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DEPARTMENT OF MECHANICAL ENGINEERING AND MECHANICS
SCHOOL OF ENGINEERING
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA 23508

OPTIMAL CURE CYCLE DESIGN FOR AUTOCLAVE PROCESSING OF THICK COMPOSITES LAMINATES: A FEASIBILITY STUDY

By

Jean W. Hou, Principal Investigator

Progress Report
For the period January 15 to October 15, 1985

Prepared for
National Aeronautics and Space Administration
Langley Research Center
Hampton, VA 23665

Under
Research Grant NAG-1-561
Robert M. Baucom, Technical Monitor
MD-Polymeric Materials Branch

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OLD DOMINION UNIVERSITY RESEARCH FOUNDATION

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

TABLE OF CONTENTS - continued

LIST OF FIGURES - continued

INTRODUCTION

The research progress in the project "Optimal Cure Cycle Design for Autoclave Processing of Thick Composite Laminates: A Feasibility Study," during the period of January to October, may be reported separately in three aspects; namely:

1. design sensitivity analysis for the chemical-kinetic reaction during prepreg processing, while the temperature is considered as a design variable,

2. finite element analysis for the thermal system of heat conduction coupled with the chemical-kinetic reaction during prepreg processing,

3. design sensitivity analysis for the thermal system of heat conduction coupled with the chemical-kinetic reaction during prepreg processing, while the temperature of cure cycle is considered as a design variable.

The chemical-kinetic reaction of Hercules 3501 during autoclave processing has been modelled and expressed in terms of an equation of degree of cure:

$$\dot{\alpha} = \begin{cases} (K_1 + K_2\,\alpha)\,(1 - \alpha)\,(B - \alpha) & \alpha \leq 0.3 \\ K_3\,(1 - \alpha) & \alpha > 0.3 \end{cases} \qquad (1)$$

where B is constant, and K_1, K_2 and K_3 are functions of temperature. Note that the rate of cure presents discontinuity at $\alpha = 0.3$. The design sensitivity calculation of transient problems with discontinuous derivative is theoretically difficult. In addition, it is numerically difficult to precisely monitor the critical time at which the discontinuity occurs. The research results in this regard have been documented in Appendix A. In a

summary, one first studied the effect of the accuracy of the critical time evaluation on the accuracy of the thermal design sensitivity analysis. It showed that the design sensitivity calculated by the adjoint variable technique is not sensitive to the accuracy of the critical time evaluation. Next, the adjoint variable technique was employed to find the thermal design sensitivity numerically. Two approaches were developed. One maintains the jump condition. The other uses a logic function to smoothly approximate the discontinuity within a smalll region. Both approaches showed good results. Nevertheless, the latter one is to be used for further study. The reason is that the $\dot{\alpha}$ is a function of time as well as position; therefore, it is numerically difficult to keep track of the $\dot{\alpha}$ discontinuity at every spatial position.

The second stage of research is devoted to the computer code development for the simulation of a heat conduction model coupled with a chemical-kinetic model during prepreg processing. The equation for the chemical-kinetic model is already given in equation 1. In addition, the heat condction equation is given as

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} + \rho H_R \dot{\alpha} \qquad (2)$$

where ρ is the mass density, c is the coefficient of heat capacity, k is the heat conduction coefficient, and H_R is the heat generated by cured resin.

The finite element discretization is introduced to convert the initial-boundary value equations (1) and (2) into a set of first order differential equations. This set of equations are then solved simultaneously by a numerical integration code called DE. To preserve analysis accuracy, the temperature and the degree of cure are subjected to the same numerical error control during the numerical integration.

Two numerical example have been performed. One simulates the autoclave processing of 192 ply prepregs with 32% Hercules resin content. The resin flow can be neglected in this example, because the resin content is low. To focus on the heat conduction and the chemical-kinetic models, the measured temperature on the surfaces of the composite laminate are used as boundary temperature, instead of the temperature of cure cycle. Although the heat flux, induced by the heat convection of autoclave air temperature, is neglected, the numerical result is in an excellent agreement with Loo's data, as shown in figure 1. The long CDC computer time (17,056 CPU seconds) is required to to analyze a complete cycle of autoclave processing. This may be because the autoclave processing needs a long real time (275 minutes) to perform. In addition, the numerical integration requires small time step size becuase the system equations are quite "stiff".

The second example is taken from the results of compression modelling of composite laminates [1]. The research was done in General Motor Research Center. The degree of cure of resin in term of temperature is given as

$$\dot{\alpha} = (K_1 + K_2 \alpha^m)(1 - \alpha)^n \qquad (3)$$

where m and n are constants, and K_1 and K_2 are functions of temperature. Note that neither $\dot{\alpha}$ discontinuity nor resin flow are needed to be considered in this example. The developed computer code can be used to solve equations 2 and 3 without difficulties. The results calculated are close to those published, as shown in figures 2 and 3.

In the third stage, one concentrates on the derivation of the thermal design sensitivities of temperature uniformity related to the change of surface temperature. Note that the temperature on the surface of prepreg is called the surface temperature which is controlable and is considered as a

design variable. Moreover, the goal of the optimal design is to achieve a uniform temperature distribution across the thickness of the laminates. The performance index of the temperature uniformity, ψ, may be defined as the least square of the deviation between the pointwise temperature and the average temperature as:

$$\psi = \int_{t_o}^{t_f} \left[\int_o^h T^2\, dz - \left(\int_o^h T\, dz\right)^2/h\right] dt \qquad (4)$$

where T is the temperature distribution and h is the thickness of the laminate.

Two methods have been developed to analyze the thermal design sensitivity. One is the adjoint variable method. The other is the approach of direct differentiation.

Using the adjoint method, the design derivative of the temperature uniformity is derived as

$$\frac{d\psi}{dT_c} = \int_{t_o}^{t_f} \int_o^h \left(-u \frac{\partial f}{\partial T_c} - \rho H_R \lambda \frac{\partial f}{\partial T_c}\right) dz\, dt \qquad (5)$$

where f is the right side of equation 3 and the adjoint variable λ and u are solved by the following equations:

$$\rho c\dot{\lambda} = - k \frac{\partial^2 \lambda}{\partial z^2} - u \frac{\partial f}{\partial T} - \rho H_R \lambda \frac{\partial f}{\partial T} - \frac{2}{h} \int_o^h T dz$$

$$\dot{u} = u \frac{\partial f}{\partial \alpha} + \rho H_k \lambda \frac{\partial f}{\partial \alpha}$$

with homogeneous boundary conditions and terminal conditions defined at $t = t_f$. The above equations are coupled linear equations which can be solved by the same computer code developed for the thermal analysis discussed

previously.

Using the direct differentiation, equation 4 can be taken for derivatives with design variable, T_c, directly as

$$\frac{d\psi}{dT_c} = 2 \int_{t_o}^{t_f} \left[\int_o^h T\, T'\, dz - \int_o^h T\, dz \cdot \int_o^h T'\, dz/h \right] dt \qquad (6)$$

where $T' \equiv dT/dT_c$ can be obtained by taking the derivatives of equations 2 and 3 as

$$\rho c \frac{\partial T'}{\partial t} = k \frac{\partial^2 T'}{\partial z^2} + \rho H_R \dot{\alpha}'$$

and

$$\dot{\alpha}' = \frac{\partial f}{\partial \alpha} \alpha' + \frac{\partial f}{\partial T} T'$$

with homogeneous boundary and initial conditions. Again, the f in the above equations denotes the right side of equation 3 and $\alpha' \equiv d\alpha/dT_c$. The perturbation of the performance index, $\Delta\psi$, due to the change of the design variable, ΔT_c, can be approximated by the design derivative, $d\psi/dT_c$, i.e.,

$$\Delta\psi \cong \frac{d\psi}{dT_c} \cdot \Delta T_c \qquad (7)$$

where the actual change $\Delta\psi$ can be obtained by the finite difference scheme, i.e.,

$$\Delta\psi = \psi(T_c + \Delta T_c) - \psi\,(T_c) \qquad (8)$$

The combination of the preceding two equations provides a good mean to check the accuracy of the thermal design sensitivity. As listed in Table 1, the actual changes are calculated for various perturbation of design variable, ΔT_c, based on equation 8; and the last two columns indicated the change of ψ predicted by methods presented in equations 5 and 6. Using the compression molding of a polyester [1] as an example, it is noted that the

direct differentiation method is superior to the adjoint method in this study. The direct differentiation method provides a better evaluation of the actual change of the performance index. Besides, the approach of direct differentiation provides the time histories of design derivatives $d\psi/dT_c$, dT/dT_c and $d\alpha/dT_c$, as shown in figures 4 to 6, respectively. It is of great interest to observe that the change of the control temperature has significant effect on the temperature uniformity only when the operational time of processing is over 100 seconds. The figures dT/dT_c and $d\alpha/dT_c$ confirm this observation.

Conclusions

Two goals listed in the proposal have been achieved, namely, the thermal analysis and the calculation of thermal sensitivity. A finite element program for the thermal analysis and design derivatives calculation for temperature distribution and the degree of cure has been developed and verified. It is found that the direct differentiation is the best approach for the thermal design sensitivity analysis. In addition, the approach of the direct differentiation provides time histories of design derivatives which are of great value to the cure cycle designers. The approach of direct differentiation is to be used for further study, i.e., the optimal cycle design.

Reference

1. Barone, M. E. and Caulk, D. A., "The Effect of Deformation and Thermoset Cure on Heat Conduction in a Chopped-Fiber Reinforced Polyester During Compression Molding," Int. J. Heat Mass Transfer, Vol. 22, pp. 1021-1032, 1979.

Table 1 Thermal Design Sensitivity Analysis for Compression Molding

Mold Temp.	Cost Function	Actual Change	$\psi' \Delta T_c^*$	$\psi' \Delta T_c^{**}$
423°K	21019.648	-----	-----	-----
422°K	20501.695	517.95	341.97	501.051
418°K	18157.462	2862.186	1720.32	2505.257
413°K	16137.194	4882.45	3445.93	5010.514
408°K	14772.308	6247.34	5160.96	7515.771
403°K	13479.446	7540.20	6881.28	10021.028
393°K	11083.596	9936.05	10321.92	15031.542
428°K	23238.107	2218.46	1720.32	2505.251
433°K	25042.554	4022.90	3440.64	5010.514

*Calculated by the adjoint variable method

**Calculated by the direct differentiation

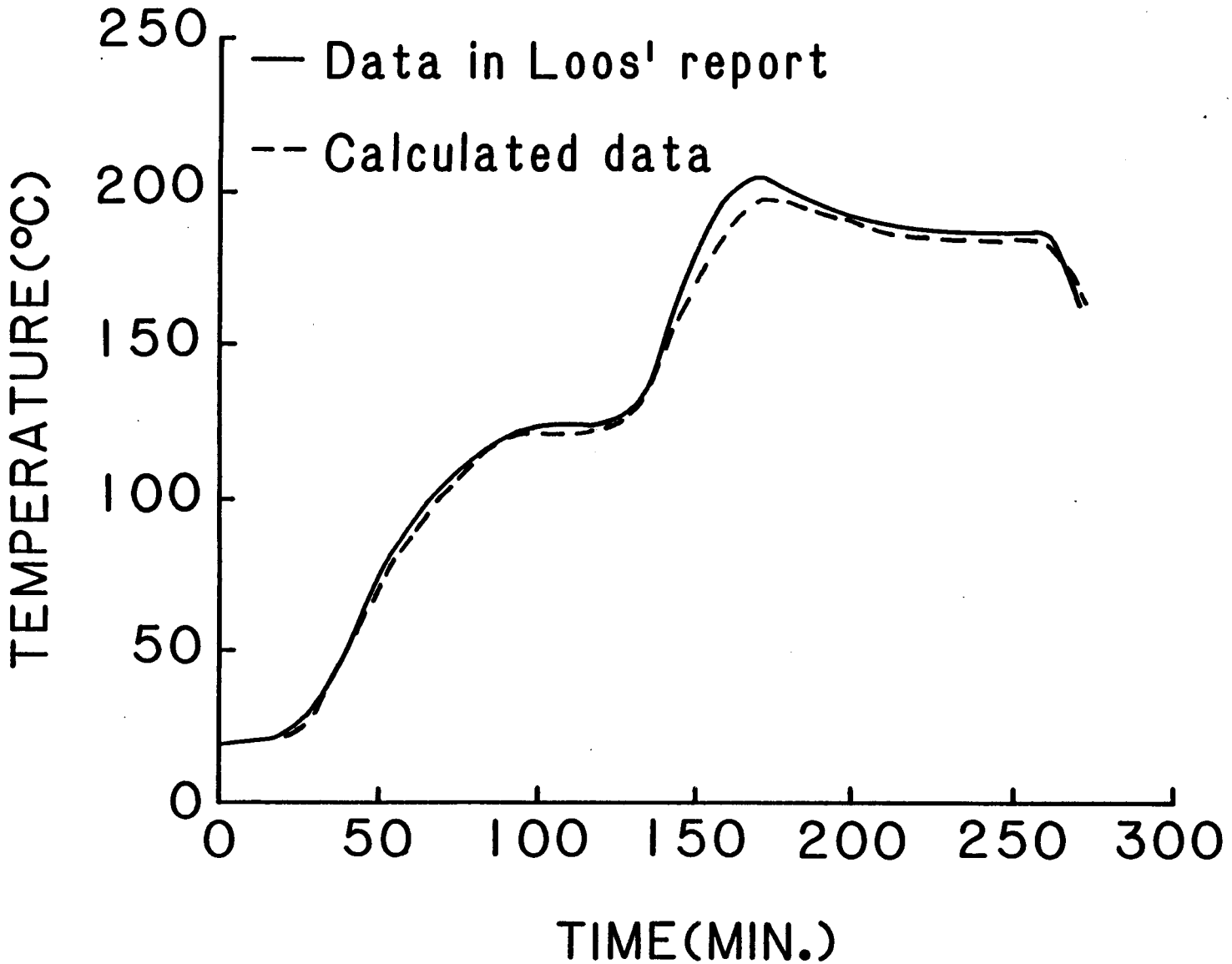

Figure 1. Temperature Profile at the Center of Laminate.
Solid Line -- Data in Loos' Report
Discrete Points -- Calculated Data

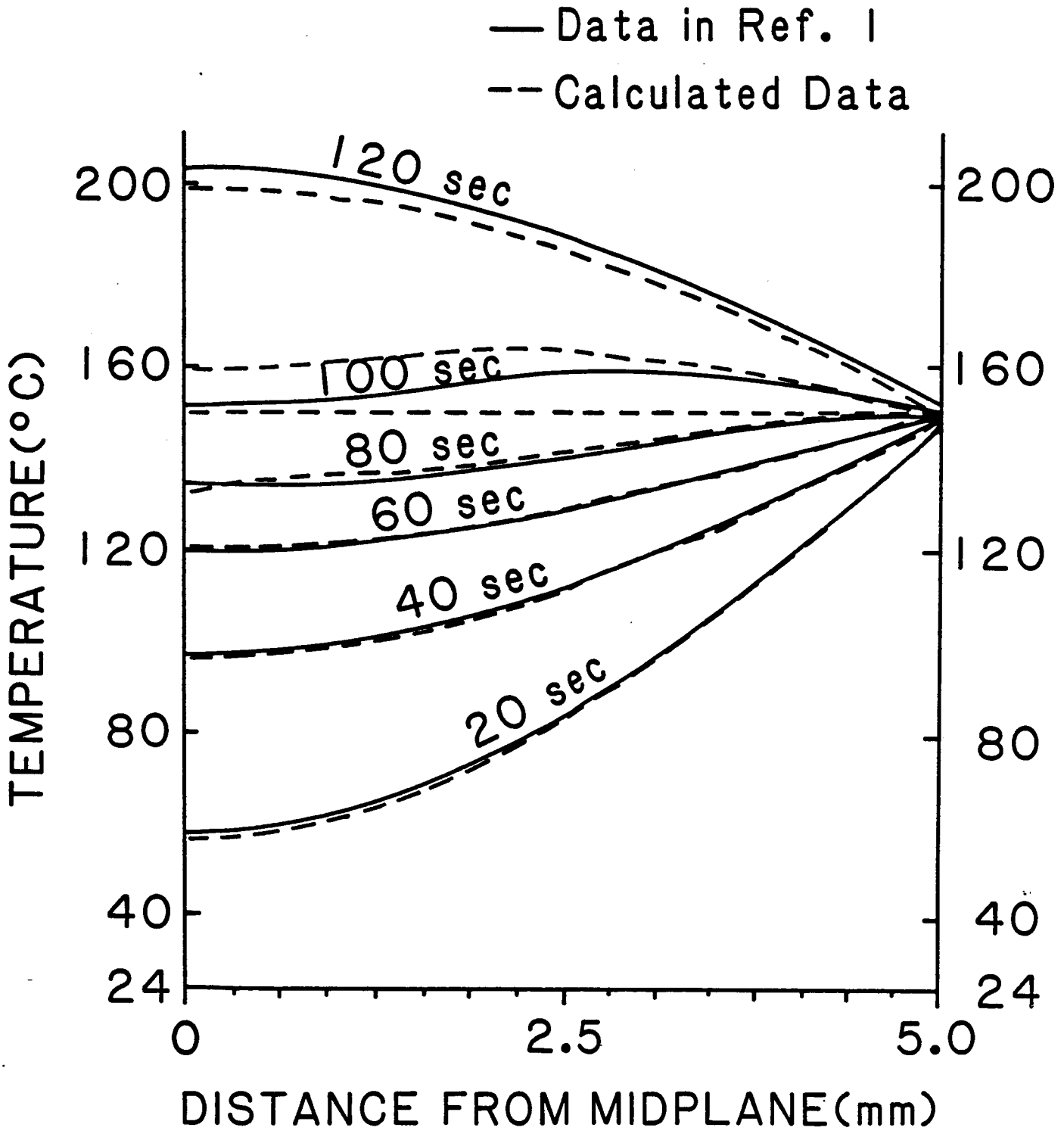

Figure 2. Temperature Profiles for 10-mm Thick Sheet.

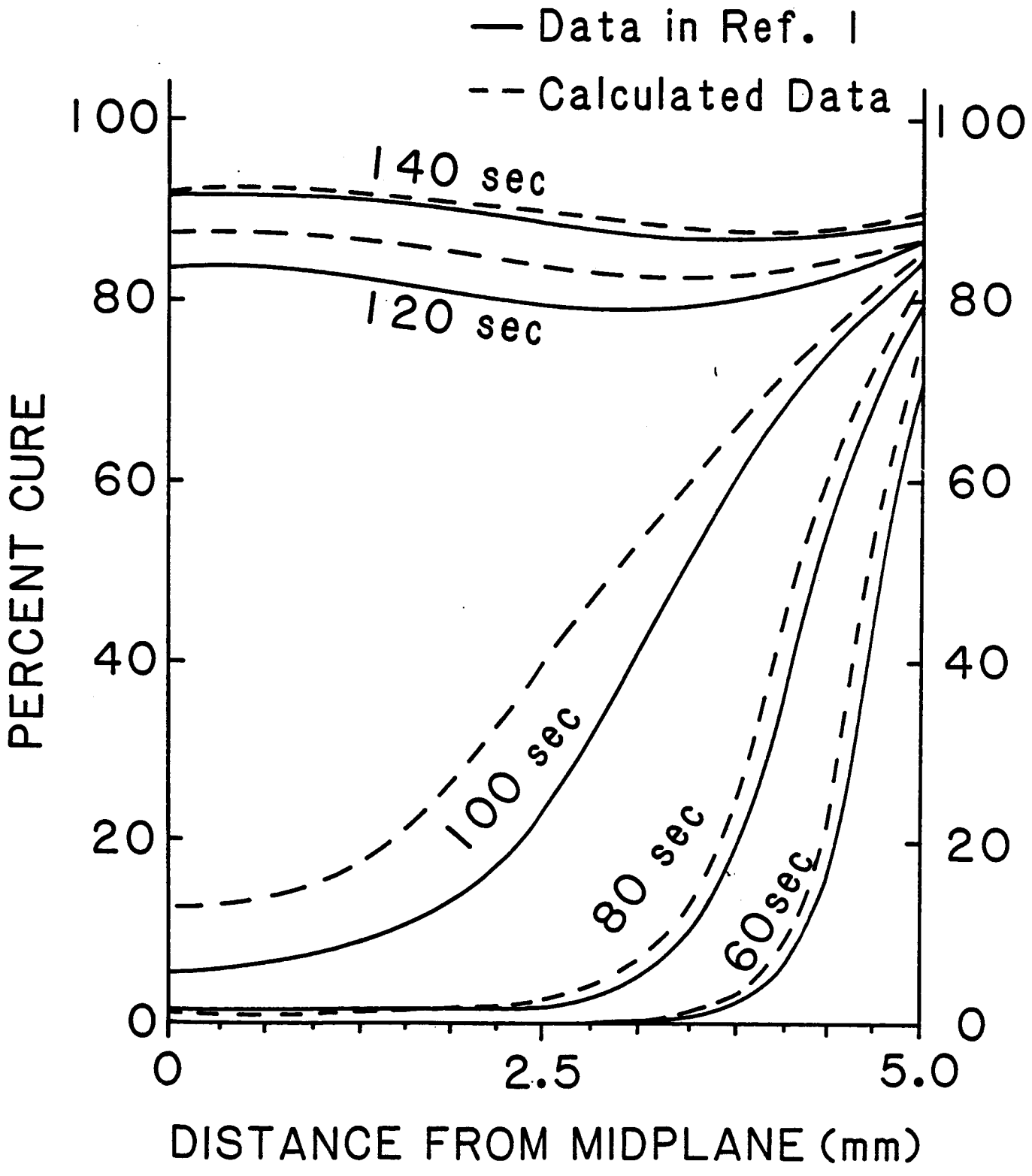

Figure 3. Cure Profiles for 10-mm Thick Sheet.

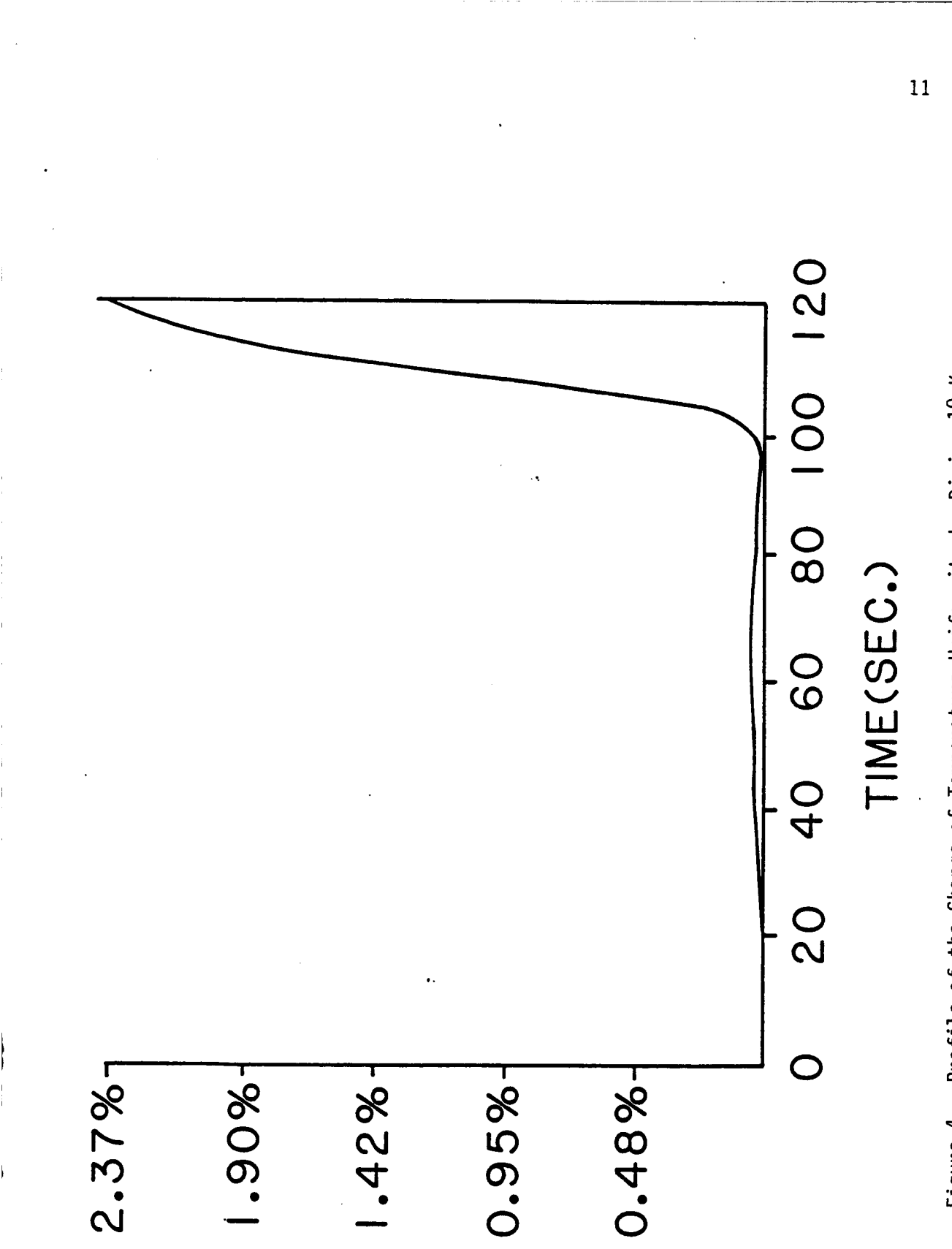

Figure 4. Profile of the Change of Temperature Uniformity by Rising 1^{o} K Mold Temperature.

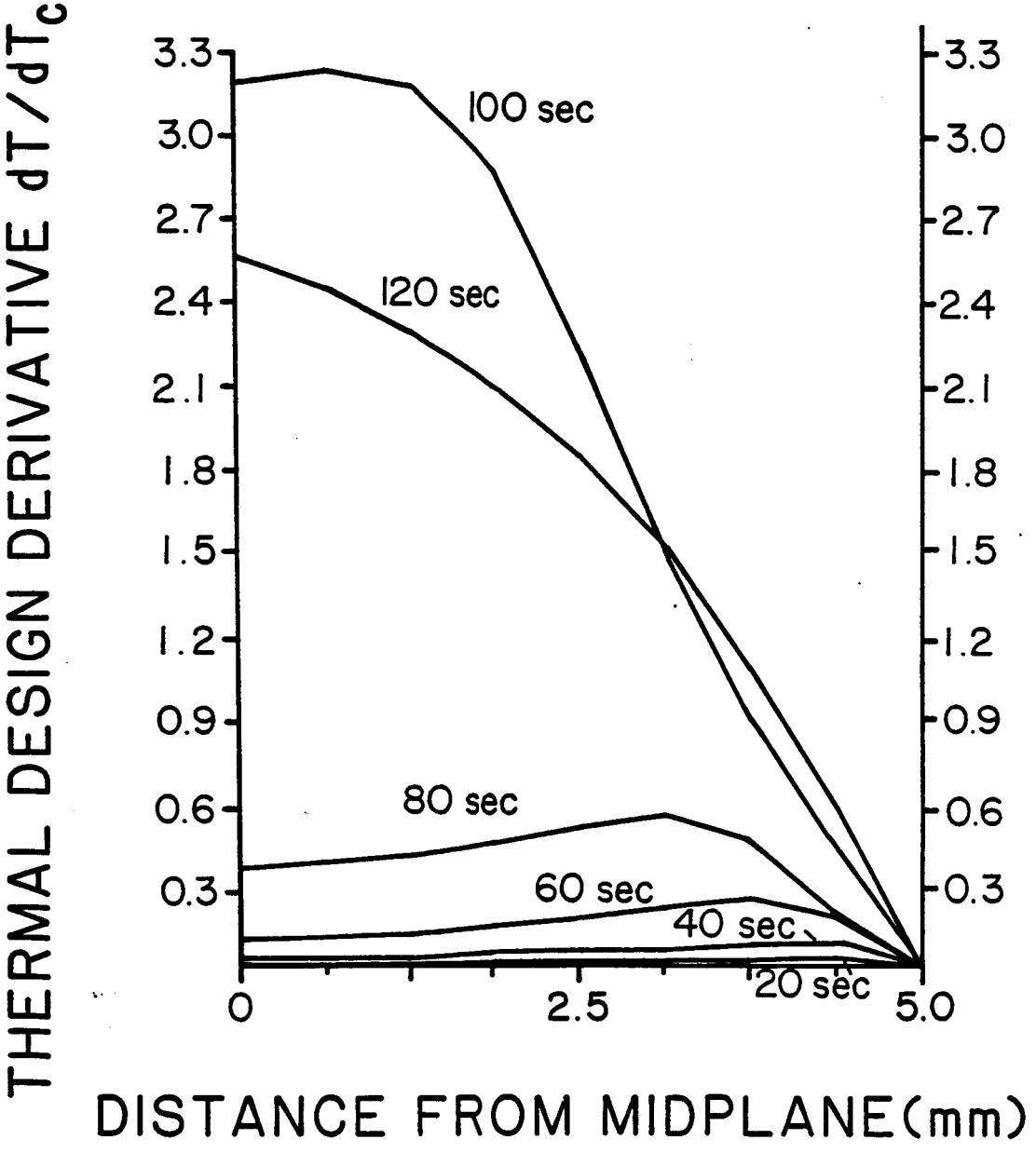

Figure 5. Profiles of Thermal Design Derivatives of Temperature with Respect to Mold Temperature.

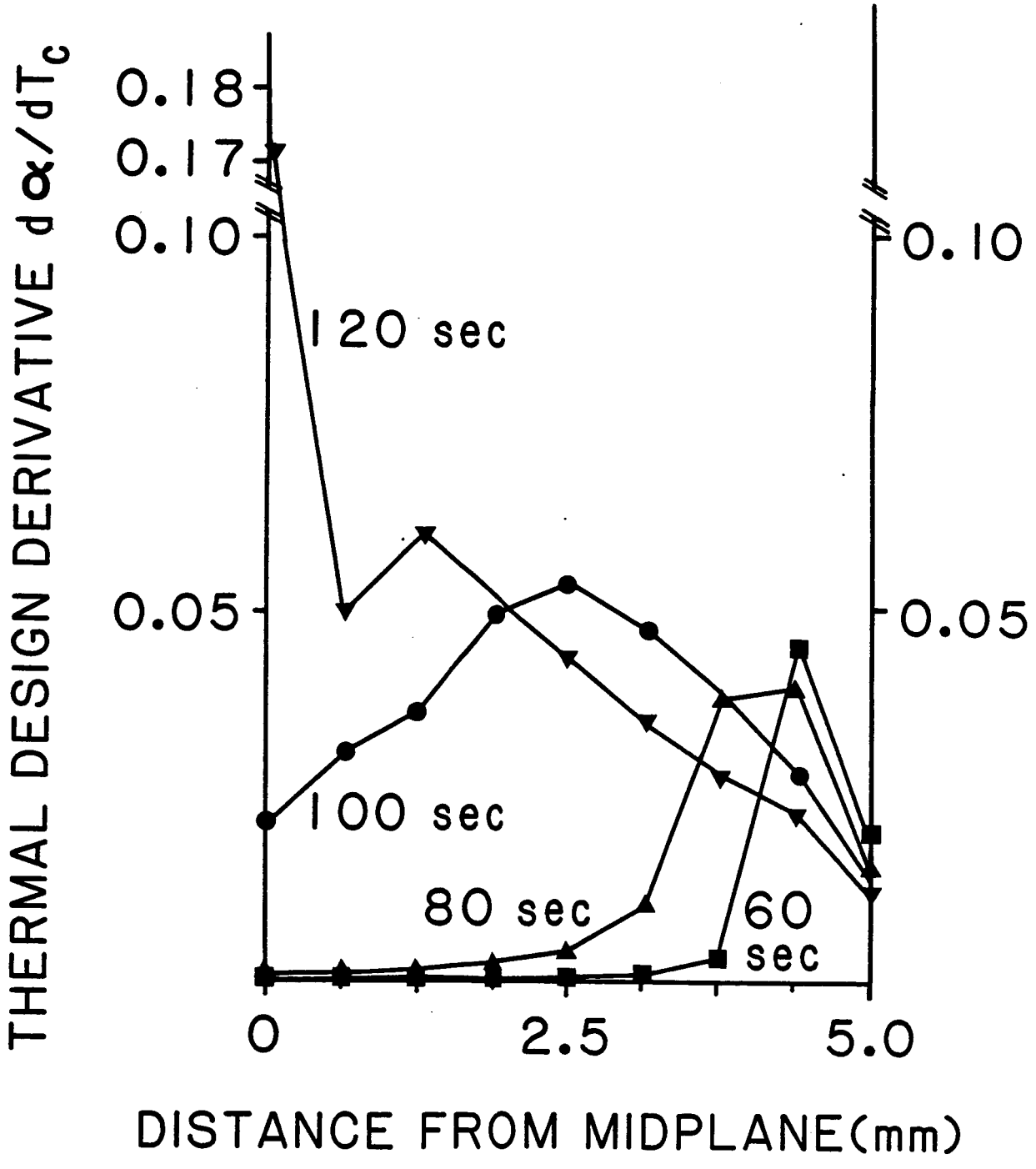

Figure 6. Profiles of Thermal Design Derivatives of Percent Cure with Respect to Mold Temperature.

APPENDIX A

NUMERICAL STUDIES ON THE DESIGN SENSITIVITY CALCULATION OF TRANSIENT PROBLEMS WITH DISCONTINUOUS DERIVATIVES

SUMMARY

The aim of this study is to find a reliable numerical algorithm to calculate design sensititivty of transient problem with discontinous derivatives. The finite difference method and the adjoint variable technique using both Simpson's rule and DE program, a predicator - corrector algorithm, are investigated. It is shown that the design sensitivity calculated by the finite difference method is quite sensitive to the numerical errors. Nevertheless, the design sensitivity calculated by the adjoint variable technque is relatively stable against various numerical integrations and time steps. It is concluded that the adjoint variable technique in conjunction with the DE program with appropriate truncation error control provides very satisfactory numerical results.

I. INTRODUCTION

The derivative of the thermal response with respect to the design variable is usually called thermal design derivative or sensitivity. The information of design derivative is not only very useful for the trade-off design but it is also required for the iterative design optimization.

The calculation of design derivatives in thermal problems has attracted research interest in such areas as design of space structure subject to temperature constraints [1], and chemical process control [2].

For the problems of interest, the state equation is usually expressed as

$$\dot{z} = f(b, z, t), \qquad o \leq t \leq \tau \tag{1}$$

with initial condition

$$z(b, o) = z_o \tag{2}$$

where a dot denotes differentiation with time, t, b is the design variables and z_0 is prescribed initial condition. The state function z(b, t) is a function of time and design variable. Although the design variable b is generally a function of time, in the following discussion, it is listed as a constant parameter for simplicity.

Four different methods [1]; the Green's function, finite difference, direct differentiation,and adjoint variable technique, are currently used in the calculation of thermal design sensitivity, i.e., dz/db. Haftka [1, 3] indicated that the numerical integration scheme (explicit or implicit) used to solve Eq. 1 is an important factor in detemining the computational efficiency and accuracy of thermal design sensitivity for the problem with continuous derivative $\dot{z}$.

On the other hand it is not uncommon in engineering applications that $\dot{z}$ or the function f(b, z, t) defined in Eq. 1 exhibits discontinuities. The critical time at which the discontinuity happens is usually monitored by the state variable z. Engineering examples can be found in the multi-stage control problem [4], control of chemical kinetics [5], and the mechanical system with intermittent motion [6, 7]. The intermittent motion is characterized by the occurence of nearly discontinuous force and velocity caused by impulsive force, impact, mass capture, and mass release. The optimal design problems of mechanisms with intermittent motion have been discussed by Huang, Huag and Andrews [6]. Their method is based on the identification of critical times at which discontinuities in forces or velocities occur. Jump conditions of those discontinuities are employed in an adjoint variable approach for the calculation of design sensitivity coefficients. Ehle and Haug [7] introduced the "logical function" to smoothly approximate discontinuities. An example in their work shows that time step and

the size of transient zone used for discontinuity approximation have significant effect on the accuracy of design sensitivity calculation.

It is the objective of this study to investigate the numerical accuracy of design sensitivity calculation, focused on the numerical integration schemes and the approximation of of critical time.

II. Design Sensitivity Analysis

A functional is given as

$$\psi = \int_0^\tau g(z(t), b, t)\, dt \tag{3}$$

where τ is the terminal time which is assumed to be independent of the design variable b. The state variable z(t) is governed by the state equations as follows:

$$\dot{z} = f = \begin{cases} f_1 (z(t), b, t) ; & \text{when } z(t) < c \\ f_2 (z(t), b, t) ; & \text{when } z(t) > c \end{cases} \tag{4}$$

with initial condition

$$z(o) = z_o \tag{5}$$

The constant c of jump condition in Eq. 4 is assumed again to be independent on design variable. It is obvious that the state variable z(t) and the critical time $\bar{t}$ at which $z(\bar{t}) = c$ depend on the design variable b because z(t) is the solution of Eq. 4. In other words, z and $\bar{t}$ can be defined as z(t, b) and $\bar{t}(b)$, respectively. The problem of interest is to determine the design sensitivity of functional ψ. The variation of functional ψ with respect to the design variable is defined as

$$\delta\psi = \lim_{\varepsilon \to 0} \frac{\psi(t, b+\varepsilon\delta b) - \psi(t, b)}{\varepsilon}$$

$$= \frac{d\psi(t, b+\varepsilon\delta b)}{d\varepsilon}\bigg|_{\varepsilon=0} \qquad (6)$$

$$= \psi' \, \delta b$$

where δb is the perturbation of design variable and ψ' is defined as $d\psi/db$. The variation of state function, δz, can be defined by a similar fashion.

According to the definition of variation and Leibnitz's rule, the variation of functional is derived as

$$\delta\psi = \int_0^{\tau} \left(\frac{\partial g}{\partial z} \delta z + \frac{\partial g}{\partial b} \delta b\right) dt + \left(g\Big|_{\bar{t}^-} - g\Big|_{\bar{t}^+}\right) \delta\bar{t} \qquad (7)$$

Note that, because of the dependence of b, $\delta z = (\partial z/\partial b)\delta b$ and $\delta\bar{t} = (\partial\bar{t}/\partial b)\delta b$. The last term of above equation can be dropped provided that the continuity assumption of g at $\bar{t}$ is maintained. The variations, δz and $\delta\bar{t}$ can be determined by using the equality of Eq. 4 and the jump condition $z(\bar{t}) = c$. However, by careful selection of the adjoint equation, it is not necessary to obtain explicit expressions for δz and $\delta\bar{t}$ in order to obtain the variation $\delta\psi$.

In accordance with the equality of Eq. 4, it is evident that

$$0 = \int_0^{\tau} \lambda(\dot{z}-f) \, dt$$

$$= \int_0^{\bar{t}^-} \lambda(\dot{z}-f_1) \, dt + \int_{\bar{t}^+}^{\tau} \lambda \, (\dot{z}-f_2) \, dt \qquad (8)$$

for an arbitrary function $\lambda(t)$ and the design variable b. The variation of the preceding functional yields:

$$0 = \int_0^{\bar{t}^-} \delta\lambda(\dot{z}-f_1)\,dt + \int_{\bar{t}^+}^{\tau} \delta\lambda\,(\dot{z}-f_2)\,dt$$

$$+ \int_0^{\bar{t}^-} \lambda(\delta\dot{z} - \frac{\partial f_1}{\partial b}\,\delta b - \frac{\partial f_1}{\partial z}\,\delta z)\,dt + \int_{\bar{t}^+}^{\tau} \lambda(\delta\dot{z} - \frac{\partial f_2}{\partial b}\,\delta b - \frac{\partial f_2}{\partial z}\,\delta z)\,dt$$

$$+ \lambda(\dot{z} - f_1)\Big|_{\bar{t}^-}\,\delta\bar{t} - \lambda(\dot{z} - f_2)\Big|_{\bar{t}^+}\,\delta\bar{t} \qquad (9)$$

Note that the summation of first two terms should be zero because the equality of Eq. 8 is also true for an arbitrary $\delta\lambda$. Furthermore, it is understood that the critical time $\bar{t}$ depends on design variable implicitly through the relation $z(\bar{t}, b) = c$. Thus, employing the Leibnitz's rule, the variation $\delta\bar{t}$ appears in the derivation. However, these two boundary terms may be dropped out because $\dot{z} - f_1$ and $\dot{z} - f_2$ are equal to zero when the time t approaches to $\bar{t}^-$ and $\bar{t}^+$, respectively, according to Eq. 4. After simplification and integration by parts, the preceding equation can be rewritten as

$$0 = \int_0^{\bar{t}^-} \lambda\,(\delta\dot{z} - \frac{\partial f_1}{\partial b}\,\delta b - \frac{\partial f_1}{\partial z}\,\delta z)\,dt + \int_{\bar{t}^+}^{\tau} \lambda\,(\delta\dot{z} - \frac{\partial f_2}{\partial b}\,\delta b - \frac{\partial f_2}{\partial z}\,\delta z)\,dt$$

$$= \int_0^{\bar{t}^-} [(-\dot{\lambda} - \frac{\partial f_1}{\partial z})\,\delta z - \lambda\,\frac{\partial f_1}{\partial b}\,\delta b]\,dt + \int_{\bar{t}^+}^{\tau} [(-\dot{\lambda} - \frac{\partial f_2}{\partial z})\,\delta z$$

$$- \lambda\,\frac{\partial f_2}{\partial b}\,\delta b]\,dt + \lambda\delta z\Big|_0^{\bar{t}^-} + \lambda\,\delta z\Big|_{\bar{t}^+}^{\tau} \qquad (10)$$

Note that the operators "δ" and "$\cdot$" are exchangable provided that z is a continuous function of b and t in the time domains $0 \leq t < \bar{t}^-$ and $\bar{t}^+ < t \leq \tau$. The initial condition $z(b,0) = z_0$ is assumed to be independent on the design variable. Consequently, $\delta z = 0$ at $t = 0$. As to the total

variation of the jump condition $z(b,\bar{t}) = c$, it is derived as $\dot{z}\delta\bar{t} + \delta z = 0$ or $\delta z = -\dot{z}\delta\bar{t}$ for t approaches to either $\bar{t}^-$ or $\bar{t}^+$. The boundary terms in Eq. 10 can then be rearranged as

$$\begin{aligned}
&\lambda\delta z\Big|_0^{\bar{t}^-} + \lambda\delta z\Big|_{\bar{t}^+}^{\tau} \\
&= -\lambda\dot{z}\Big|_{\bar{t}^-}\delta\bar{t} + \lambda\dot{z}\Big|_{\bar{t}^+}\delta\bar{t} + \lambda\delta z\Big|_{\tau} \\
&= \left[-(\lambda f_1)\Big|_{\bar{t}^-} + (\lambda f_2)\Big|_{\bar{t}^+}\right]\delta\bar{t} + \lambda\delta z\Big|_{\tau}
\end{aligned}$$

Adding Eqs. 7 and 10 up, one has the variation of the functional ψ as

$$\begin{aligned}
\delta\psi = &\int_0^{\bar{t}^-}\left(-\dot{\lambda} - \frac{\partial f_1}{\partial z} + \frac{\partial g}{\partial z}\right)\delta z\, dt + \int_{\bar{t}^+}^{\tau}\left(-\dot{\lambda} - \frac{\partial f_2}{\partial z} + \frac{\partial g}{\partial z}\right)\delta z\, dt \\
&+ \int_0^{\bar{t}^-}\left(\frac{\partial g}{\partial b} - \lambda\frac{\partial f_1}{\partial b}\right)\delta b\, dt + \int_{\bar{t}^+}^{\tau}\left(\frac{\partial g}{\partial b} - \lambda\frac{\partial f_2}{\partial b}\right)\delta b\, dt \\
&+ \lambda\,\delta z\Big|_{\tau} \\
&+ \left[(\lambda f_2 - g)\Big|_{\bar{t}^+} - (\lambda f_1 - g)\Big|_{\bar{t}^-}\right]\delta\bar{t} \qquad (11)
\end{aligned}$$

Since λ still retains its arbitrariness, the only unknowns in the last formulation are δz and $\delta\bar{t}$. One may now specify the variable λ in such a way that all of terms associated with δz and $\delta\bar{t}$ are dropped. Defining the following adjoint equations:

$$\dot{\lambda}_1 = -\frac{\partial f_1}{\partial z} + \frac{\partial g}{\partial z}, \qquad 0 < t < \bar{t} \qquad (12)$$

$$\dot{\lambda}_2 = -\frac{\partial f_2}{\partial z} + \frac{\partial g}{\partial z}, \qquad \bar{t} < t < \tau \qquad (13)$$

with terminal conditions:

$$\lambda_2(\tau) = 0 \tag{14}$$

and

$$\lambda_1(\bar{t}) = [\lambda_2(\bar{t})\, f_2 - g\big|_{\bar{t}^+} + g\big|_{\bar{t}^-}]/f_1 \quad \text{for } f_1(\bar{t}) \neq 0 \tag{15}$$

Finally, the combination of Eqs. 11-15 provides a simple formula for $\delta\psi$,

$$\delta\psi = \int_0^{\bar{t}^-} \left(\frac{\partial g}{\partial b} - \lambda_2 \frac{\partial f_1}{\partial b}\right) \delta b \, dt + \int_{\bar{t}^+}^{\tau} \left(\frac{\partial g}{\partial b} - \lambda_2 \frac{\partial f_2}{\partial b}\right) \delta b \, dt \tag{16}$$

If the design variable is a parameter instead of a function, the general expression of Eq. 16 can be simplified to yield the design sensitivity,

$$\frac{d\psi}{db} = \int_0^{\bar{t}^-} \left(\frac{\partial g}{\partial b} - \lambda_1 \frac{\partial f_1}{\partial b}\right) dt + \int_{\bar{t}^+}^{\tau} \left(\frac{\partial g}{\partial b} - \lambda_2 \frac{\partial f_2}{\partial b}\right) dt \, .$$

Example 1 The state equation is given as

$$\dot{z} = \begin{cases} b^2 t^2, & 0 \leq z < 1440 \\ bt, & 1440 < z \end{cases}$$

with initial condition $z(b,0) = 0$.

Given the functional ψ as

$$\psi_1 = \int_0^{\tau} z^2 \, dt,$$

the derivative $d\psi/db$ is simply obtained as

$$\frac{d\psi_1}{db} = \int_0^{\bar{t}} 2\lambda_1 \, bt^2 \, dt + \int_{\bar{t}}^{\tau} \lambda_2 b \, dt,$$

where the adjoint variables λ_1 and λ_2 are determined by the adjoint equations

$$\begin{cases} \lambda_1 = -2z, & 0 \leq t < \bar{t} \\ \lambda_2 = -2z, & \bar{t} < t \leq \tau \end{cases}$$

with terminal conditions,

$$\begin{cases} \lambda_2(\tau) = 0 \\ \lambda_1(\bar{t}) = \lambda_2(\bar{t})/(b\bar{t}), & \text{at } t = \bar{t} \end{cases}$$

If the design variable and the total time interval are assigned as $b = 400$ and $\tau = 2$, it follows that the critical time $\bar{t}$ is exactly equal to $\bar{t} = 0.3$ for jump condition $z(\bar{t}) = 1440$ and the design sensitivity is obtained as $d\psi/db = 5598.3$. The state variable and adjoint variable can be solved analytically. They are plotted in Fig. 1. The jumps of $\dot{z}$ and λ are indicated.

Example 2 A model of chemical kinetics is investigated here. The relation between the degree of cure α and the reaction or cure rate $\dot{\alpha}$ during the curing process of Graphite/Epoxy composite is determined experimentally as [5],

$$\dot{\alpha} = \begin{cases} f_1(\alpha, T, t) = (K_1+K_2\alpha)\ (1-\alpha)\ (B-\alpha), & 0 \leq \alpha < 0.3 \\ f_2(\alpha, T, t) = K_3(1-\alpha), & 0.3 \leq \alpha \end{cases} \qquad (17)$$

with initial condition $\alpha(0) = 0$ and the following definitions

$$K_1 = \Delta A_1\ \text{Exp}\ (-\Delta E_1/RT)$$

$$K_2 = \Delta A_2\ \text{Exp}\ (-\Delta E_2/RT)$$

$$K_3 = \Delta A_3\ \text{Exp}\ (-\Delta E_3/RT)$$

where ΔA_1, ΔA_2, ΔA_3, ΔE_1, ΔE_2, ΔE_3, R and B are material constants [5], and T is °K temperature. The problem is to analyze the sensitivity of a functional of α with respect to the temperature, i.e., $d\psi/dT$ where ψ is defined as

$$\psi_2 = \int_o^\tau \alpha^2 \, dt$$

The adjoint equation is derived as

$$\begin{aligned} \dot{\lambda}_1 &= 2\alpha + \lambda_1 (K_1 + K_1 B - K_2 B + 2K_2 B\alpha + K_2\alpha - 2K_1\alpha - K_2\alpha^2), \\ &\qquad\qquad 0 < t < \bar{t} \\ \dot{\lambda}_2 &= 2\alpha - K_3\lambda_2, \qquad\qquad \bar{t} < t < \tau \end{aligned} \tag{18}$$

with terminal conditions,

$$\lambda_2 (\tau) = 0 \qquad , \text{ at } t = \tau,$$

$$\lambda_1 (\bar{t}) = \frac{-\lambda_2(\bar{t})\, K_3}{K_1\alpha^2 - K_1 B + K_2\alpha^2 + B\, K_2\alpha^2 - 2K_2\alpha^3} \quad , \text{ at } t = \bar{t} \, .$$

In addition, the variation of functional ψ_2, $d\psi_2/dT$, is given as

$$\frac{d\psi_2}{dT} = \int_o^{\bar{t}} (-\lambda_1 \frac{\partial f_1}{\partial T}) \, dt + \int_{\bar{t}}^{\tau} (-\lambda_2 \frac{\partial f_2}{\partial T}) \, dt \tag{19}$$

It is not easy to solve Eqs. 17 and 18 analytically. Instead, they are solved numerically in the next section. And $d\psi_2/dT$ in Eq. 19 is evaluated by a numerical integration method.

As mentioned earlier, the discontinuous derivative can be replaced by a logical function $L(z,\varepsilon)$ which smoothly approximates a Heaviside step function H,

$$H = \begin{cases} 1 & z>o \\ 0 & z<o \end{cases}$$

within a given region $o<z<\varepsilon$ for a small number ε. The logical function $L(z,\varepsilon)$ is defined as [7]:

$$L(z,\varepsilon) = \frac{1}{2} \cdot \frac{|z|^{2n+1} + z^{2n+1}}{|z|^{2n+1} + \frac{1}{2}\left[|z-\varepsilon|^{2n+1} - (z-\varepsilon)^{2n+1}\right]} \qquad (20)$$

where n is an integer selected so as to ensure the continuity of the derivative up to order d, i.e., $2n+1 > d$. The n is taken as 1 in this study. Note that the values of logical function $L(z,\varepsilon)$ are 0, $1/2$ and 1 for $z=0, \varepsilon/2$ and ε, respectively. The differential equation, equation 4, can be combined into a single function by using the logical function $L(z,\varepsilon)$ as

$$\dot{z} = f_1 [1 - L(z-c,\varepsilon)] + f_2 \cdot L(z-c,\varepsilon) .$$

Since L is a smooth function, there is no discontinuity in the $\dot{z}$ of the preceding equation. Thus, the formulation of the design sensitivity analysis can be simplified a great deal.

The design derivative of function ψ_2, defined in the example 2, can be easily obtained by using the standard adjoint variable technique:

$$\frac{d\psi_2}{dT} = \int_0^{\tau} \left[- \frac{\partial f_1}{\partial T} (1-L)\lambda - \frac{\partial f_2}{\partial T} L\lambda \right] dt \qquad (21)$$

where the adjoint variable λ satifies the following adjoint equation:

$$\dot{\lambda} + \left[\frac{2f_1}{\partial\alpha} (1-L) - f_1 \frac{\partial L}{\partial\alpha} + \frac{\partial f_2}{\partial\alpha} L + f_2 \frac{\partial L}{\partial z} \right] \lambda + 2\alpha = o \qquad (22)$$

with terminal condition

$$\lambda(\tau) = o .$$

With the definition of $L(\alpha-0.3,\varepsilon)$ Eq, 20, the derivative $\partial L/2\alpha$ is not

difficult to calculate.

Although using a logical function to smooth the derivative discontinuity, one may avoid the need to identify the critical time of jump condition, yet the selection of ϵ , the domain where the logical function is defined, introduces a new difficulty. The numerical results listed in Table 4.b are obtained by integrating Eqs. 20 - 22. To obtain these results, the report time step required in DE program is given as $\Delta T=0.05$.

III. Numerical Considerations

The calculation of the design sensitivity of thermal system with discontinous derivatives encounters in numerical difficulties as expected. Numerical errors arise not only in solving the state equation but also in identifying the critical time of jump condition.

There are two numerical integration schemes employed here to solve the state and adjoint equations discussed in the preceding section. One is the Simpson's method, the other is DE program [8] using the Adams family of formulas.

Since the truncation error of Simpson's method is proportional to the fourth order derivative of unknown function, it provides exact integration for solving equation in the first example.

The DE program is one of predictor-corrector integration algorithm using Adams family of formulas. The truncation error is controlled by varying both the step size and the order of the method. The truncation error at time step t_{n+1} is required to satisfy

$$|\text{trunc}| \leq \text{ABSERR} + \text{RELERR} \cdot |z_n|$$

where the z_n is the solution of differential equation at t_n and the values ABSERR and RELERR are supplied by the user. The DE program is quite easy to be used and has capability to manage moderate stiff equation which happens commonly in the problem of chemical kinetics.

The critical time $\bar{t}$ at which the jump condition occurs is determined by selecting the time grid point closest to the condition $z(\bar{t}) = c$ for a given constant c and state variable z. Thus, the accuracy of $\bar{t}$ strongly depends on the step size.

The cost function and design derivative obtained by the adjoint variable technique of the first example are examined first. The comparisons between different numerical integrations used to solve equations, as well as time step and bounds of errors are listed in Table 1. It is indicated that all of them provide satisfactory results. Since b is taken as 400 in this calculation, $\bar{t}$ is exactly 0.3. Therefore, there is no approximation error at all on the critical time $\bar{t}$. Note that when the DE program is used for solving the state and adjoint equations, the cost function $\psi(\tau) = \int_0^\tau \alpha^2 \, dt$ is solved by an additional differential equation $\dot{\psi} = \alpha^2$.

To investigate possible sources of errors in the numerical calculations of thermal design derivatives, the change of cost functional with respect to different perturbation size of design variables are listed in Table 2. The design derivatives, ψ', in Table 2 are obtained by using the finite difference method and adjoint variable techniques with different numerical integration algorithms. It shows that the finite difference method, the adjoint variable techniques with Simpson's rule and with DE program introducing error bounds less than 10E-4 exhibit quite a deviation against the exact calculation. The major source of error might be the miscalculation of $\bar{t}$ in the analysis.

As an example, when b is reduced to 399.9 (0.025% change) the difference between cost functions evaluated exactly, 5293504.6, and evaluated by the Simpson's rule, 6194664.7, soars up to 901160 (17%). This big discrepency results from the numerical prediction of critical time $\bar{t}$ which should be 0.299 analytically instead of 0.3 numerically. Although the error of $\bar{t}$ is small, it happens in a neighborhood of steep $\dot{z}$ which causes significant error of z. Moreover, this error is squared and accumulated through t = 0.3 to t = 2.0.

It has been shown in Table 2 that the accuracy of the design sensitivity calculated by the adjoint variable technique is less sensitive to different numerical integration schemes than the accuracy of the cost functional evaluation does. To see the effect of the miscalculation of $\bar{t}$ on the accuracy of the design sensitivity calculated by the adjoint variable technique, various $\bar{t}$'s, which is supposed to be 0.3 analytically, are used for the design sensitivity calculation. The results are listed in Table 3. It is clearly shown that the adjoint variable approach is quite insensitive, compared to the finite difference method, to the numerical errors arising in the analysis and in the estimation of $\bar{t}$ at the jump conditions.

In example 2, neither state variable z nor critical time $\bar{t}$ has analytical solution. The design sensitivities listed in Table 4.a are calculated by the finite difference method and the adjoint variable technique with DE program. It is again shown that the adjoint variable technique provides a more stable solution than the finite difference method does, against numerical errors. The jumps of state variable and adjoint variable for example 2 are indicated clearly in Fig. 2.

Furthermore, the numerical results listed in Table 4.b are obtained by using the logic function approximation and by integrating Eqs. 20-22. The accuracy of the approach is also quite satisfactory.

IV. Conclusions and Remarks

The calculation of design sensitivity is discussed for the thermal transient problem with discontinuous derivative. The numerical difficulties depend on the approximation error of integration and the evaluation of the critical time of jump condition.

Because of the simplicity, it is a very common practice in the optimal

design community that the finite difference approach is used as a standard reference to check the accuracy of design sensitivity calculations. However, it is revealed in this investigation that the finite difference method may provide very unreliable information of design sensitivity. On the other hand, the adjoint variable technique using numerical integration algorithm with varied step size and error control performs satisfactorily in the design sensitivity analysis. Finally, it is also suggested in this investigation that the design sensitivity analysis can be used as an accuracy indicator for analyzing the transient problems with discontinuous derivatives.

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Table A1. Comparisons of Design Sensitivity Calculations of Example 1 at b = 400

Cost and gradient	Exact	D. E., Δt=0.01		Simpon's Rule	
		ERR=1.E-4	ERR=1.E-8	Δt=0.01	Δt=0.0001
ψ	5294072.	5294578.	5294073.	5294073.	5294049.
ψ'	6041.7	6046.	6035.7	6036.	6036.2

Table A2. Perturbation of Cost Function

(a) Exact Integration based on the given critical time $\bar{t}$

δb	ψ	$\Delta\psi$*	$\psi'\delta b$**	$\bar{t}$
0.1	5294641.	568.2	604.1	0.3
1	5299760.	5687.2	6041.7	0.3
4	5316879.7	22807.	24166.8	0.3
10	5351383.7	57311.	60417.	0.3
20	5409692.	115619.2	120834.	0.3
40	5530494.8	236422.1	241668.	0.29
-0.1	5293504.6	-568.1	-604.1	0.3
-1	5283205.2	-10867.5	-6041.7	0.31
-4	5265617.6	-28455.0	-24166.8	0.31
-10	5230743.3	-63329.4	-60417.	0.31
-20	5168474.0	-125598.6	-120834.	0.32
-40	5047690.4	-246382.3	-241668.	0.33

* by the finite difference method

** by using the adjoint variable technique

(b) Design Sensitivity by Using DE Program

	ERR = 1.E - 4				ERR = 1.E - 8			
δb	ψ	$\Delta\psi$	$\psi' \delta b$	$\bar{t}$	ψ	$\Delta\psi$	$\psi' \delta b$	$\bar{t}$
0.1	5296769.	2191.	604.6	0.3	5294676.	603.	603.5	0.3
1	5301065.	6487.	604.6	0.3	5300109.	6036.	6435.7	0.3
4	5335334.	40756.	24184.	0.3	5318213.	24140.	24143.1	0.3
10	5357658.	63080.	60460.	0.3	5354408.	60335.	60357.8	0.3
20	5417215.	122637.	120920.	0.3	5414704.	120631.	120715.6	0.3
40	5650796.	356218.	241840.	0.29	5535266.	241193.	241431.2	0.29
-0.1	5295286.	708.	-604.6	0.3	5293469.	-604.	-603.5	0.3
-1	5288646.	-5932.	-6046.	0.31	5288036.	-6037.	-6035.7	0.31
-4	5270086.	-24492.	-24184.	0.31	5269922.	-24151.	-24143.1	0.31
-10	5233724.	-60854.	-60460.	0.31	5233674.	-60399.	-60357.8	0.31
-20	5175668.	-11890.	-120920.	0.32	5173186.	-120887.	-120715.6	0.32
-40	5052250.	-242328.	-241840.	0.33	5051821.	-242252.	-241431.2	0.33

(c) Design Sensitivity Calculated by Using Simpson's Rule

	$\Delta t = 0.01$				$\Delta t = 0.001$			
δb	ψ	$\Delta\psi$	$\psi'\delta b$	$\bar{t}$	ψ	$\Delta\psi$	$\psi'\delta b$	$\bar{t}$
0.1	5298884.2	4811.0	603.6	.3	5298888.9	4839.3	603.6	0.300
1	5342381.0	48307.8	6036.	.3	5342384.0	48335.0	6036.2	0.300
4	5489298.6	195225.5	24144.	.3	5402432.1	108383.1	24145	0.298
10	5792261.9	498188.7	60360.	.3	5432358.5	138309.5	60362.5	0.295
20	6324608.9	1030535.8	120720.	.29	5467981.4	173932.4	120725.	0.290
40	6369644.1	1075571.0	241440.	.28	5578684.0	284635.0	241450.	0.282
-0.1	6194664.7	900591.5	-603.6	.3	5374019.6	79970.6	-603.6	0.300
-1	6143693.8	849620.7	-6036.	.3	5330111.5	36062.5	-6036.2	0.301
-4	5976044.6	681971.4	-24144.	.3	5352527.6	58478.6	-24145.	0.302
-10	5651040.9	356967.7	-60360.	.31	5307599.7	13550.7	-60362.5	0.305
-20	5993670.1	699596.9	-120720.	.31	5218612.9	-75436.0	-120725.	0.310
-40	5710638.8	416565.6	-241440.	.32	5064800.8	-229248.1	-241450	0.322

Table A3. Effect of $\bar{t}$ Miscalculation on Design Sensitivity Calculation

(a) DE Program

	ERR = 1.E - 4			ERR = 1.E - 8		
$\bar{t}$	0.29	0.30	0.31	0.29	0.30	0.31
ϕ'	5854.95	6046.96	6265.71	5843.81	6035.93	6259.06

(b) Simpson's Rule

	Δt = 0.01			Δt = 0.001		
$\bar{t}$	0.29	0.30	0.31	0.299	0.300	0.301
ϕ'	5833.32	6036.33	6272.18	6014.13	6036.25	6058.71

Table A4. Design Sensitivity Analysis of Example 2 at T=475°K and $\delta T = 1^0K$

(a) Adjoint variable method with jump condition

ERROR	ΔT	$\Delta\phi^*$	$\phi' \delta T^*$
1.E - 8	0.005	-0.149048	-0.193377
1.E - 8	0.05	-0.149048	-0.193916
1.E - 4	0.005	-0.155362	-0.193810
1.E - 4	0.05	-0.111411	-0.194819

(b) Adjoint variable method with logical function

ERROR	ε^{**}	$\Delta\phi^*$	$\phi\delta T^*$
1.E - 8	0.00017	-0.14921	-0.15202
1.E - 8	0.00009	-0.14921	-0.15195
1.E - 4	0.00017	-0.1119	-0.15179
1.E - 4	0.00009	-0.1119	-0.15139

* The temperature is changed from 475°K to 474°K.

** The domain where the logical function is defined.

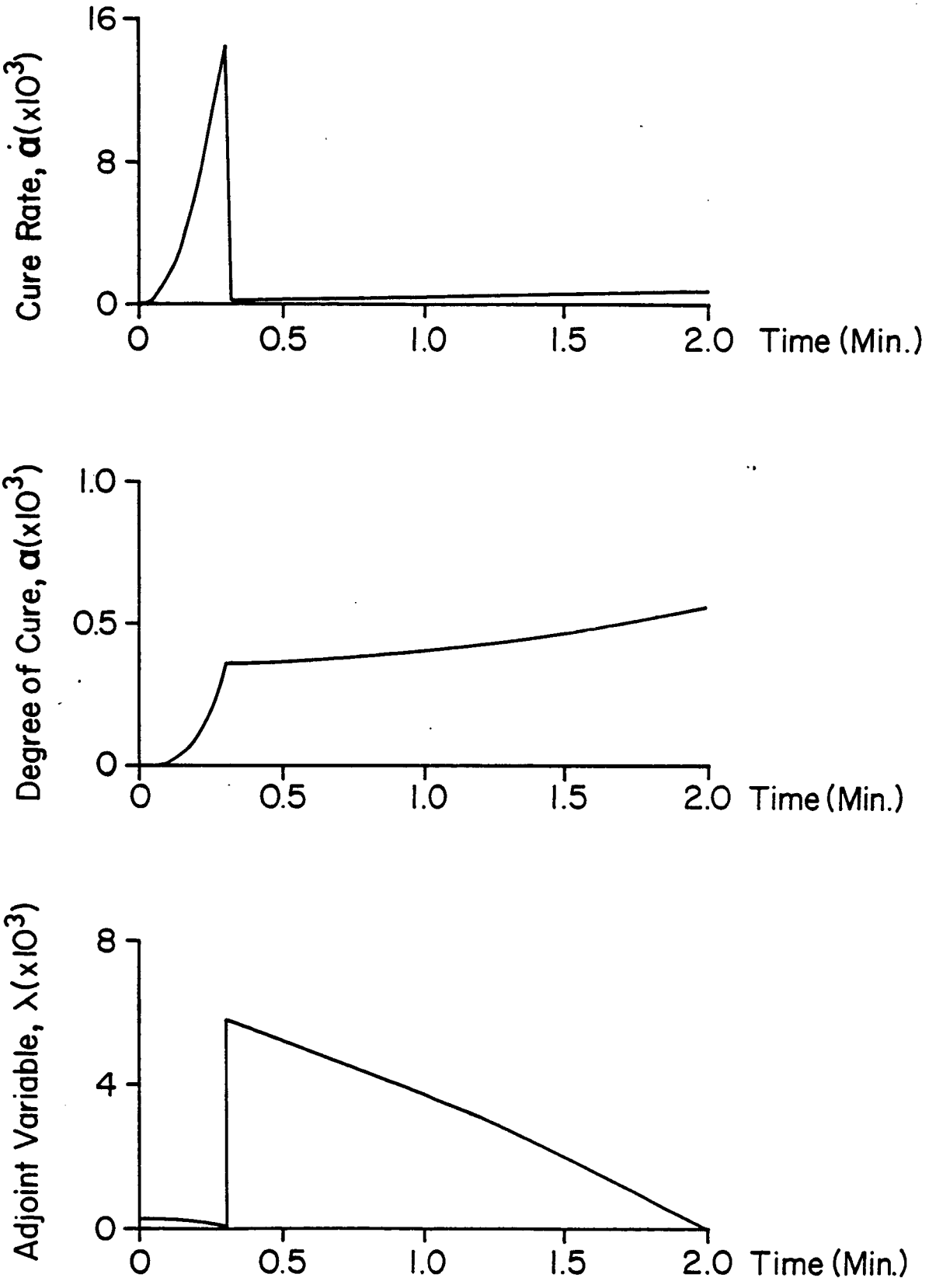

Figure A1. State Variable and Adjoint Variable for Example 1.

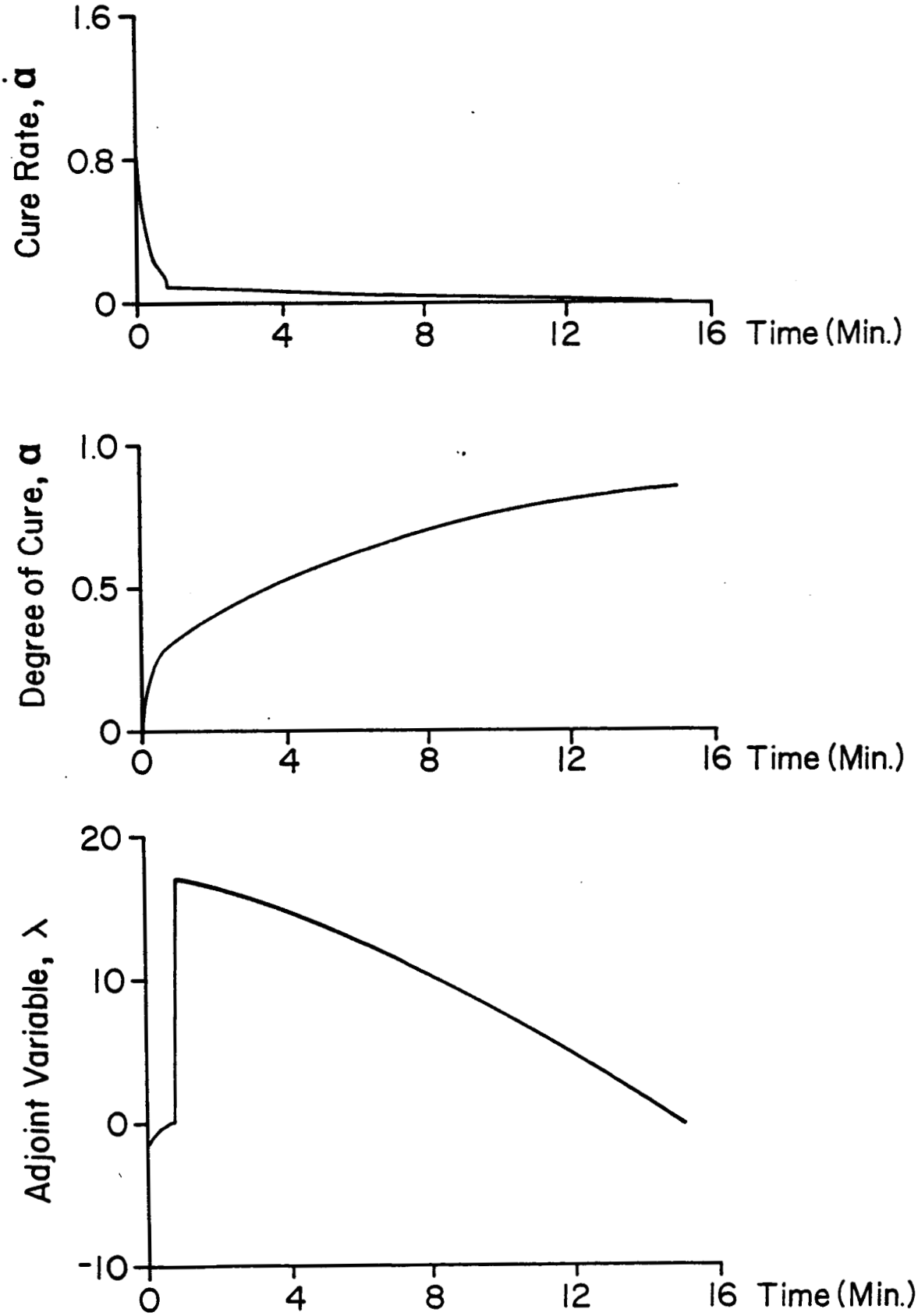

Figure A2. State Variable and Adjoint Variable for the Curing Process.