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J. of Heat Transfer **106**, 483 (1984).

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SIMULATION OF RAPID HEATING IN FUSION REACTOR FIRST WALLS
USING THE GREEN'S FUNCTION†

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†Submitted to J. of Heat Transfer

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Abstract

The solution of the heat conduction problem in moving boundary conditions is very important in predicting accurate thermal behavior of materials when very high energy deposition is expected. Such high energy fluxes are encountered on first wall materials and other components in fusion reactors. A numerical method has been developed to solve this problem by the use of the Green's function. A comparison is made between this method and a finite difference one. The comparison in the finite difference method is made with and without the variation of the thermophysical properties with temperature. The agreement between the Green's function and the finite difference method is found to be very good.

A. Introduction

The rapid heating of fusion first wall components either due to x-ray and ion debris deposition in ICF reactors or during a plasma dump in magnetic fusion reactors may lead to melting and subsequently to intense evaporation. As a result, an accurate analysis of this heat conduction problem requires the solution of a two moving boundaries problem. A moving face where vaporization occurs becomes one boundary in addition to the moving internal boundary between the liquid and solid. Because of the moving boundaries and the difference between the properties of the liquid and solid states of the same material, the distribution is nonlinear.

The solution of the heat conduction equation in moving boundary conditions is presented by the use of the Green's function method. A comparison between the Green's function solution and a finite difference solution developed in previous studies⁽³⁾ is also presented. This comparison with finite difference methods is made with and without the variation of the thermal properties with temperature.

B. Formulation of the Heat Conduction Problem

Consider the first wall as a semi-infinite medium. This is reasonable in view of the short heat penetration depth during a plasma disruption or target debris deposition in ICF reactors. Under a heat flux $F(t)$, the temperature distribution $T(x,t)$ must then satisfy the heat conduction equation:

$$\rho c \frac{\partial T}{\partial t} - \nabla \cdot k \nabla T = \dot{q}(x,t) \quad (1)$$

where: ρ = density
 c = specific heat

k = thermal conductivity

$\dot{q}(x,t)$ = volumetric energy deposition rate.

All the thermophysical properties are functions of the local temperature. The boundary conditions are that $T(x,t) \rightarrow T_{\text{back}} = \text{constant}$ for large depth distances x , and on the surface $x = 0$,

$$F(t) = -k(T_v) \frac{\partial T}{\partial x} + \rho(T_v)L_v v(T_v) + \sigma\epsilon(T_v^4 - T_0^4) \quad (2)$$

where $T_v(t) = T(0,t)$, L_v is the heat of vaporization, and $v(T_v)$ is the velocity of the receding surface. This velocity is a function of the instantaneous surface temperature and other materials parameters. Furthermore, the radiative heat transfer term contains the Stefan-Boltzmann constant, σ , ϵ is the emissivity of first wall material, and the surface temperature of the cold portion of the first wall is T_0 . For the radiative heat loss, it is assumed that parts of the first wall (mainly in magnetic fusion reactors) not struck by the plasma dump remain at the steady state temperature T_0 . In ICF reactors this term goes to zero since a microexplosion reaction is assumed to be symmetrical.

The general heat-conduction equation with constant thermal properties can be written as:

$$\rho c \frac{\partial T}{\partial t} - k \nabla^2 T = \dot{q}(x,t) \quad (3)$$

where ρ , c , k are independent of temperature. For a semi-infinite medium, the Green's function is given by:

$$G(x,t,x',t') = \frac{1}{2\sqrt{\pi\alpha(t-t')}} \left\{ e^{-\frac{(x-x')^2}{4\alpha(t-t')}} + e^{-\frac{(x+x')^2}{4\alpha(t-t')}} \right\} \quad (4)$$

where α is the thermal diffusivity. The general solution for the temperature rise due to any deposition function is given by⁽⁴⁾

$$T(x,t) = \int_{t'} \int_{x'} \frac{1}{\rho c} \dot{q}(x',t') G(x,t,x',t') dx' dt' . \quad (5)$$

If the heating is continued long enough and at a sufficiently high rate, significant vaporization may occur from the surface assuming that the melting material stays in place. It is necessary to account for the receding surface at the interface between vapor and solid or liquid. This can be done by introducing a moving coordinate system:

$$z(t) = x - s(t) \quad (6)$$

for which the surface always remains at $z = 0$. Transforming the heat conduction Eqs. (1) or (3) to this moving frame gives

$$\rho c \left(\frac{\partial T}{\partial t} + \frac{\partial T}{\partial z} \cdot \frac{dz}{dt} \right) - \nabla \cdot k \nabla T = \dot{q}(z,t) \quad (7)$$

where
$$\frac{dz}{dt} = - \frac{ds(t)}{dt} = - v(t) \quad (8)$$

$v(t)$ = velocity of the receding surface. Substituting Eq. (8) into Eq. (7) gives

$$\rho c \frac{\partial T}{\partial t} - \rho c v(t) \frac{\partial T}{\partial z} - \nabla \cdot k \nabla T = \dot{q}(z,t) . \quad (9)$$

The main difference in this equation is that it includes the convective term $v(t) \frac{\partial T}{\partial z}$. This term is important in the case of intensive evaporation if we are to obtain accurate calculations of the temperature. The velocity of the receding surface, i.e. $v(t)$, is a highly nonlinear function of temperature. The surface boundary condition is then given by

$$F(t) = -k \left. \frac{\partial T}{\partial z} \right|_{z=0} + \rho L_V v(t) + \sigma \epsilon (T_V^4 - T_0^4) \quad (10)$$

where: $v(t)$ is again the velocity of the receding surface,

$F(t)$ is the incident heat flux.

Equation (9) can be written as

$$\rho c \frac{\partial T(z,t)}{\partial t} - k \nabla^2 T(z,t) = \dot{q}(z,t) + \rho c v(t) \frac{\partial T(z,t)}{\partial z} . \quad (11)$$

The right-hand side of Eq. (11) consists of the volumetric energy deposition function and a convective term $\rho c v(t) \frac{\partial T}{\partial z}$ which could be treated as a part of the deposition function. Then Eq. (11) can be written as

$$\rho c \frac{\partial T(z,t)}{\partial t} - k \nabla^2 T(z,t) = \dot{q}'(z,t) \quad (12)$$

where

$$\dot{q}'(z,t) = \dot{q}(z,t) + \rho c v(t) \frac{\partial T(z,t)}{\partial z} . \quad (13)$$

The solution for the temperature rise due to the deposition function given by Eq. (13) and boundary condition in Eq. (10) is given by⁽⁵⁾

$$T(z,t) = \int_{t'} \int_{x'} \frac{1}{\rho c} \dot{q}'(z',t) G(z,t,z',t') dz' dt' - \alpha \int_{t'} dt' G(z,t,0,t') \frac{\partial T(0,t')}{\partial z} . \quad (14)$$

From Eq. (10) the gradient of the temperature can be represented by

$$k \frac{\partial T(0,t)}{\partial z} = \rho L_v v(t) + \sigma \epsilon (T_v^4 - T_0^4) - F(t) . \quad (15)$$

Substituting Eqs. (15) and (13) into Eq. (14) yields

$$T(z,t) = \frac{1}{\rho c} \int_{t'} \int_{x'} (\dot{q}'(z',t') + \rho c v(t') \nabla T(z',t')) G(z,t,z',t') dz' dt' + \frac{1}{\rho c} \int_{t'} G(z,t,0,t') (F(t') - \rho L_v v(t') - \sigma \epsilon (T_v^4 - T_0^4)) dt' \quad (16)$$

where: $\nabla T(z,t) = \frac{\partial T(z,t)}{\partial z}$

$$T_v = T(0,t) .$$

The difficulty in calculating the temperature rise from Eq. (16) is that both $v(t)$ and $\nabla T(z,t)$ are functions of the current temperatures which are unknown. This is also true for the radiative heat transfer term in the second integral of Eq. (16). Although calculating the surface velocity, $v(t)$, requires only the knowledge of the surface temperature, the term $\nabla T(z,t)$ requires the current temperature distribution throughout the entire space.

A good approximation for the solution of Eq. (16) is to use numerical techniques developed in Ref. (2). Assuming that we divide space and time into many divisions, the solution for the temperature increase is given by:

$$\begin{aligned}
T(x_n, t_n) = & \sum_{t'_i=0}^{t_{n-1}} w_i \Delta t_i \int_0^{\infty} \frac{1}{\rho C} [\dot{q}(x', t'_i) + \rho c v(t'_i) \nabla T(x', t')] G(x_n, t_n, x', t'_i) dx' \\
& + w_n \Delta t_n \lim_{t'_i \rightarrow t_n} \int_0^{\infty} \frac{1}{\rho C} [\dot{q}(x', t'_i) + \rho c v(t'_i) \nabla T(x', t'_i)] G(x_n, t_n, x', t'_i) dx' \\
& + \frac{1}{\rho C} \sum_{t'_i=0}^{t_{n-1}} \Delta t_i [F(t'_i) - \rho L_V v(t'_i) - \sigma \epsilon (T^4(0, t'_i) - T_0^4)] G(x_n, t_n, 0, t'_i) \\
& + \frac{1}{\rho C} \Delta t_n [F(t_n) - \rho L_V v(t_n) - \sigma \epsilon (T^4(0, t_n) - T_0^4)] \frac{1}{2\sqrt{\pi \alpha \Delta t_n}} e^{-\frac{x_n^2}{4\alpha \Delta t_n}}
\end{aligned} \tag{17}$$

where: $T(x_n, t_n)$ is the temperature at any point x_n and time t_n

w_i is a weighting factor depending on the method of integration
 Δt_i incremental time.

In this last integral the Green's function possesses a singularity at $t'_i \rightarrow t_n$. To avoid this singularity, first we integrate from $t'_i = 0$ up to $t'_i = t_{n-1}$ and the last term in this integration is treated separately. Also

$$\Delta t_n \ll \Delta t_i \tag{18}$$

and

$$t_{n-1} = t_n - \Delta t_n. \tag{19}$$

It can be shown that⁽¹⁾

$$\lim_{\epsilon \rightarrow 0} \frac{1}{2\sqrt{\pi \alpha \epsilon}} e^{-\frac{(x-x')^2}{4\alpha \epsilon}} \longrightarrow \delta(x - x') \tag{20}$$

where $\delta(x - x')$ is the cronial δ -function. The last term of the first integral in Eq. (17) can then be written as

$$w_n \Delta t_n \int_0^{\infty} \frac{1}{\rho c} [\dot{q}(x', t'_i) + \rho c v(t'_i) \nabla T(x', t'_i)] \lim_{t'_i \rightarrow t_n} G(x_n, t_n, x', t'_i) \\ = w_n \Delta t_n \int_0^{\infty} \frac{1}{\rho c} [\dot{q}(x', t'_i) + \rho c v(t'_i) \nabla T(x', t'_i)] [\delta(x - x') + \delta(x + x')] dx' .$$

Also note that

$$\int f(x', t) \delta(x - x') dx' = f(x, t)$$

$$\int f(x', t) \delta(x + x') dx' = f(-x, t) .$$

Then substituting Eq. (20) in Eq. (17) the temperature rise in Eq. (17) reduces to:

$$T(x_n, t_n) = \dots + w_n \Delta t_n \frac{1}{\rho c} [\dot{q}(x_n, t_n) + \rho c v(t_n) \nabla T(x_n, t_n)] + \frac{1}{\rho c} \sum_{t'_i=0}^{t_{n-1}} \Delta t_i [F(t'_i) \\ - \rho L v(t'_i) - \sigma \epsilon (T^4(0, t'_i) - T_0^4)] G(x_n, t_n, 0, t'_i) \\ + \frac{1}{\rho c} [F(t_n) - \rho L v(t_n) - \sigma \epsilon (T^4(0, t_n) - T_0^4)] \frac{1}{2\sqrt{\pi\alpha}} e^{-\frac{x_n^2}{4\alpha\Delta t_n}} \sqrt{\Delta t_n} \quad (21)$$

where $\int_0^{\infty} dx' \dot{q}(x', t_n) \delta(x_n - x') = \dot{q}(x_n, t_n)$ and $\int_0^{\infty} dx' \nabla T(x', t_n) \delta(x_n - x') = \nabla T(x_n, t_n)$ since $\dot{q}(-x_n, t_n) = 0$ and $\nabla T(-x_n, t_n) = 0$.

Again the R.H.S. of Eq. (21) contains terms which are functions of the current unknown temperature. These can be approximated by using the temperatures from the previous time step which are known. By choosing the increments between time steps small enough, the solution of Eq. (21) yields an accurate approximation to the integral Eq. (16). These choices always involve a compromise between accuracy and computer time.

The solution of Eq. (21) is implemented in the computer code A*THERMAL.⁽²⁾ This equation can be used to determine the thermal response of fusion first walls both in inertial and in magnetic confinement reactors due to any kind of incident radiation, such as laser, x-rays, heat flux or ions (light or heavy) for inertial confinement and plasma ions in magnetic confinement reactors.

C. Test Case

To test the accuracy of the solution for the moving boundary problem developed in this study, a comparison with the finite difference methods is made. An example of the plasma disruption cases⁽³⁾ is considered where 400 J/cm^2 is deposited in a carbon first wall in 20 ms. The comparison is made between the finite difference with and without the variations of the thermal properties with temperature. In the Green's function methods it is assumed that the thermal properties are constant and equal to those of the finite difference with constant properties. Perturbation methods to account for the variation of thermal properties with temperature in the Green's function methods are developed in Ref. (1). A solution for the two moving boundaries problem where the material could change phase beside the surface moving boundary using the Green's function is also contained in the computer code A*THERMAL.

D. Results and Discussion

The surface temperature as a function of the deposition time for the three methods, i.e. finite difference with variable properties, finite difference with constant properties, and the Green's function is shown in Fig. 1. The agreement between the Green's function and the finite difference with constant properties is very good as is seen from Fig. 2. The little difference between the two methods, which is less than 3%, could be explained by the size of the time step chosen for each method. The size of the time step for

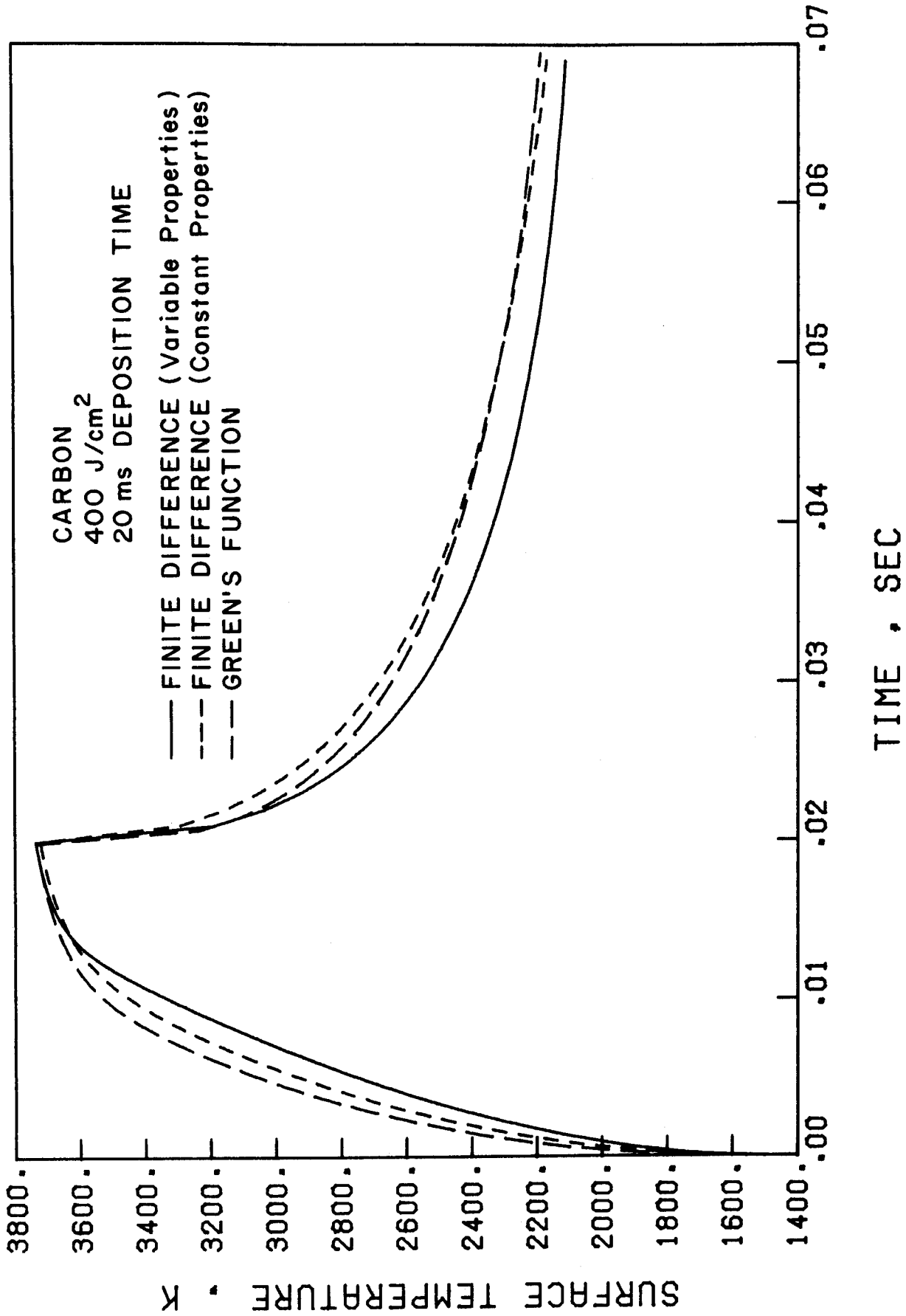


Figure 1 Comparison of surface temperature rise for carbon for 400 J/cm² deposited in 20 ms by different methods.

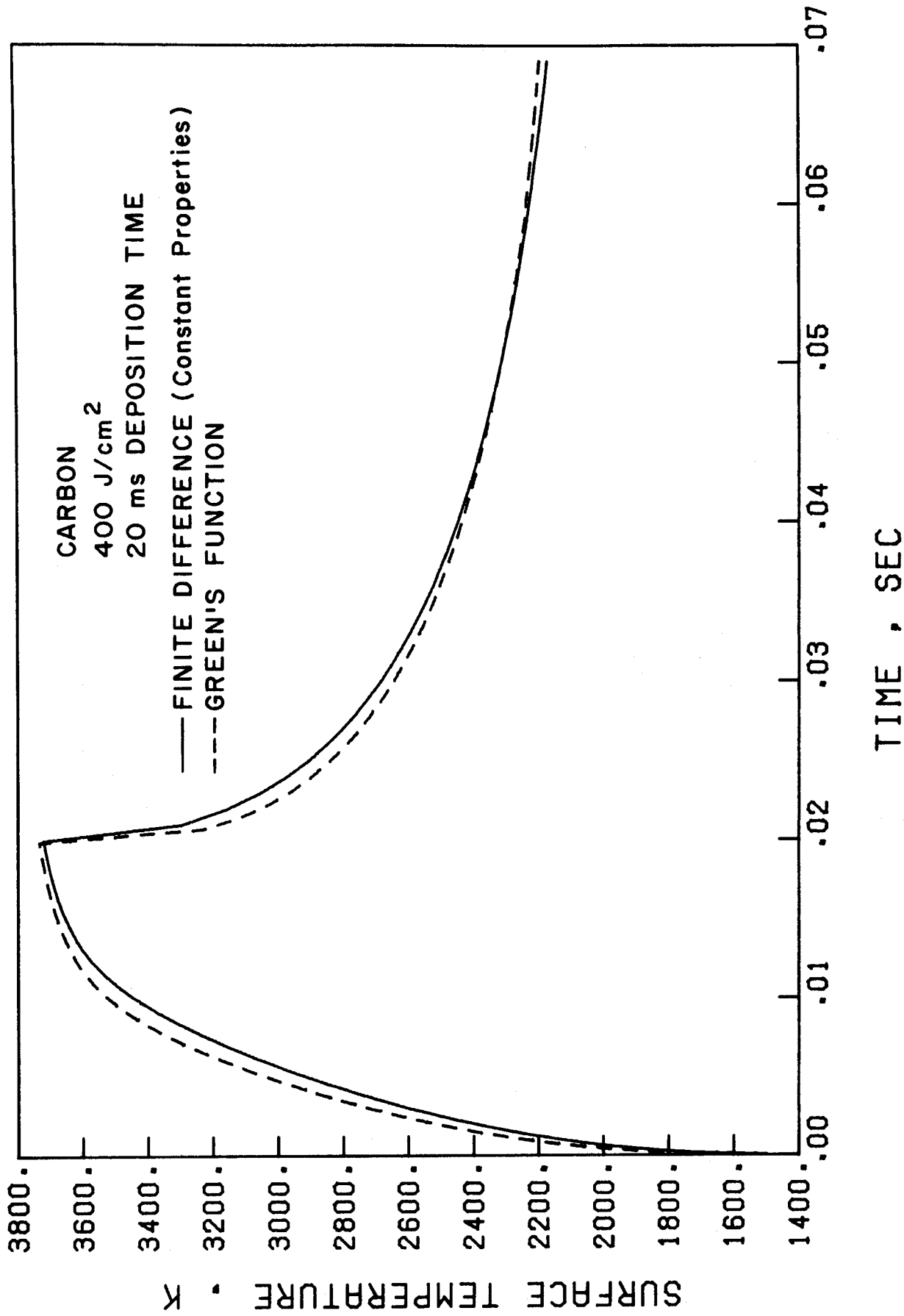


Figure 2 Surface temperature rise for carbon by finite difference and Green's function methods.

Green's function problem is much larger than that for finite difference. This is chosen to keep the computer cost for the two problems relatively the same. The Green's function method required more calculations than the finite difference but with a much larger time step. The effect of the variation of thermal properties on the surface temperature can also be seen from Fig. 1. The constant thermal properties chosen for the Green's function and the finite difference was an average over a high temperature range. Because the lower the temperature, the higher the conductivity for carbon, the finite difference with variable properties has lower temperature than the other two methods either at earlier time in the pulse or at longer times after the end of the disruption.

The velocity of the receding surface, $v(t)$, as a function of time for the three methods of calculation is shown in Fig. 3. The lower surface velocity at earlier times for the finite difference with variable properties is due to the lower surface temperature because of higher thermal conductivity. The difference between the finite difference with constant properties and the Green's function is illustrated in Fig. 4. The agreement between the two methods is considered very good. The slightly higher velocity predicted by the Green's function is due to the slightly higher surface temperature. Because of the highly nonlinear dependence of the surface velocity on the surface temperature, the difference between the surface velocity calculation by the Green's function and by the finite difference methods is larger than the difference in calculating the surface temperature.

The amount of the total material vaporized can be estimated by integrating the velocity of the receding surface over the pulse duration time. Figure 5 shows the amount of carbon vaporized as calculated by the three

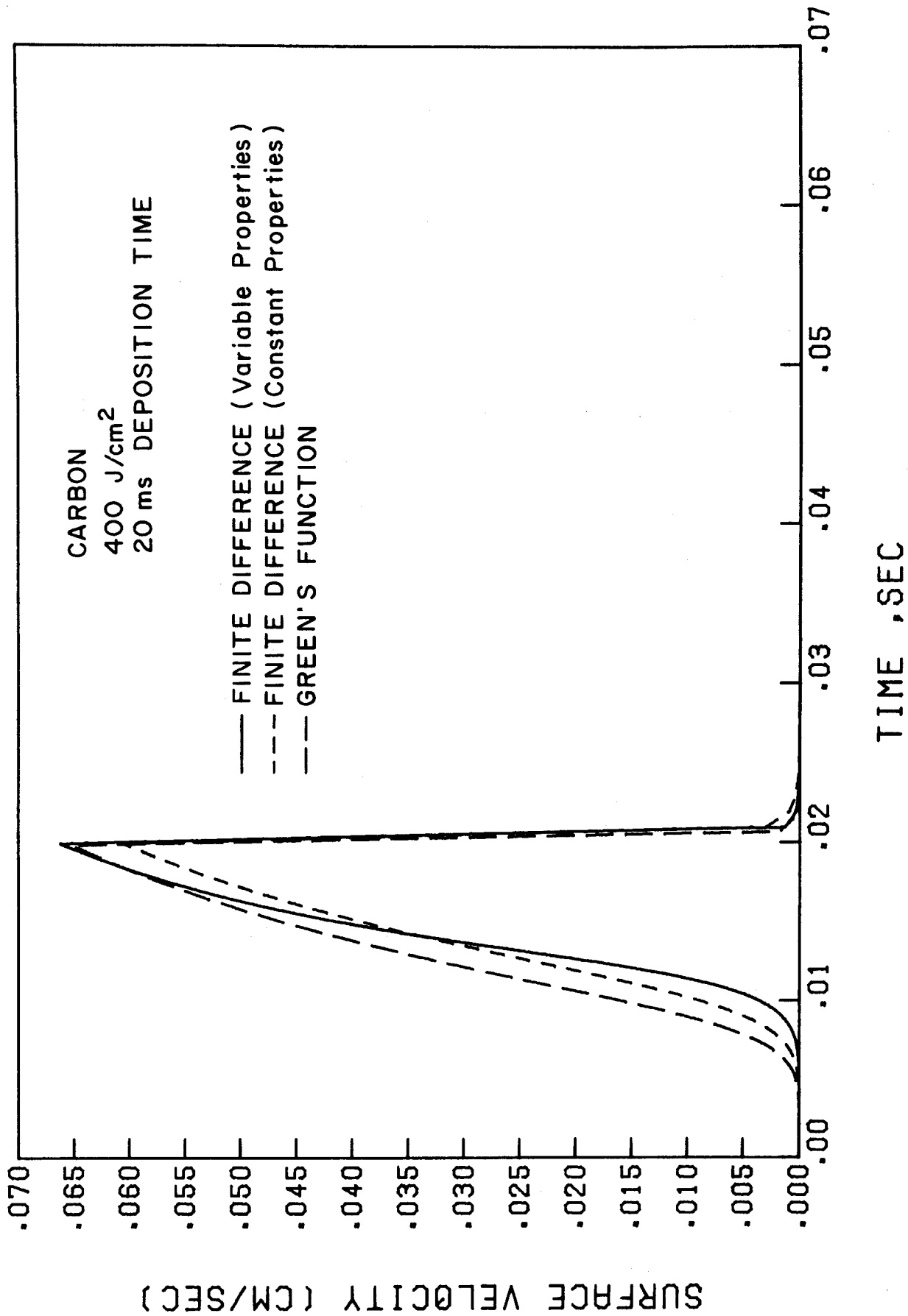


Figure 3 Carbon surface velocity for 400 J/cm² deposited in 20 ms by different methods.

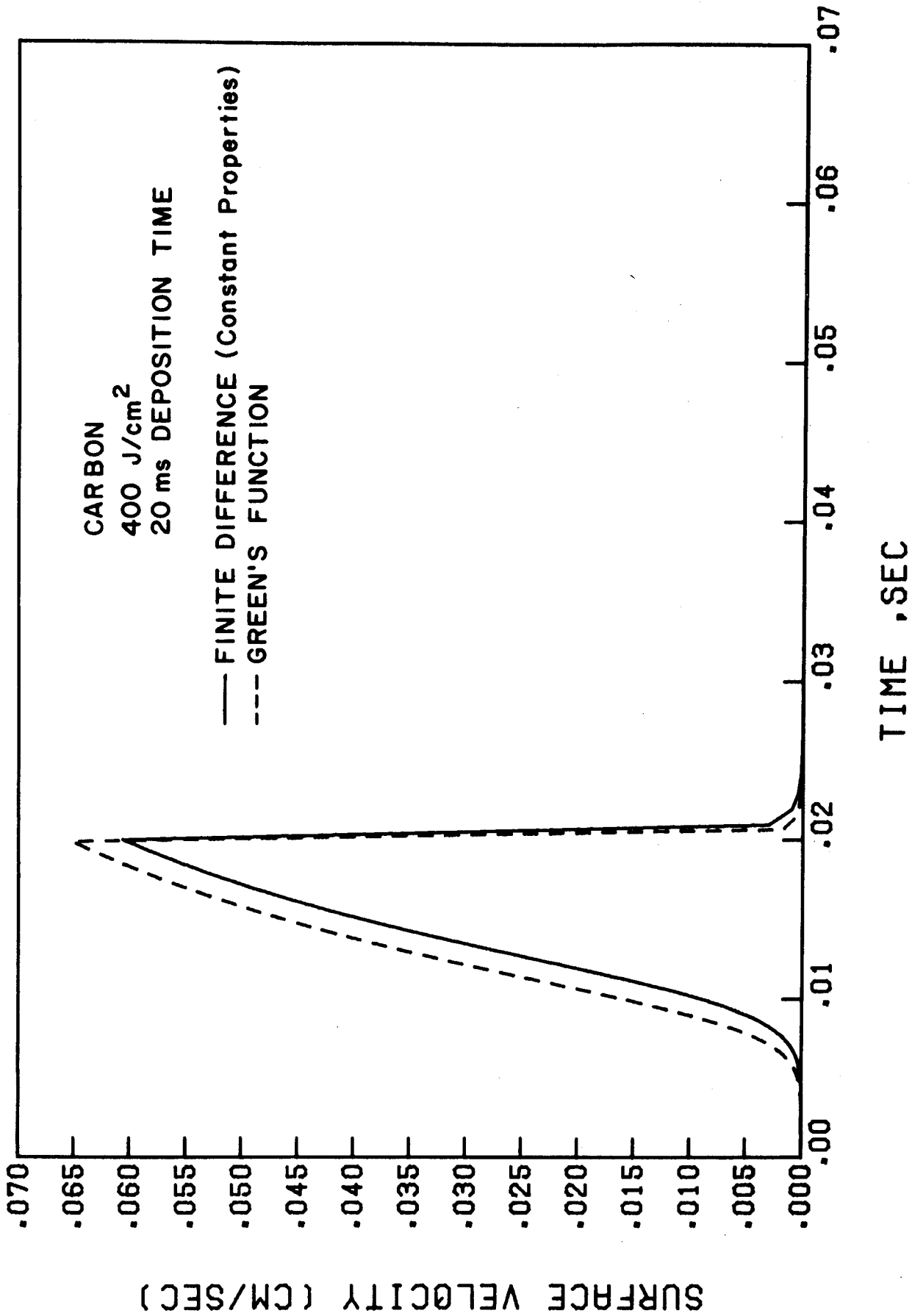


Figure 4 Surface velocity of carbon for 400 J/cm² deposited in 20 ms with finite difference and Green's function methods.

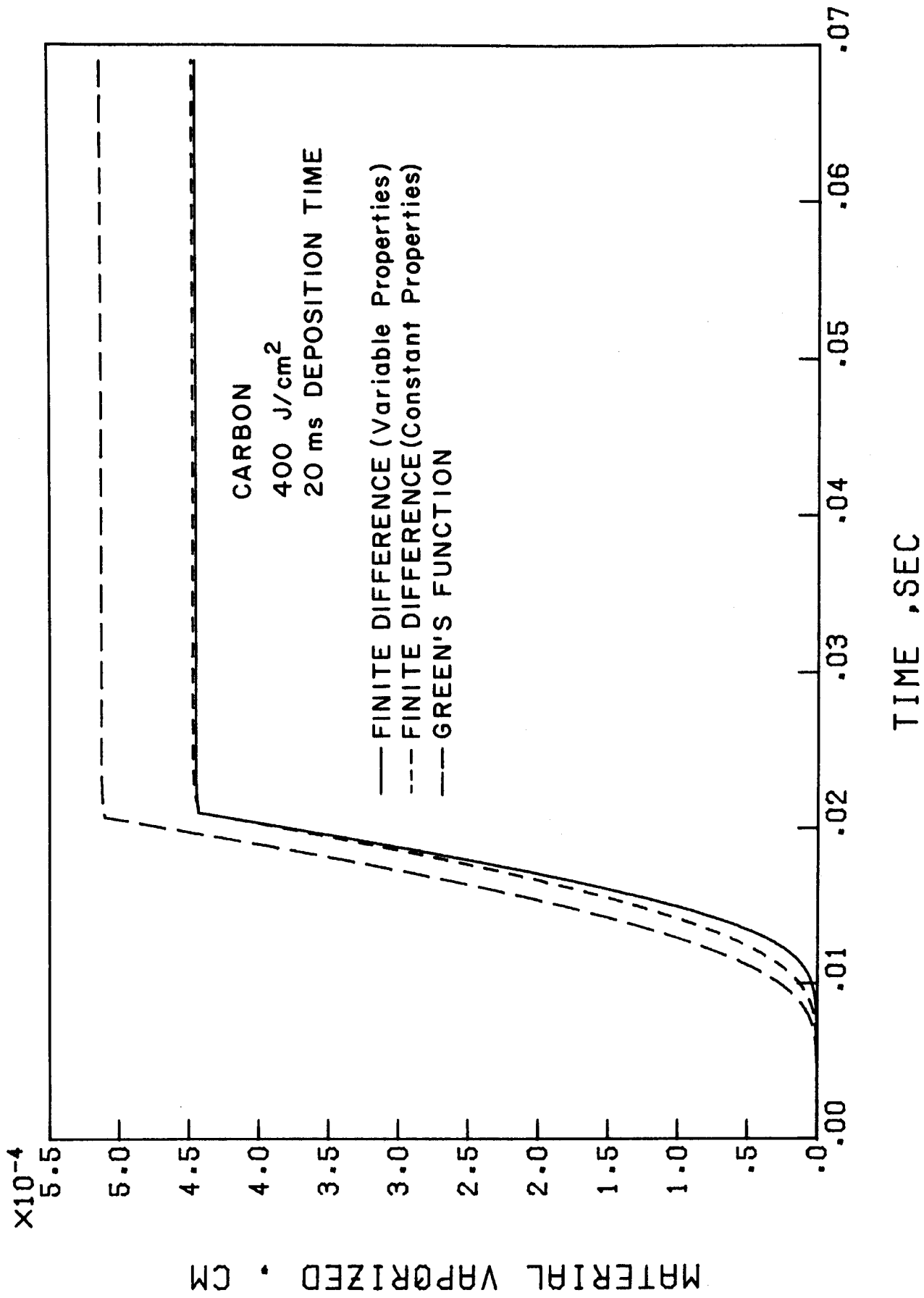


Figure 5 Evaporated material from carbon by different methods.

different methods. The good agreement between both the finite difference methods, i.e. with and without the variation of thermal properties, is not because of the insignificance of the variation of the thermal properties with temperature, but rather because of the chosen value for the constant properties. This can be seen from Fig. 4 where although the velocity of the surface for the variable properties is lower at earlier times of the pulse, it becomes higher than the velocity for the constant properties near the end of the pulse. This has the effect of producing almost equal material vaporized from carbon for these two methods. On the other hand, Fig. 6 shows about 10% higher total material vaporized by the Green's function methods than the finite difference with constant properties. Although the surface temperature calculated using the Green's function is only slightly higher than that calculated by the finite difference and even lower after the end of the disruption time, the strong dependence of the evaporated material on the surface temperature and the integration of the surface velocity over all the pulse duration causes larger differences. After the end of the pulse the temperature drops very fast to where there is no significant vaporization occurring. So the slightly lower surface temperature calculated by the Green's function after the end of the pulse will not affect the total material evaporated.

The temperature distribution inside the bulk of the first wall material is also calculated using the three methods. Figures 7 through 10 show the temperature distribution of carbon at distance $x = 14$ and 70 microns from the surface. Because of the lower temperature inside the material the difference (at $x = 14$ and 70 microns) between the finite difference with variable properties is larger than the difference between the other two methods. The larger the distance into the material the lower the temperature and the larger the

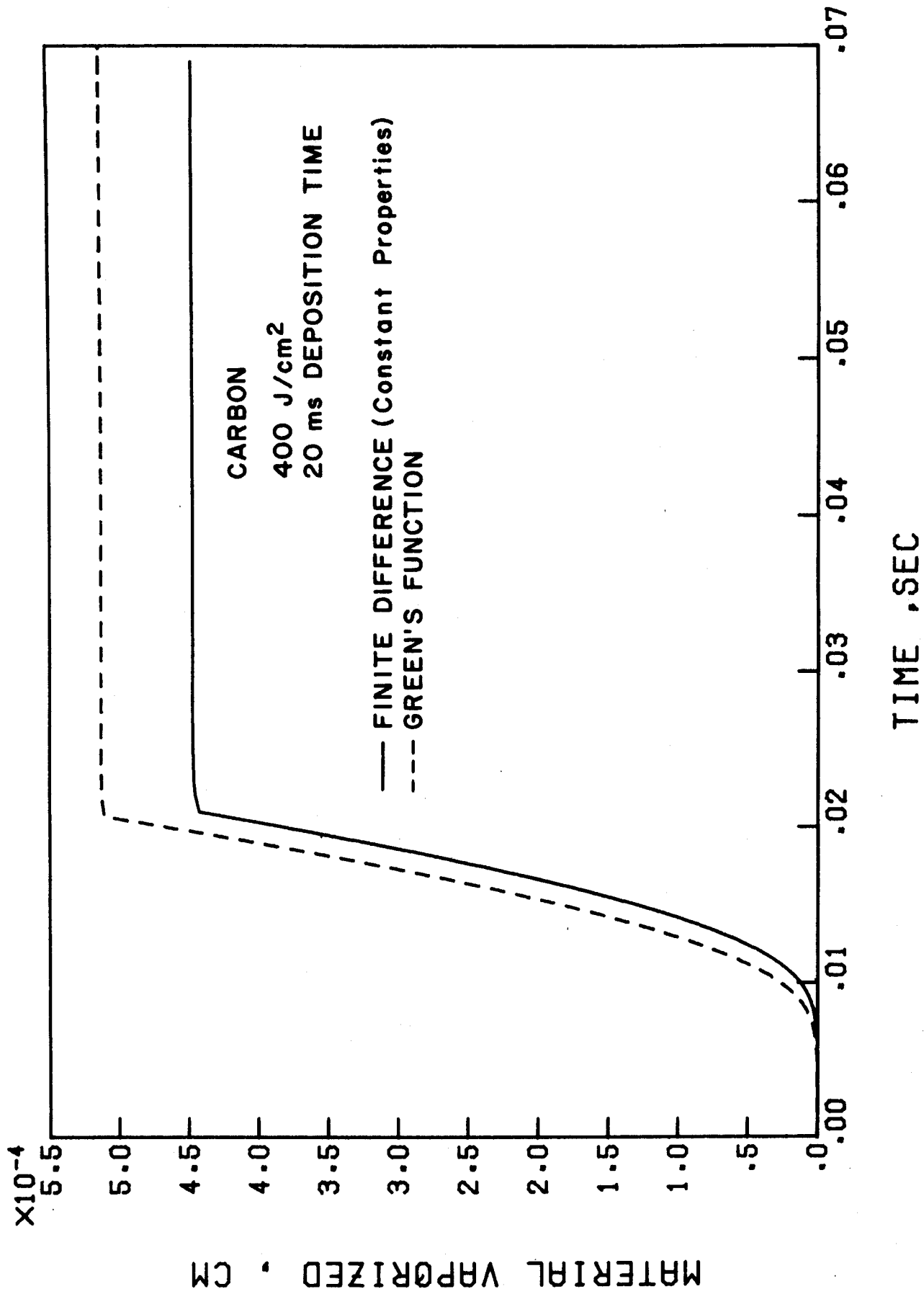


Figure 6 Carbon material evaporated as calculated by finite difference and Green's function methods.

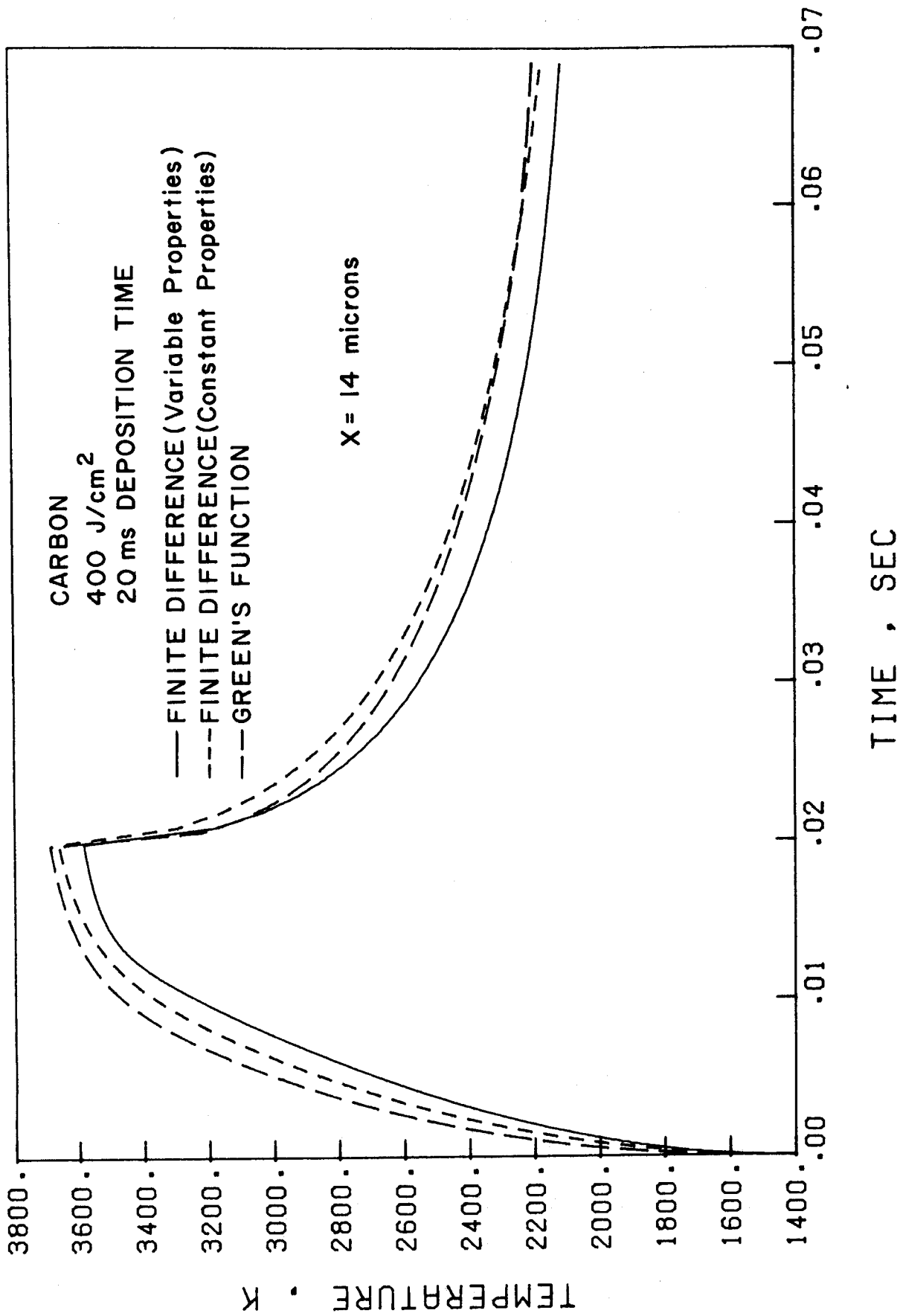


Figure 7 Comparison of temperature rise for carbon for 400 J/cm² deposited in 20 ms by different methods at x = 14 microns.

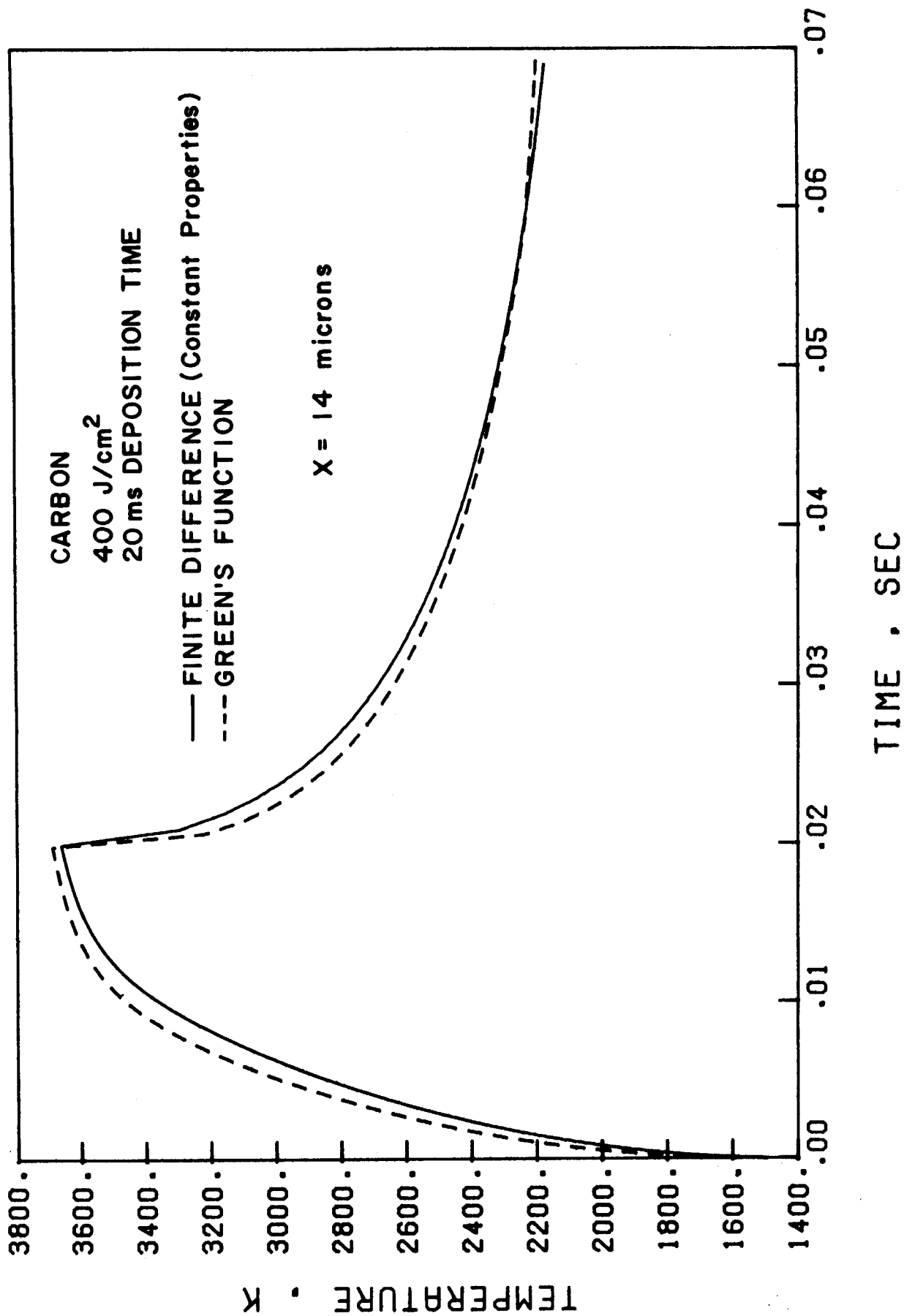


Figure 8 Temperature rise of carbon at $x = 14$ microns by finite difference and Green's function methods.

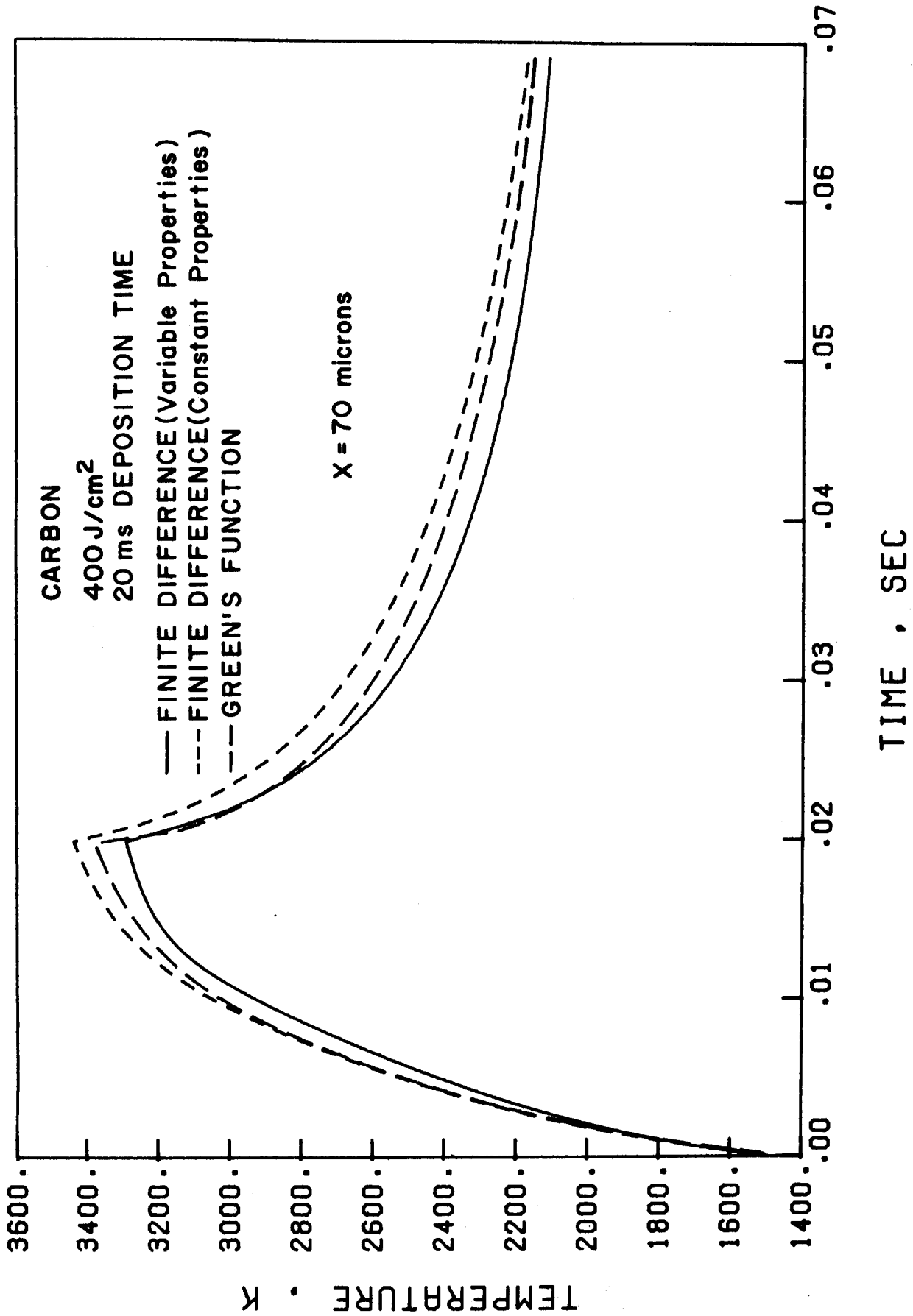


Figure 9 Comparison of temperature rise for carbon for 400 J/cm² deposited in 20 ms by different methods at x = 70 microns.

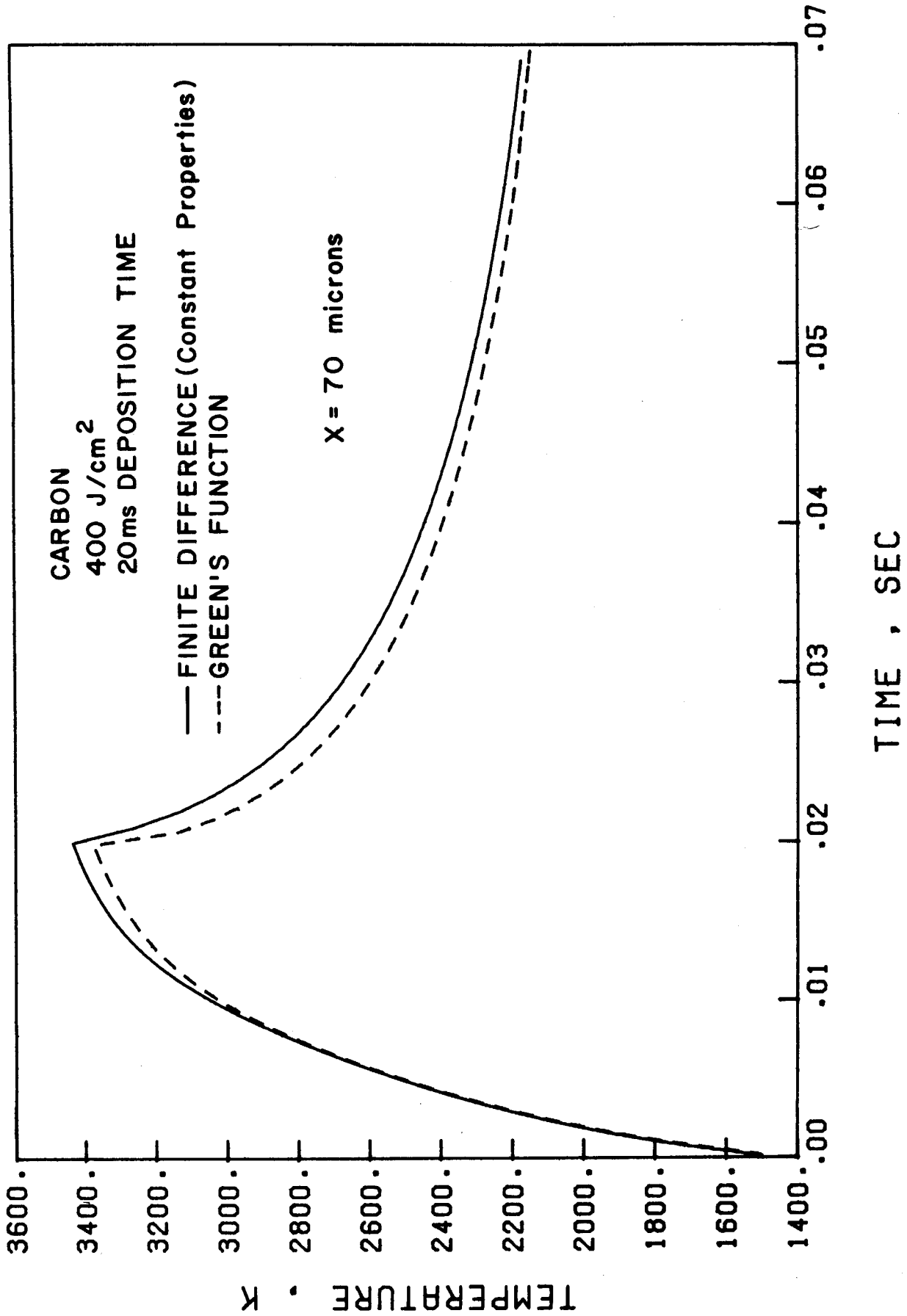


Figure 10 Temperature rise of carbon at $x = 70$ microns by finite difference and Green's function methods.

effect of the thermal properties. The agreement between Green's function and the finite difference with constant properties at larger distances into carbon is still very good as can be seen from Figs. 8 and 10.

E. Conclusions

A method has been developed to solve the heat conduction problem with moving boundaries and other boundary conditions by the use of the Green's function. The agreement of this solution with the method of the finite difference to solve the same problem is seen to be very good. The variation of the thermal properties with temperature can be very important in calculating accurate temperatures, especially in the case of very high energy depositions or if the material undergoes a change of phase. This is because of the larger differences between the solid and liquid phase properties. Because of the highly nonlinear dependence of the receding surface velocity on the surface temperature, a small change in calculating the surface temperature could result in large differences in the surface velocity and consequently larger differences in calculating the total material removed from the surface by evaporation.

Acknowledgment

Support for this work has been provided by the U.S. Department of Energy, Los Alamos National Laboratory, the Japan Atomic Energy Research Institute (JAERI), and the Wisconsin Electric Utilities Research Foundation (WEURF).

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