can be found at $(i,j,n+1)$ or moving a step to the right in one time increment

P_o : probability that a particle at $(i,j,n-1)$ can be found at $(i,j,n+1)$ or returning to the same position in two time steps

P_y^- and P_y^+ are given interpretations similar to P_x^- and P_x^+

Moreover, Kaplan points out that these probability coefficients must satisfy two conditions (4:460):

1. No probability or coefficient can be negative
2. The sum of the probabilities or coefficients cannot exceed unity

By simply adding the coefficients found in Equation (1), condition two is found to be satisfied. However, condition one implies that P_0 must be non-negative which occurs only when

$$R \leq 1/4$$

The method then predicts that oscillations may occur when R is greater than $1/4$ and is in agreement with the coefficient method.

Accuracy of Methods

Since finite difference methods are "built" by neglecting the higher order terms of its Taylor series representation, truncation error is inevitable. The Dufort-Frankel scheme possesses truncation error of order $H^2 + \Delta t^2 + (\Delta t/H)^2$ (7:157). An improvement in the truncation error of the Saul'ev method can be realized by using Equations (2a) and (2b) in an alternating fashion (7:199). If each is used alone, the error is of order $(H + \Delta t^2)$ (7:199). When used together in alternating directions, the error is reduced to order $H^2 + \Delta t^2 + (\Delta t/H)^2$ (7:199).

The truncation error for the exponential scheme is not listed in the literature. However, an approximation can be found by noting that for certain values of f , Equation (3) is equivalent to other conventional finite difference schemes with known truncation error. With f equal to 0.5, Equation (3) corresponds to the Crank-Nicolson method (9:29). An f of 1.0 similarly leads to the fully implicit formulation (9:29). Further, it is easily verified that for large values of R , f approaches 1.0 in value. Conversely, as R is made arbitrarily small, f approaches 0.5. Thus, for small values of R , the exponential scheme should have truncation error approaching the Crank-Nicholson ($H^2 + \Delta t^2$) (10:189) and at large R , that of the fully implicit ($H^2 + \Delta t$) (10:189).

In addition to truncation error, oscillatory behavior can cause considerable inaccuracy. Substantial errors are then predicted for both the Dufort-Frankel and Saul'ev methods for large values of R .

Because the computer can retain only a finite number of digits, round-off errors are introduced. As the number of computations are increased, the round-off error may grow, possibly nullifying any accuracy advantage gained by refining time step or mesh size (6:15).

Error Analysis

To determine the accuracy associated with each finite difference method, maximum and root mean square errors were computed. Root mean square error was calculated according to (12:1023-1024).

$$\text{Erms} = \sum_{j=1}^J \sum_{i=1}^I [(T_a(i,j,n) - T(i,j,n))^2 / IJ]^{1/2}$$

where

$T_a(i,j,n)$ = analytical solution at point (i,j,n)

$T(i,j,n)$ = finite difference solution at point (i,j,n)

I = number of nodes in x direction

J = number of nodes in y direction

The maximum error at any nodal point was also calculated. This gives an indication of overall grid accuracy and is computed as

$$\text{Emax} = \max | T_a(i,j,n) - T(i,j,n) |$$

IV. Numerical Results

Numerical solutions obtained by the Dufort-Frankel, Saul'ev, and exponential schemes are presented. Two sample problems, each with a known analytical solution, are solved using each method. In addition, solutions obtained by the fully implicit method are provided for comparison. The sample problems and their analytical solutions are first presented. Next, oscillatory behavior is investigated for all methods. Finally, root mean square (Erms) and maximum (Emax) error are given to quantify solution accuracy.

Problem #1

The first problem and its analytical solution were successfully used in a previous thesis to investigate oscillatory behavior of the Peaceman-Rachford alternating direction implicit method (6:18-19). The problem is:

$$\frac{\partial T(x,y,t)}{\partial t} = \frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2}$$

with

$$T(x,y,0) = 0$$

and

$$T(x,0,t) = T(x,1,t) = T(1,y,t) = T(0,y,t) = 400$$

for

$$0 < x < 1 \quad \text{and} \quad 0 < y < 1$$

The analytical solution is (6:19):

$$T(x,y,t) = 400 (1-f(x,y,t))$$

where

$$f(x,y,t) = g(x,t) h(y,t)$$

$$g(x,t) = \sum_{n=1}^{\infty} \frac{4}{n\pi} \exp(-n^2\pi^2 t) \sin(n\pi x)$$

$$h(y,t) = \sum_{n=1}^{\infty} \frac{4}{n\pi} \exp(-n^2\pi^2 t) \sin(n\pi y)$$

$$n = 1, 3, 5 \dots$$

Problem #2

The second problem considered is:

$$\frac{\partial T(x,y,t)}{\partial t} = \frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2}$$

with

$$T(x,y,0) = 0$$

$$T(x,0,t) = T(0,y,t) = T(1,y,t) = 0; \quad T(x,1,t) = 400$$

where

$$0 < x < 1 \quad \text{and} \quad 0 < y < 1$$

This problem is identical to one found in Myers solved for the steady state case (8:127). The solution for the transient case is found to be:

$$T(x,y,t) = f(x,y,t) + g(x,y)$$

where

$$f(x,y,t) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} B_{mn} \sin(m\pi x) \sin(n\pi y) \exp(-(n^2\pi^2 + m^2\pi^2)t)$$

$$n = 1, 2, 3, \dots$$

$$m = 1, 2, 3, \dots$$

and

$$g(x,y) = \frac{4}{\pi} \sum_{l=1}^{\infty} [(\sin(l\pi x) \sinh(l\pi y)) / (l \sinh(l\pi))]$$

$$l = 1, 3, 5, \dots$$

$$B_{mn} = -4 \int_0^1 \int_0^1 g(x,y) \sin(n\pi y) \sin(m\pi x) dx dy$$

The steady state solution, $g(x,y)$, is found in Myers (8:129). The transient portion is found by separation of variables and superposition (1:130).

Oscillatory Solutions

Solutions for each method were computed using a square grid with $H = \Delta x = \Delta y = 0.1$ (Figure 2). To graphically display oscillatory behavior, solutions for nodes 57 and 41 are shown for selected values of R and corresponding time step ΔT . Temperatures are listed in degrees. The specific unit, whether $^{\circ}\text{K}$ or $^{\circ}\text{C}$ will obviously follow from the choice of thermal diffusivity (α), here equal to one.

Problem #1

As predicted in Chapter III, oscillatory solutions were found for both the Dufort-Frankel (DF) and Saul'ev (SV) difference methods when particular values of R were utilized. Figures 3 and 4 demonstrate the oscillations produced by the DF for $R = 1.0$. Although the oscillations decrease with time, they are still large enough (> 100 degrees) to render the solution unusable. For values of R below 0.25, only steady, smooth behavior was observed. Figures 5 and 6 show the DF scheme to be free of oscillations for $R = 0.2$.

The Saul'ev approximation was found to be free of oscillations for $R = 1.0$ (Figures 7 and 8). However, oscillatory behavior became evident when R was increased to 5.0 (Figure 9). This was to be expected since the "threshold" for oscillations in the SV ($R = 0.5$) is higher than in the DF method ($R = 0.25$).

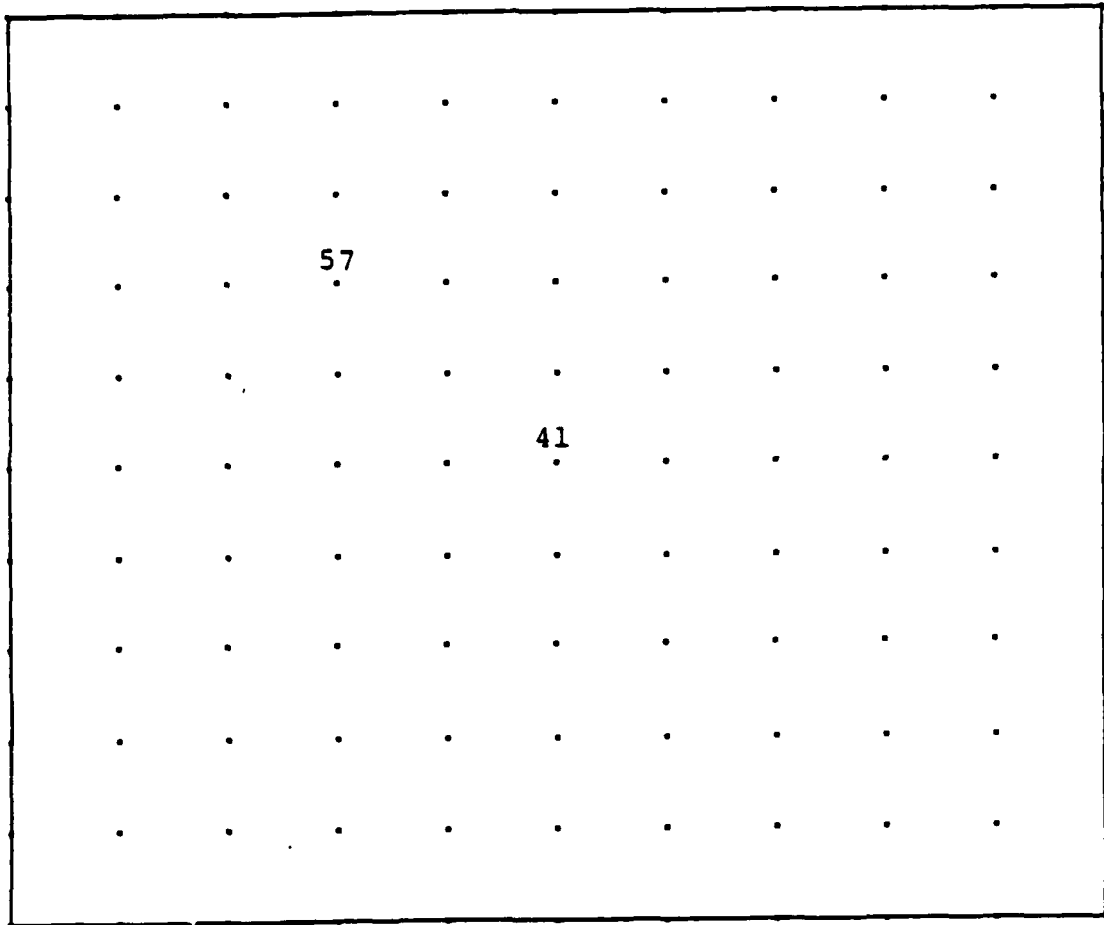


FIG 2. FINITE DIFFERENCE GRID IMPOSED ON
A UNIT SQUARE ($H = 0.1$)

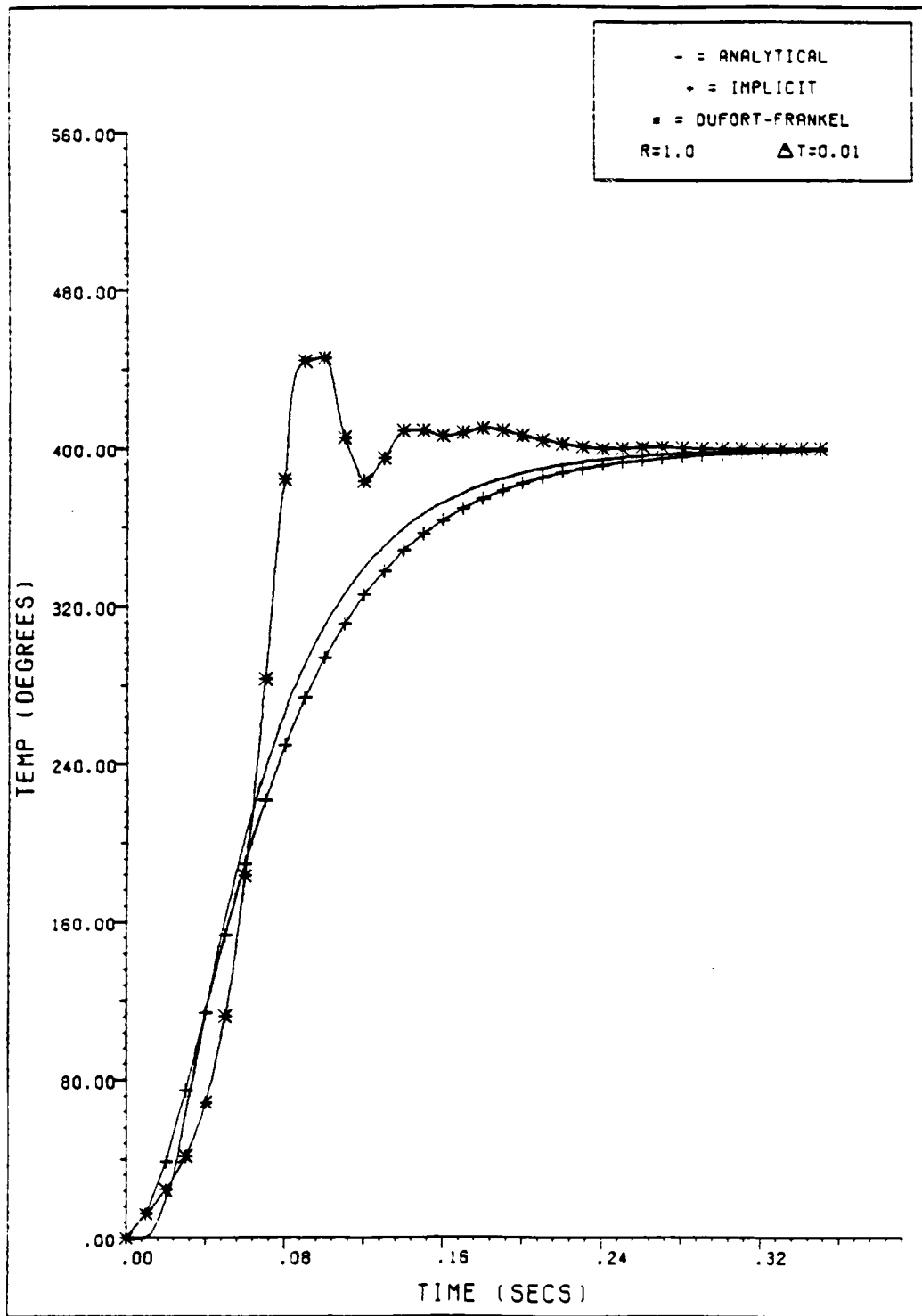


FIG 3. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 41)

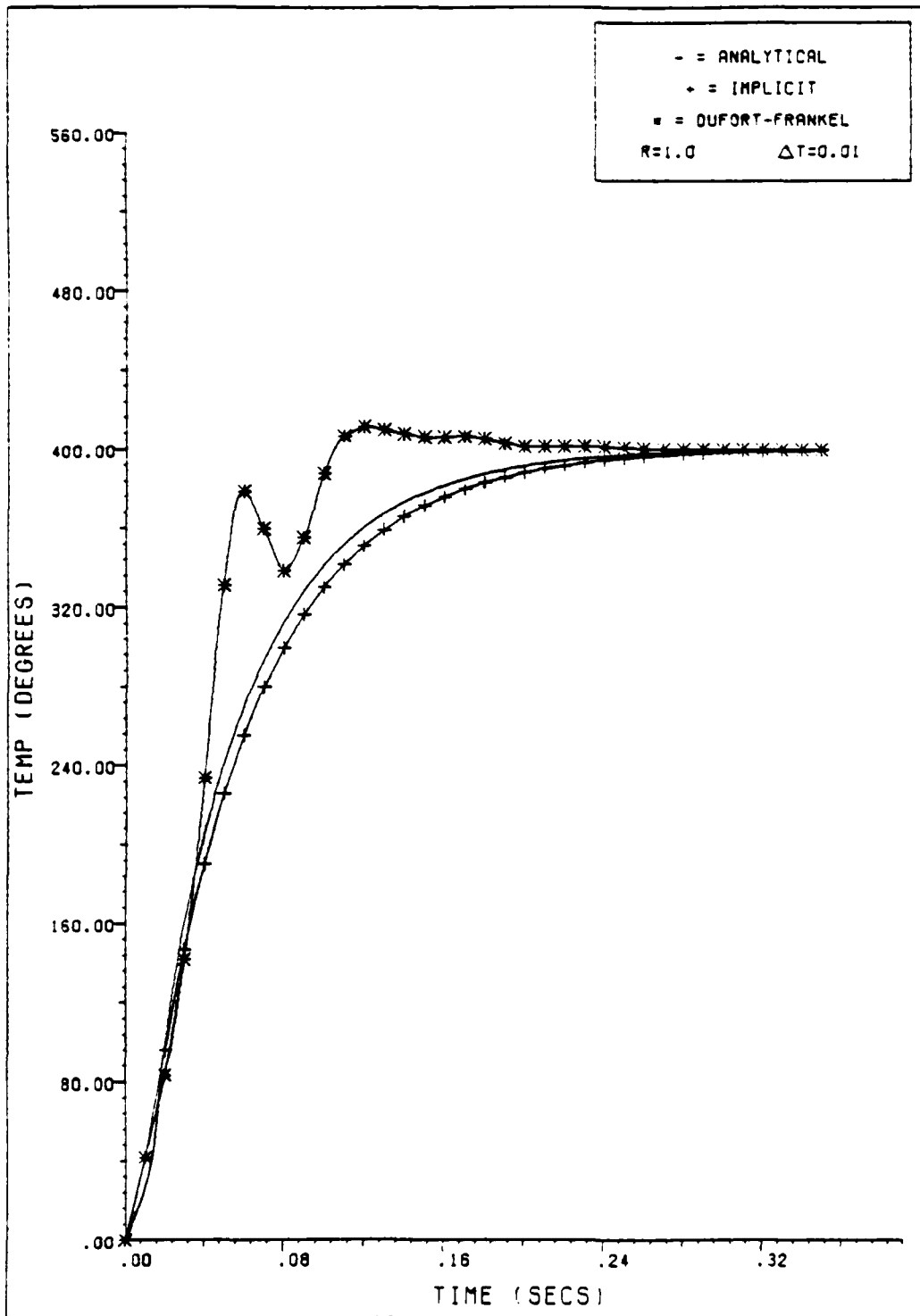


FIG 4. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 57)

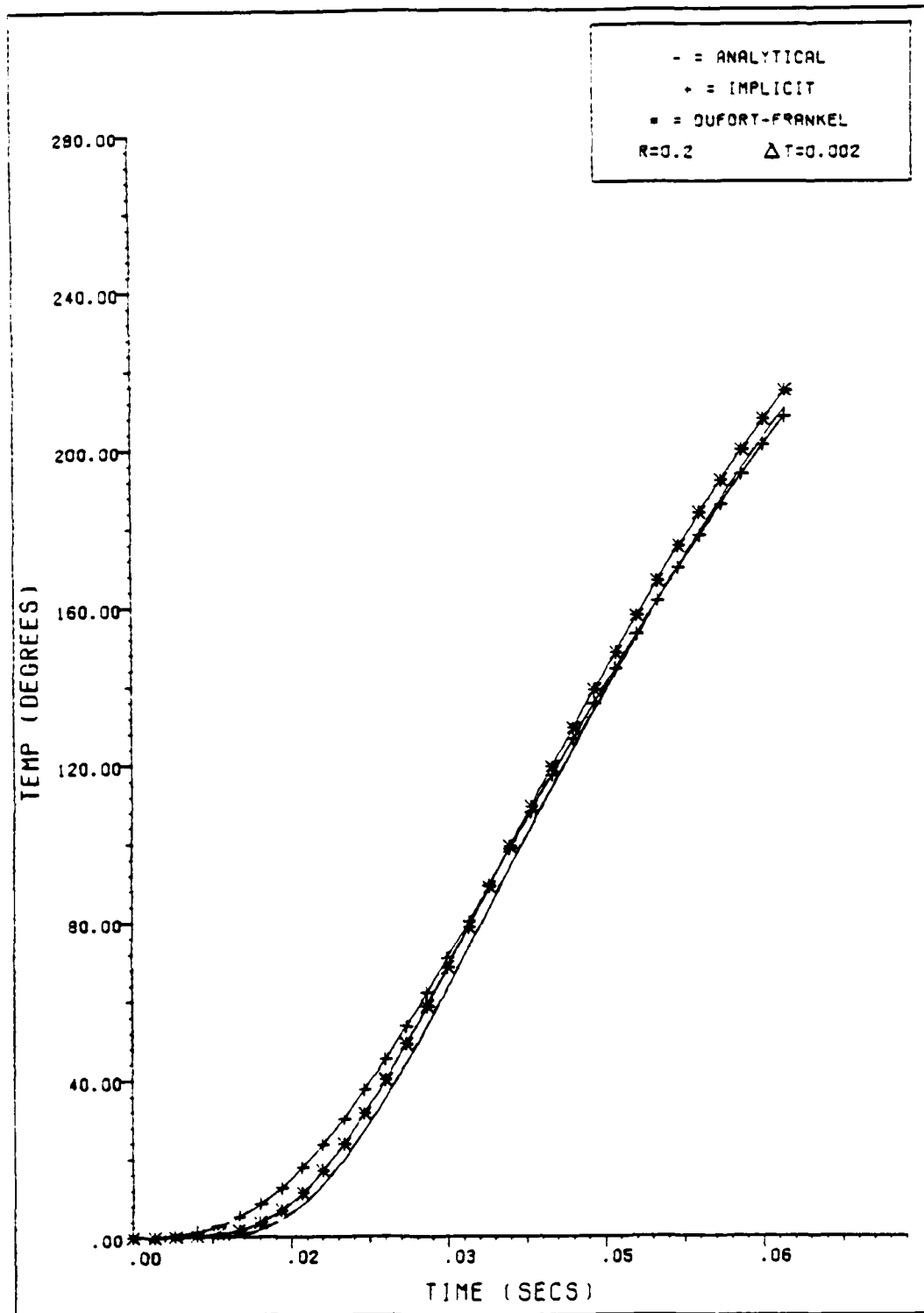


FIG 5. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 4)

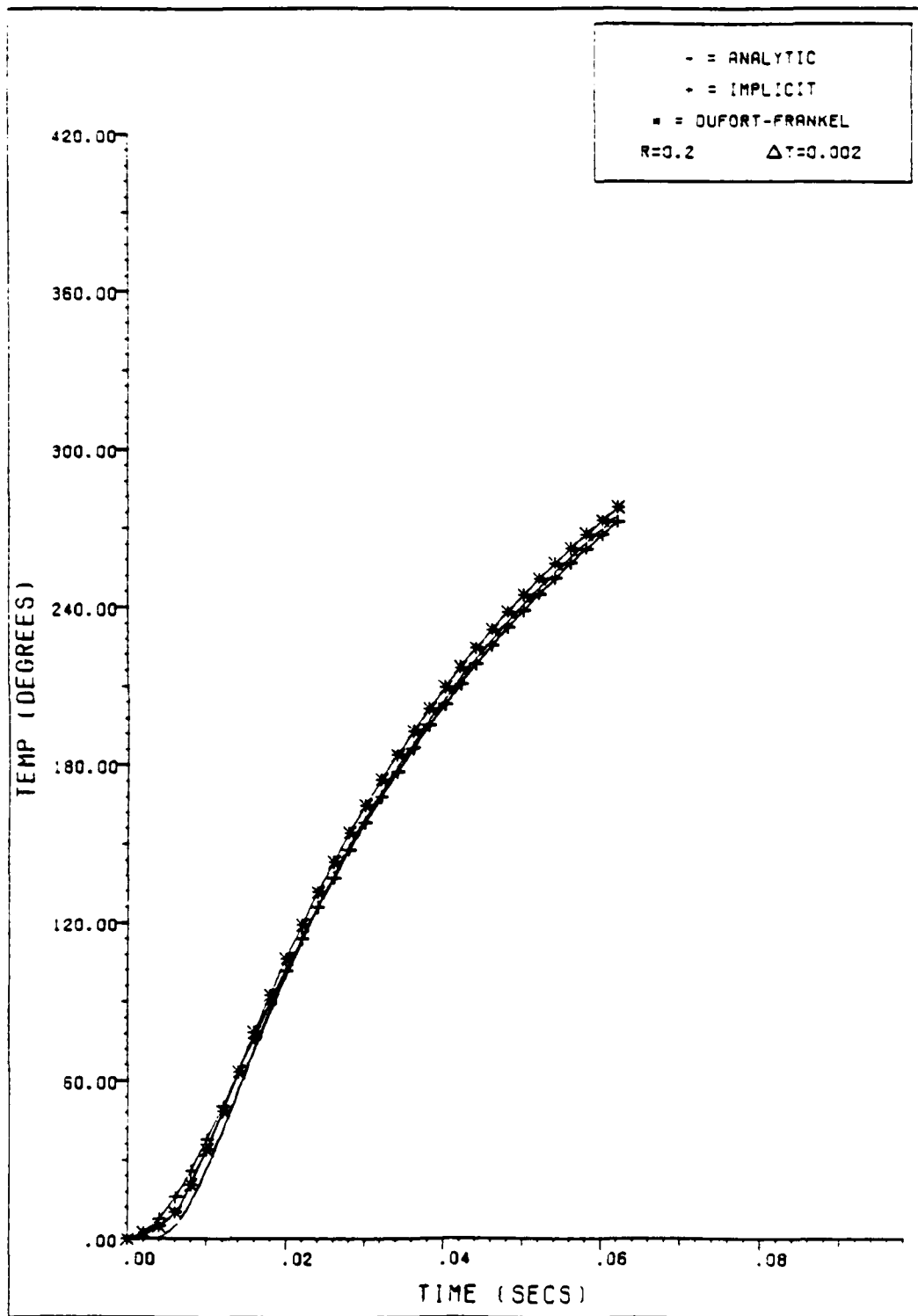


FIG 6. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 57)

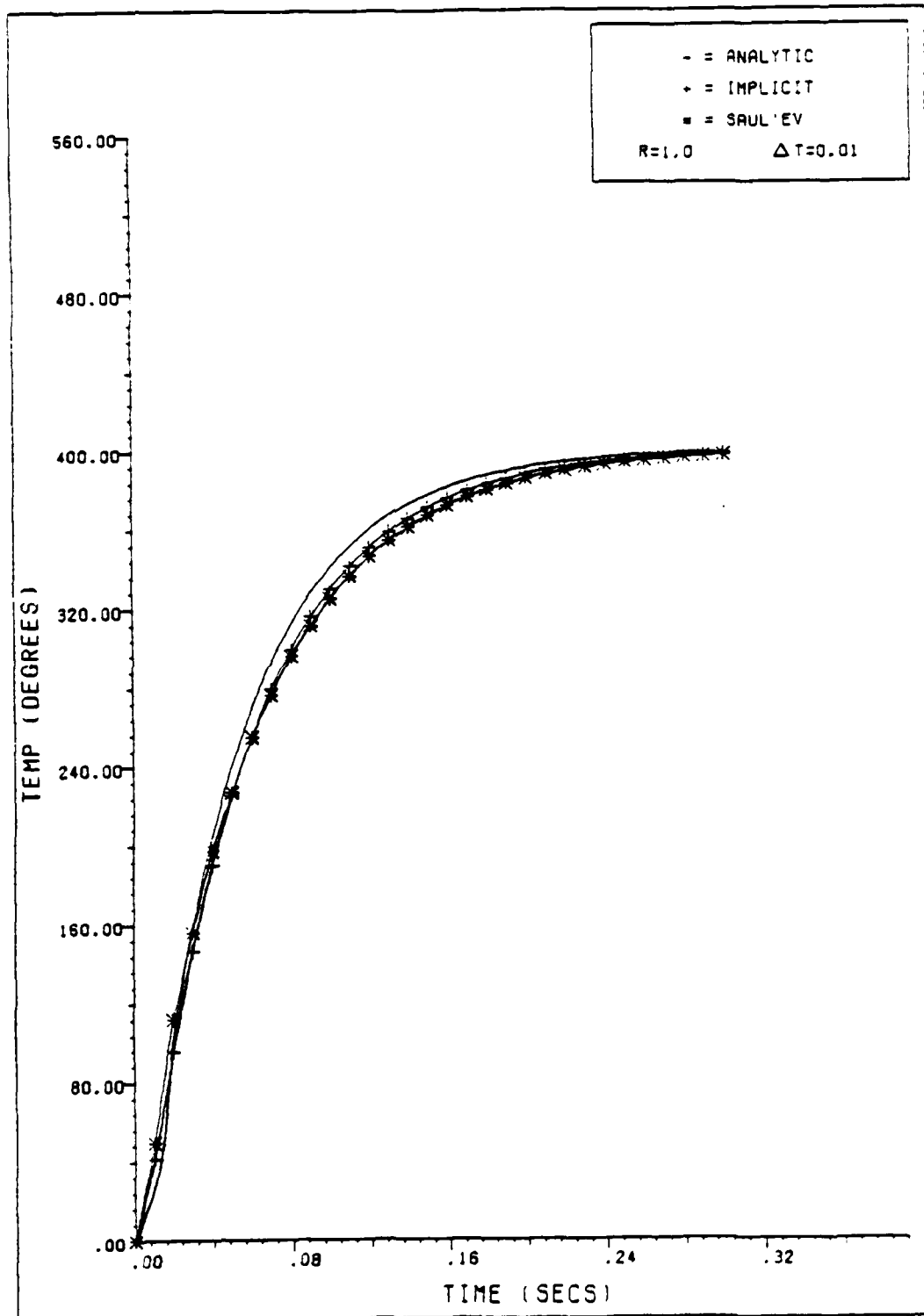


FIG 7. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 57)

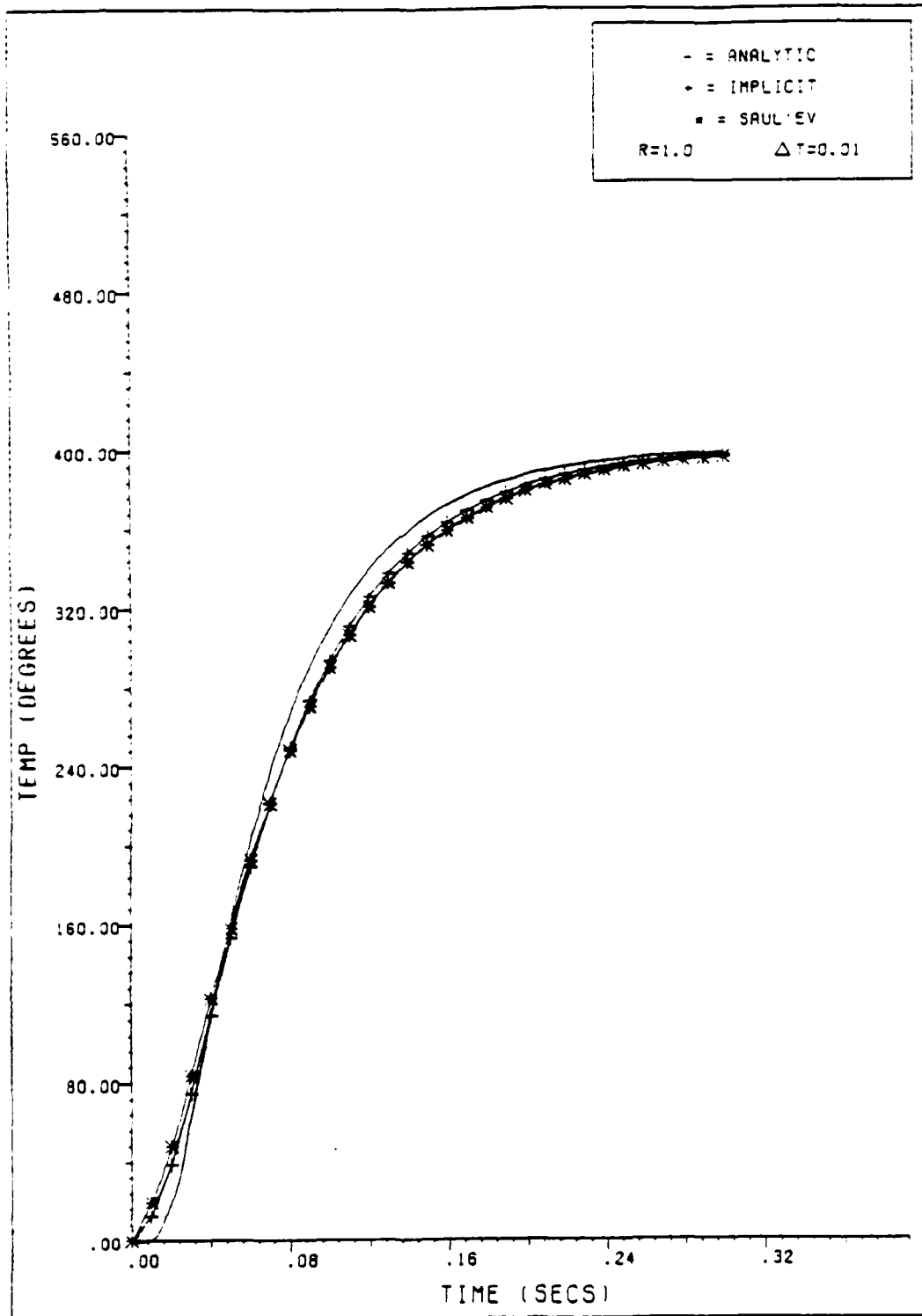


FIG 8. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 41)

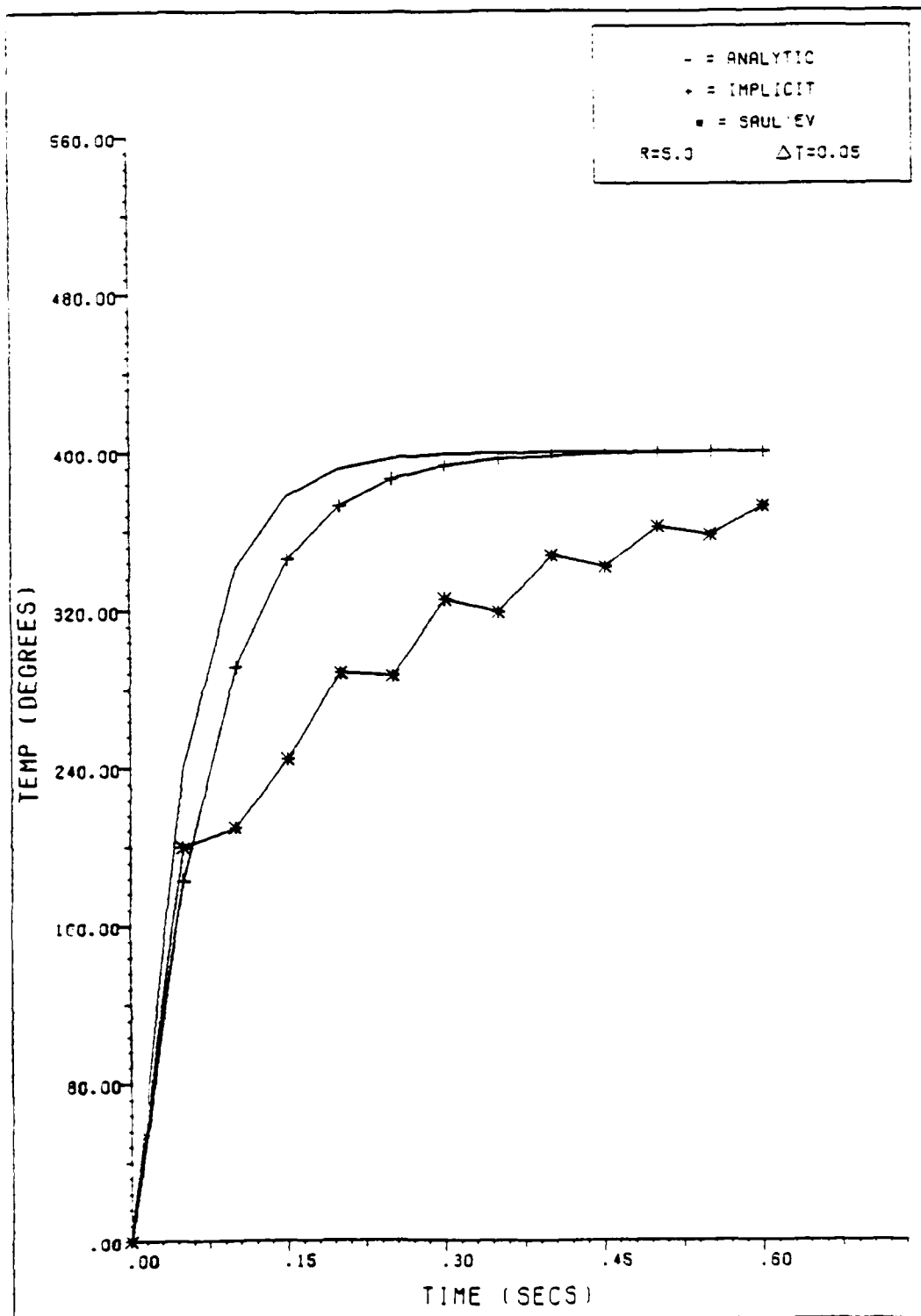


FIG 9. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 57)

Oscillatory behavior could not be induced in the exponential scheme (EXP) no matter how large the time step. Figures 10 and 11 show the solution for $R = 1.0$. Solutions for $R = 10.0$ ($\Delta T = 0.1$) are displayed in Figures 12 and 13. Again, the solutions are free of numerical fluctuations.

Problem #2

In general, problem #2 results confirmed the previous findings. Namely, that both the DF and SV methods produce oscillatory solutions for values of R in the ranges predicted. Numerical oscillations are again seen for the DF method at $R = 1.0$. A comparison of Figures 2 and 4 with Figures 14 and 15 reveal similar oscillations that decrease with time.

Unlike before, the SV scheme now displays small oscillations for $R = 1.0$ (Figures 16 and 17). When the value of R is increased to 5.0, the oscillations grow in magnitude and gross error results. However, stability is maintained since the oscillations decay with time (Figure 18).

Once again, the exponential method produced only smooth, steady solutions for all values of R . Figures 19 and 20 show the solution to be non-oscillatory for $R = 1.0$. Note also that the solution is generally more accurate than the implicit method.

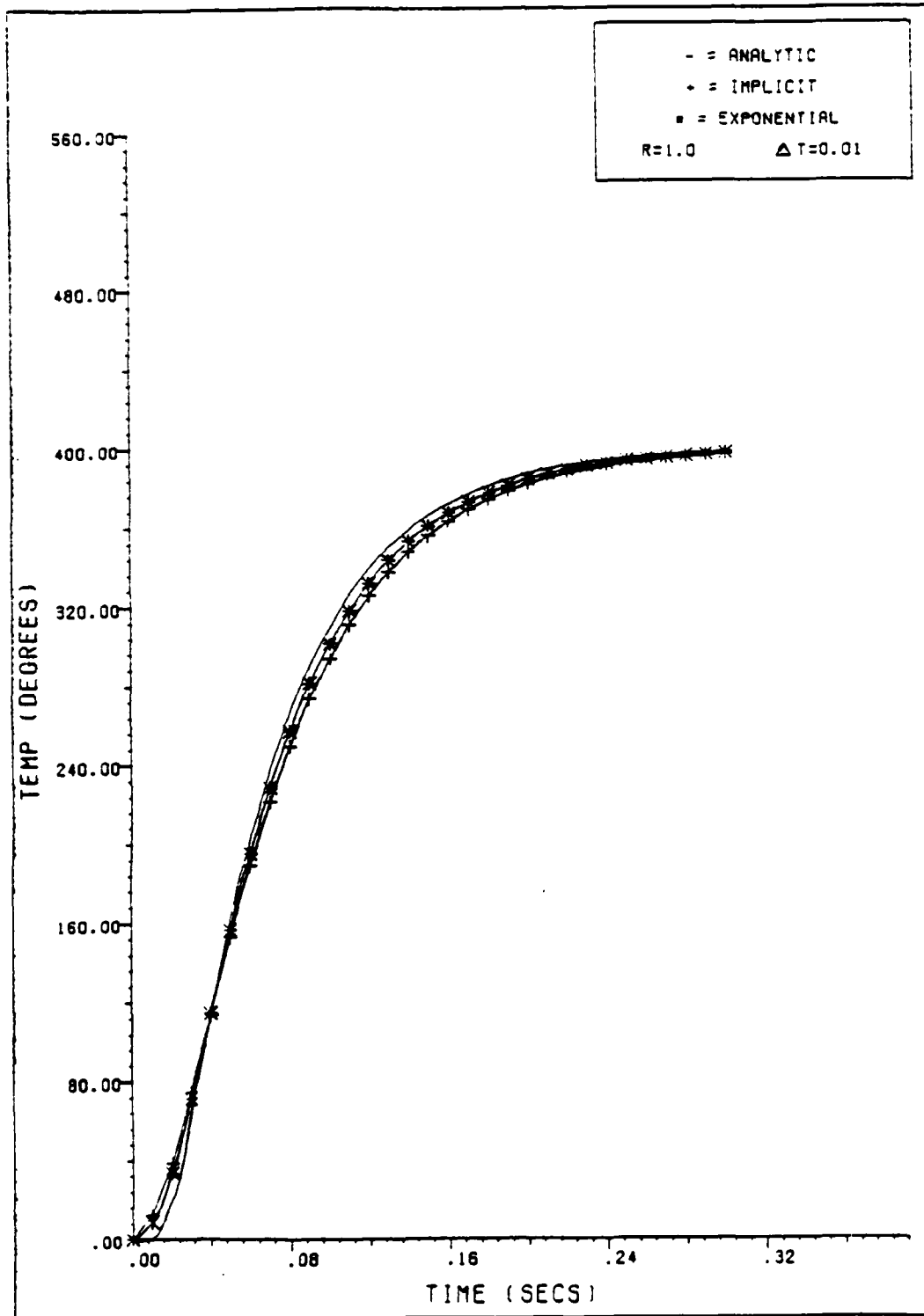


FIG 10. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 41)

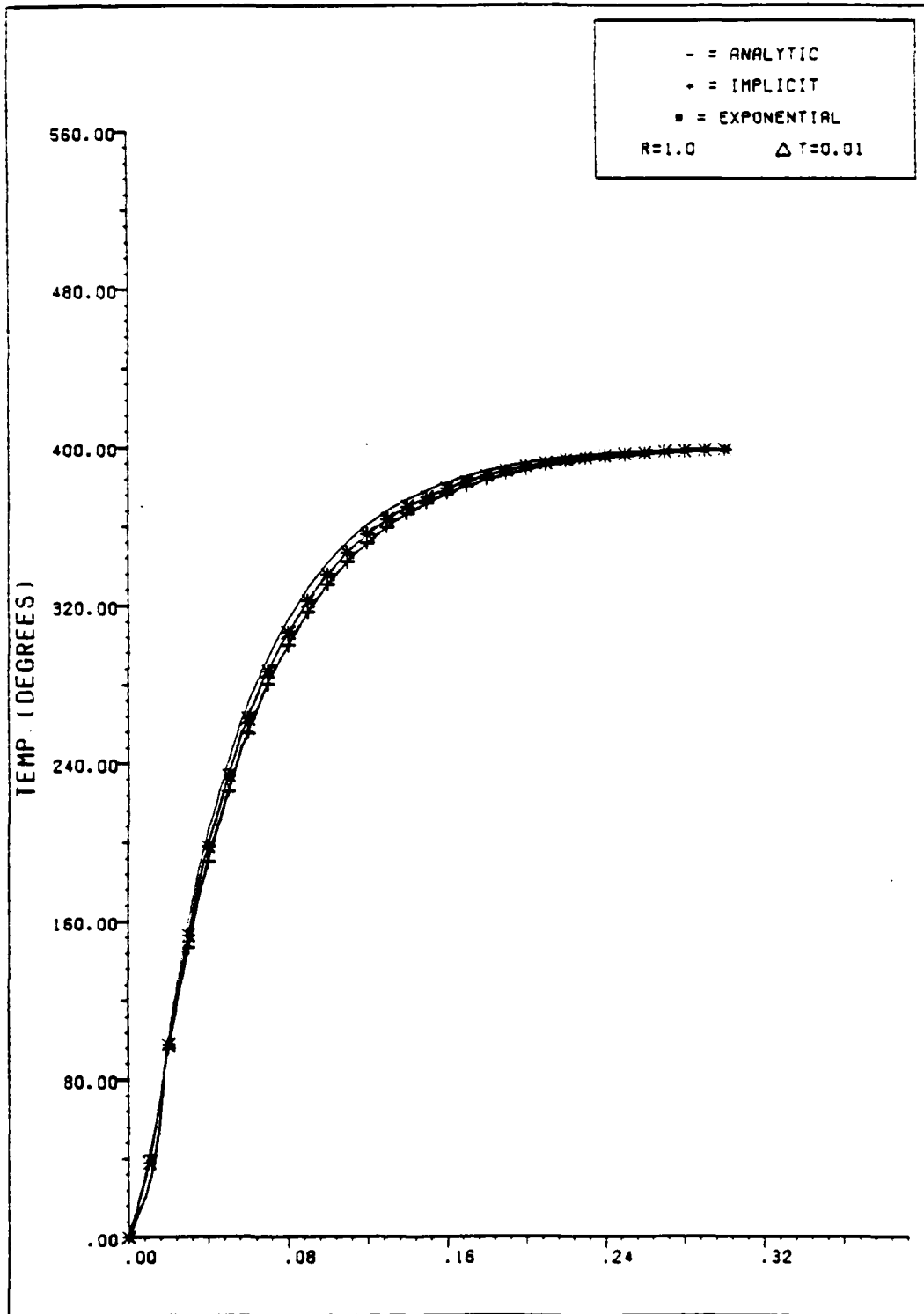


FIG 11. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 57)

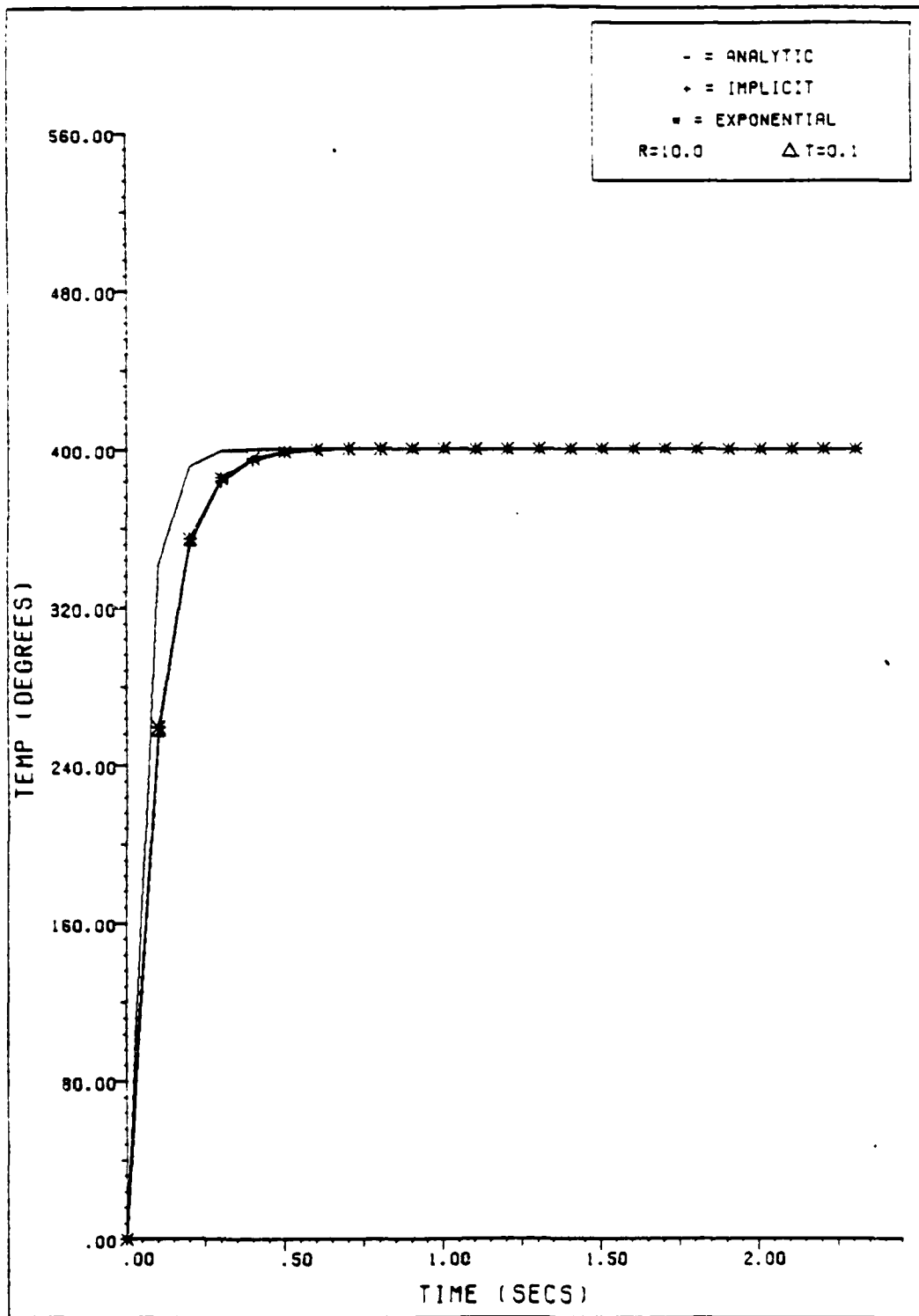


FIG 12. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 41)

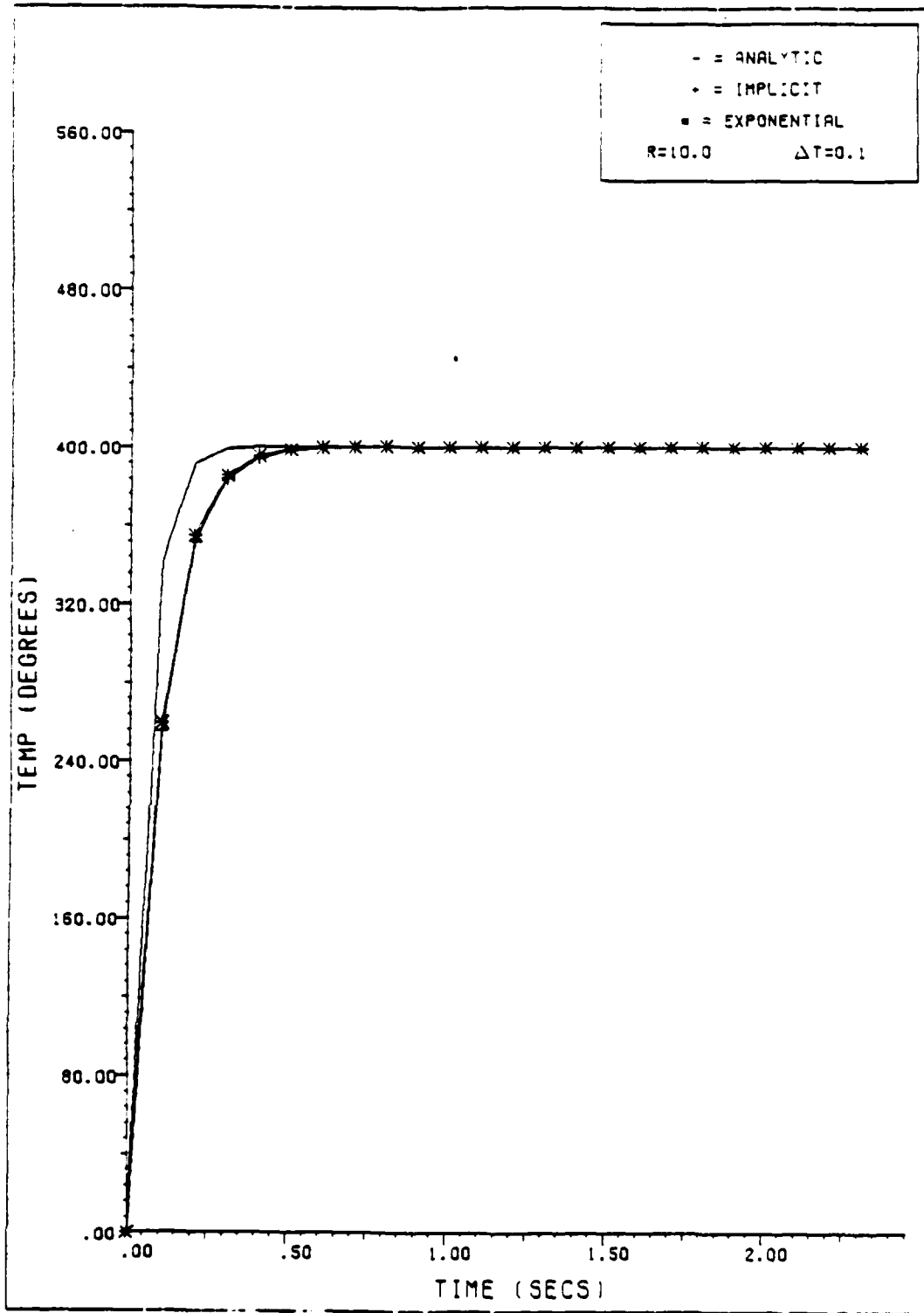


FIG 13. NUMERICAL SOLUTIONS PROBLEM #1 (NODE 57)

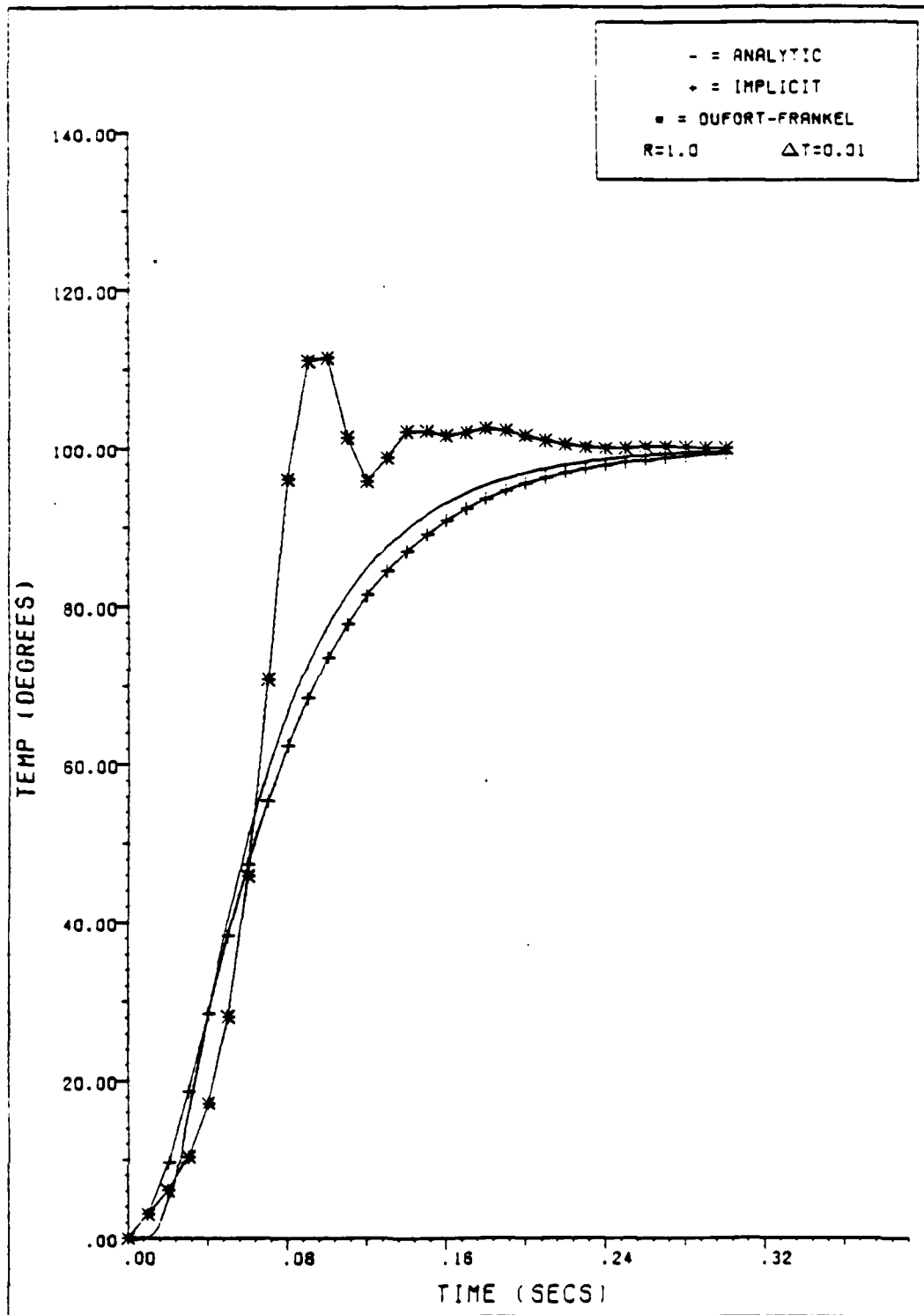


FIG 14. NUMERICAL SOLUTIONS PROBLEM #2 (NODE 41)

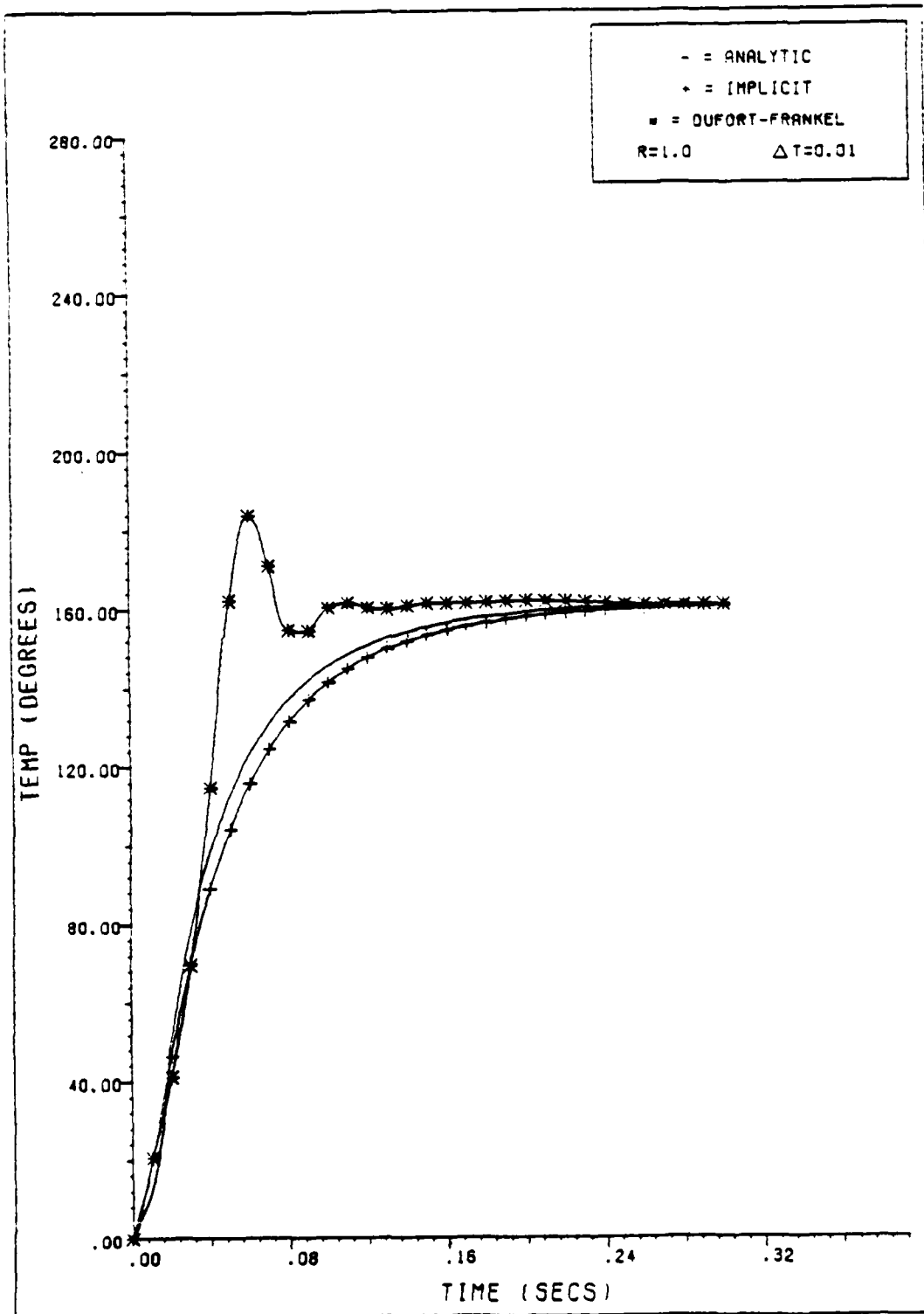


FIG 15. NUMERICAL SOLUTIONS PROBLEM #2 (NODE 57)

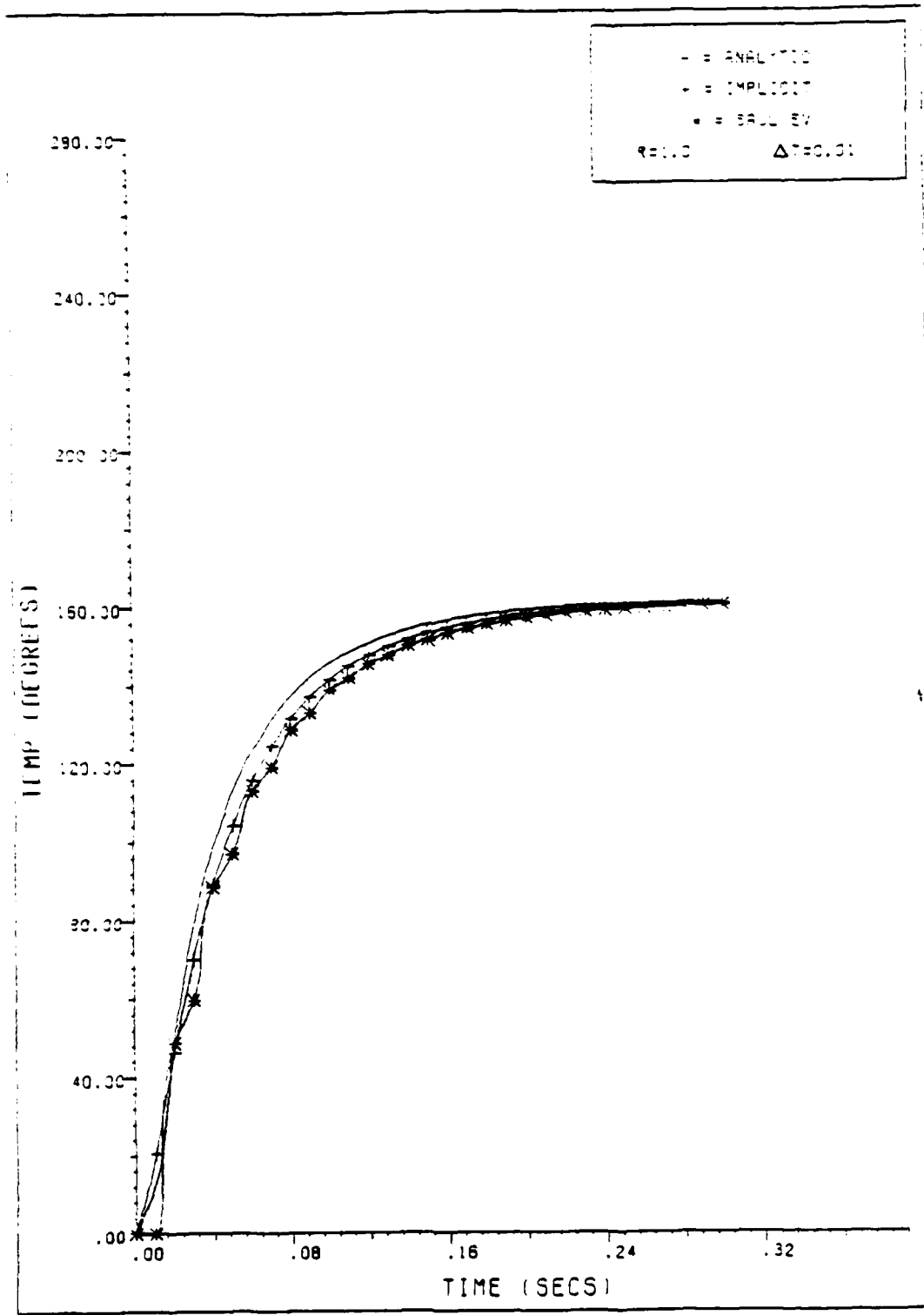


FIG 16. NUMERICAL SOLUTIONS PROBLEM #2 (NODE 57)

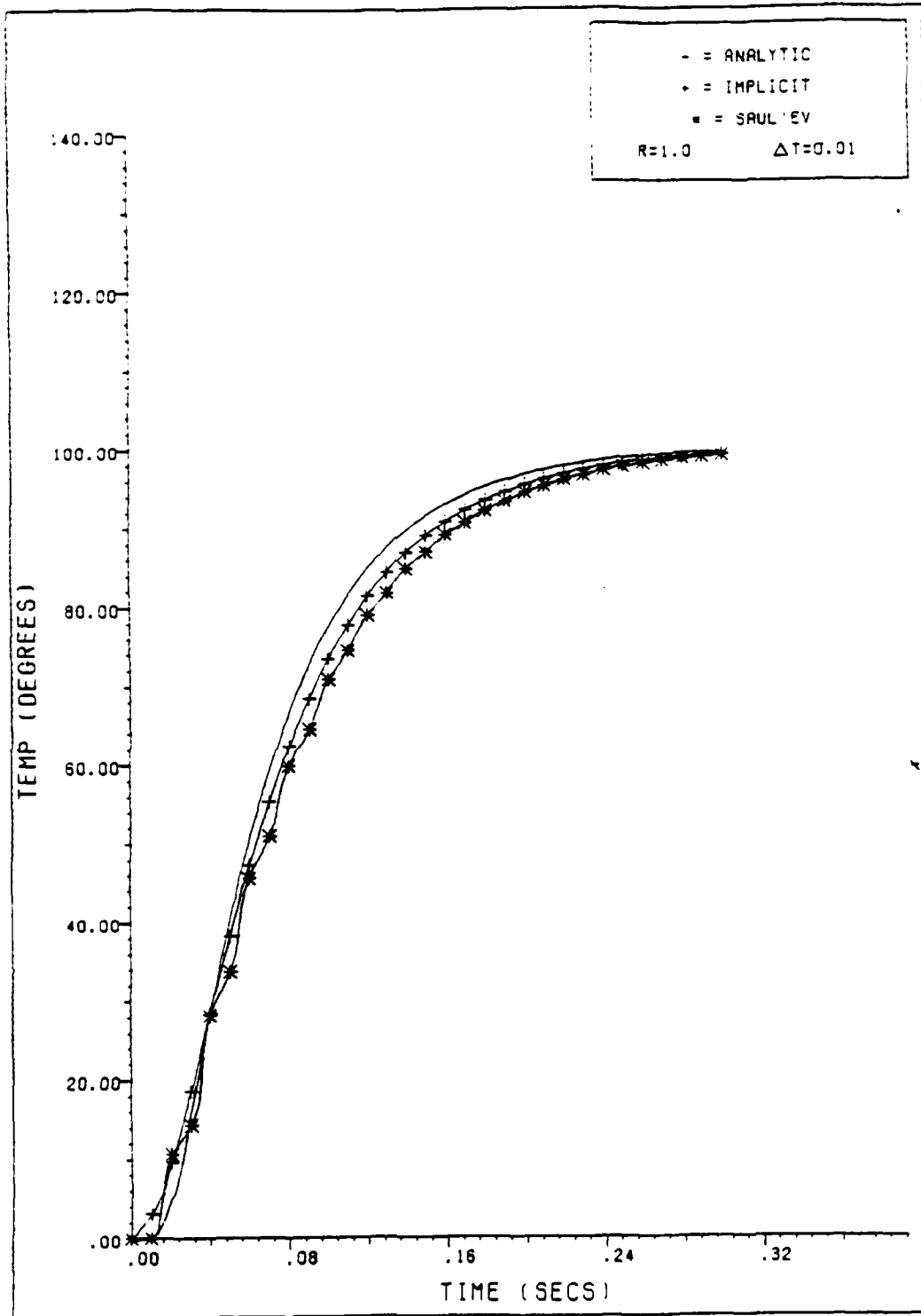


FIG 17. NUMERICAL SOLUTIONS PROBLEM #2 (NODE 41)

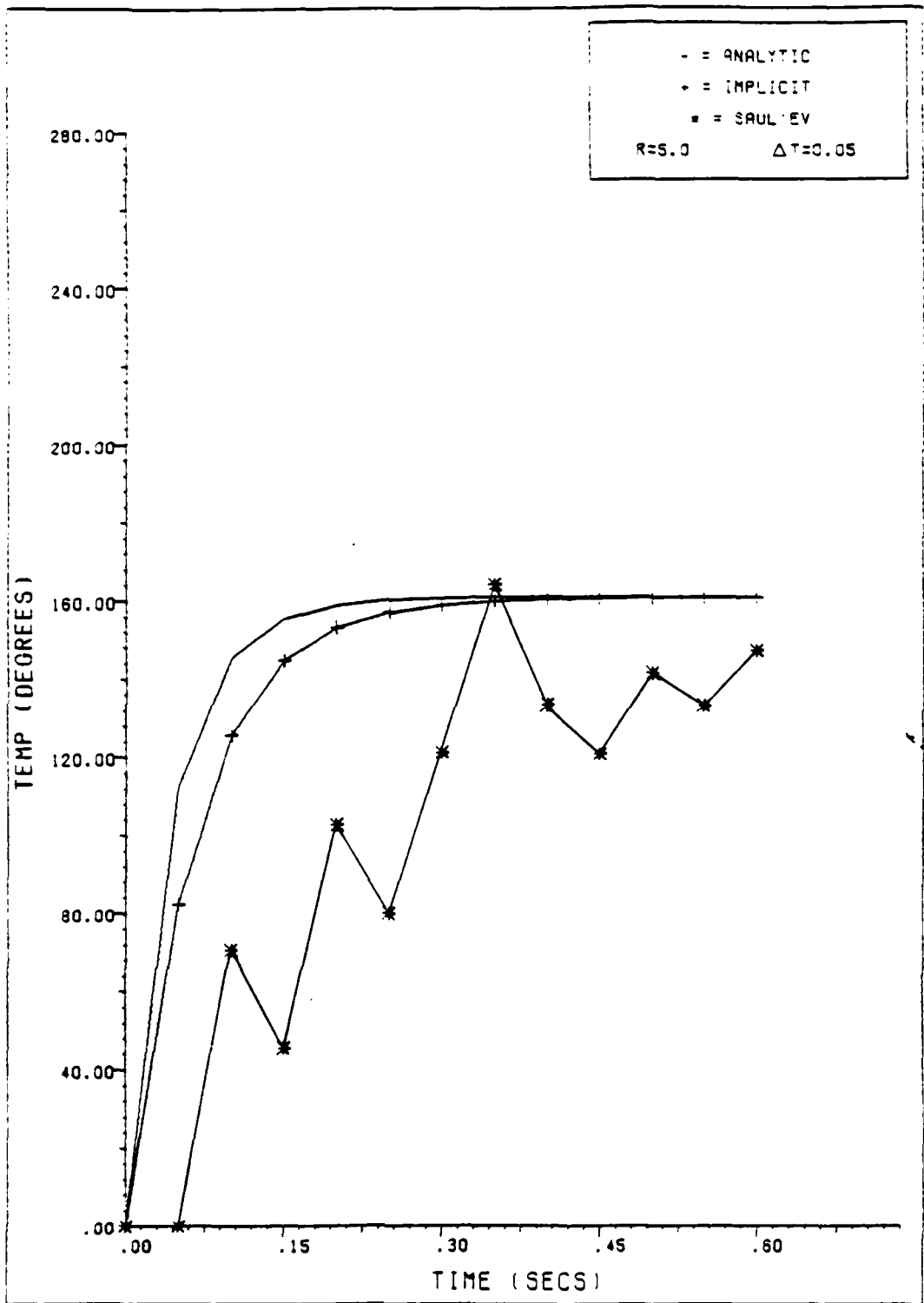


FIG 18. NUMERICAL SOLUTIONS PROBLEM #2 (NODE 57)

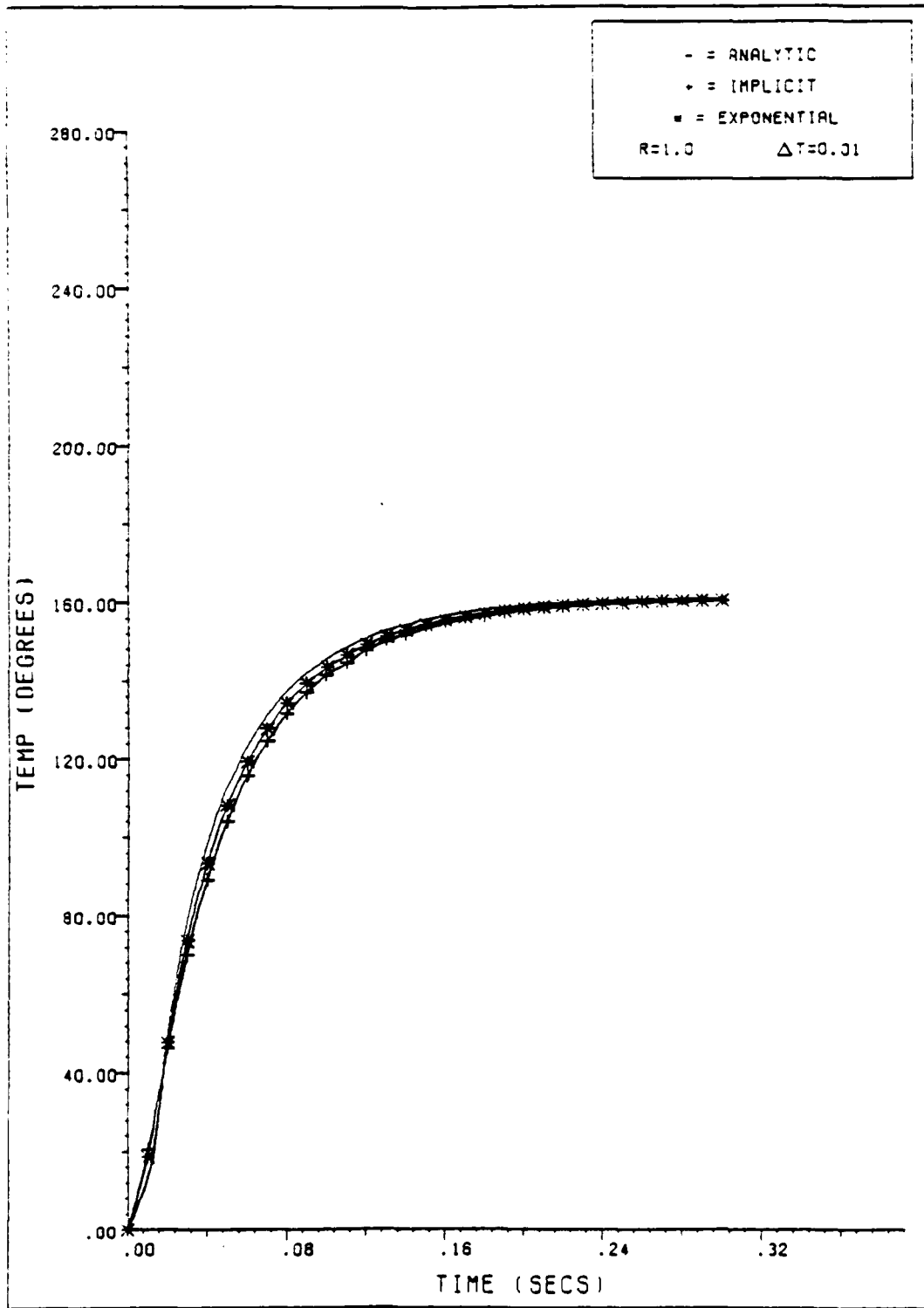


FIG 19. NUMERICAL SOLUTIONS PROBLEM #2 (NODE S7)

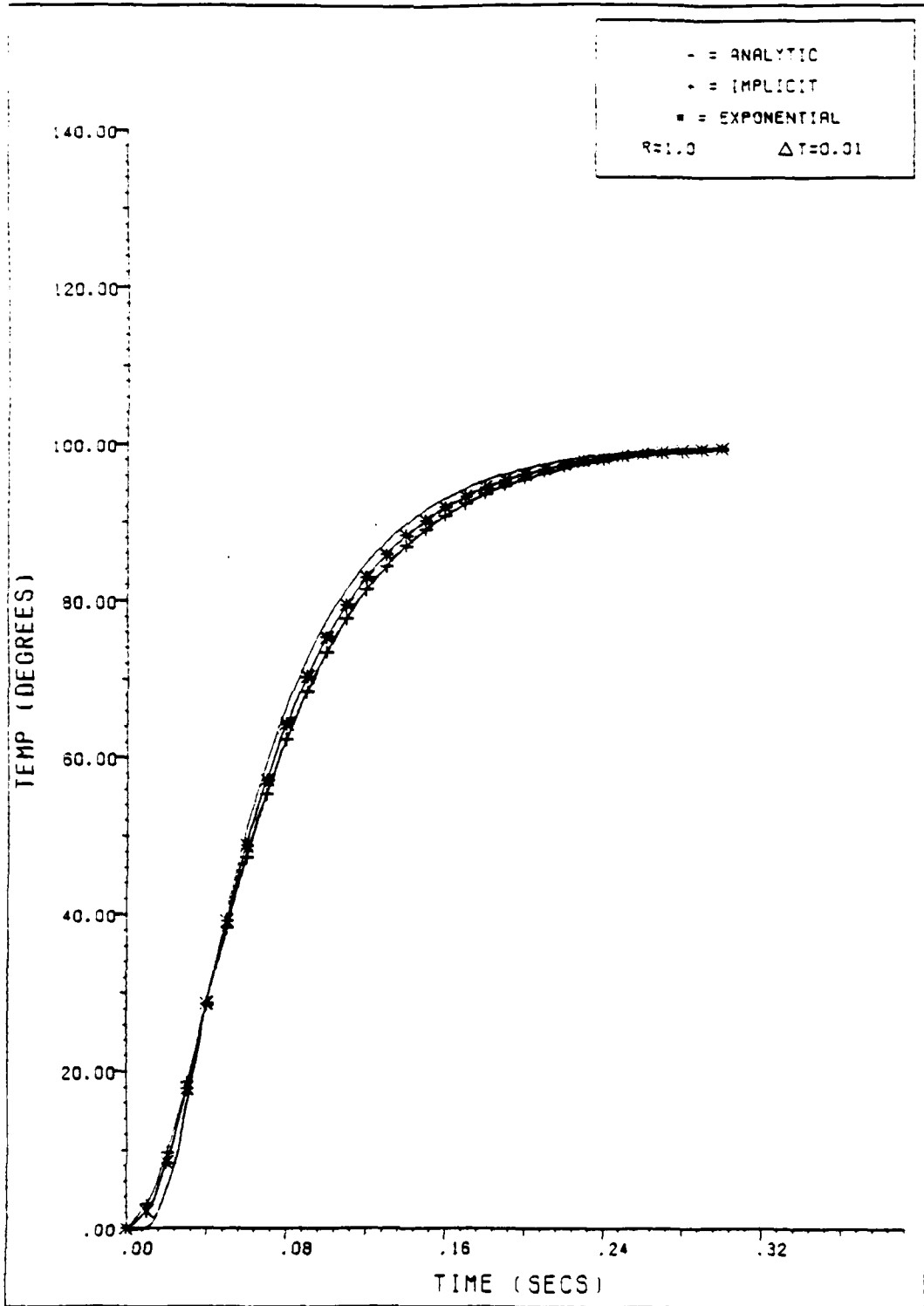


FIG 20. NUMERICAL SOLUTIONS PROBLEM #2 (NODE 41)

Accuracy of Solutions

To quantitatively examine the effects of oscillations and other errors, root mean square error (Erms) and maximum error (Emax) were calculated. For a mesh spacing of $H = 0.1$, problem #1 solutions proved to be more accurate. By suitably reducing the time step, errors of less than one degree could be realized. No matter how small a time step was used, solutions to problem #2 were, at best, accurate to within only three degrees. These deviations occurred primarily along the grid boundaries. An attempt to reduce this error by halving the mesh size resulted in even larger error. This phenomenon may occur when large numbers of arithmetic operations cause the accumulation of round-off error to become significant. Thus, to examine the effect of mesh size on truncation error, additional solutions were found for a grid spacing of $H = 0.2$.

Root Mean Square Error

In both problems, the exponential method demonstrated superior accuracy for time steps greater than 0.005 seconds. This was not surprising since this method possesses the least truncation error at small time steps ($H^2 + \Delta t^2$) while enjoying accuracy similar to the fully implicit at large time steps ($H^2 + \Delta t$).

The DF and SV schemes are comparable to the EXP when time steps less than 0.001 seconds are used. More often than not, all methods outperform the fully implicit

method for small time steps. The DF scheme is superior to the SV for time steps below 0.001 seconds. Above this value, the SV scheme is more accurate. Dufort and Frankel point out an optimum value of time step for their difference method. For fixed H, truncation error will be minimized when a time step of $\Delta t = H^2/\sqrt{12}$ is utilized (3:142). For the mesh considered (H = 0.1), this corresponds to a time step of approximately 0.003 seconds. Figure 22 suggests that minimum Erms exist for the DF method when time steps of 0.001 seconds are used.

Maximum Error

Maximum error, calculated at $t = 0.1$ and $t = 0.3$ seconds, is displayed in Figures 25-32. The effect of doubling the mesh size can be seen in Figures 26, 28, 30, and 32. Again, because the exponential scheme does not oscillate, its performance is superior for values of R greater than 0.5.

The DF scheme produced good results for problem #1 ($E_{max} < \text{one degree}$) when small values of R were used. Generally, the DF was more accurate than the SV for values of R less than 0.25. For values of R between 0.25 and 0.5, the SV method was more accurate. Both methods become virtually unusable for R greater than 1.0 where solutions are found to be between 10 and 100 degrees in error. Even though the exponential solution retained superior accuracy

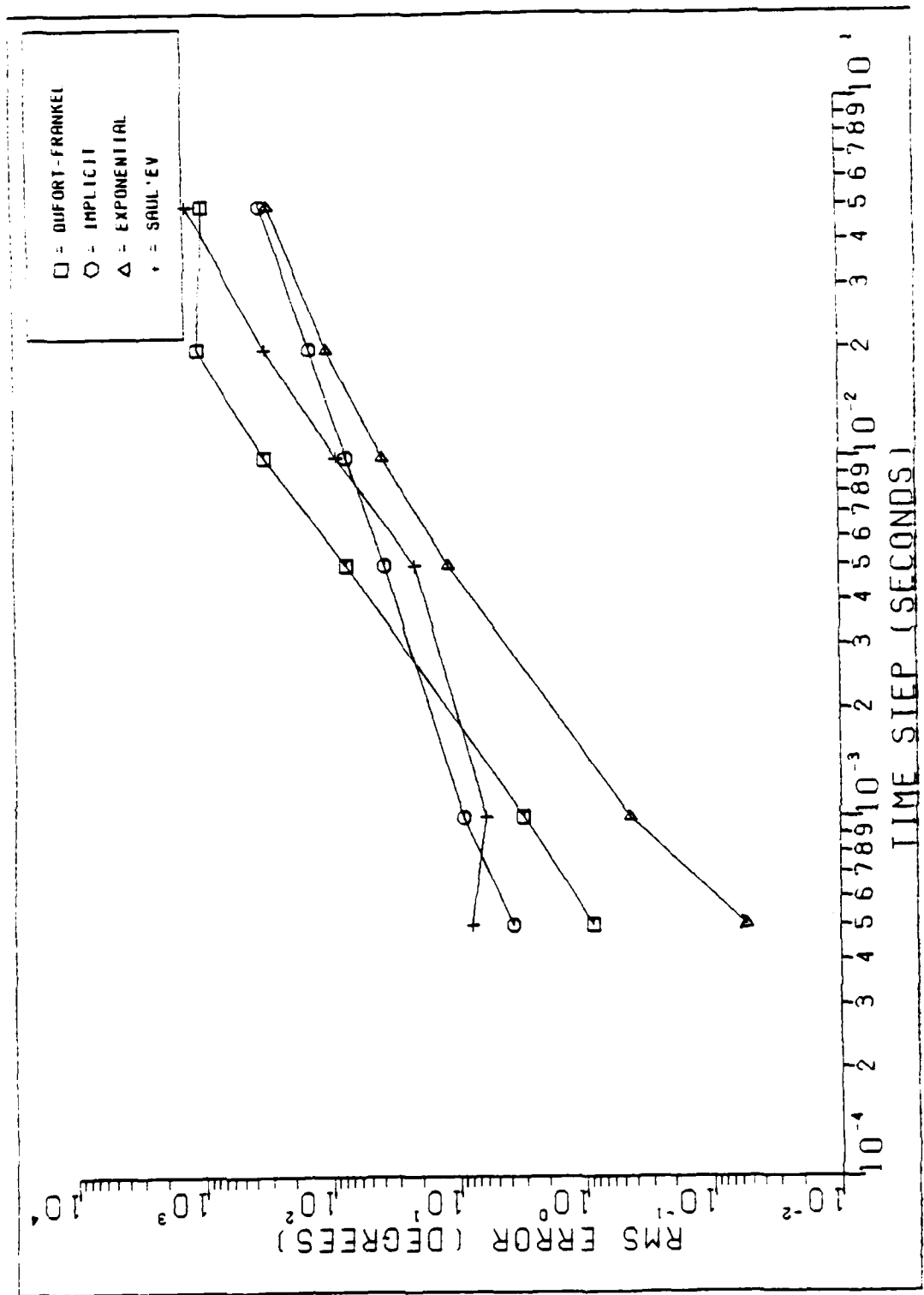


FIG 21. ERROR VS TIME STEP PROBLEM #1 T=0.1 SECS

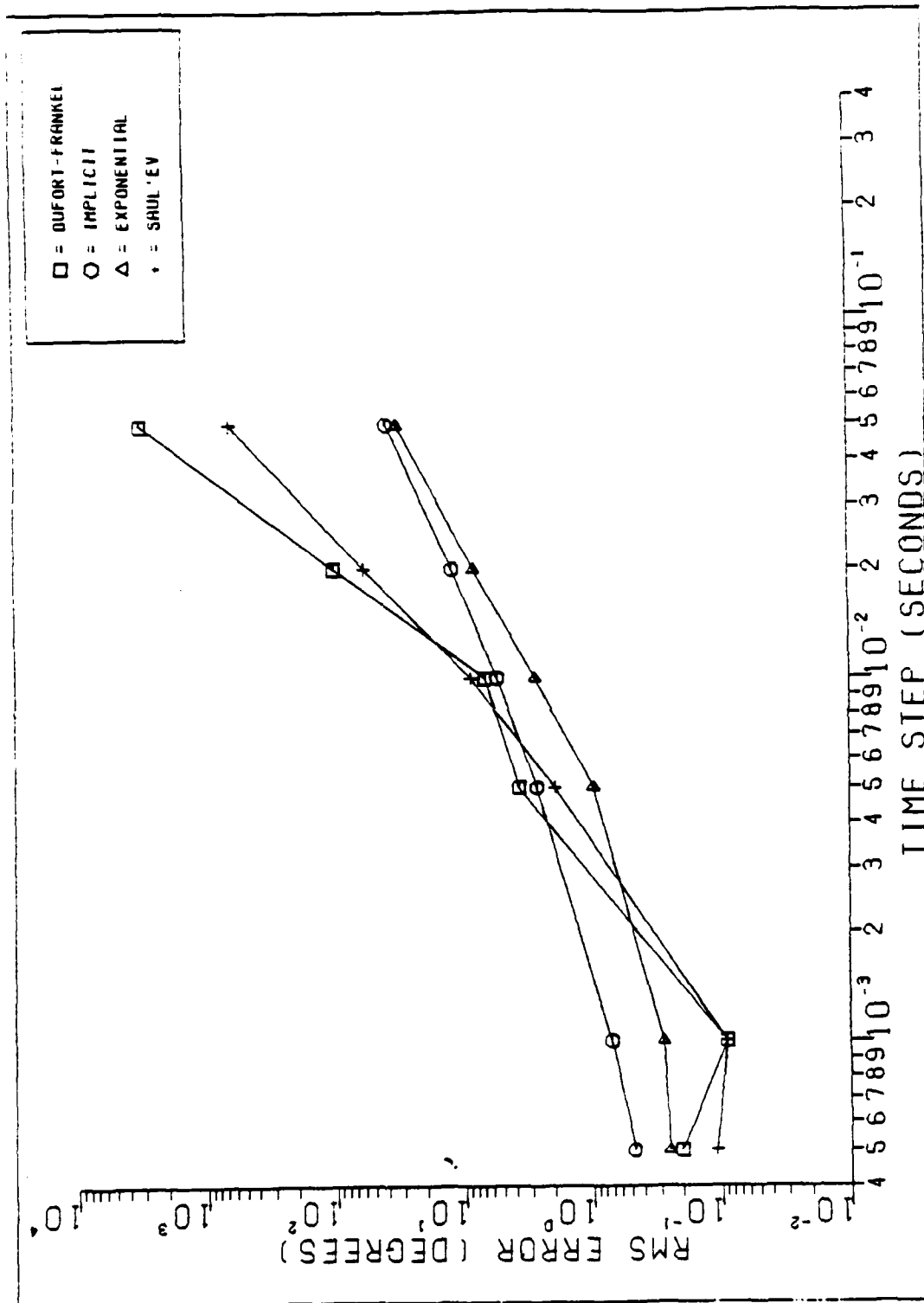


FIG 22. ERROR VS TIME STEP PROBLEM #1 T=0.3 SECS

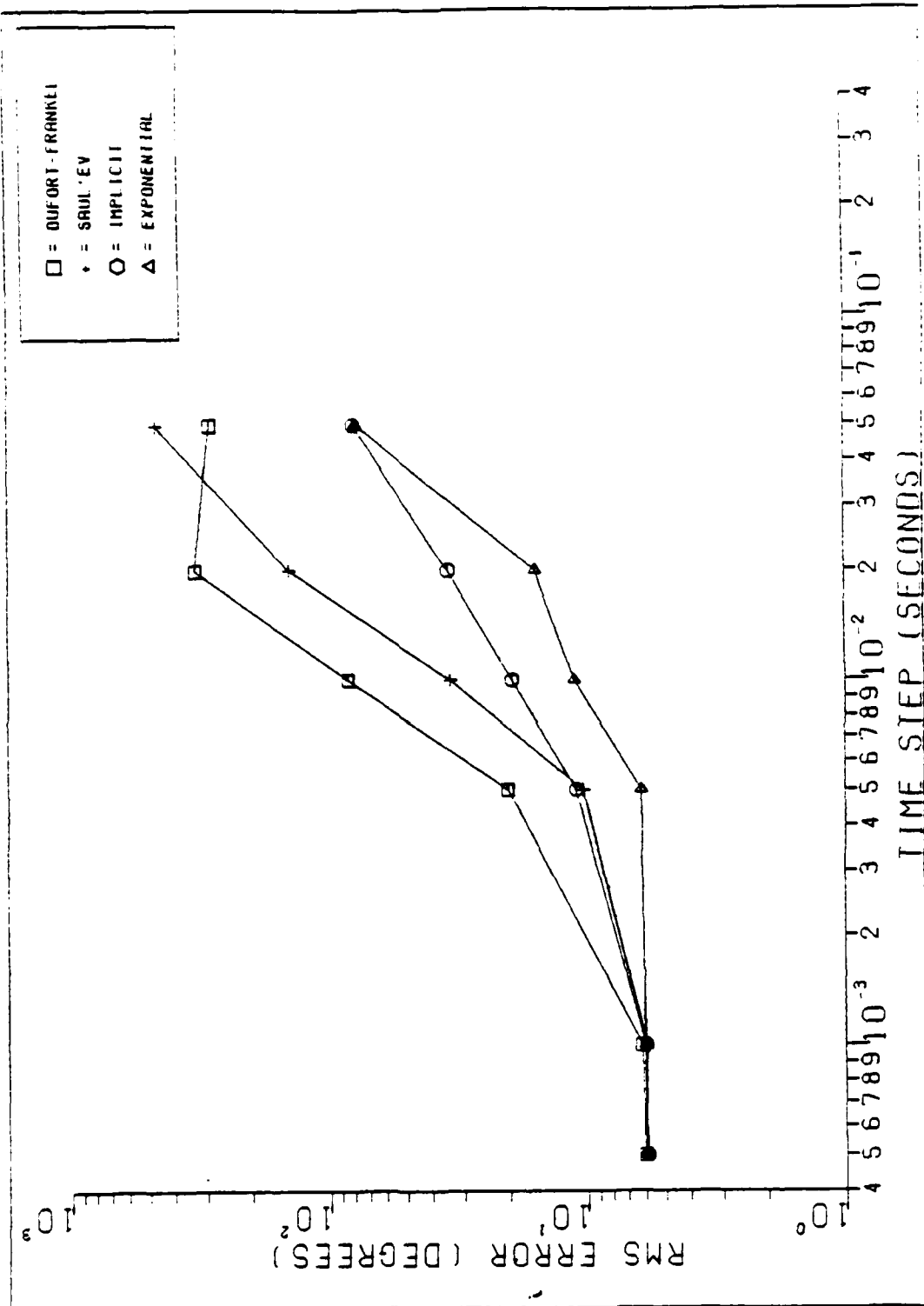


FIG 23. ERROR VS TIME STEP PROBLEM #2 T=0.1 SECS

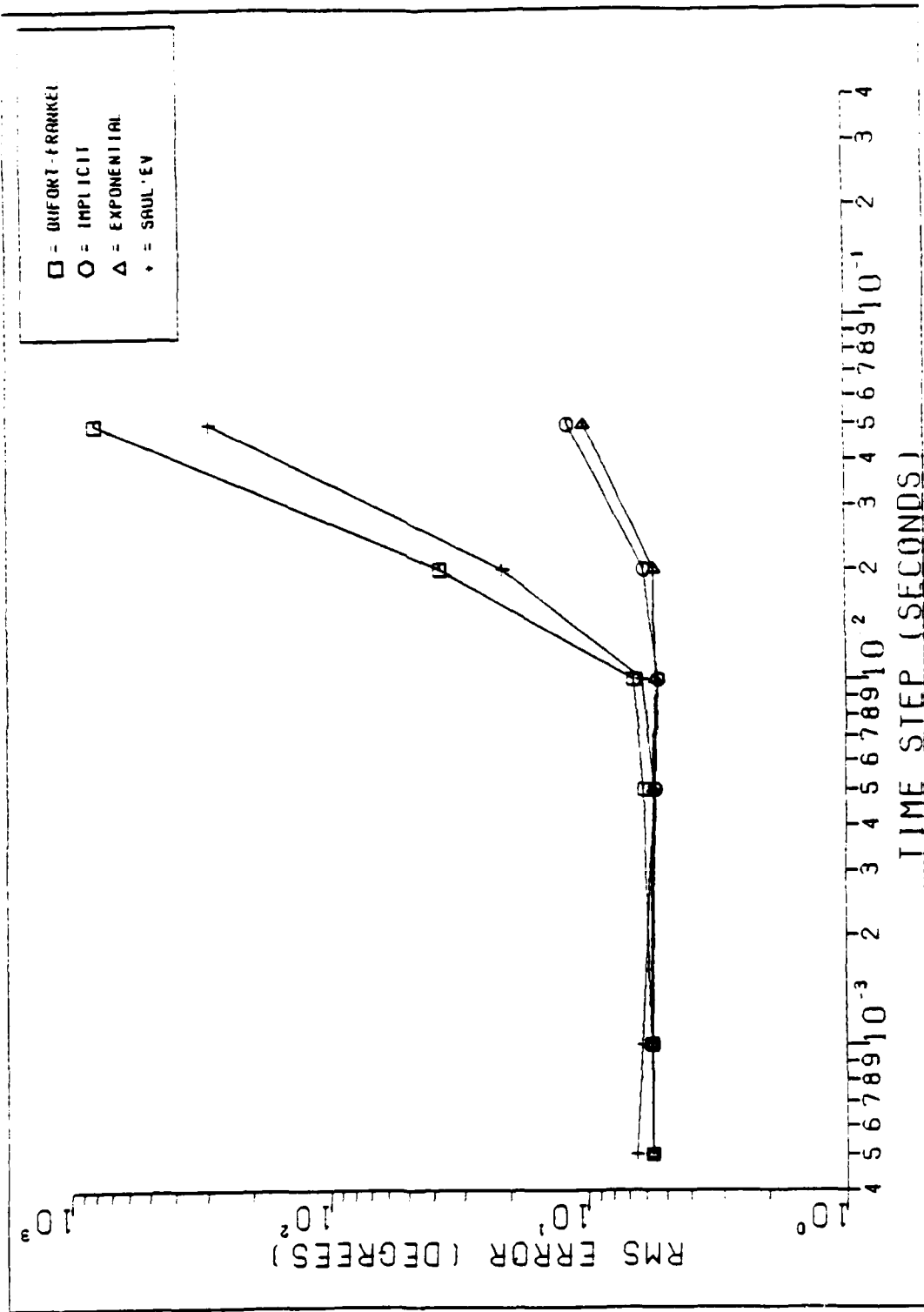


FIG 24. ERROR VS TIME STEP PROBLEM #2 T=0.3 SECS

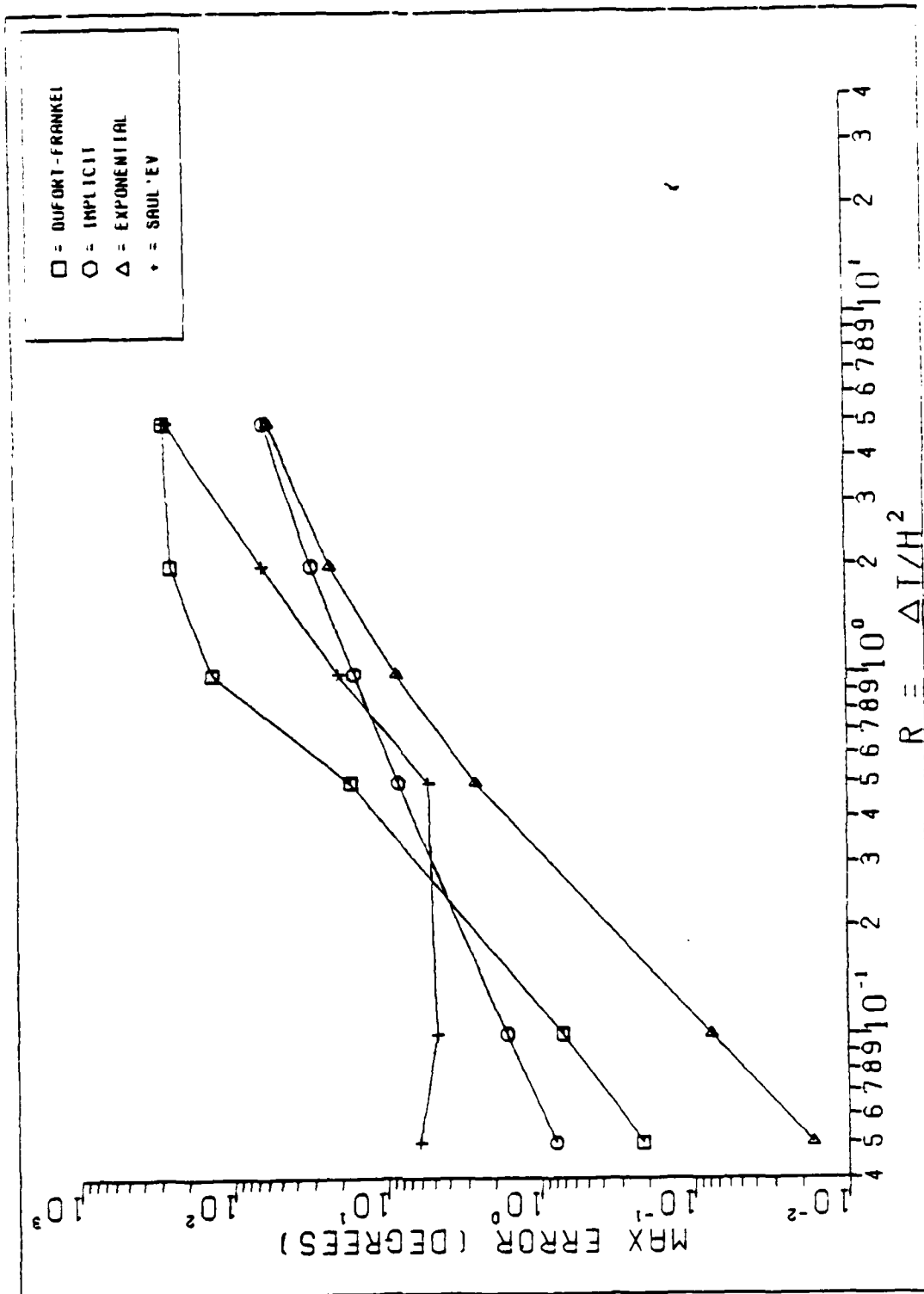


FIG 25. MAX ERROR VS R PROBLEM #1 T=0.1 H=0.1

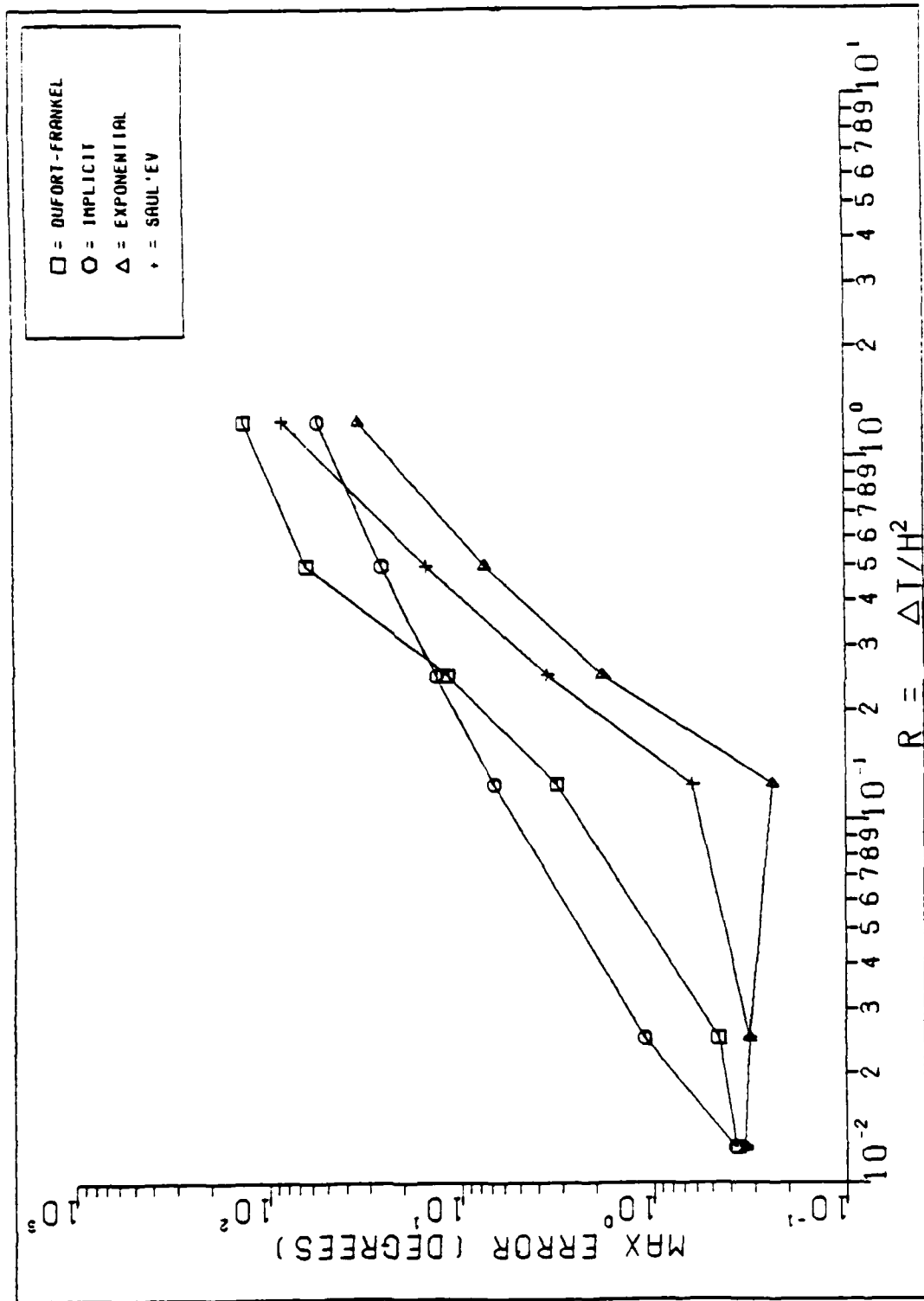


FIG 26. MAX ERROR VS R PROBLEM #1 T=0.1 H=0.2

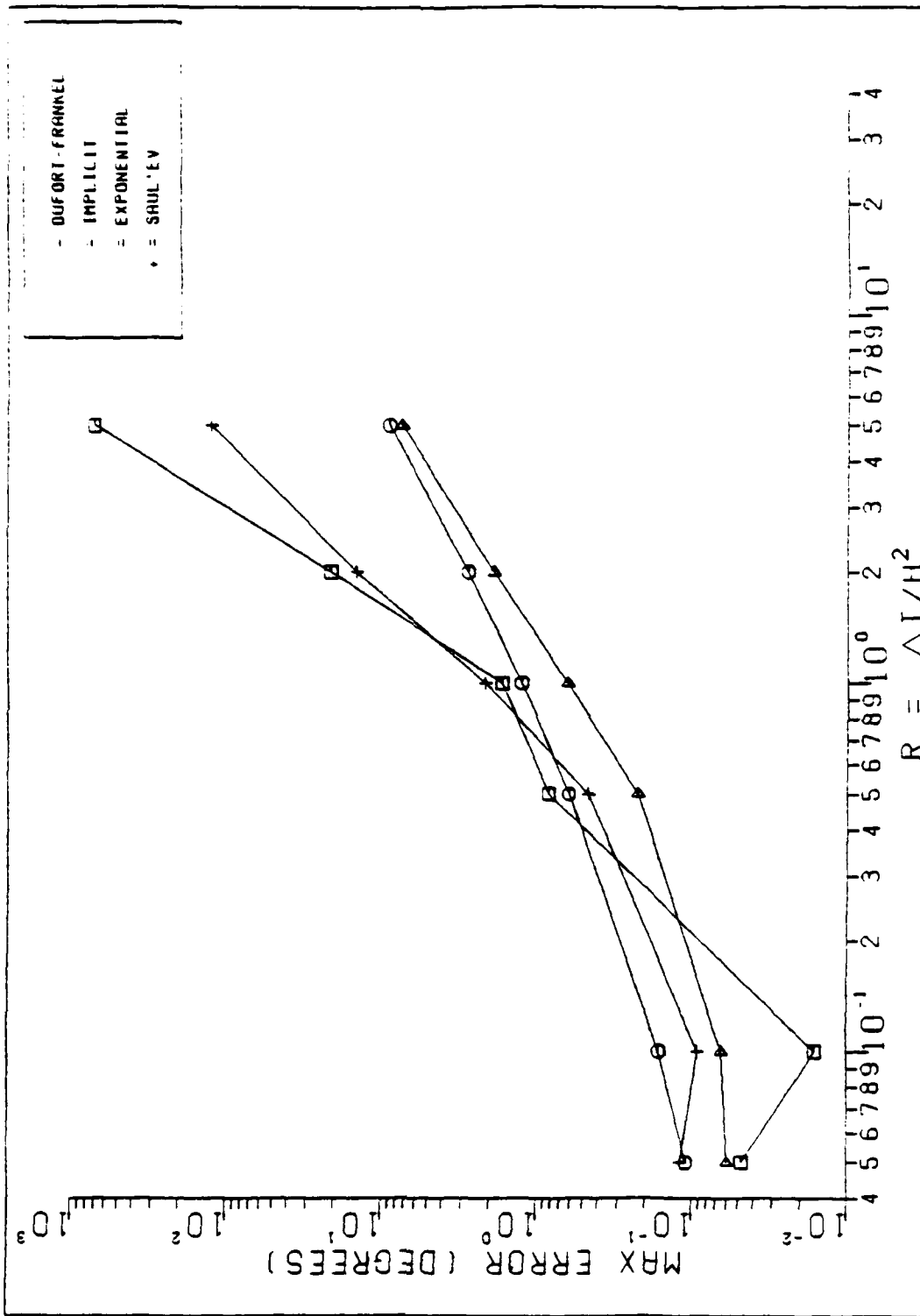


FIG 27. MAX ERROR VS R PROBLEM #1 T=0.3 H=0.1

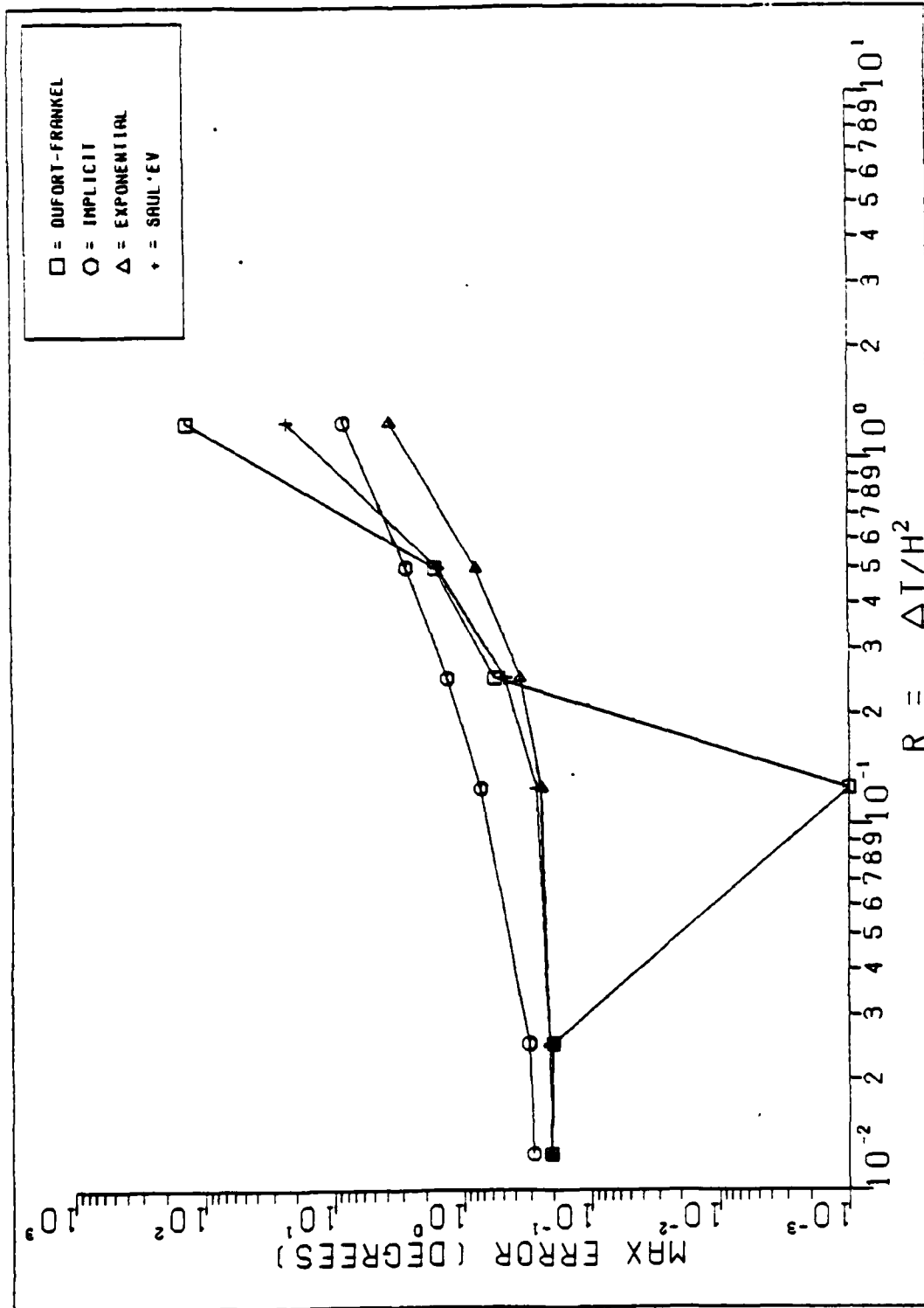


FIG 28. MAX ERROR VS R PROBLEM #1 T=0.3 H=0.2

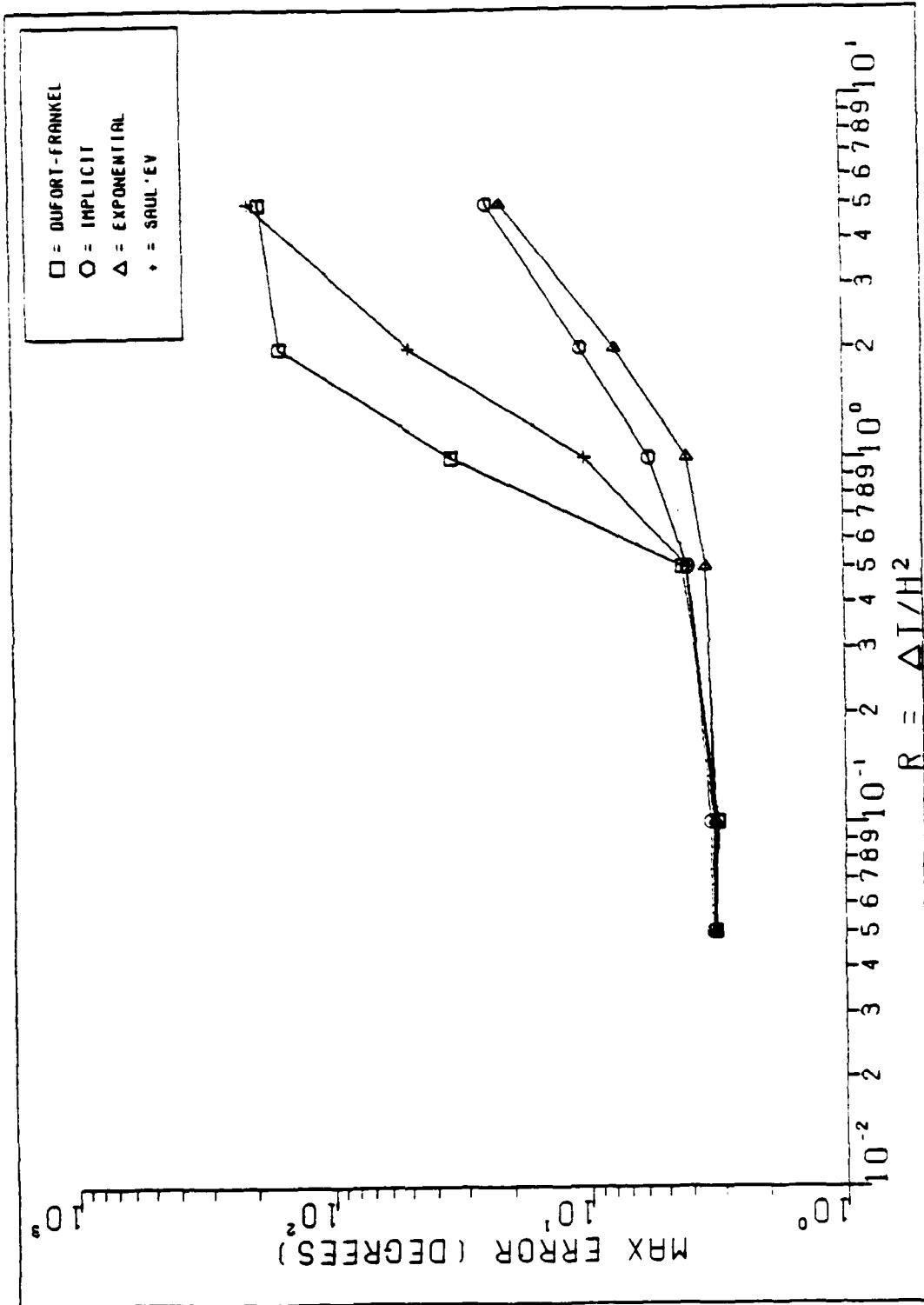


FIG 29. MAX ERROR VS R PROBLEM #2 T=0.1 H=0.1

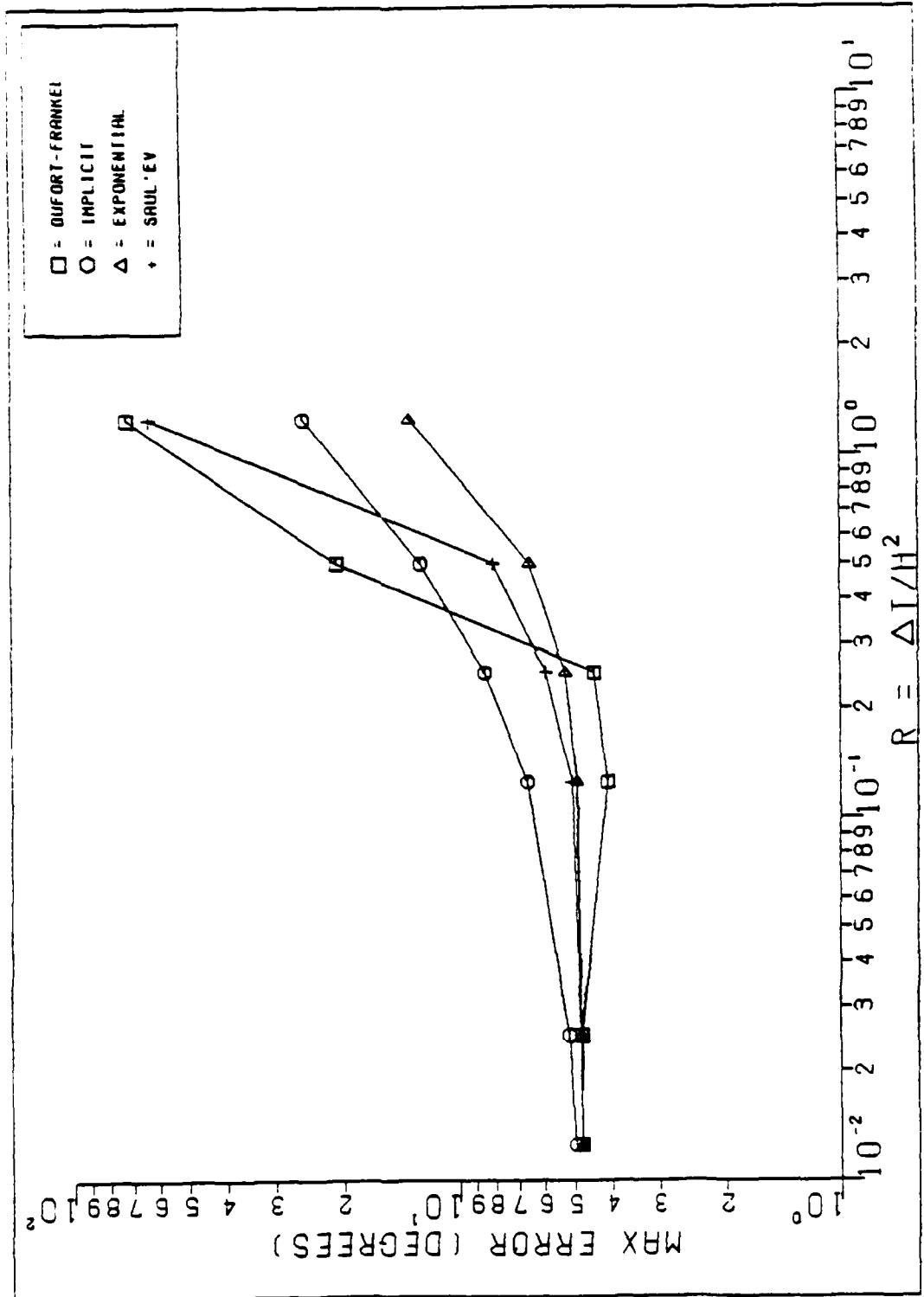


FIG 30. MAX ERROR VS R PROBLEM #2 T=0.1 H=0.2

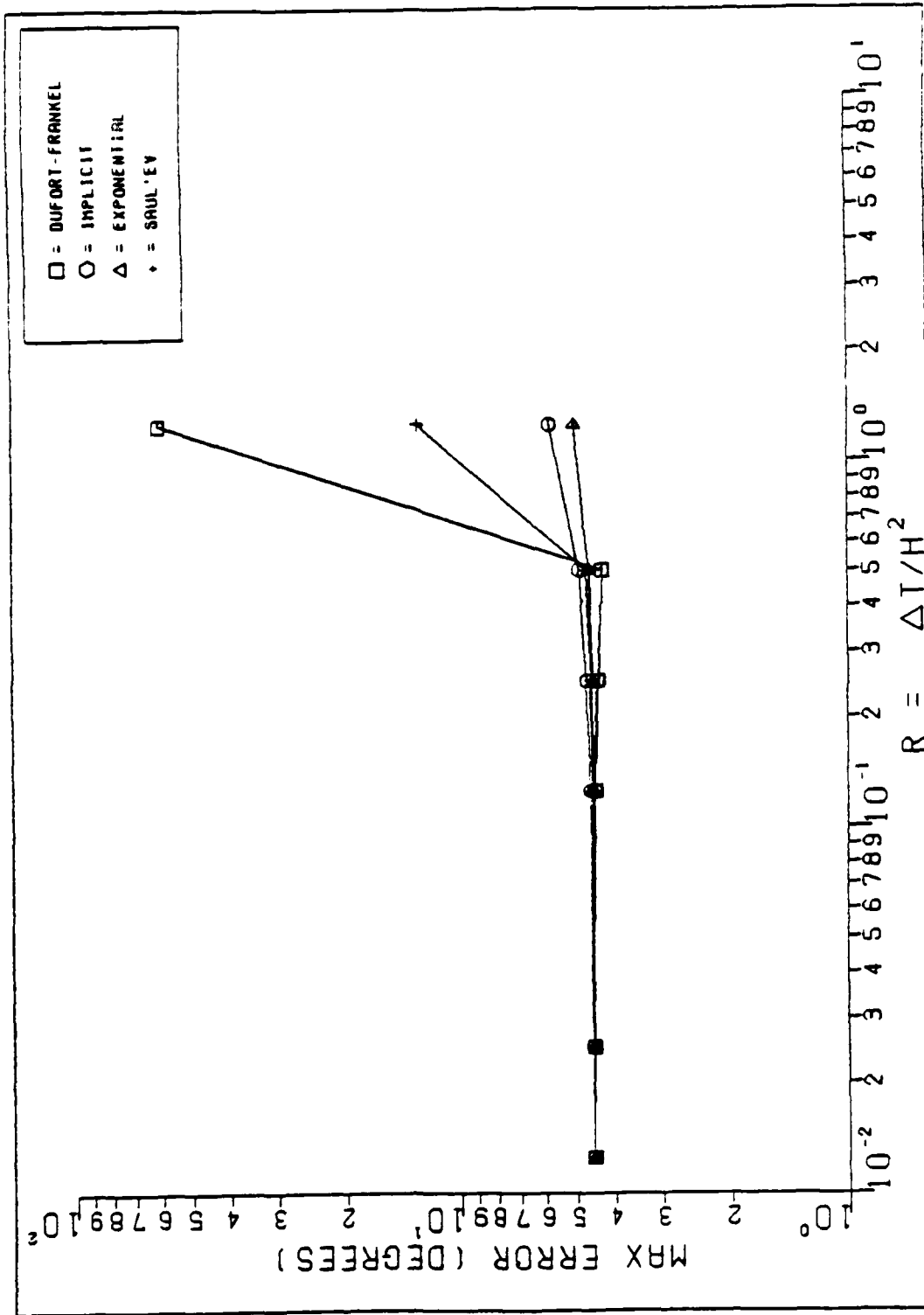


FIG 32. MAX ERROR VS R PROBLEM #2 T=0.3 H=0.2

for large R, only those solutions for R less than 1.0 are accurate enough for most engineering applications.

An increase in mesh size should result in a larger truncation error for all methods. For the same R, solutions found with $H = 0.1$ yield more accurate results in all cases. The effect of doubling the mesh size while the time step is held constant can be easily demonstrated. The DF method possesses truncation error of order $H^2 + \Delta t^2 + (\Delta t/H)^2$. For $t = 0.0005$ and $H = 0.1$ an error of $1.003E-02$ is predicted. When H is increased to 0.2 , an expected error of $4.0007E-02$ results. The ratio of predicted errors is then $(4.0007E-02)/(1.003E-02)$ or 3.99 . Figure 27 shows an error of 0.047 for the DF scheme when $R = 0.05$ ($t = 0.0005$, $H = 0.1$). The error corresponding to this time step on Figure 28 occurs at $R = 0.0125$ ($t = 0.0005$, $H = 0.2$) and has a value of 0.207 . The ratio of these two errors is $(0.207/0.047)$ or, approximately 4.40 .

The effect of oscillatory behavior on solution accuracy is readily apparent from Figures 29 and 31. The SV and DF solutions are reasonably accurate ($E_{max} < 5$ degrees) until R becomes greater than 0.5 . Above $R = 1.0$, oscillatory behavior of both methods results in significant error.

The performance of the fully implicit method was about what was expected. It was superior to the DF and SV methods for large time steps. This is because the truncation error for the DF and SV methods is of order

$H^2 + \Delta t^2 + (\Delta t/H)^2$ and order $H^2 + \Delta t$ for the fully implicit method (10:189). This also explains why the DF and SV schemes are more accurate than the fully implicit method at smaller time steps. The exponential method was superior to the fully implicit scheme for small time steps and roughly comparable at large time steps. Again, if the truncation error of the exponential scheme is approximated by that of the Crank-Nicolson at small R , and that of the fully implicit at large R , this behavior is expected.

Time Required for Computations

All numerical solutions were calculated using a 24 bit, Harris 800 computer. To compare the amount of central processor unit (CPU) time required for each method, problem #1 was solved using the largest time step for which a maximum error of less than one degree resulted. This method of comparison is identical to one used in a previous paper where the performance of several finite difference methods was also of interest (6:52).

Of the explicit methods, the SV was the fastest. The choice of the fully implicit method to bootstrap the DF scheme to the first time level caused it to be slower than the SV. The EXP was slowest since a matrix equation of order N , the number of nodes, had to be solved for each iteration.

For the coarser mesh, Figure 33 shows all methods to be roughly the same. Both the DF and SV required 30 iterations to achieve the desired level of accuracy. The EXP required only 15 iterations due to its superior accuracy at larger time steps.

When the mesh size was halved, an obvious speed advantage resulted for the SV (Figure 34). The larger matrix equations that resulted caused the EXP and DF methods to be considerably slower. Even though the EXP again required half as many iterations, the SV scheme proved faster.

It is realized that the grid sizes used here are somewhat coarse. But as the mesh is refined, the SV should increase its speed advantage. Of course, if $R=1/4$ is used to calculate the first time level of the DF, the method reduces to a two level formula and no additional scheme is needed for bootstrapping. Interestingly, the apparent advantage of utilizing larger time steps did not result in a computationally faster algorithm for the EXP.

CPU TIME REQUIRED $H = 0.2 \quad t = 0.3$

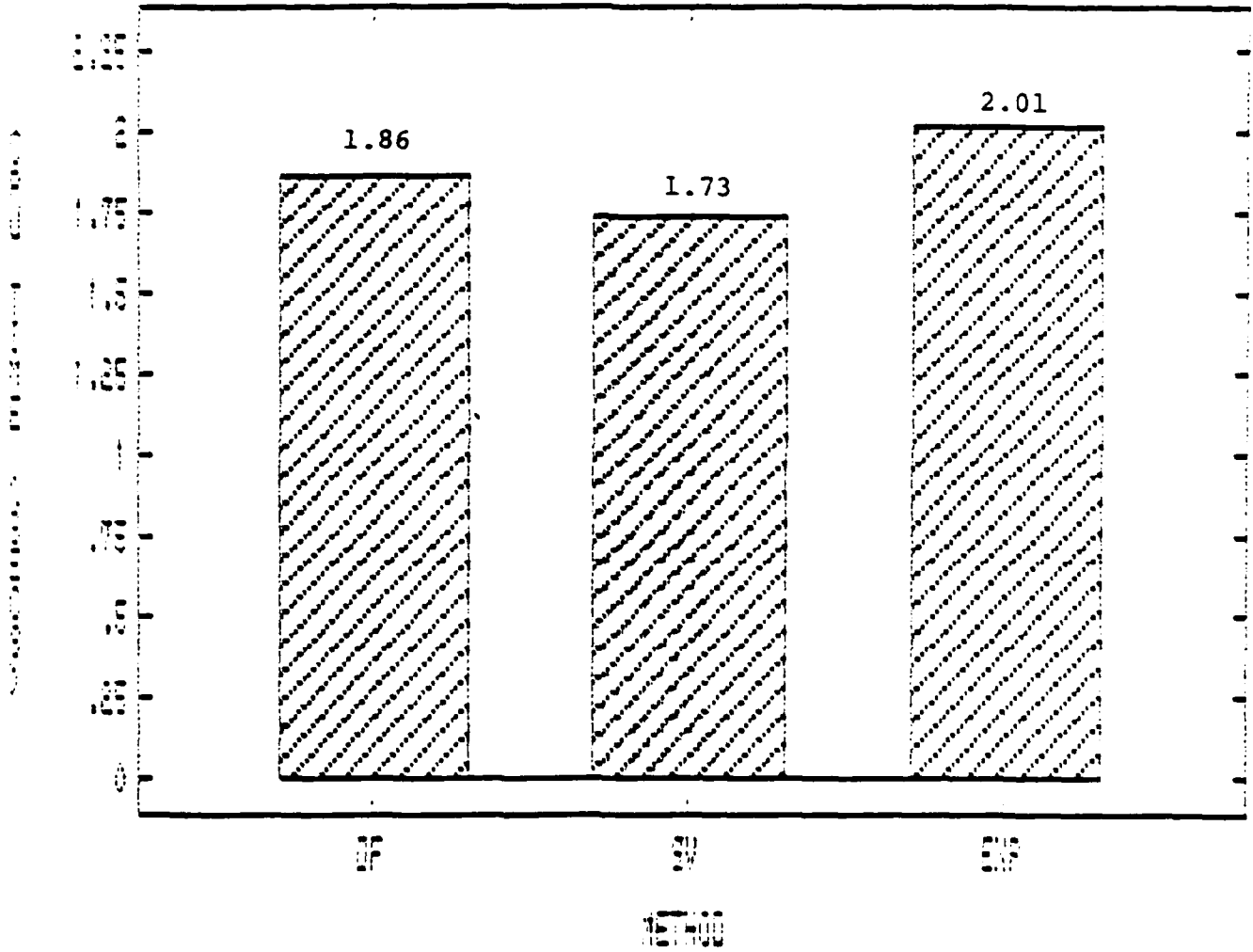


FIG 33. CPU TIME REQUIRED $H = 0.2 \quad t = 0.3$

CPU TIME REQUIRED $H = 0.1$ $t = 0.3$

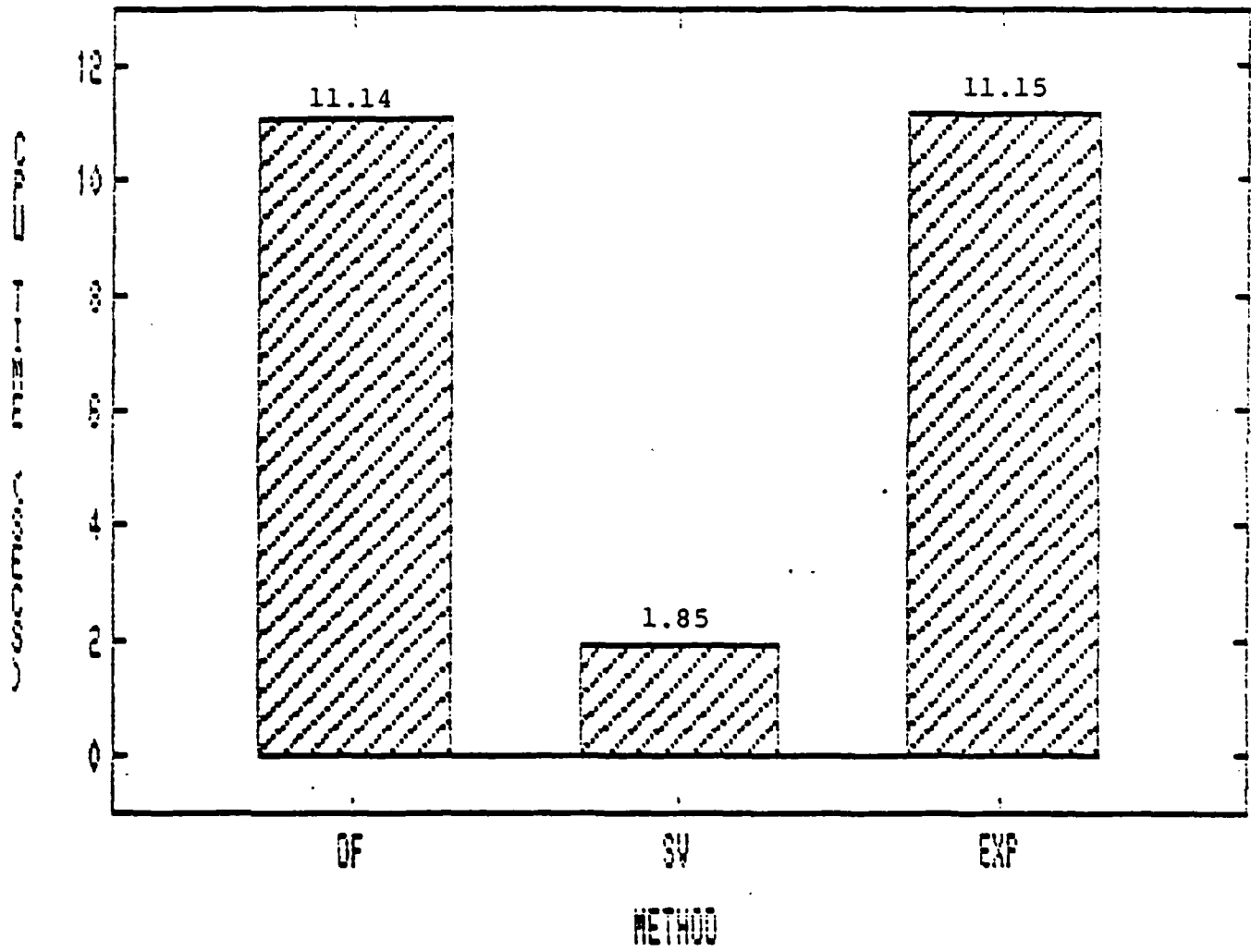


FIG. 34. CPU TIME REQUIRED $H = 0.1$ $t = 0.3$

V. Conclusions and Recommendations

Conclusions

Numerical oscillations resulted in both the DF and SV schemes for the values of R predicted. In both cases, stability was maintained since the oscillations decreased with time. For the same R, the SV generally experienced less violent oscillations. The oscillations were usually large enough to destroy the solution in both methods with $R > 1.0$. As predicted, the EXP did not oscillate for any size time step.

In problem #1, at early times ($t = 0.1$ secs), the EXP retained good accuracy ($E_{max} < 1$ degree) for values of R up to 0.1. The scheme displayed marginal accuracy ($E_{max} < 10$ degrees) for values of R between 0.1 and 1.0. The exponential was more accurate than the fully implicit method for small time steps. For large R ($R > 1.0$), the fully implicit and exponential methods were roughly the same. For small R, the explicit methods and EXP were about equal. The DF demonstrated good accuracy for $R < 0.25$. Above this value, the SV was consistently the more accurate.

At later times, the explicit solutions became more accurate as the oscillations decayed. The SV and DF were now accurate to within one degree for values of R up to

0.5 ($t = 0.3$ secs). Above $R = 0.5$, the SV was more accurate. In problem #1, the EXP retained good accuracy for R up to 1.0. Although the EXP was the most accurate above $R = 1.0$, errors greater than 10 degrees still existed.

Of the explicit methods, the SV was the fastest computationally. The use of the fully implicit method to bootstrap the DF scheme, caused it to be fairly slow for an explicit method. Even though the exponential method could use a larger time step without sacrificing accuracy, the burden of solving simultaneous equations by Gaussian elimination caused it to require the most CPU time.

Recommendations

As a result of this study, the following are proposed:

1. Generalize Myer's matrix approach to oscillatory behavior to include all nodes.
2. Investigate the use of the probabilistic method to determine the stability condition of implicit finite difference schemes.
3. Extend the exponential method to three dimensions and check for oscillatory solutions.
4. Apply the methods studied here to problems having derivative or mixed boundary conditions.
5. Compare the accuracy of the exponential method with that of the variable-weighted implicit method (7:161) for both small and large time steps.

6. Determine if the truncation error of the exponential scheme can be expressed in terms of R . If so, an optimum value of time step may be realized resulting in greater accuracy.

Appendix A: Derivation of the Dufort-Frankel
Finite Difference Method

To derive the Dufort-Frankel method in two dimensions, first consider Richardson's explicit approximation (7:238):

$$\frac{T(i,j,n+1) - T(i,j,n-1)}{2\Delta t} = \frac{T(i+1,j,n) - 2T(i,j,n) + T(i-1,j,n)}{\Delta x^2} + \frac{T(i,j+1,n) - 2T(i,j,n) + T(i,j-1,n)}{\Delta y^2}$$

This formulation is known to be unconditionally unstable (7:238). If the $T(i,j,n)$ term is replaced by $(1/2)(T(i,j,n+1) + T(i,j,n-1))$ the unconditionally stable Dufort-Frankel scheme results:

$$T(i,j,n+1)(1+4R) = 2R[T(i+1,j,n) + T(i-1,j,n) + T(i,j+1,n) + T(i,j-1,n)] + (1-4R)T(i,j,n-1)$$

where

$$R = \Delta t/H^2$$

$$\Delta x = \Delta y = H$$

Appendix B: Matrix Analysis of Oscillations in the Exponential Difference Method

Myer's matrix approach to predicting oscillatory behavior will be applied to the exponential scheme in two dimensions. In addition, a four nodal point grid and homogeneous Dirichlet boundary conditions are assumed.

To begin, a difference equation is written for each node of the grid. The resulting system of four equations can then be written as:

$$\underline{A} \bar{u}^{(n+1)} = \underline{B} \bar{u}^{(n)}$$

Here, \underline{A} and \underline{B} represent coefficient matrices, while $\bar{u}^{(n+1)}$ and $\bar{u}^{(n)}$ are column matrices of temperatures at times $(n+1)$ and (n) respectively. Further, the eigenvalues of $\underline{A}^{-1} \underline{B}$ will determine the oscillatory behavior of the system (8:285) and are found from the relation (8:285)

$$\det(\underline{A}^{-1} \underline{B} - \lambda \underline{I}) = 0$$

Myers shows that this is equivalent to the expression (8:285)

$$\det(\underline{B} - \lambda \underline{A}) = 0$$

Hence, the eigenvalues of $(\underline{B} - \lambda \underline{A})$ determine the oscillatory behavior of the system. If Equation (3) is

applied to a four nodal point grid with homogeneous Dirichlet boundary conditions, the following matrix results for $(\underline{B} - \lambda \underline{A})$:

$$\begin{bmatrix} X - \lambda Y & C + \lambda D & C + \lambda D & 0 \\ C + \lambda D & X - \lambda Y & 0 & C + \lambda D \\ C + \lambda D & 0 & X - \lambda Y & C + \lambda D \\ 0 & C + \lambda D & C + \lambda D & X - \lambda Y \end{bmatrix}$$

where

$$X = 1 - 4R(1-f)$$

$$Y = 1 + 4Rf$$

$$C = R(1-f)$$

$$D = Rf$$

The determinant can be simplified using the following techniques (4):

Subtracting the last row from the first yields

$$\begin{bmatrix} X - \lambda Y & 0 & 0 & -(X - \lambda Y) \\ C + \lambda D & X - \lambda Y & 0 & C + \lambda D \\ C + \lambda D & 0 & X - \lambda Y & C + \lambda D \\ 0 & C + \lambda D & C + \lambda D & X - \lambda Y \end{bmatrix}$$

Subtracting the third row from the second and factoring results in

$$(X - \lambda Y)^2 \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ C + \lambda D & 0 & X - \lambda Y & C + \lambda D \\ 0 & C + \lambda D & C + \lambda D & X - \lambda Y \end{bmatrix}$$

Adding the first column to the last yields

$$(X - \lambda Y)^2 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ C + \lambda D & 0 & X - \lambda Y & 2(C + \lambda D) \\ 0 & C + \lambda D & C + \lambda D & X - \lambda Y \end{bmatrix}$$

Developing the determinant about the first row results in

$$(X - \lambda Y)^2 \begin{bmatrix} 1 & -1 & 0 \\ 0 & X - \lambda Y & 2(C + \lambda D) \\ C + \lambda D & C + \lambda D & X - \lambda Y \end{bmatrix}$$

Adding the first column to the second and again developing about the first row yields

$$(X - \lambda Y)^2 \begin{bmatrix} X - \lambda Y & 2(C + \lambda D) \\ 2(C + \lambda D) & X - \lambda Y \end{bmatrix}$$

For the value of the determinant to be zero, the following relations must be true

$$(X - \lambda Y)^2 = 0$$

$$(X - \lambda Y) = + 2(C + \lambda D)$$

$$(X - \lambda Y) = - 2(C + \lambda D)$$

The first relation produces two identical eigenvalues, (X/Y) or:

$$(1-4R(1-f))/(1+4Rf) = \exp (-4R)$$

The second and third relations respectively yield

$$\lambda_3 = 1 - (6R/(1+6Rf))$$

and
$$\lambda_4 = 1 - (2R/(1-2Rf))$$

It is easily verified that all eigenvalues are less than one in modulus and that λ_4 is the spectral radius. For all values of R, λ_4 is positive and less than unity, hence, no oscillations are predicted.

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The two dimensional transient heat (diffusion) equation with Dirichlet boundary conditions was solved using the Dufort-Frankel, Saul'ev, and, Exponential (Power-law) finite difference schemes. All methods were investigated for oscillatory behavior and comparisons of accuracy made.

To predict the time step at which oscillatory behavior would occur, the coefficient, matrix, and probabilistic methods of stability analysis were utilized. At time steps greater than the square of the mesh divided by the thermal diffusivity, oscillatory solutions were apparent in both the Dufort-Frankel and Saul'ev schemes. The exponential method, as predicted, did not oscillate for any size time step.

Although the exponential scheme was the most accurate at large time steps, the solution still contained enough error to be unusable in many engineering applications. At small time steps, all methods were more accurate than the fully implicit formulation.

The exponential method was found to be the slowest computationally. The Saul'ev scheme proved to be the fastest while still achieving the required degree of accuracy.

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