



**Numerical Methods for Calculating the
Temperature Increase in Inertial Confinement
Fusion Reactor First Walls**

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***FUSION TECHNOLOGY INSTITUTE
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Introduction

The temperature response of a material exposed to thermonuclear radiation may be determined when the time and space dependent energy deposition functions are known. Typically, the Green's function is used to determine the thermal response of the first wall material.⁽¹⁾ The object of this paper is to discuss a new method of using the Green's function to solve the heat conduction equation which avoids the singularities unique to this problem. A comparison is made between this calculation and a previous one⁽²⁾, which did not treat the singularities, and corrections to the previous calculation⁽²⁾ will be presented.

Finally, an approximate analytical solution for the non-linear heat-conduction equation, in which thermal properties vary with temperature, will be discussed.

Direct Deposition Model

The general heat-transfer equation is given by⁽³⁾

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

where: ρ is the density of the material

c is the specific heat

k is the thermal conductivity

and these properties vary with temperature. For the case of constant thermal properties, this equation reduces to:

$$\rho_0 c_0 \frac{\partial T}{\partial t} - k_0 \nabla^2 T = \dot{q}(x,t) \quad (2)$$

where ρ_0 , c_0 , k_0 are independent of temperature.

The general solution for the temperature rise due to any deposition function can be obtained from the theory of Green's functions providing that the thermal properties do not vary with temperature and assuming that the Green's function is known:

$$T(x,t) = \int_{t'} \int_{x'} \frac{1}{\rho c} \dot{q}(x',t') G(x,t,x',t') dx' dt' \quad (3)$$

where: $\dot{q}(x,t)$ is the volumetric energy deposition rate

$G(x,t,x',t')$ is the Green's function.

For a semi-infinite medium, with insulated boundary, the Green's function is given by⁽³⁾

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

where α is the thermal diffusivity.

Unfortunately, problems arise when we try to perform the last integral in Eq. (3) either analytically or numerically. The Green's function possesses a singularity at $t' \rightarrow t$ and $x' \rightarrow x$. A method will be discussed to avoid these singularities when the integration is done analytically or numerically.

First, if we want to integrate analytically, then

$$T(x,t) = \int_{t'=0}^t \int_{x'=0}^{\infty} \frac{1}{\rho c} \dot{q}(x',t') G(x,t,x',t') dx' dt' .$$

At $t' \rightarrow t$ the Green's function has a singularity. To avoid that we integrate from $\int_{t'=0}^{t-\epsilon} + \int_{t-\epsilon}^t$ and take the limit when $\epsilon \rightarrow 0$, i.e.

$$\begin{aligned}
T(x,t) &= \int_0^{t-\epsilon} \int_{x'} \frac{1}{\rho c} \dot{q}(x',t') G(x,t,x',t') dx' dt' \\
&+ \lim_{\epsilon \rightarrow 0} \int_{t-\epsilon}^t \int_{x'} \frac{1}{\rho c} \dot{q}(x',t') G(x,t,x',t') dx' dt' \quad .
\end{aligned} \tag{5}$$

It can be shown that

$$\lim_{\epsilon \rightarrow 0} \frac{1}{2\sqrt{\pi\alpha\epsilon}} e^{-\frac{(x-x')^2}{4\alpha\epsilon}} \rightarrow \delta(x - x') \quad (\text{see Appendix A})$$

since

$$\begin{aligned}
T(x,t) &= \int_0^{t-\epsilon} \int_{x'} \frac{1}{\rho c} \dot{q}(x',t') G(x,t,x',t') dx' dt' \\
&+ \int_{t-\epsilon}^t \int_{x'} \frac{1}{\rho c} \dot{q}(x',t') \lim_{\epsilon \rightarrow 0} G(x,t,x',t') dx' dt' \quad .
\end{aligned} \tag{6}$$

Then the second part of the last integral can be written as:

$$= \int_{t-\epsilon}^t dt' \int_0^{\infty} \frac{1}{\rho c} \dot{q}(x',t') [\delta(x - x') + \delta(x + x')] dx' \tag{7}$$

$$= \int_{t-\epsilon}^t dt' [\dot{q}(x,t') + \dot{q}(-x,t')] \tag{8}$$

where: $\dot{q}(-x,t') = 0$.

Equation (8) then becomes

$$= \int_{t-\epsilon}^t dt' \dot{q}(x,t') \approx \dot{q}(x,t) \int_{t-\epsilon}^t dt \approx \epsilon \dot{q}(x,t) = 0$$

as $\epsilon \rightarrow 0$. Substituting this result into Eq. (6) we find

$$T(x,t) = \int_0^{t-\epsilon} dt' \int_0^{\infty} \frac{1}{\rho c} \dot{q}(x',t') G(x,x',t,t') dx' \quad (9)$$

The last integral can be performed analytically for reasonable deposition functions $\dot{q}(x,t)$, and we can then take the limit when $\epsilon \rightarrow 0$.

In most practical cases, it is difficult to find an easy analytic deposition function so that performing this integration analytically becomes very complicated. This usually means that in order to accommodate different spectra, it is necessary to do the integration numerically. Assuming that we divide space and time into many divisions, the solution for the temperature increase is given by:

$$T(x_n,t_n) = \sum_{t'_i=0}^{t_n} w_i \Delta t_i \int_0^{\infty} \frac{1}{\rho c} \dot{q}(x',t'_i) G(x_n,t_n,x',t'_i) dx' \quad (10)$$

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 will be treated separately, i.e.,

$$\begin{aligned}
T(x_n, t_n) &= \sum_{t'_i=0}^{t_{n-1}} w_i \Delta t_i \int_0^{\infty} dx' \frac{1}{\rho c} \dot{q}(x', t'_i) G(x_n, t_n, x', t'_i) \\
&+ w_n \Delta t_n \lim_{t'_i \rightarrow t_n} \int_0^{\infty} \frac{1}{\rho c} \dot{q}(x', t'_i) \frac{1}{2\sqrt{\pi\alpha(t_n - t'_i)}} \\
&\times \left\{ e^{-\frac{(x_n - x')^2}{4\alpha(t_n - t'_i)}} + e^{-\frac{(x_n + x')^2}{4\alpha(t_n - t'_i)}} \right\} dx' .
\end{aligned} \tag{11}$$

As before,

$$\begin{aligned}
T(x_n, t_n) &= \sum_{t'_i=0}^{t_{n-1}} w_i \Delta t_i \int_0^{\infty} dx' \frac{1}{\rho c} \dot{q}(x', t'_i) G(x_n, t_n, x', t'_i) \\
&+ w_n \Delta t_n \int_0^{\infty} dx' \frac{1}{\rho c} \dot{q}(x', t_n) \{ \delta(x_n - x') + \delta(x_n + x') \}
\end{aligned} \tag{12}$$

$$\begin{aligned}
T(x_n, t_n) &= \sum_{t'_i=0}^{t_{n-1}} w_i \Delta t_i \int_0^{\infty} \frac{1}{\rho c} \dot{q}(x', t'_i) G(x_n, t_n, x', t'_i) dx' \\
&+ w_n \Delta t_n \dot{q}(x_n, t_n) .
\end{aligned} \tag{13}$$

Care should be taken in choosing the time increments. For more accurate results the last time increment should be very small, i.e.

$$\Delta t_n \ll \Delta t_i \quad , \quad i \neq n$$

and

$$t_{n-1} = t_n - \Delta t_n$$

so that the approximation of the Green's function by a δ -function is reasonable.

Thus, by this method we avoided the Green's function singularities and for any given deposition function we can calculate the temperature increase at any point and at any time.

The solution of the last equation (13) is contained in the computer code A*THERMAL⁽⁴⁾. When the deposition function, $\dot{q}(x,t)$, is directly used in the solution it is called the direct deposition method. Since the solutions for different models of the energy deposition discussed by Hunter⁽⁵⁾ in the computer code T*DAMEN⁽⁶⁾ did not contain corrections for these singularities, we have included the complete and correct solution for any deposition function in the code, A*THERMAL.⁽⁴⁾ The modified methods will be discussed here and the difference in the results obtained directly from the deposition function will be illustrated.

Simple Deposition Model

For low energy ions, where the energy loss can be expressed with a modified Lindhard model, the volumetric energy deposition rate can be written as,⁽²⁾

$$\dot{q}(x,t) = f(t) g(x) \tag{14}$$

$$\text{and } \left. \begin{aligned} g(x) &= \left(\frac{A_1}{t} - A_2 x\right) & x < x_{\max} \\ &= 0 & x > x_{\max} \end{aligned} \right\} \tag{15}$$

where $f(t)$ is the incident particle flux

x_{\max} is the maximum range of the ions

A_1, A_2 are constants.

The temperature rise due to this deposition function can be obtained by performing the integral,

$$T(x,t) = \int_{t'} f(t') \int_{x'} \left(\frac{A_1}{t'} - A_2 x' \right) G(x,t,x',t') dx' dt' \quad (16)$$

To solve this integral by methods developed in this paper, the temperature at any point x_n and time t_n is given by

$$T(x_n, t_n) = \sum_{t'=t_i}^{t_{n-1}} w_i f(t_i) \Delta t_i \int_{x'=0}^{x_{\max}} \frac{1}{\rho c} \left(\frac{A_1}{t'} - A_2 x' \right) G(x_n, t_n, x', t') dx' \quad (17)$$

$$+ w_n \Delta t_n f(t_n) \lim_{t' \rightarrow t_n} \int_0^{x_{\max}} \left(\frac{A_1}{t'} - A_2 x' \right) G(x_n, t_n, x', t') dx' \quad .$$

The second integral can be reduced to

$$= w_n \Delta t_n f(t_n) \int_0^{x_{\max}} \left(\frac{A_1}{t'} - A_2 x' \right) \{ \delta(x_n - x') + \delta(x_n + x') \} dx'$$

where $\delta(x + x') = 0$ since $x' > 0$

$$\begin{aligned} &= w_n \Delta t_n f(t_n) \left(\frac{A_1}{t_n} - A_2 x_n \right) && x_n < x_{\max} \\ &= 0 && x_n > x_{\max} \end{aligned} \quad (18)$$

Then the complete solution is given by

$$T(x_n, t_n) = \sum_{t'=t_i}^{t_{n-1}} w_i f(t_i) \Delta t_i \int_{x'=0}^{x_{\max}} \frac{1}{\rho C} \left(\frac{A_1}{t'} - A_2 x' \right) G(x_n, t_n, x', t') dx' \quad (19)$$

$$+ \begin{cases} w_n \Delta t_n f(t_n) \left(\frac{A_1}{t_n} - A_2 x_n \right) & x_n < x_{\max} \\ 0 & x_n > x_{\max} \end{cases}$$

Uniform Deposition Model

The work of Frank et al. (6) considered the response of an infinite half space subject to a uniform spatial and temporal energy deposition as shown in Fig. 1. The solution was only given for the resulting surface temperature as a function of time. Hovingh(7,8) used the same deposition assumption, but evaluated the temperature numerically with the Chart-D Code. The response at any time and position was derived by Hunter,(1) but the numerical solution for the time integral used in the T*DAMEN code did not treat the singularities correctly. In this study, the complete solution using numerical integration for the time integral to allow different spectra is derived below. The deposition function is given by

$$\dot{q}(x, t) = \frac{F(t)}{\delta(t)} \frac{1}{K}$$

where: $F(t)$ = incident energy/unit area

$\delta(t)$ = deposition region

K = deposition duration.

The temperature rise is then give by

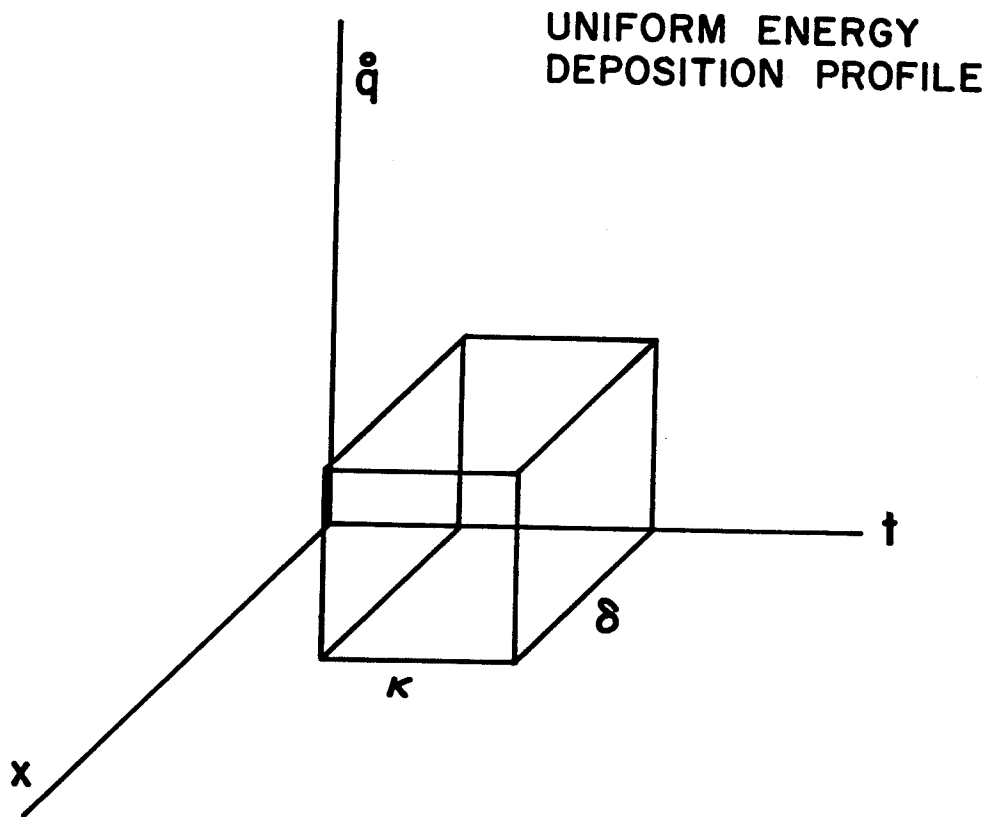


Figure 1

$$T(x,t) = \frac{1}{\rho c} \int_{t'} \frac{f(t')}{K\delta(t')} dt' \int_0^{\delta} G(x,t,x',t') dx' \quad (20)$$

The spatial integral can be reduced to⁽³⁾

$$\int_0^{\delta} G(x,t,x',t') dx' = \frac{1}{2} \left[\operatorname{erf} \left(\frac{\delta - x}{2\sqrt{\alpha(t-t')}} \right) + \operatorname{erf} \left(\frac{\delta + x}{2\sqrt{\alpha(t-t')}} \right) \right] \quad (21)$$

where: erf = error function.

Then,

$$T(x,t) = \frac{1}{2} \frac{1}{\rho c} \int_{t'} \frac{f(t')}{K\delta(t')} \left[\operatorname{erf} \left(\frac{\delta - x}{2\sqrt{\alpha(t-t')}} \right) + \operatorname{erf} \left(\frac{\delta + x}{2\sqrt{\alpha(t-t')}} \right) \right] dt' \quad (22)$$

$$k = t' \quad t < K \quad .$$

Now to integrate numerically with respect to time

$$T(x_n, t_n) = \frac{1}{2} \sum_{t_i=0}^{t_{n-1}} \frac{1}{\rho c} w_i \Delta t_i \frac{f(t_i)}{t_i \delta(t_i)} \left[\operatorname{erf} \left(\frac{\delta - x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) + \operatorname{erf} \left(\frac{\delta + x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) \right] \quad (23)$$

$$+ \frac{1}{2} \frac{1}{\rho c} \frac{f(t_n)}{t_n \delta(t_n)} w_n \Delta t_n \operatorname{Lim}_{t_i \rightarrow t_n} \left\{ \operatorname{erf} \left(\frac{\delta - x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) + \operatorname{erf} \left(\frac{\delta + x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) \right\}$$

since

$$\lim_{t_i \rightarrow t_n} \operatorname{erf} \left(\frac{\delta - x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) = \begin{cases} \operatorname{erf}(\infty) = 1 & \text{if } x_n < \delta \\ \operatorname{erf}(-\infty) = -1 & \text{if } x_n > \delta \end{cases}$$

and $\lim_{t_i \rightarrow t_n} \operatorname{erf} \left(\frac{\delta + x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) = \operatorname{erf}(\infty) = 1$

and the last term reduces to

$$\begin{aligned} &= \frac{1}{\rho c} w_n \Delta t_n \frac{f(t_n)}{K\delta(t_n)} & x_n < \delta \\ &= 0 & x_n > \delta \end{aligned}$$

This result could also be obtained directly from the Green's function since

$$\lim_{t_i \rightarrow t_n} \int_0^{\delta} G(x_n, t_n, x', t_i) dx' = \int_0^{\delta} \{\delta(x_n - x') + \delta(x_n + x')\} dx' = 1$$

Then, the temperature rise is given by

$$T(x_n, t_n) = \frac{1}{2} \frac{1}{\rho c} \sum_{t_i=0}^{t_n-1} w_i \Delta t_i \frac{f(t_i)}{K\delta(t_i)} \left[\operatorname{erf} \left(\frac{\delta - x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) + \operatorname{erf} \left(\frac{\delta + x_n}{2\sqrt{\alpha(t_n - t_i)}} \right) \right]$$

$$\begin{aligned} &\frac{1}{\rho c} w_n \Delta t_n \frac{f(t_n)}{K\delta(t_n)} & x_n < \delta & \quad (24) \\ &+ \{ \\ &0 & x_n > \delta \end{aligned}$$

General Deposition Model

In this model, first developed by Hunter,⁽²⁾ the deposition function is transformed into the general form of a polynomial with coefficients determined by the energy of the ion, i.e.,

$$\dot{q}(x,t) = f(t) g(x) \quad (25)$$

where

$$g(x) = \sum_{i=0}^4 C_i x^i \quad (26)$$

and C_i are in general functions of time. The solution for the temperature will be given by

$$T(x,t) = \int_{t'} f(t') \int_{x'} \frac{1}{\rho c} \left(\sum_{i=0}^4 C_i x'^i \right) G(x,t,x',t') dx' dt' . \quad (27)$$

The spatial integral becomes the evaluation of the following sequence

$$S_i = \frac{C_i}{\sqrt{\pi}} \int \left(\frac{x'^i}{A} e^{-\frac{(x'-x)^2}{A^2}} + \frac{x'^i}{A} e^{-\frac{(x'+x)^2}{A^2}} \right) dx' \quad (28)$$

where

$$A = 2\sqrt{\alpha(t-t')} .$$

The solutions for these S_i integrals are given in reference (9). The complete solution for the temperature rise is then

$$T(x,t) = \int dt' \frac{f(t')}{\rho c} \frac{1}{\sqrt{\pi}} \sum C_i S_i \Big| \text{evaluated at limits of } x' . \quad (29)$$

The spatial contribution is contained in the evaluation of the function $\sum C_N S_N$ at the limits of the deposition region while the temporal contribution can be done numerically to allow for arbitrary spectra.

In the general deposition profile, the deposition function is divided into three regions as shown in Fig. 2. Each region has different coefficients C_i 's. The temperature rise can be written as

$$T(x,t) = \int dt' \frac{f(t')}{\rho c} \frac{1}{\sqrt{\pi}} \left\{ \sum_{i=0}^4 C_{1i} S_i \Big|_{III} + \sum_{i=0}^4 C_{2i} S_i \Big|_{II} + \sum_{i=0}^4 C_{3i} S_i \Big|_{I} \right\} \quad (30)$$

where: C_{1i} = the coefficient of the deposition function in region I

$S_i|_I$ = the value of the function S_i at the limits of region I.

It is now possible to integrate numerically over time by the methods developed in this paper. The temperature rise at any point x_n and time t_n is given by

$$T(x_n, t_n) = \frac{1}{\rho c} \sum_{t_i=0}^{t_n-1} w_i \Delta t_i f(t_i) \left\{ \sum_{i=0}^4 C_{3i} S_i \Big|_{x'=x_M} + \sum_{i=0}^4 C_{2i} S_i \Big|_{x'=x_H} + \sum_{i=0}^4 C_{1i} S_i \Big|_{x'=x_L} \right\} + \frac{1}{\rho c} w_n \Delta t_n f(t_n) \lim_{t_i \rightarrow t_n} \int g(x') G(x_n, t_n, x', t') dx' \quad (31)$$

The second integral can be written as:

GENERAL ENERGY DEPOSITION PROFILE

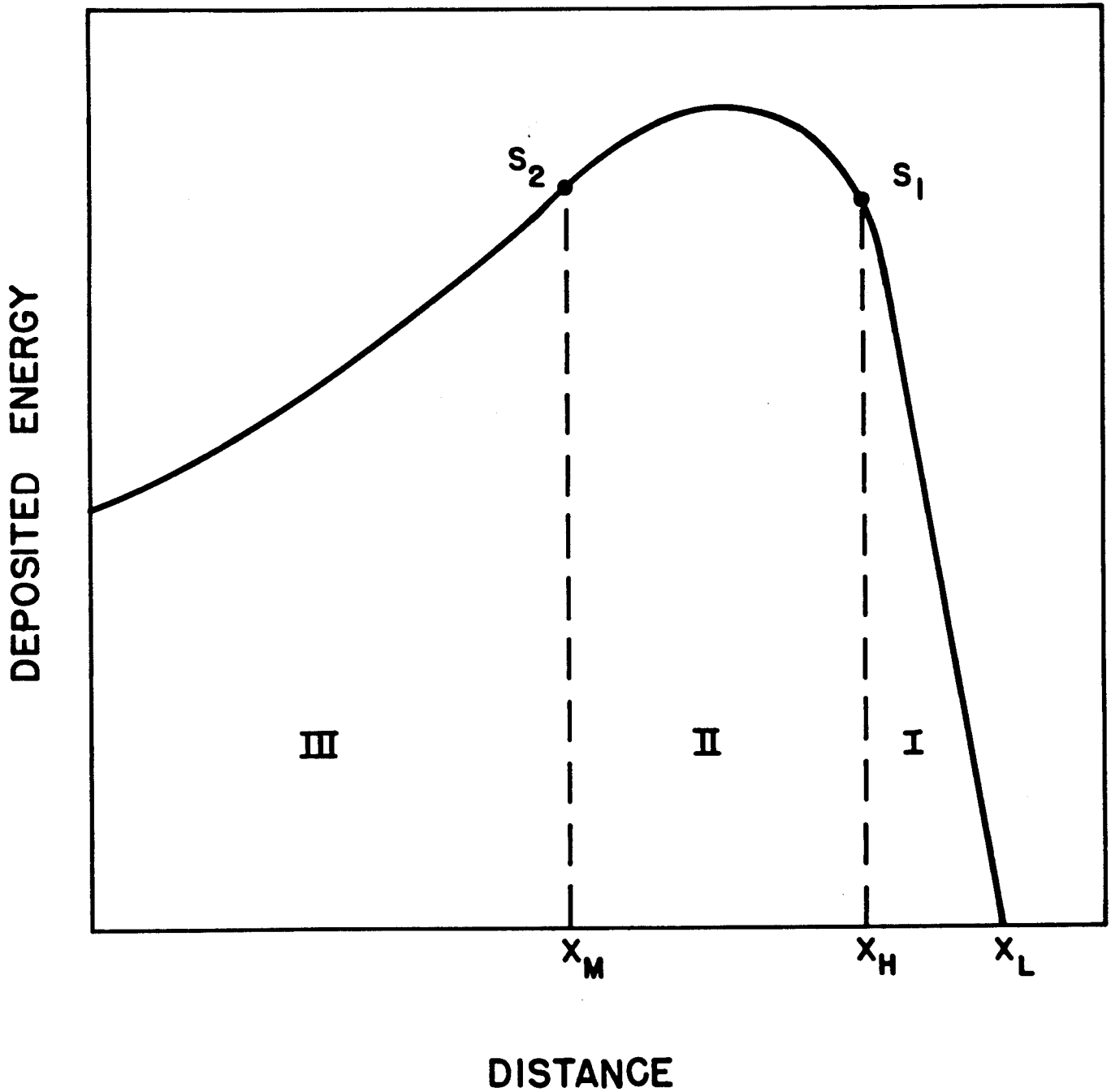


Figure 2

$$\begin{aligned}
&= \frac{1}{\rho C} w_n \Delta t_n f(t_n) \left\{ \left(\int_0^{x_M} \sum_i C_{3i} x'^i + \int_{x_M}^{x_H} \sum_i C_{2i} x'^i \right. \right. \\
&\quad \left. \left. + \int_{x_H}^{x_L} \sum_i C_{1i} x'^i \right) \delta(x' - x_n) dx' \right. \\
&= \frac{1}{\rho C} w_n \Delta t_n f(t_n) \left[\left\{ \begin{array}{ll} \sum_{i=0}^4 C_{3i} x_n^i & 0 < x_n < x_M \\ 0 & \text{otherwise} \end{array} \right\} \right. \\
&\quad \left. + \left\{ \begin{array}{ll} \sum_i C_{2i} x_n^i & x_M < x_n < x_H \\ 0 & \text{otherwise} \end{array} \right\} \right. \\
&\quad \left. + \left\{ \begin{array}{ll} \sum_i C_{1i} x_n^i & x_H < x_n < x_L \\ 0 & \text{otherwise} \end{array} \right\} \right] . \quad (32)
\end{aligned}$$

Results and Conclusions

In this section, we compare the differences between the methods developed in this paper with previous calculations.^(1,2) Two examples are considered in this study. In these examples we calculate the thermal response of a material, for example a first wall in an inertial confinement fusion reactor, due to a given spectrum of incident ions.

In the first example we considered hydrogen ions with a 5 keV Maxwellian spectrum incident on an aluminum wall. Figure 3 shows the energy deposition rate of hydrogen ions into aluminum. It can be seen that the range of hydrogen is about 0.3 micron. Figure 4 shows a comparison of the time dependent

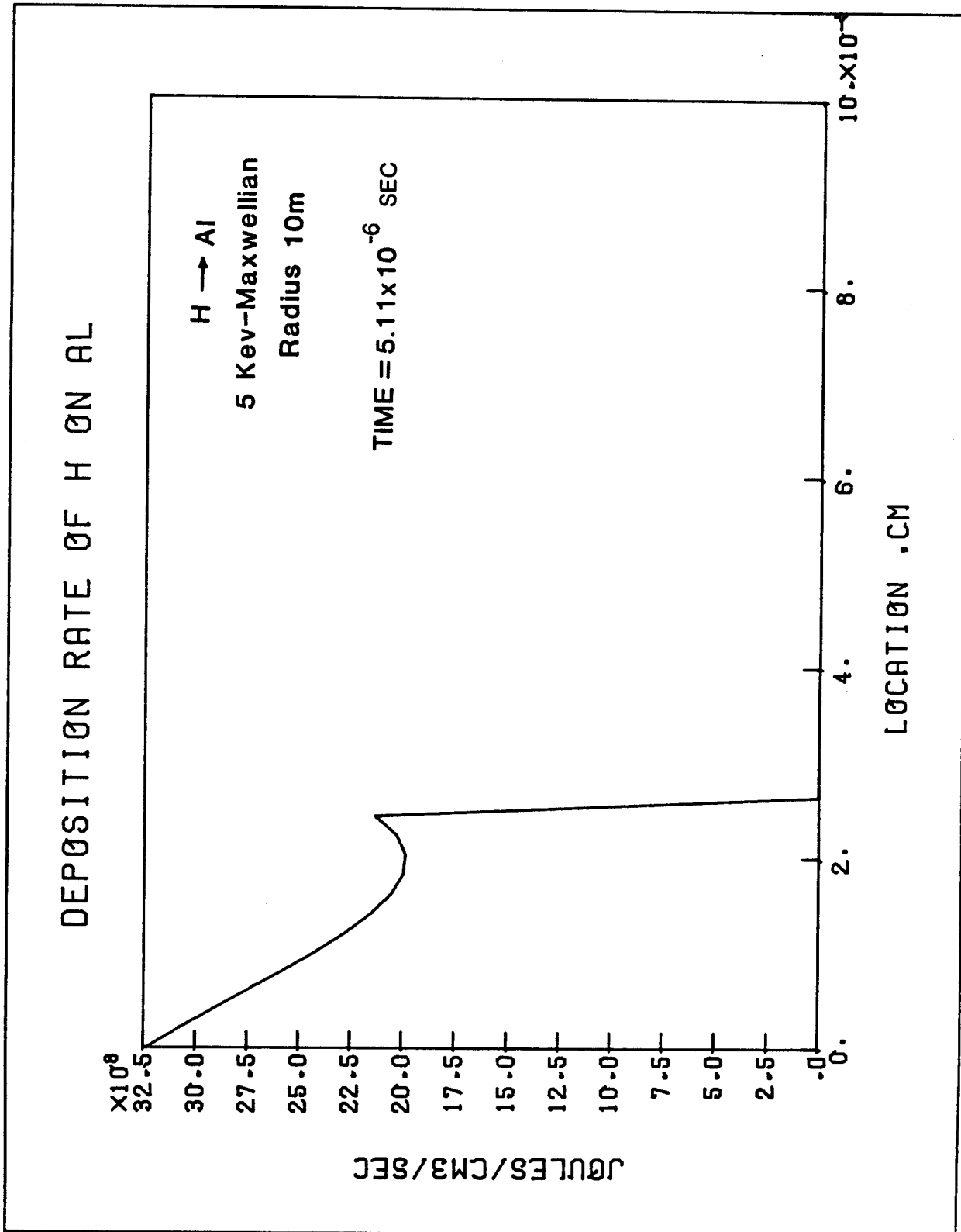


Figure 3

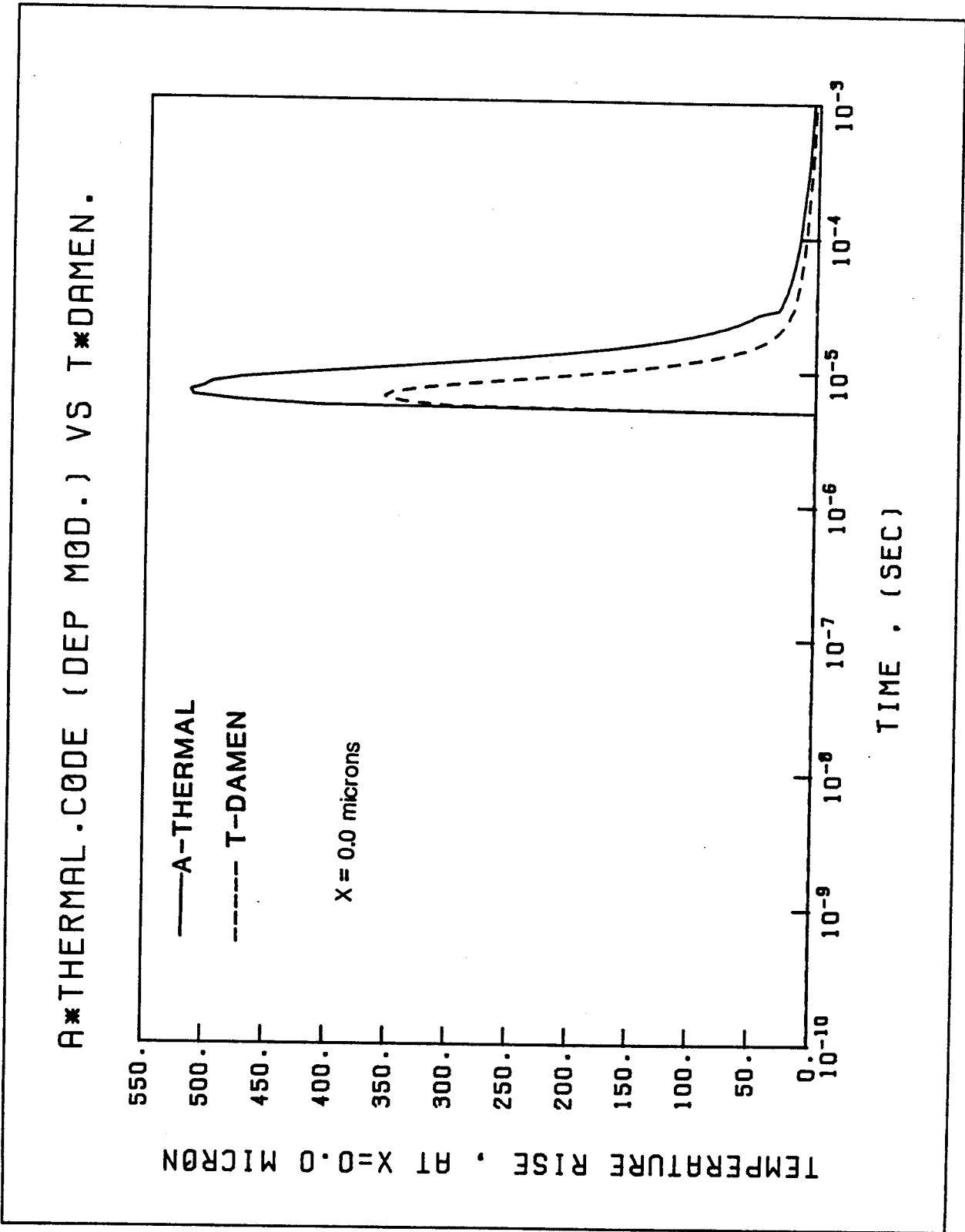


Figure 4

temperature response of the Al surface as predicted by the A*THERMAL and T*DAMEN codes. The same deposition function given in Fig. 1 was used by the two codes. The difference between the two codes with respect to the peak temperature rise at the surface is about 30%, being lower for the T*DAMEN code. The direct deposition model, developed earlier in this paper, was used to compare with the general deposition model of T*DAMEN.

Figure 5 shows a comparison between the codes A*THERMAL and T*DAMEN both using the simple deposition model discussed before. A*THERMAL, using the correct solution of the simple deposition model, yields almost the same result as the direct deposition model shown in Fig. 4. Again the T*DAMEN estimation is about 30% lower than that predicted by the A*THERMAL code. As mentioned before, these differences arise from the improper treatment of the Green's function singularities when integrating numerically over time.

Figure 6 shows a comparison between the direct deposition model and the correct solution of the simple and the general deposition models, developed in this paper. The agreement among these different models is fairly good except that the simple deposition model underestimates the temperature rise at later times because of the simplicity of the model.

A comparison between the codes A*THERMAL and T*DAMEN in calculating the temperature rise at 0.5 micron (beyond the end of range of the hydrogen) from the Al surface is shown in Fig. 7. The comparison is made using the same model, i.e., the simple deposition model. It is noted that at $x = 0.5$ micron, both codes agree fairly well. This can be explained by noting from Fig. 3 that there is no deposition at $x = 0.5$ micron and all hydrogen ions are stopped within a distance of 0.3 micron. This means that

A*THERMAL . VS T*DAMEN . CODE (MOD . 1)

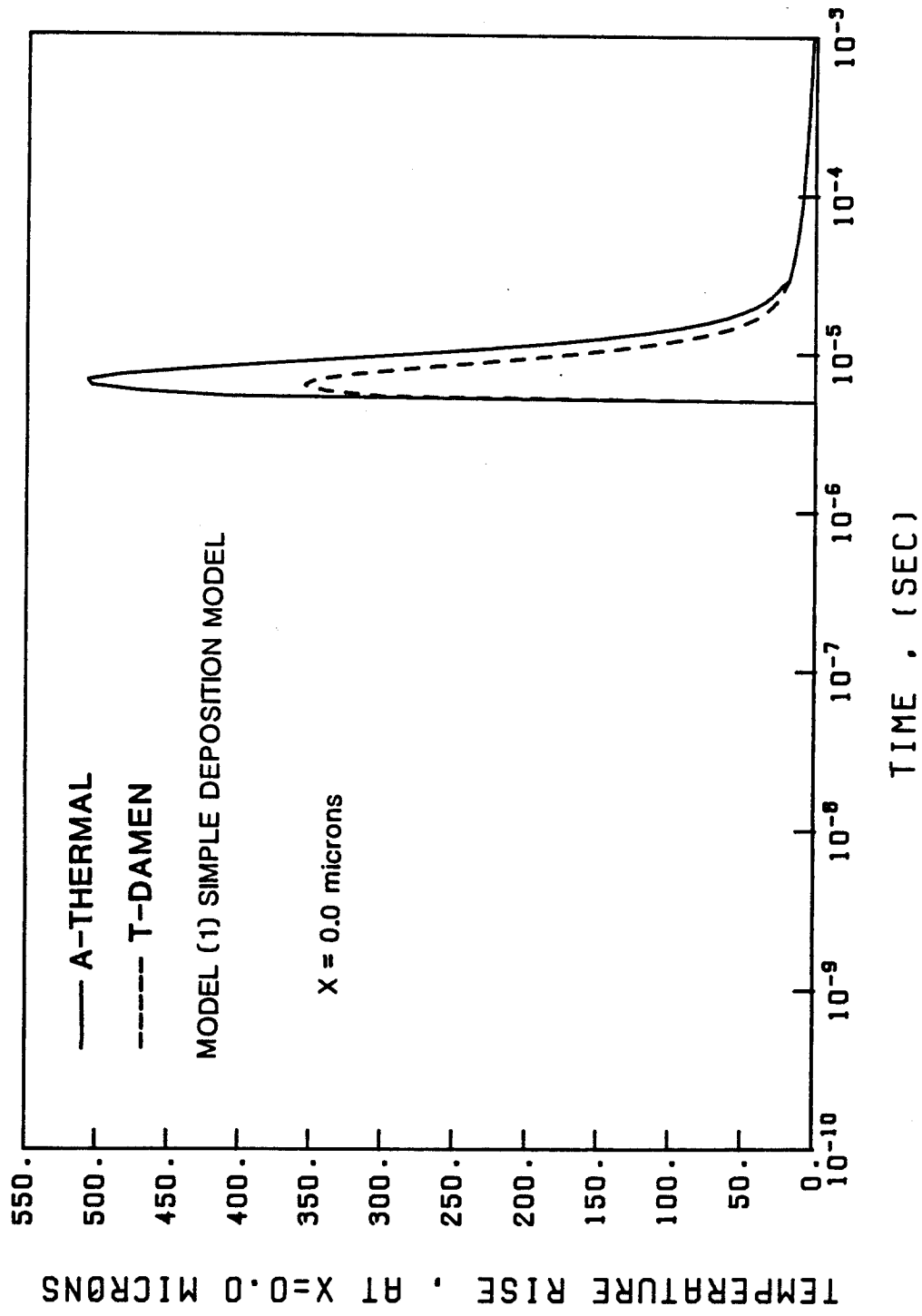


Figure 5

A* THERMAL CODE (DIFFERENT MODELS)

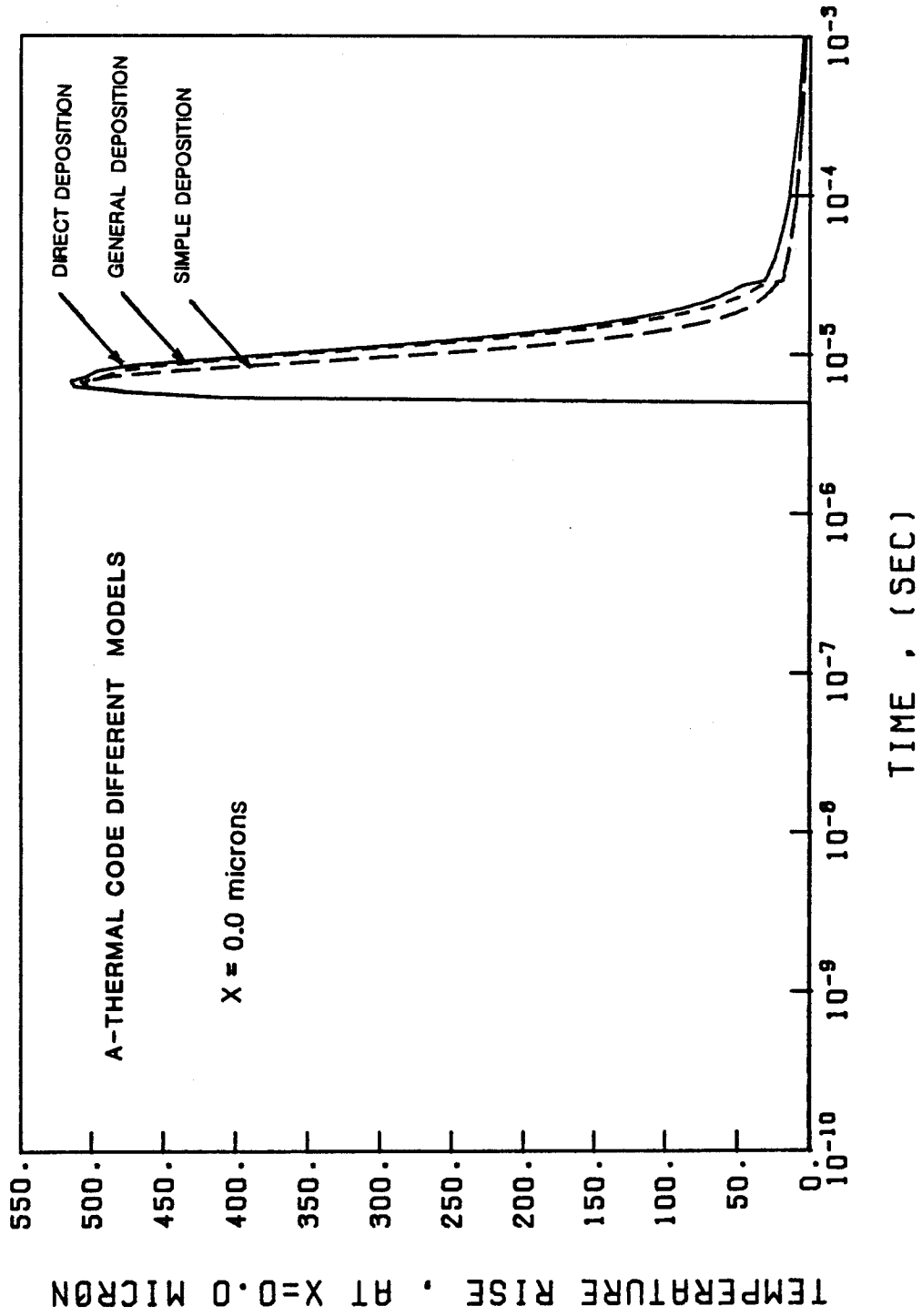


Figure 6

A* THERMAL . VS T* DAMEN . CODE (MOD. 1)

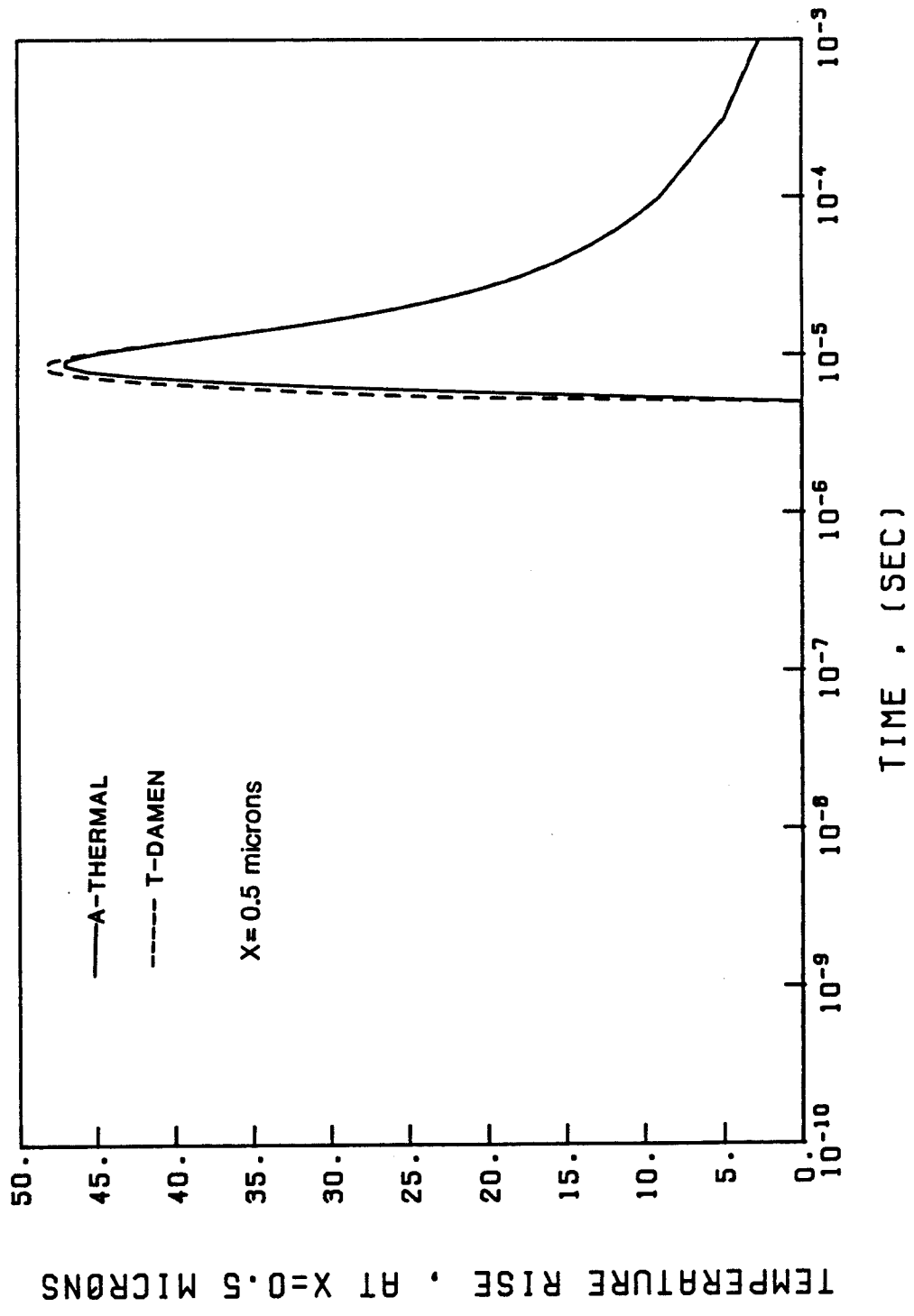


Figure 7

$$\dot{q}(x = 0.5 \text{ micron}, t) = 0$$

and the correction due to the Green's function singularity goes to zero.

Another example to illustrate these differences uses Ta ions incident on an Al wall. The tantalum spectrum is assumed to be 905 keV Maxwellian. Figure 8 shows the energy deposition rate as a function of distance into Al wall and Fig. 9 shows the deposition rate as a function of time. In this calculation of the temperature rise of Al, it is assumed that no phase change takes place, i.e., as if Al were to stay as a solid; phase change and vaporization are currently under consideration. Figure 10 represents the temperature rise of an Al first wall surface as calculated from the codes A*THERMAL and T*DAMEN. In these cases T*DAMEN overestimates the temperature rise by about 20%, compared to an underestimation of about 30% due to incident hydrogen ions. This is again because of the improper treatment of the Green's function singularities. Figure 11 shows a comparison between the direct deposition model and the modified general deposition model in the A*THERMAL code. The agreement is very good.

Approximate Solution for the Nonlinear Heat Conduction Equation Using the Methods of Green's Function

In this section, we consider the case where the thermal properties vary with temperature. In most cases, it is a good approximation to assume that the thermal properties, i.e. thermal conductivity and specific heat vary linearly with temperature,

$$k = k_0(1 + bT) \tag{33}$$

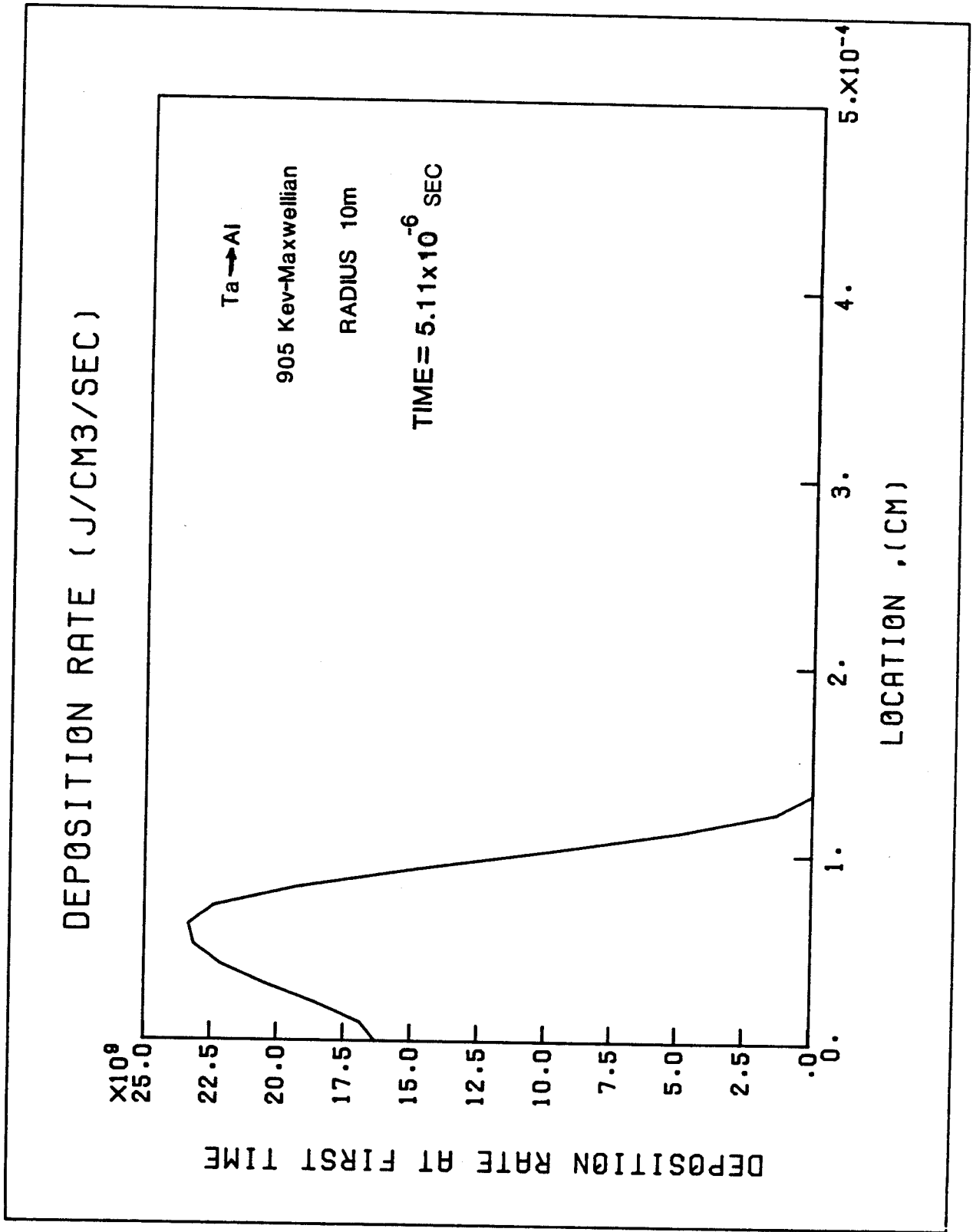


Figure 8

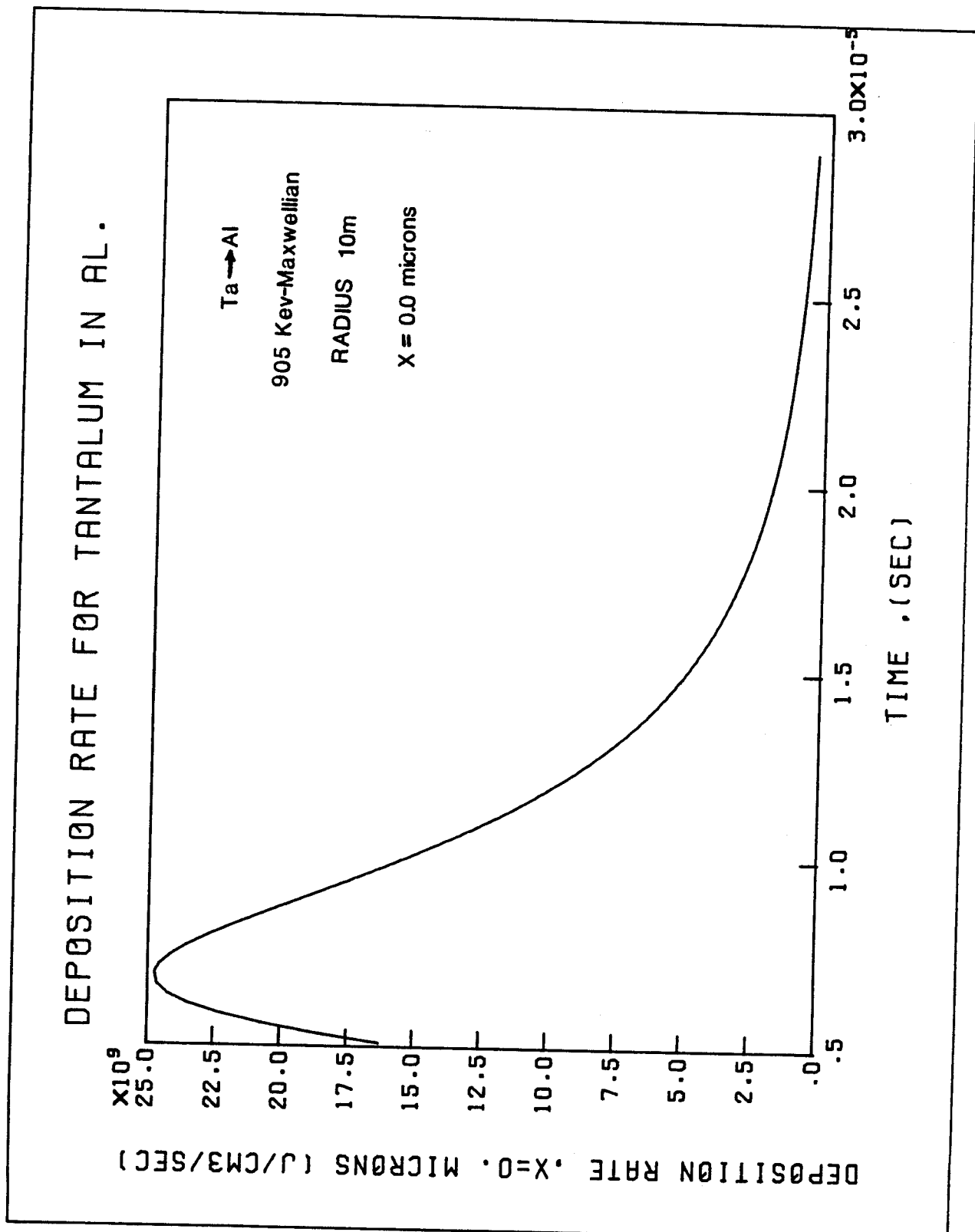


Figure 9

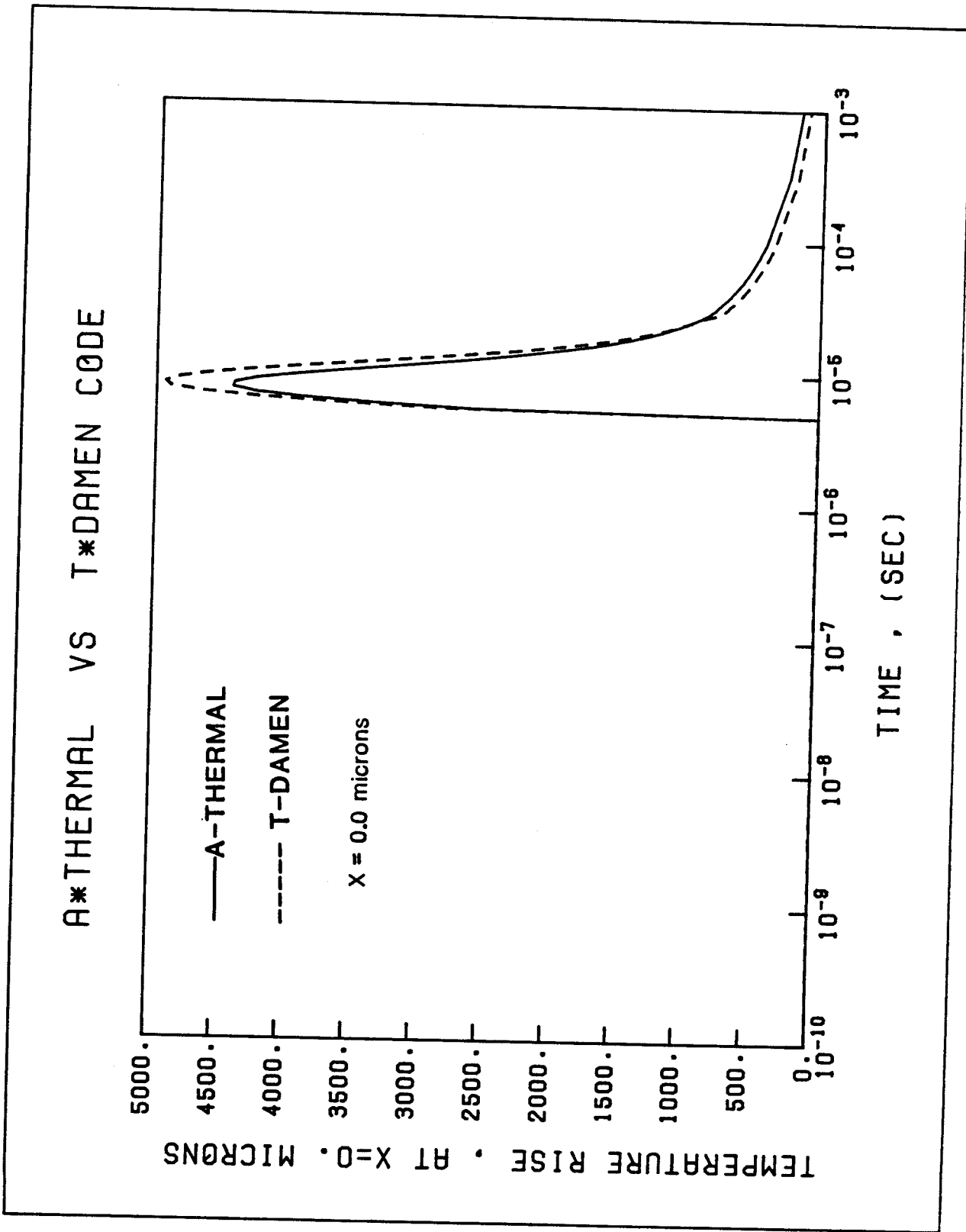


Figure 10

A* THERMAL CODE (DEP MOL VS GEN MOD)

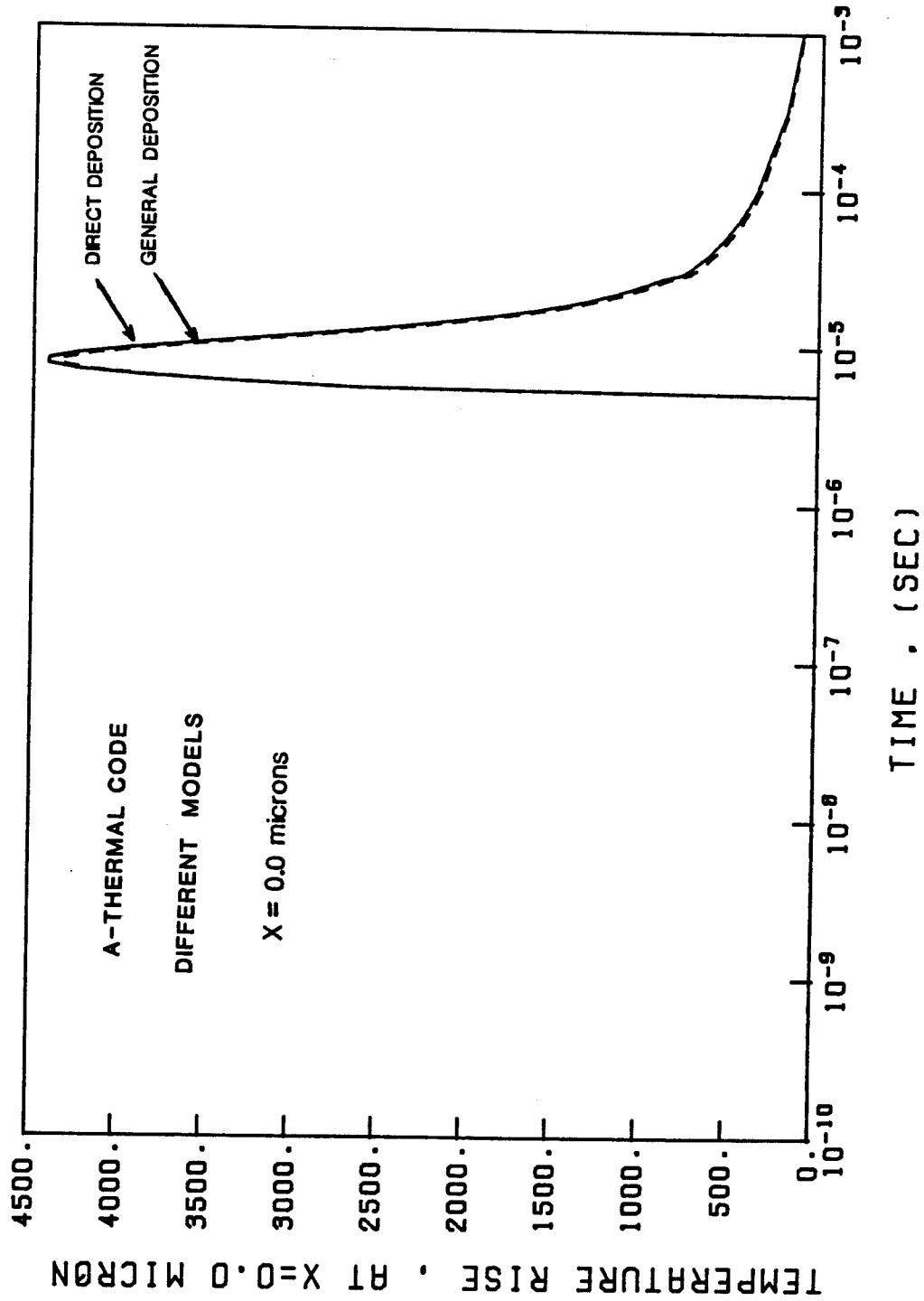


Figure 11

$$C = C_0(1 + aT) \quad (34)$$

where a, b are constants. If the density ρ varies too with temperature, we can use

$$\rho C = \rho_0 C_0(1 + a_1 T) \quad .$$

Substituting Eqs. (33) and (34) into Eq. (1) yields

$$\rho C_0(1 + aT) \frac{\partial T}{\partial t} - k_0 \nabla \cdot (1 + bT) \nabla T = \dot{q}(x, t)$$

$$\rho C_0 \frac{\partial T}{\partial t} - k_0 \nabla^2 T = \dot{q}(x, t) + [bk_0 \nabla \cdot (T \nabla T) - a\rho C_0 T \frac{\partial T}{\partial t}]$$

$$\text{or} \quad \rho C_0 \frac{\partial T}{\partial t} - k_0 \nabla^2 T = \dot{q}(x, t) + bf_1(x, t) - af_2(x, t) \quad (35)$$

where

$$f_1(x, t) = k_0 \nabla \cdot (T \nabla T) = k_0 [T \nabla^2 T + (\nabla T)^2] \quad (36)$$

$$f_2(x, t) = \rho C_0 T \frac{\partial T}{\partial t} = \rho C_0 T \dot{T} \quad . \quad (37)$$

Using first order perturbation methods^(10,11) the solution of Eq. (35) can be obtained by analogy to the solution of Eq. (2). That is

$$T_1(x, t) = T(x, t) + bF_1(x, t) - aF_2(x, t) \quad (38)$$

where $T(x,t)$ is the solution for the heat conduction equation with constant thermal properties, i.e.

$$T(x,t) = \int_{t'} \int_{x'} \frac{\dot{q}(x',t')}{\rho C_0} G(x,t,x',t') dx' dt' \quad (39)$$

$$F_1(x,t) = \alpha_0 \int_{t'} \int_{x'} \nabla \cdot (T_1 \nabla T_1) G(x,t,x',t') dx' dt' \quad (40)$$

$$F_2(x,t) = \int_{t'} \int_{x'} T_1(x',t') \dot{T}_1(x',t') G(x,t,x',t') dx' dt' \quad (41)$$

where $\alpha_0 = \frac{k_0}{\rho C_0}$.

Since $F_1(x,t)$ and $F_2(x,t)$ are functions of $T_1(x,t)$ which is not known, these integrals cannot be performed. However, it is a good approximation to set $T_1(x,t) = T(x,t)$ in these integrals, i.e. the solution for the same equation but for constant properties. This solution $T(x,t)$ is usually known exactly for many cases in heat conduction.

So, substituting $T_1(x,t) = T(x,t)$ in Eqs. (40), (41) yields

$$F_1(x,t) \approx \alpha_0 \int_{t'} \int_{x'} \nabla \cdot (T \nabla T) G(x,t,x',t') dx' dt' \quad (42)$$

$$F_2(x,t) \approx \int_{t'} \int_{x'} T(x',t') \dot{T}(x',t') G(x,t,x',t') dx' dt' \quad (43)$$

To simplify the term $\nabla \cdot (T \nabla T)$ in Eq. (42), we make use of the vector relations⁽¹³⁾

$$\nabla \cdot \psi a = a \nabla \psi + \psi \nabla \cdot a$$

i.e.

$$G \nabla \cdot (T \nabla T) = \nabla \cdot (G T \nabla T) - T \nabla T \nabla G$$

also

$$\int_{\text{vol.}} G \nabla \cdot (T \nabla T) dx' = \int_{\text{vol.}} \nabla \cdot (G T \nabla T) dx' - \int_{\text{vol.}} T \nabla T \nabla G dx' .$$

But

$$\int_{\text{vol.}} \nabla (G T \nabla T) dv = \oint_{\text{surface}} G T \nabla T ds$$

assuming that we have an insulated face, i.e. $\nabla T(0,t) = 0$. Then,

$$\int_{\text{vol.}} \nabla (G T \nabla T) dv = \oint G T \nabla T ds = 0 .$$

So, the function $F_1(x,t)$ reduces to

$$F_1(x,t) = - \alpha_0 \int_{t'} \int_{x'} T(x',t') \nabla T(x',t') \nabla G(x,t,x't') dx' dt' \quad (44)$$

which is now easier to calculate. Substituting in Eq. (38), the first order solution to account for variation of thermal properties with temperature is given by

$$\begin{aligned}
T_1(x,t) = T(x,t) - b\alpha_0 \int_{t'} \int_{x'} T(x',t') \nabla T(x',t') \nabla G(x,t,x',t') dx' dt' \\
- a \int_{t'} \int_{x'} T(x',t') \dot{T}(x',t') G(x,t,x',t') dx' dt' .
\end{aligned}
\tag{45}$$

Now to solve the last equation numerically using the techniques discussed earlier, we will integrate both integrals numerically over time from $t_i = 0$ to $t_i = t_{n-1}$, and the last term will be treated separately, i.e.

$$\begin{aligned}
F_1(x_n, t_n) &= \sum_{t_i=0}^{t_{n-1}} w_i \Delta t_i \int_{x'} T(x',t') \nabla T(x',t') \nabla G(x,t,x',t') dx' \\
&+ \lim_{t_i \rightarrow t_n} w_n \Delta t_n \int_{x'} T(x',t') \nabla T \nabla G dx' \\
&= \dots + w_n \Delta t_n \int_{x'} T(x',t') \nabla T \lim_{t_i \rightarrow t_n} \nabla G dx'
\end{aligned}
\tag{46}$$

from the theory of δ -functions:

$$\lim_{t_i \rightarrow t_n} \nabla G \rightarrow \nabla \delta(x_n - x')$$

$$F_1(x_n, t_n) = \dots + w_n \Delta t_n \int T(x',t') \nabla T(x',t') \nabla \delta(x_n - x') dx'$$

$$\int f(x') \nabla \delta(x - x') dx' = \nabla f(x)$$

$$F_1(x_n, t_n) = \dots + w_n \nabla t_n \nabla (T(x_n, t_n) \nabla T(x_n, t_n))
\tag{47}$$

from vector relationships⁽¹²⁾

$$\nabla(\mathbf{a} \cdot \mathbf{b}) = (\mathbf{a} \cdot \nabla)\mathbf{b} + (\mathbf{b} \cdot \nabla)\mathbf{a} + \mathbf{a} \times (\nabla \times \mathbf{b}) + \mathbf{b} \times (\nabla \times \mathbf{a})$$

last two terms equal 0 for one dimensional geometry, i.e.

$$\nabla(\mathbf{T} \cdot \nabla \mathbf{T}) = \mathbf{T} \cdot \nabla \nabla \mathbf{T} + \nabla \mathbf{T} \cdot \nabla \mathbf{T}$$

$$= \mathbf{T} \nabla^2 \mathbf{T} + (\nabla \mathbf{T})^2$$

$$\text{and } \nabla^2 \mathbf{T} = \frac{1}{\alpha_0} \dot{\mathbf{T}}(x,t) - \dot{\mathbf{q}}(x,t)/k_0 \quad .$$

Substituting in $F_1(x,t)$, yields

$$\begin{aligned} F_1(x_n, t_n) &= \sum_{t_i=0}^{t_{n-1}} w_i \Delta t_i \int_{x'} \mathbf{T}(x', t') \nabla \mathbf{T}(x', t') \nabla G(x, t, x', t') dx' \\ &+ w_n \Delta t_n \left\{ \left[\frac{1}{\alpha_0} \mathbf{T}(x_n, t_n) \dot{\mathbf{T}}(x_n, t_n) - \frac{\dot{\mathbf{q}}(x_n, t_n) \mathbf{T}(x_n, t_n)}{k_0} \right] \right. \\ &\left. + (\nabla \mathbf{T}(x_n, t_n))^2 \right\} \quad . \end{aligned} \quad (48)$$

And for the second integral, i.e.

$$\begin{aligned} F_2(x, t) &= \int_{t'} \int_{x'} \mathbf{T}(x', t') \dot{\mathbf{T}}(x', t') G(x, t, x', t') dx' dt' \\ F_2(x_n, t_n) &= \sum_{t_i=0}^{t_{n-1}} w_i \Delta t_i \int_{x'} \mathbf{T}(x', t') \dot{\mathbf{T}}(x', t') G(x, t, x', t') dx' \\ &+ \lim_{t_i \rightarrow t_n} w_n \Delta t_n \int_{x'} \mathbf{T}(x', t') \dot{\mathbf{T}}(x, t) G(x, t, x', t') dx' \end{aligned} \quad (49)$$

$$\begin{aligned}
F_2(x_n, t_n) &= \sum_{t_i=0}^{t_{n-1}} w_i \Delta t_i \sum_{x_i} T(x_i, t_i) \dot{T}(x_i, t_i) G(x_n, t_n, x_i, t_i) \Delta x_i' \\
&\quad + \lim_{t_i \rightarrow t_n} w_n \Delta t_n \int_{x'} T(x', t') \dot{T}(x', t') G(x_n, t_n, x', t') dx' \\
&= \dots + w_n \Delta t_n \int_{x'} T(x', t') \dot{T}(x', t') \delta(x_n - x') dx' \\
F_2(x_n, t_n) &= \dots + w_n \Delta t_n T(x_n, t_n) \dot{T}(x_n, t_n) \quad . \quad (50)
\end{aligned}$$

And finally the temperature at any point x_n , and time t_n for linear variations of thermal properties can be given by

$$T_1(x_n, t_n) = T(x_n, t_n) - bF_1(x_n, t_n) - aF_2(x_n, t_n) \quad . \quad (51)$$

However, in the solution for $T_1(x, t)$ we do not have to evaluate both functions $F_1(x, t)$ and $F_2(x, t)$. It can be shown that the sum of these two functions, i.e. $F_1(x, t) + F_2(x, t)$ is a solution for a medium in which the thermal properties, specific heat and thermal conductivity, vary in the same way. That is, this is the solution for constant thermal diffusivity α .

The solution for constant thermal diffusivity, but with C and k varying with temperature in the same way, can be shown⁽³⁾ to be of the same form as that for constant thermal diffusivity where both C and k are constants. The initial and boundary conditions will be changed.

Suppose

$$\rho C_0 \frac{\partial T}{\partial t} - k_0 \nabla^2 T = \dot{q}(x, t) \quad (2)$$

has the solution $T(x,t)$ with the boundary conditions,

$$T(L,t) = H$$

$$T(x,0) = h \quad .$$

To get the solution for the equation

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

where

$$C/C_0 = k/k_0 = 1 + \mu T \quad (\text{where } \mu \text{ is either a or b})$$

C_0 and k_0 are calculated at any arbitrary temperature T_0 . If we write

$$T' = \int_{T_0}^T (1 + \mu T) dT \quad (52)$$

where T_0 is any arbitrary temperature, one can easily show that the equation satisfied by T' is obtained from (2) on replacing T by T' , providing that the initial and boundary values of T' , say h' and H' , are obtained by setting h and H as the upper limits of the integral.

So, the solution $T'(x,t)$ also is equal to:

$$T'(x,t) = F_1(x,t) + F_2(x,t) \quad . \quad (53)$$

Since the values of $T'(x,t)$ are easily obtained, it is only necessary to perform one integral $F_1(x,t)$ or $F_2(x,t)$ to get the solution $T_1(x,t)$ that we are

looking for, i.e.

$$\begin{aligned} T_1(x,t) &= T(x,t) - bF_1(x,t) - aF_2(x,t) \\ &= T(x,t) - b[T'(x,t) - F_2(x,t)] - aF_2(x,t) \end{aligned}$$

$$T_1(x,t) = T(x,t) - bT'(x,t) - (a - b) F_2(x,t) \quad (54)$$

or $T_1(x,t) = T(x,t) - aT'(x,t) + (a-b) F_1(x,t) \quad . \quad (55)$

Now, only $F_1(x,t)$ or $F_2(x,t)$ need to be evaluated. This is useful especially when one of these functions gets complicated as in the case of a non-insulating face of the first wall.

In some cases, the variations of thermal properties with temperature may be very large over the range from room temperature up to the melting point and these variations must be taken into account. Problems involving phase transformations might account for large variations since, most of the time, the thermal properties undergo a wide variation at the transformation temperature.

As an example to illustrate the methods discussed in this paper, consider the case of hydrogen ions incident on Al as a first wall. The thermal properties of Al, i.e. specific heat and thermal conductivity, are fitted linearly with temperature. Figure 12 shows the temperature rise in the Al surface with and without the variation of thermal properties with temperature; there is about a 10% decrease in the maximum temperature when considering the variation of thermal properties with temperature. At lower temperatures, the differences are very small, and the variations of thermal properties with

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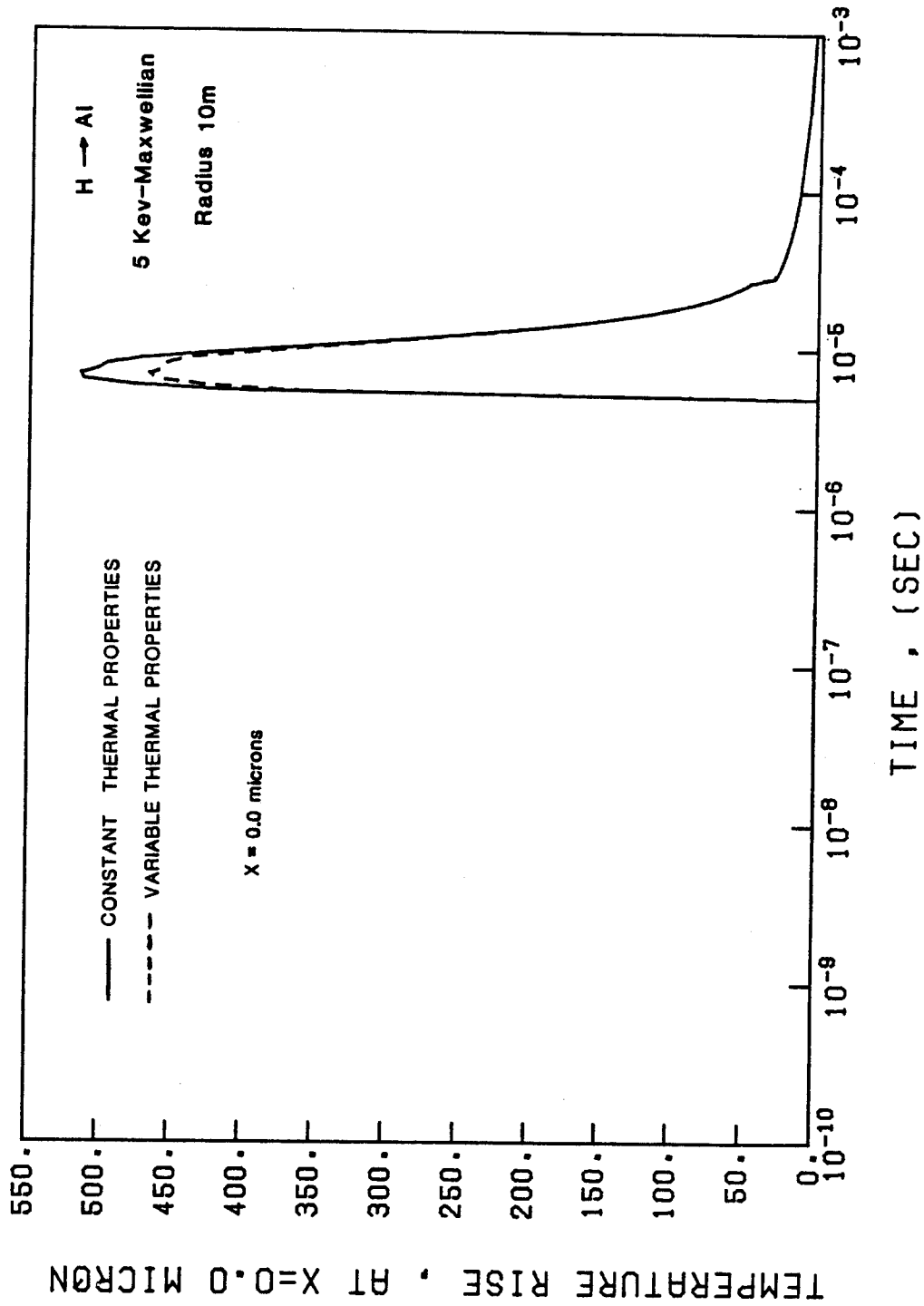


Figure 12

temperature can be neglected (Fig. 13). At higher temperatures the differences become larger and the variations of thermal properties must be included.

Conclusion

The temperature rise due to ion energy deposition into a first wall material has been calculated using the methods of Green's function. A new method has been developed to avoid the singularities associated with the Green's function. Several models for calculating the temperature increase are discussed using this new method. A large difference in the temperature rise in the regions where there is an energy deposition is noticed between the model calculation and a previous similar calculation where the singularities of the Green's function have not been treated properly. An approximate solution for the non-linear heat-conduction equation in which the specific heat and the thermal conductivity vary linearly with temperature is discussed. The effect of the variation of the thermal properties over wide temperature fluctuations could be substantial and should be included.

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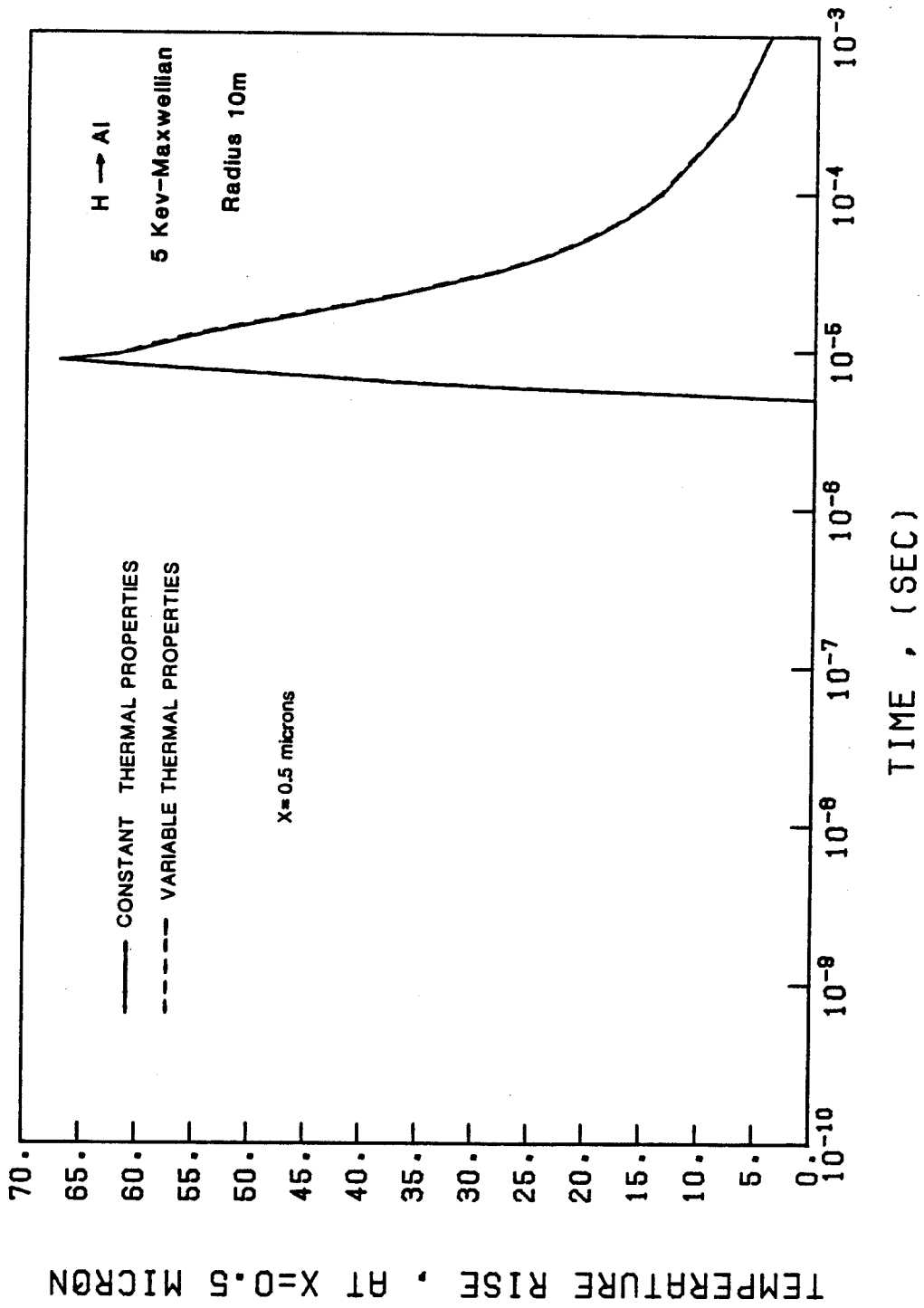


Figure 13

Appendix A

To show that the Green's function for the thermal response of a semi-infinite medium behaves like a δ -function, consider the function

$$\Delta(x) = \frac{1}{\sqrt{\pi b}} e^{-x^2/b} \quad , \quad b = 4\alpha(t - t') \quad .$$

We want to show that

$$\lim_{b \rightarrow 0} \Delta(x) = \delta(x)$$

i.e.

$$\lim_{b \rightarrow 0} \frac{1}{\sqrt{\pi b}} e^{-x^2/b} = \delta(x) \quad .$$

To evaluate the total area under the curve of this function, i.e.

$$\int_{-\infty}^{\infty} \Delta(x) \, dx = \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi b}} e^{-x^2/b} \, dx \quad ,$$

substitute $y = x^2/b$ $dy = 2x/b \, dx$, i.e.

$$dx = \frac{b}{2\sqrt{by}} \, dy \quad .$$

Substitute

$$\int_{-\infty}^{\infty} \Delta(x) dx = 2 \int_0^{\infty} \frac{1}{\sqrt{\pi b}} e^{-y} \frac{\sqrt{b}}{2} y^{-1/2} dy = \frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-y} y^{-1/2} dy$$

$$= \frac{1}{\sqrt{\pi}} \Gamma\left(\frac{1}{2}\right)$$

where Γ = gamma function(13)

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

i.e.

$$\int_{-\infty}^{\infty} \Delta(x) dx = 1$$

or
$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi b}} e^{-x^2/b} dx = 1$$

which is equivalent to $\int_{-\infty}^{\infty} \delta(x) dx = 1$. We conclude that

$$\lim_{t \rightarrow t'} \frac{1}{\sqrt{4\pi\alpha(t-t')}} e^{-\frac{(x-x')^2}{4\alpha(t-t')}} = \delta(x-x') \quad .$$

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