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Computational Experience With an Explicit Difference Scheme for a One Phase Stefan Problem

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D. G. Wilson

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COMPUTATIONAL EXPERIENCE WITH AN EXPLICIT DIFFERENCE SCHEME FOR A ONE PHASE STEFAN PROBLEM

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COMPUTATIONAL EXPERIENCE WITH AN EXPLICIT DIFFERENCE SCHEME FOR A ONE PHASE STEFAN PROBLEM

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ABSTRACT

The purpose of this paper is to compare the results of a computational scheme of Rose, A Method for Calculating Solutions of Parabolic Equations With a Free Boundary, Math. Comp. 14 (1960), 249-256, with the known analytic solution of a single phase Stefan problem with constant boundary temperature. Rose's scheme was implemented in FORTRAN on a DEC PDP-10. Computations were performed for Stefan numbers St = .01, .1, 1, 10, and 100. Three relative mesh sizes ($\gamma = DT/(DX)^2 = 1/2, 1/6,$ and $1/25$) were used. For each St, the relative mesh size had very little effect on accuracy. However, taking $\gamma = 1/25$ resulted in dramatically increased computing time. The relative errors of temperature were large near the phase change front.

Introduction.

In the following we examine the accuracy of the method of Rose [2] for the melting of a semi-infinite solid slab initially at its critical temperature, due to an imposed constant surface temperature. In dimensionless variables, our model takes the form:

(1) $u_t = u_{xx}$, for $0 < x < \Sigma(t)$, $0 < t < TMAX$;

(2) $u(0,t) = 1$, for $0 < t < TMAX$;

(3) $u(\Sigma(t),t) = 0$, for $0 < t < TMAX$;

(4) $\dot{\Sigma}(t) = -St\, u_x(\Sigma(t),t)$, for $0 < t < TMAX$;

(5) $\Sigma(0) = 0$;

(6) initially the slab is all solid.

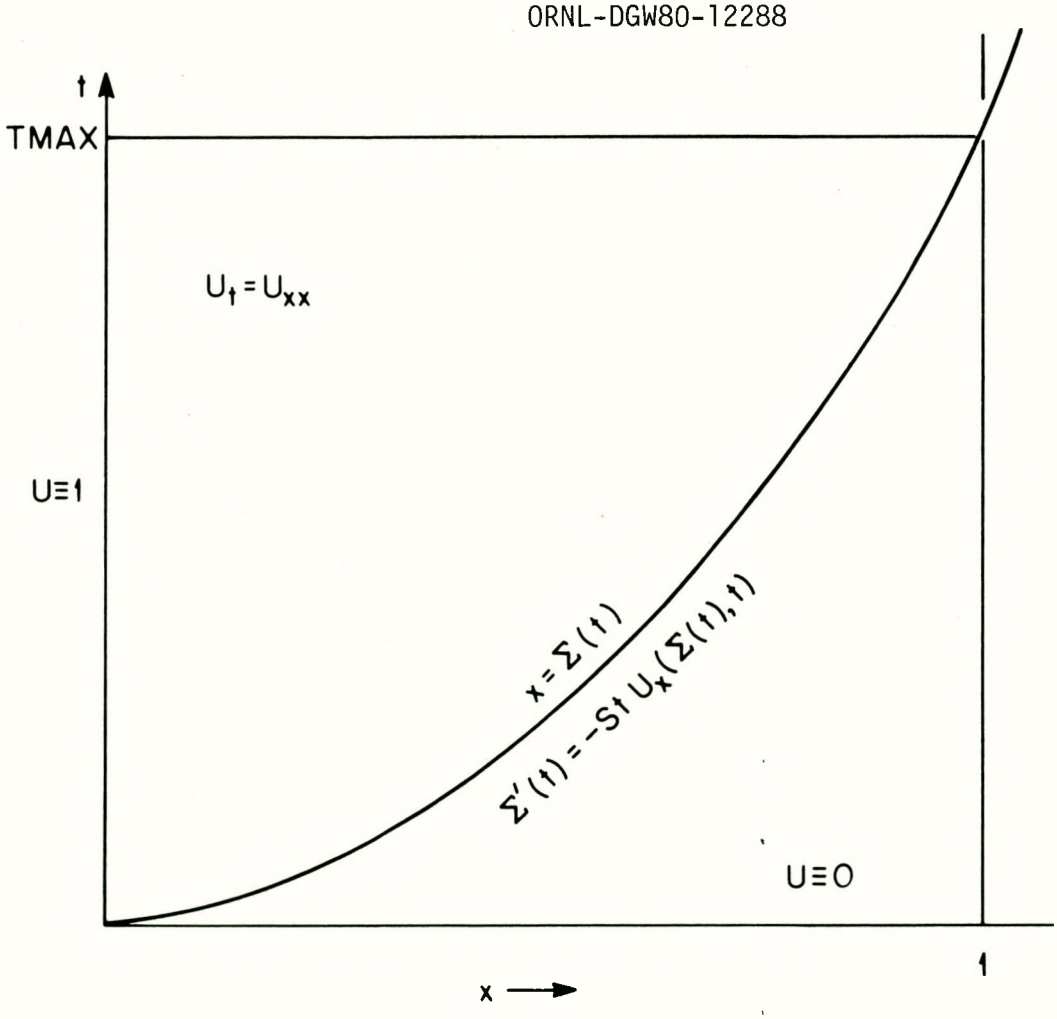

Figure 1. Phase front of one dimension semi-infinite slab, initially solid, with imposed temperature $T > T_{cr}$ on boundary.

This problem has a closed form solution, given by [1], namely

$$u(x,t) = 1 - \frac{\mathrm{erf}(x/2\sqrt{t})}{\mathrm{erf}(\lambda)}, \quad 0 \leq x \leq \Sigma(t),\ 0 < t;$$

$$\Sigma(t) = 2\lambda\sqrt{t};$$

where

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-s^2)ds$$

and λ is the unique root of

$$\lambda \exp(\lambda^2)\ \mathrm{erf}(\lambda) = St/\sqrt{\pi}.$$

Here, St (=1/H) is the Stefan number and H is the latent heat.

Rose's model takes the form

$$e_t + T_{xx} = 0, \text{ for } 0 < x < 1,\ 0 < t < TMAX;$$

$$T = \begin{cases} 0, & \text{when } 0 \leq e \leq H, \\ e-H, & \text{when } e > H; \end{cases}$$

$$e(x,0) = 0, \text{ for } 0 < x \leq 1;$$

$$T(0,t) = 1, \text{ for } 0 < t < TMAX.$$

To approximate this problem the region $0 \leq x \leq 1$, $0 \leq t \leq TMAX$, is partitioned by lines $x_i = iDX$, $0 \leq i \leq M$, and $t_n = nDT$, $0 \leq n \leq L$. The approximate solution is obtained at each of the lattice points,

(x_i,t_n). To simplify notation, let e_i^n denote $e(x_i,t_n)$ and T_i^n denote $T(x_i,t_n)$. An explicit scheme for this model is

$$e_i^{n+1} = e_i^n + \gamma\,(T_{i-1}^n - 2T_i^n + T_{i+1}^n), \quad 1 \leq i \leq M,\ 0 \leq n \leq L-1,$$

$$T_i^n = \begin{cases} 0, & \text{when} \quad 0 \leq e_i^n \leq H, \\ e_i^n - H, & \text{when} \quad H < e_i^n; \end{cases}$$

$$e_i^0 = 0, \text{ for } 1 \leq i \leq M,$$

$$T_0^n = 1, \text{ for } 0 \leq n \leq L.$$

Here $\gamma = DT/(DX)^2$ and, to guarantee stability, $0 < \gamma \leq .5$.

This system of difference equations was used to approximate the original problem. For each time level the interface, $\Sigma(t)$, was taken to be the first nodal point at which $e(x,t) \leq H$. In the notation of the discrete problem the approximate interface is given by $\Sigma_1^n = x_{I+1}$ where $e_I^n > H$ and $e_{I+1}^n \leq H$. This approximation will be referred to as Rose 1.

An improvement in the approximation of the phase interface location may be obtained by considering conservation of energy. The interface $\Sigma(t)$ satisfies

$$\Sigma(t) = St \int_0^\infty [e(x,t) - T(x,t)]dx.$$

In the approximation scheme, at the $t = t_n$ level there is a unique $i = I$ such that: for $i \leq I$, $e_i^n > H$; $e_{I+1}^n \in [0,H]$; and $e_i^n = 0$ for $i \geq I + 2$.

It is an easy exercise to show that for each n there is at most one i such that $0 < e_i^n \leq H$. Therefore, since

$$e(x,t) - T(x,t) = \begin{cases} H, & \text{for } x \leq x_I, \\ e_{I+1}^n, & \text{for } x = x_{I+1}, \\ 0, & \text{for } x \geq x_{I+2}; \end{cases}$$

we obtain

$$\Sigma(t) = St \left\{ Hx_I + \int_{x_I}^{x_{I+2}} [e(x,t) - T(x,t)]dx \right\}$$

Since e-T is known at x_i for i = I, I+1, I+2, we apply the trapazoid rule to obtain the approximation

$$\Sigma_2^n = x_I + St \left\{ [e_I^n - T_I^n] + 2[e_{I+2}^n - T_{I+1}^n] + [e_{I+2}^n - T_{I+2}^n] \right\} DX/2$$

$$= X_I + St\ H + 2\ e_{I+1}^n \} DX/2$$

$$= X_{I+1} - (DX/2) + (DX/H)e_{I+1}^n.$$

This modification will be referred to as Rose 2. Σ_2^n lies somewhere between $X_{I+1} - DX/2$ and $X_{I+1} + DX/2$.

Both schemes were programmed in FORTRAN for the DEC PDP-10.

Results.

The first thing that became apparent in the plots of the errors in the interface location approximation was the size of the errors for small time. This large error is best understood by examining figure 2. Here the actual interface (•), the Rose 1 interface (x) and the Rose 2 interface (somewhere in ——— x ———) are shown on one set of axes. The Rose 1 points and the Rose 2 lines show the

largest possible x value of the approximated interface location for that specific t level. The Rose 1 approximation cannot catch up to the actual interface until the seventh t-level, n = 7. The Rose 2 approximation may be able to reach the actual interface by the sixth t level, n = 6. The Rose 2 error may be larger than the Rose 1 error and this did occur in some cases for small t.

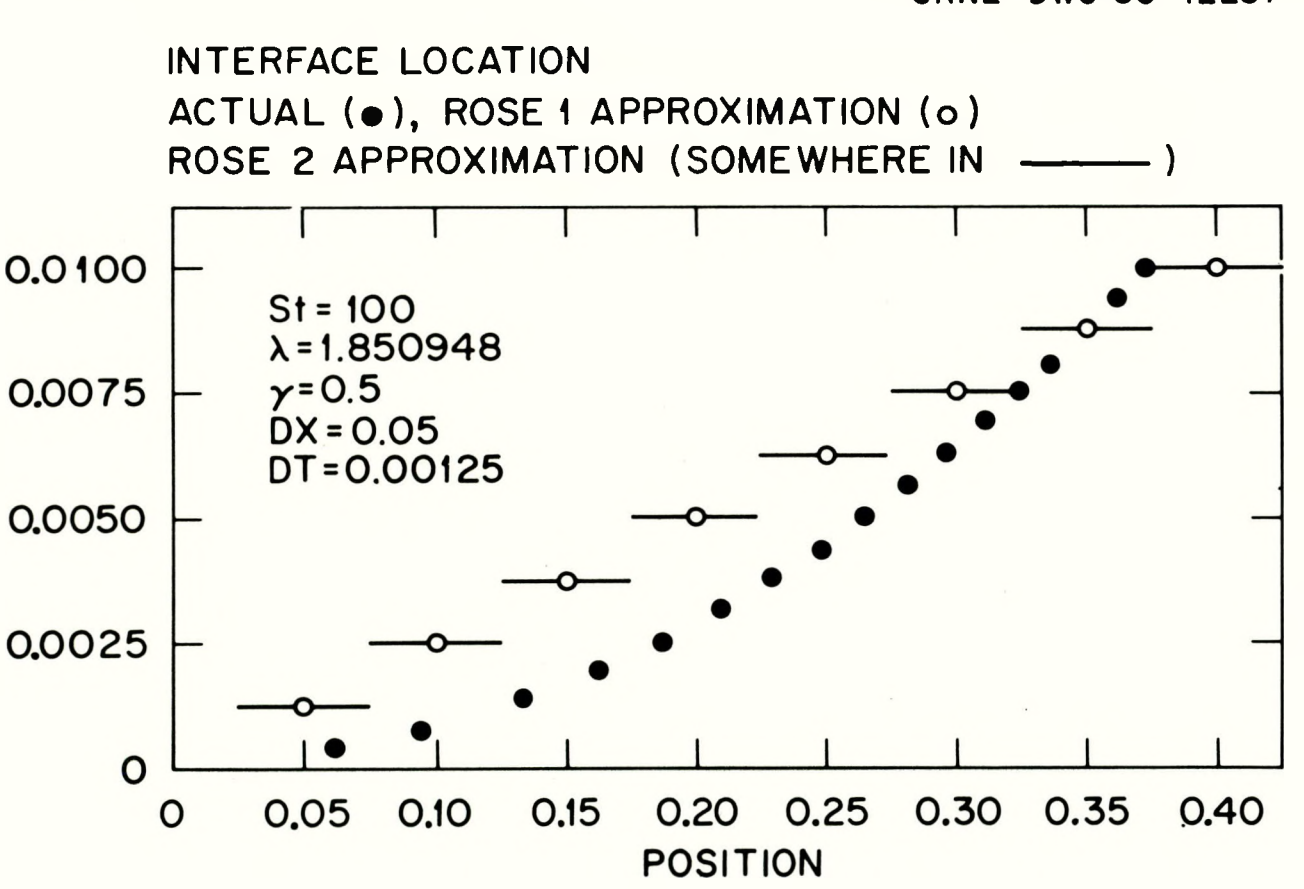

Figure 2

A complete set of plots is shown in figures 3 through 10. These correspond to St = 1, γ = .5, DX = .05 Figures 3 through 6 show the interface location and error for the Rose 1 and Rose 2 approximations. A plot of the interface, $\Sigma(t) = 2\lambda\sqrt{t}$, is superimposed on the approximations in figures 3 and 5.

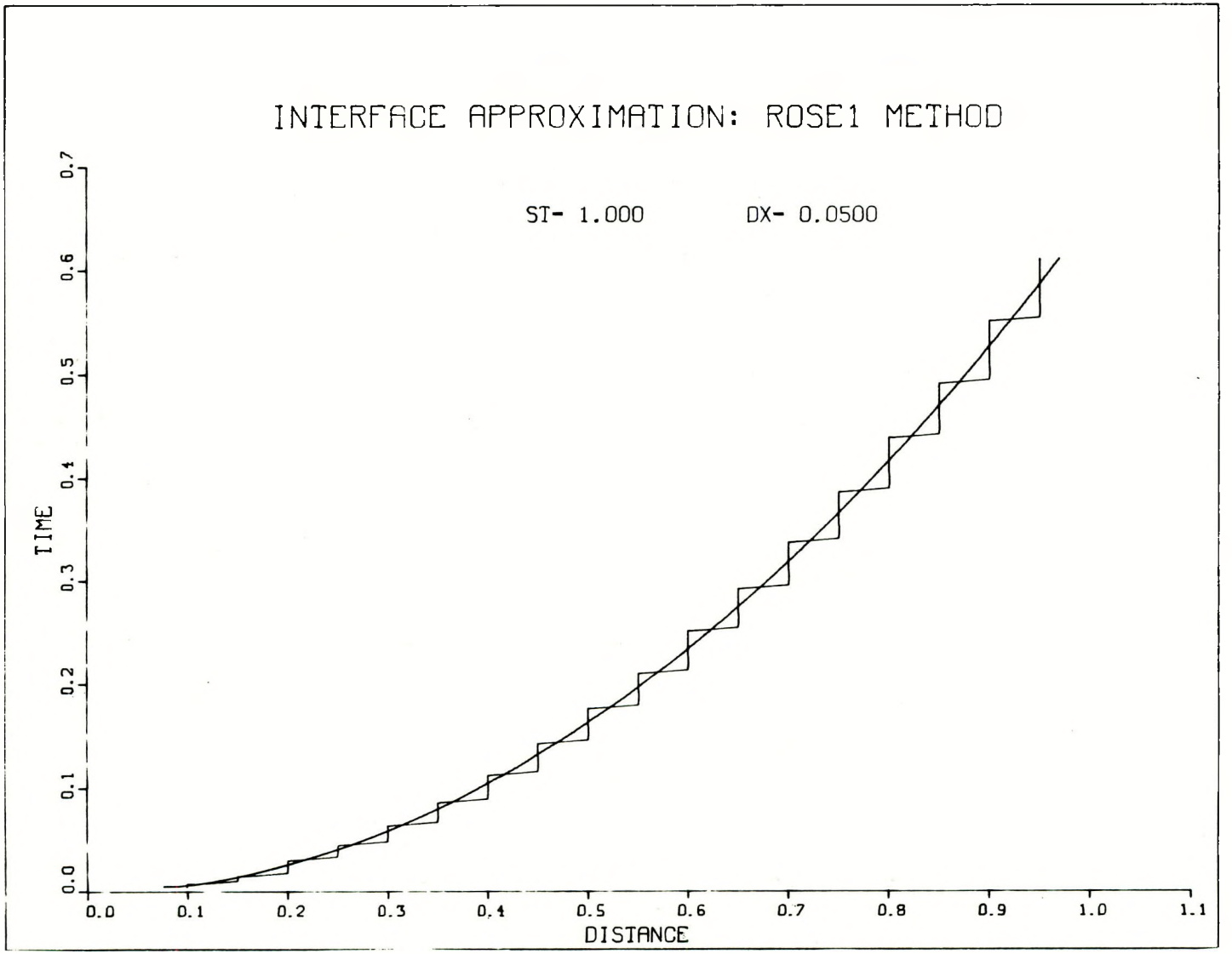

Figure 3. ROSE 1 Interface Approximation
Superimposed on $2\lambda\sqrt{t}$

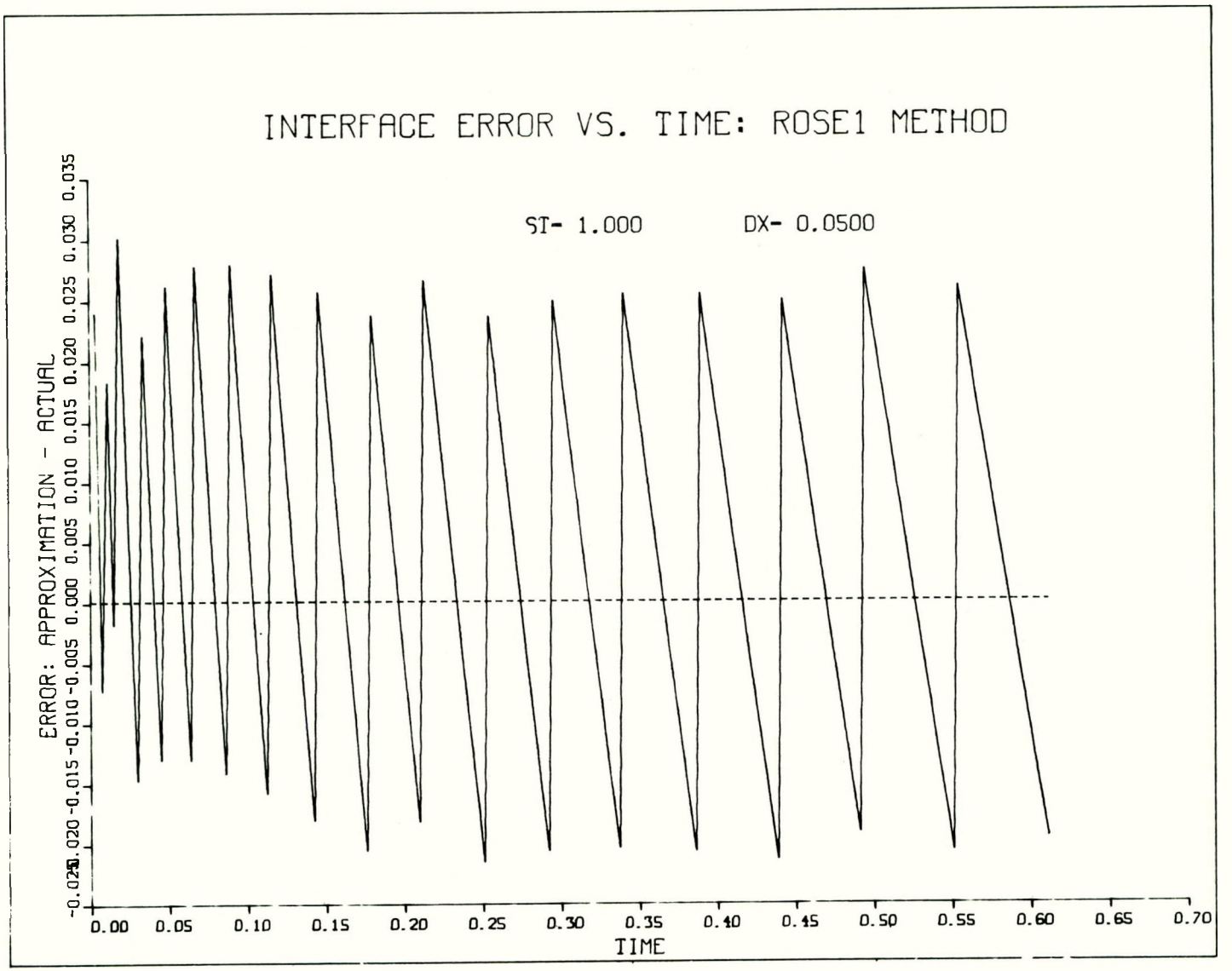

Figure 4. Error in ROSE 1 Interface Approximation

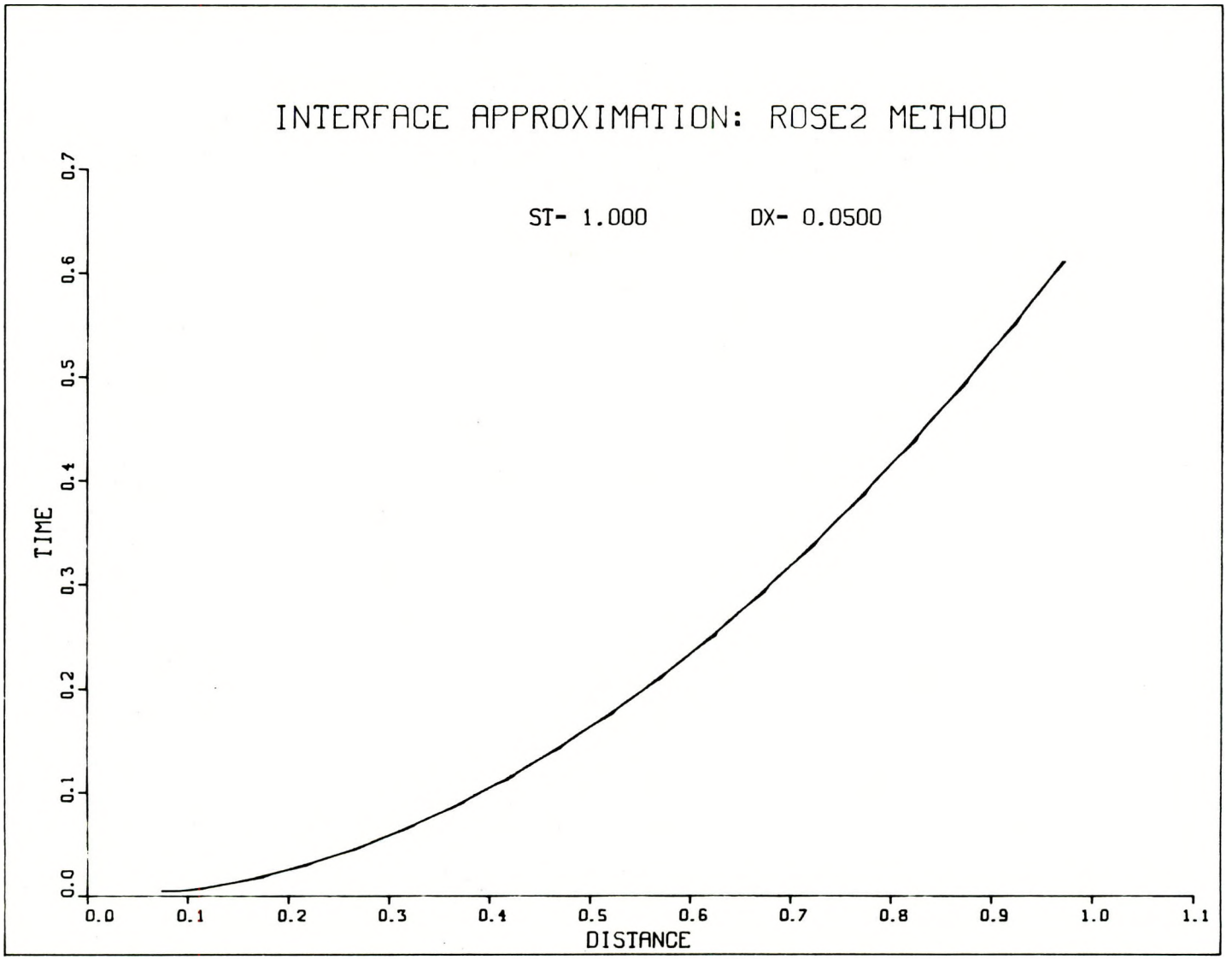

Figure 5. ROSE 2 Interface Approximation
Superimposed on $2\lambda\sqrt{t}$

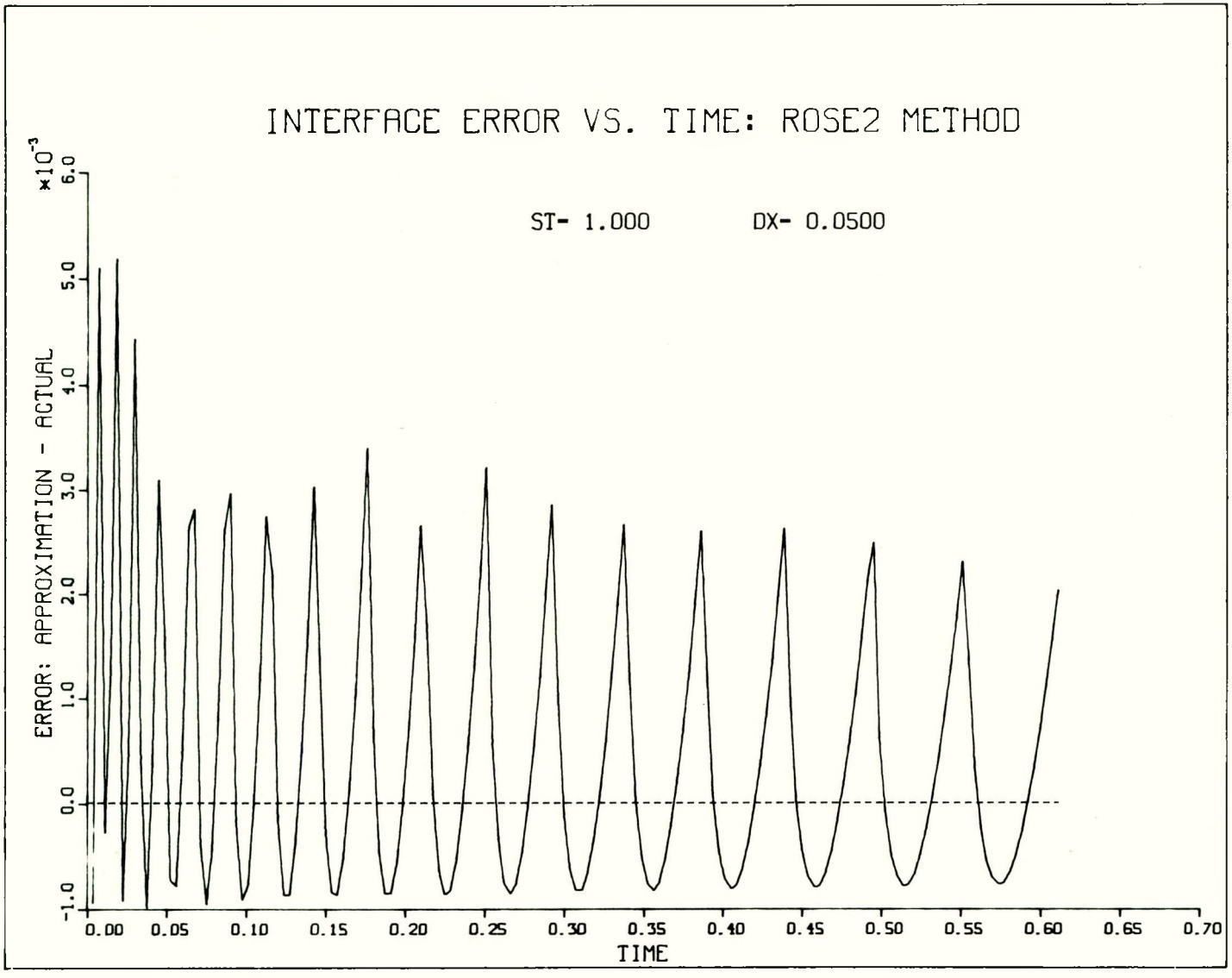

Figure 6. Error in ROSE 2 Interface Approximation

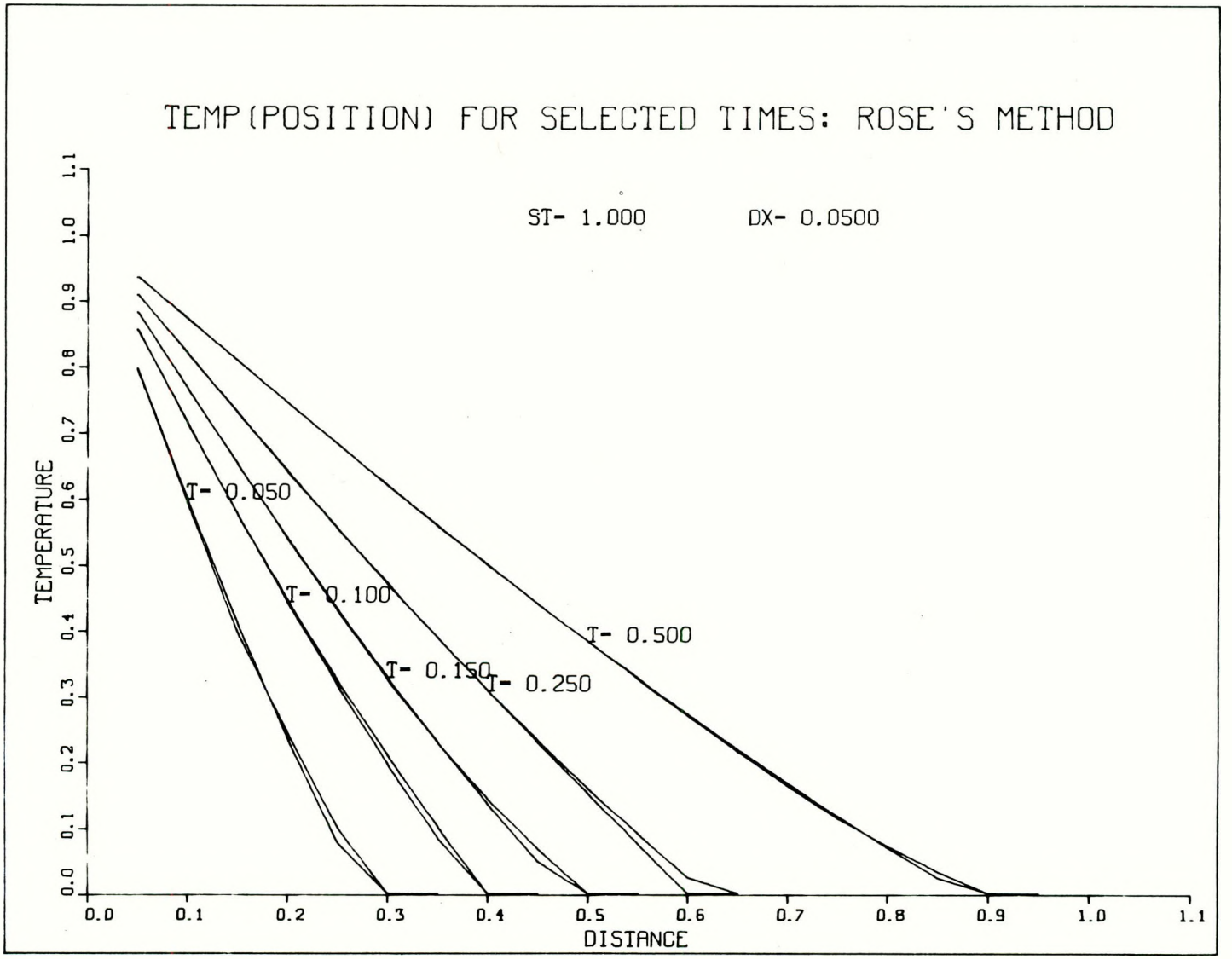

Figure 7. Temperatures as a Function of Distance at Selected Times Superimposed on $1-\mathrm{erf}(x/2\sqrt{t_i})/\mathrm{erf}(\lambda)$.

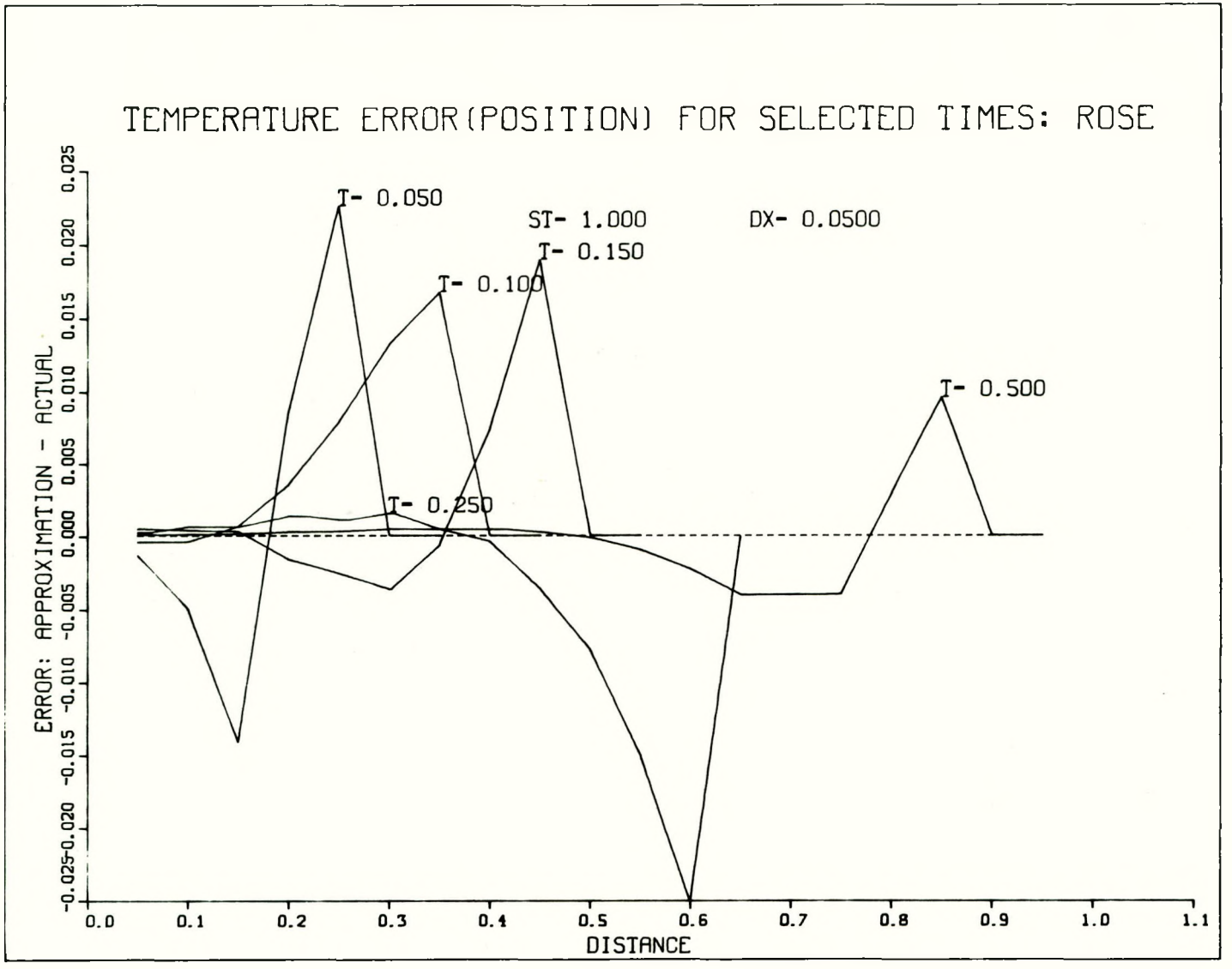

Figure 8. Errors in Temperatures as a Function of Distance

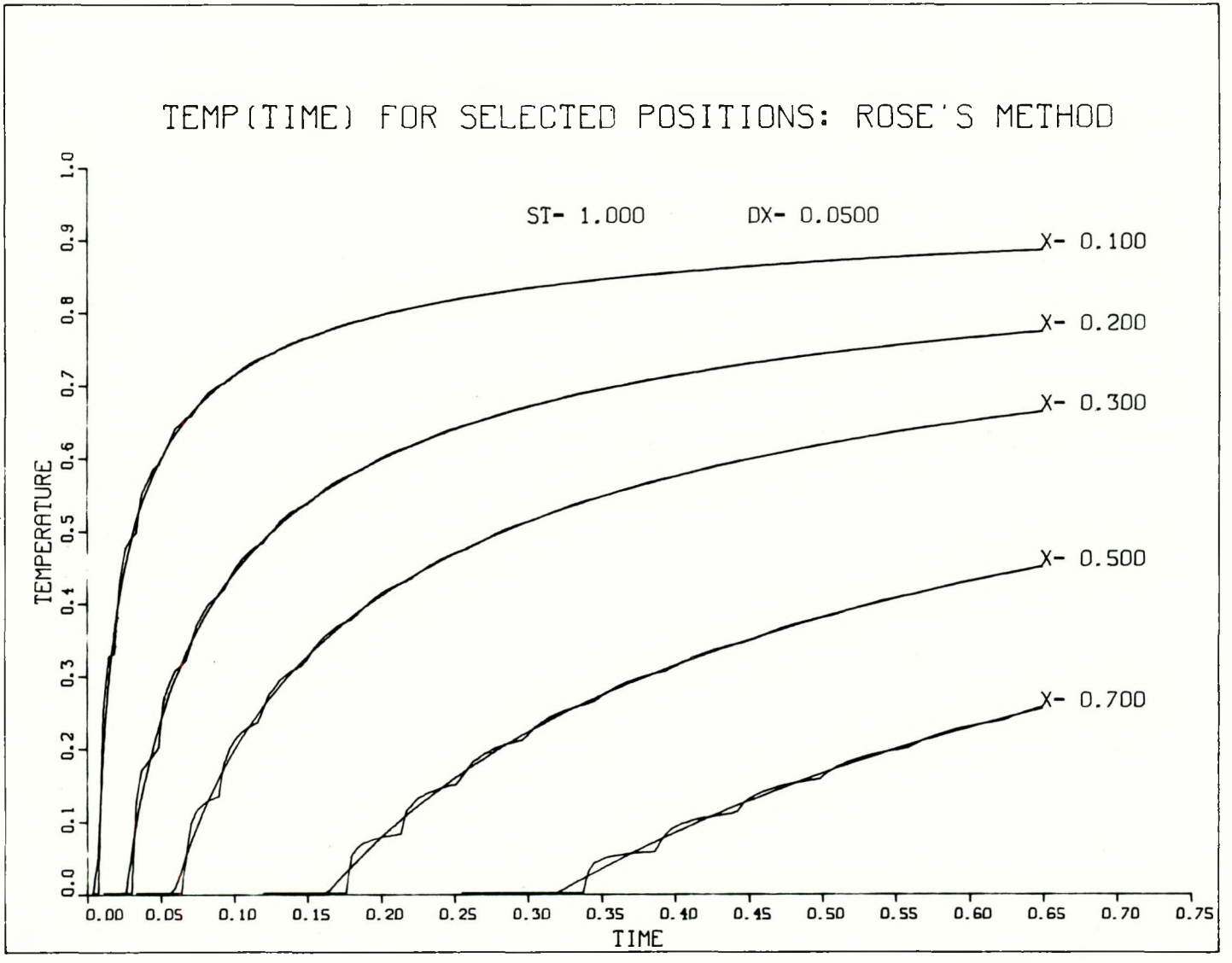

Figure 9. Temperatures as a Function of Time at Selected Positions Superimposed on $1-\mathrm{erf}(x_i/2\sqrt{t})/\mathrm{erf}(\lambda)$.

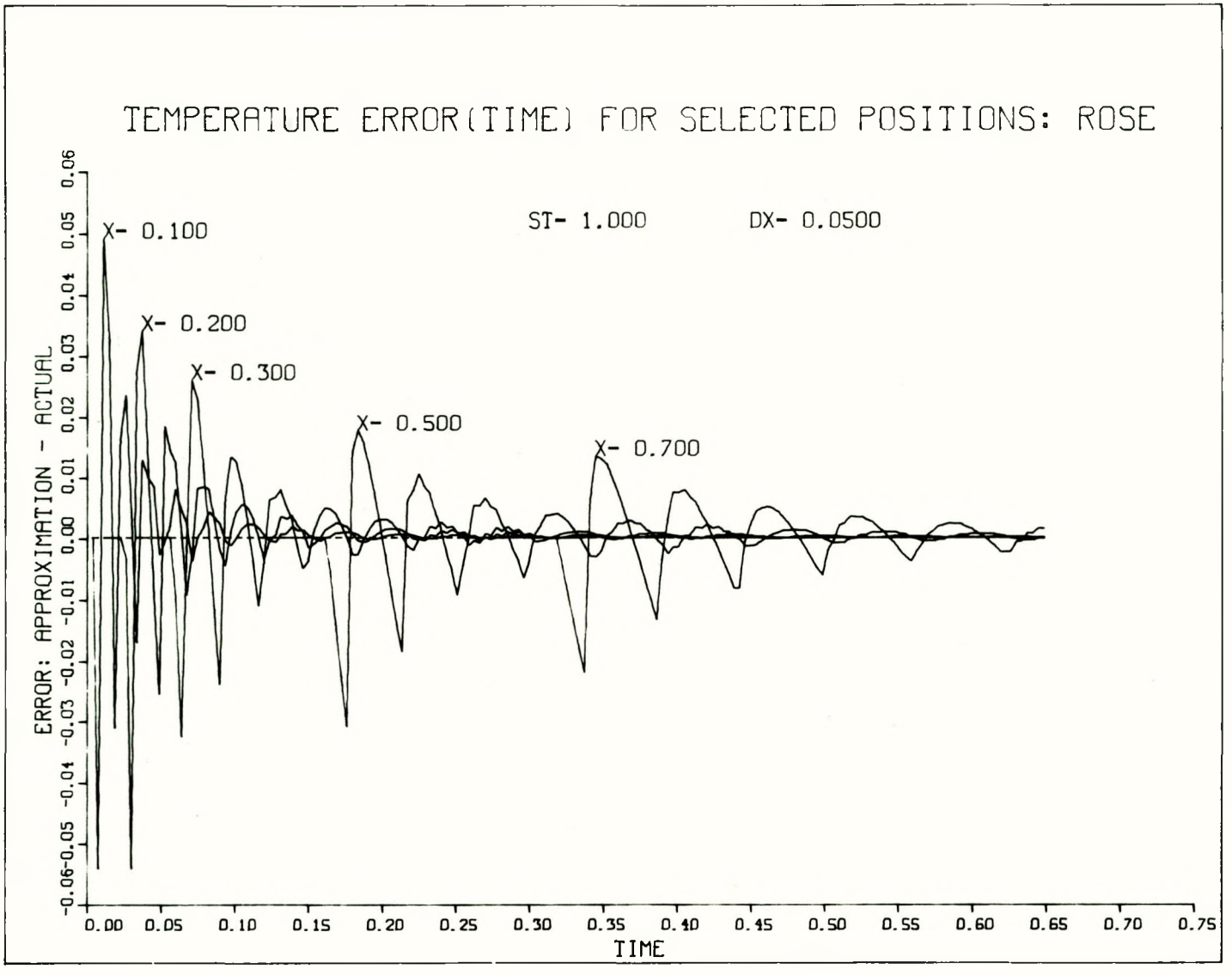

Figure 10. Errors in Temperatures as a Function of Distance.

In some plots not all t levels were plotted since the number of t levels to be plotted was limited to 200. Therefore, all points (x,t) where the error was a local maximum or local minimum were tabulated.

In table 1, corresponding to each St, γ, and technique, there are four entries. The "min. 3 valleys" is the smallest of the first three local minima, the "max. 3 peaks" is the largest of the first three local maxima, the "later min." is the smallest of the remaining local minima, and "later max." is the largest of the remaining local maxima. It is clear from table 1 that, after an initial time interval, the Rose 2 approximation is an improvement on the Rose 1 approximation.

The same program was used to compute temperatures for both the actual solution and Rose's approximation. Plots were obtained for both temperatures and errors as functions of position for five selected times. Figure 7 shows a plot of these temperatures and Figure 8 shows a plot of the errors. Plots were also obtained for temperatures and errors in temperatures as functions of time for five selected positions. Figure 9 shows a plot of these temperatures and Figure 10 shows a plot of the errors.

One important result of this analysis was the lack of dependence of the error on the choice of the Courant number, γ. The approximation of the interface by Rose 1 changed very little with any change in γ. Using Rose 2, only the form of the errors changed; that is, all errors may be positive in one case, negative in another, and

St		TYPE	Min. 3 Valleys	Max. 3 Valleys	Later Min.	Later Max.
100	1/2	Rose 1	-.035095	.007355	-.024307	.024526
		Rose 2	-.060095	-.009086	-.020526	.000000
	1/6	Rose 1	-.000620	.048871	-.014876	.038439
		Rose 2	-.000565	.023871	-.000463	.014055
	1/25	Rose 1	-.000620	.048871	-.014877	.038439
		Rose 2	.019962	.042223	.000000	.032664
1	1/2	Rose 1	-.016003	.025988	-.021969	.030776
		Rose 2	-.001150	.012994	-.000999	.005776
	1/6	Rose 1	-.015994	.033997	-.022197	.032087
		Rose 2	-.000111	.012994	-.000733	.007087
	1/25	Rose 1	-.015994	.033997	-.022197	.032087
		Rose 2	.000185	.014599	-.000672	.007240
.01	1/2	Rose 1	-.023061	.045008	-.024582	.026887
		Rose 2	.000027	.020258	.000000	.001883
	1/6	Rose 1	-.023109	.047118	-.024663	.026867
		Rose 2	.000027	.054348	-.000065	.001891
	1/25	Rose 1	-.023107	.045588	-.025056	.026887
		Rose 2	.000017	.023608	-.000420	.001482

Approximate Interface Location - Actual Interface Location
Table 1

balanced in the third even though the maximum error - minimum error remained relatively unchanged. The changes in relative error of temperature caused by changes in γ appear to be unpredictable. Since, in addition, smaller γ means longer running time, we recommend always taking $\gamma = .5$.

Temperature Error Results. The results of the temperature computations were plotted as follows:

a) For five selected times, the temperature as a function of position was plotted for the actual solution and Rose's approximation. The times chosen corresponding to each St are shown in table 2. The times t_1 will be called equivalent times since they are all approximately TMAX/10. Similarly, the times t_2, t_3, t_4, and t_5 are equivalent times.

St	TMAX	t_1	t_2	t_3	t_4	t_5
.01	50.1666	5	10	15	25	35
.1	5.1646	.5	1	1.5	2.5	3.5
1	.6502	.05	.1	.15	.25	.5
10	.1582	.02	.04	.07	.09	.12
100	.0730	.01	.02	.03	.04	.05

Five Selected Times for each St
Table 2

b) The errors (approximation - actual) as functions of position for times in a) were plotted.

c) For the five positions x = .1, .2, .3, .5, and .7, the temperature as a function of time was plotted for the actual solution and Rose's approximation.

d) The errors (approximation - actual) as functions of time for the positions in c) were plotted.

In addition, for each of the selected times, the relative error in temperature, (approximation - actual)/actual, was computed at each position where both the actual and approximate temperatures were positive. For each time, the maximum, minimum, and maximum-minimum were obtained and are recorded in table 3 for each St, γ, and time.

There are three ways to look for trends in the error. For each St and each time, changes in γ appear to affect the relative error in the St = 100 case and, to a lesser extent, in the St = 10 case. Otherwise, there seems to be little change in the relative error for changes in γ and, hence, we recommend γ = .5 to minimize cost. For each St, the relative errors appear to be unpredictable for increasing time. For each of the equivalent times t_1, ..., t_5, the relative errors again appear to be unpredictable for decreasing Stefan number.

The same error computations as discussed above were performed on the temperature as a function of time for selected positions. These results are shown in table 4. This table shows that there are no apparent trends and that the relative error is consistently high.

	St=100	St=10	St=1	St=.1	St=.01
γ	TMAX=.0730	TMAX=.1582	TMAX=.6502	TMAX=5.1646	TMAX=50.1666
	t_1=.01	t_1=.02	t_1=.05	t_1=.5	t_1= 5
1/2	.10532	.10249	.32315	.13179	.19727
1/6	.09073	.06092	.29473	.13179	.19729
1/25	.48029	.04673	.26140	.13181	
	t_2=.02	t_2=.04	t_2=.1	t_2= 1	t_2=10
1/2	.12130	.08114	.19596	.24867	.07054
1/6	.10803	.06896	.18419	.24782	.07047
1/25	.34182	.06087	.17929	.24758	
	t_3=.03	t_3=.07	t_3=.15	t_3=1.5	t_3=15
1/2	.21956	.05537	.39424	.28007	.06501
1/6	.15984	.05397	.36658	.27913	.06490
1/25	.21173	.05516	.35411	.27887	
	t_4=.04	t_4=.09	t_4=.25	t_4=2.5	t_4=25
1/2	.18762	.04571	.17005	.11116	.09581
1/6	.16437	.04326	.16920	.11105	.09597
1/25	.21179	.03929	.16957	.11094	
	t_5=.05	t_5=.12	t_5=.5	t_5=3.5	t_5=35
1/2	.59507	.96409	.43892	.27739	.39744
1/6	.16628	.40461	.42805	.27741	.39708
1/25	.28222	.31621	.41540	.27744	

$$RE(x_i) = \frac{\text{APPROXIMATE TEMP } (x_i) - \text{ACTUAL TEMP } (x_i)}{\text{ACTUAL TEMP.}(x_i)}$$

VALUES SHOWN: $\text{Max}_i\ RE(x_i) - \text{Min}_i\ RE(x_i)$

DX = .05 $\qquad DT = \gamma(DX)^2$

Table 3

Difference in Maximum and Minimum Relative Error in Temperature as a Function of Time

x	c	ST=100	ST=10	ST=1	ST=.1	ST=.01
.1	1/2	.56906	.33798	.65096	.82320	.98445
	1/6	1.92906	.22818	1.23051	1.07772	1.30479
	1/25	5.60697	.59395	1.09687	1.48052	
.2	1/2	.22708	1.25408	1.35711	1.59382	1.81882
	1/6	.30538	1.08044	1.13581	1.14812	1.43315
	1/25	4.79384	.86211	1.15986	1.50863	
.3	1/2	.27274	.89078	.52820	1.18818	1.44227
	1/6	.51367	.75855	1.27188	1.17537	1.51966
	1/25	3.32170	1.09548	1.18538	1.55399	
.5	1/2	.09544	.32635	.61037	1.60755	1.78316
	1/6	1.11720	.88610	.95313	1.59665	1.58050
	1/25	1.05086	1.09490	1.34319	1.56310	
.7	1/2	.66421	.82533	.64950	1.62041	1.65730
	1/6	.72691	.67124	1.11209	1.61443	1.78980
	1/25	1.12346	1.09208	1.35912	1.61039	

$$RE(t_n) = \frac{\text{APPROXIMATE TEMP } (t_n) - \text{ACTUAL TEMP } (t_n)}{\text{ACTUAL TEMP } (t_n)}$$

VALUES SHOWN ARE $\text{MAX}_n\ RE(t_n) - \text{MIN}_n\ RE(t_n)$

DX=.05 $\qquad DT = \gamma(DX)^2$

Table 4

Difference in Maximum and Minimum Relative Error in Temperature as a Function of Time

c	ST=100	ST+10	ST=1	ST=.1	ST=.01
1/2	13.76	15.37	17.64	33.66	184.85
1/6	16.79	17.67	22.67	69.29	531.37
1/25	17.87	23.19	43.88	238.20	

CPU Time in Seconds
Table 5

It may be of interest to know the relative amount of CPU time required. In table 5, the time required for a complete run using Rose 1 is given. A complete run consists of computation of and plotting;

a) the actual and approximate interface location;

b) the error in the interface location approximation;

c) the actual and approximate temperatures as functions of position for five selected times;

d) the error (approximation - actual) obtained in c);

e) the actual and approximate temperatures as function of time for five selected positions;

f) the error (approximation - actual) obtained in e).

These computations were obtained only at the plot points and the number of plot points was restricted to be at most 200 by uniformly distributing plot times. These run times do not include the computation of values and printing of the local maxima and minima in the interface location error. Since these times include plotting time, they should be used for comparison purposes only.

The complete run was never made for $\gamma = 1/25$ and St = .01 with a program identical with that used to get the other CPU times. This happened because this run was aborted after the time appeared to be getting very large. However, in an attempt to estimate this CPU time, a plot was made of log (log time) versus log (St). This plot is shown in figure 11 and the estimate obtained is approximately 1 hour, 45 minutes.

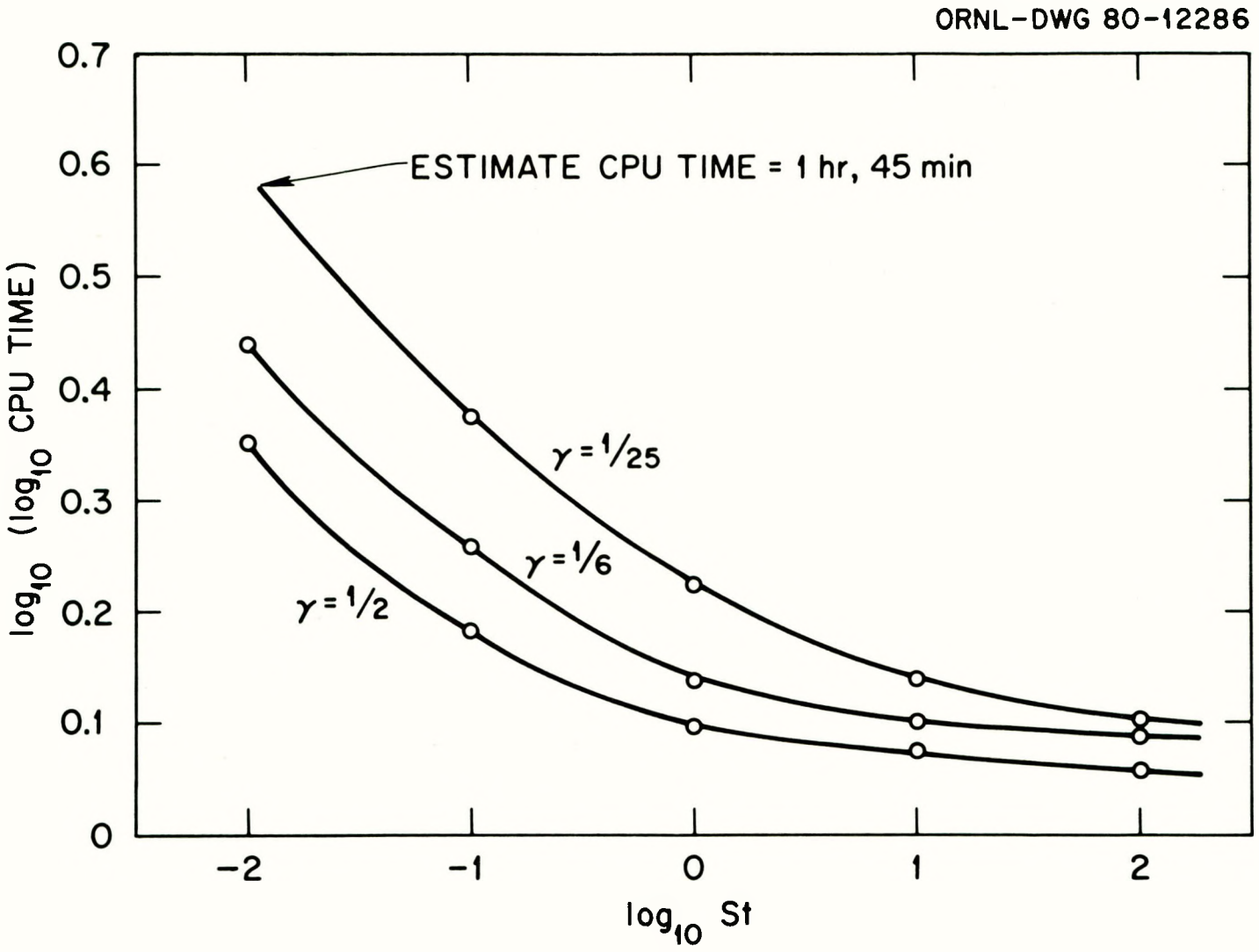

Figure 11. CPU Time Versus St to Estimate CPU Time of Case St = .01, γ = 1/25

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[2] Rose, Milton, A Method for Calculating Solutions of Parabolic Equations With a Free Boundary, Math. Comp. 14 (1960), 249-256.

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