Three-Dimensional Inverse Heat Transfer in a Composite Target Subject to High-Energy Laser Irradiation

A new numerical model is developed to simulate the 3D inverse heat transfer in a composite target with pyrolysis and outgassing effects. The gas flow channel size and gas addition velocity are determined by the rate equation of decomposition chemical reaction. The thermophysical properties of the composite considered are temperature-dependent. A nonlinear conjugate gradient method (CGM) is applied to solve the inverse heat conduction problem for high-energy laser-irradiated composite targets. It is shown that the front-surface temperature can be recovered with satisfactory accuracy based on the temperature/heat flux measurements on the back surface and the temperature measurement at an interior plane. [DOI: 10.1115/1.4006107]

Keywords: composite, inverse heat conduction problems, pyrolysis, gas flow model, temperature-dependent thermal properties

1 Introduction

Fiber-reinforced composite materials have gained wide applications in military and industry [1]. Due to unique properties such as monochromaticity and directionality, high energy laser (HEL) beams are now employed as a weapon to defeat adversary military targets. To evaluate target damage, a direct heat transfer model is required to simulate temperature transients inside a laser-irradiated composite target with known initial and boundary conditions. Currently, many theoretical models are available for this purpose. For example, Reed and Rice [2] developed a rate-dependent pyrolysis model to characterize the heat transfer in decomposing material. Chen et al. [3] used a modified Crank-Nicholson finite difference scheme to model the heat transfer process in laser-irradiated composites. Zhou et al. [4] developed a 1D nonequilibrium thermal model to predict the through-thickness transient temperature variation in a composite slab subjected to intense laser heating. The cooling effect arising from pyrolysis reaction was simulated using a two dimensional gas flow model with an assumed gas addition velocity and the microchannel shape [5].

For a solid subjected to intensive laser beam heating, the heated (front) surface is either inaccessible or too hot so that it is not suited for attaching a sensor to measure temperature response [6]. Under this circumstance, some researchers propose to determine the heated surface temperature indirectly by solving an inverse heat conduction (IHC) problem [7,8] based on the transient temperature and/or heat flux measured at the back surface. Although IHC problems have been extensively studied for different applications in the past (e.g., [9–12]), little work has been done for composite materials subjected to high energy laser heating. Though Aviles-Ramos et al. [13] developed an exact solution for the IHC in a two-layer composite material, the pyrolysis effect was not considered in their model. Recently, the authors proposed a lower-error IHC algorithm to reconstruct the front-surface heating condition of a 1D composite slab with pyrolysis effect based on the back-surface measurement information [14]. The pyrolysis outgassing model was from Ref. [4], in which the gas addition velocity and the microchannel size were assumed.

2 Inverse Heat Conduction Problem

2.1 3D Inverse Heat Conduction Model. Consider a 3D composite object with dimensions \( L \times M \times N \) as shown in Fig. 1. The Cartesian coordinate system \( O-xyz \) is set with the origin locating at a corner of the object. Initially, the object is at a uniform temperature \( T_0 \) and then is subjected to a high intensity, Gaussian laser beam \( q_{laser} \) with a 1/e radius \( c \) centered on the front surface (\( x=0 \)) from \( t=0^+ \). Before the pyrolysis occurs, only pure conduction takes place in the composite. After the temperature reaches a threshold, the composite material undergoes chemical decomposition. Meanwhile, the decomposing process gives off gaseous by-products that flow outward from the pyrolysis zone to the heated surface. Since the pyrolysis occurs only in a confined region inside the material, this pyrolysis outgassing process is approximated as a 1D compressible gas flow along the x-direction, which will be addressed in Sec. 2.2.

The direct problem in the 3D target can be expressed as follows:

\[
C(T)
\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left[ k(T) \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[ k(T) \frac{\partial T}{\partial y} \right] + \frac{\partial}{\partial z} \left[ k(T) \frac{\partial T}{\partial z} \right] + Q(x,y,z,t) + G(x,y,z,t)
\]

for \( 0 < x < L, \quad 0 < y < M, \quad 0 < z < N, \quad t > 0 \)

\[
T = T_0 \quad \text{for} \quad 0 \leq x \leq L, \quad 0 \leq y \leq M, \quad 0 \leq z \leq N, \quad t = 0
\]

\[
-k(T) \frac{\partial T}{\partial x} = q_1(y,z,t) \quad \text{for} \quad x = 0, \quad t > 0
\]

In this study, a new 3-D IHC model is formulated to recover transient heat flux and temperature at the heated surface of composite targets heated by a high energy laser. The target is assumed to be of rectangular geometry. The pyrolysis process is characterized based on a new gas flow model. The gas flow channel size and gas addition velocity are determined by the rate equation of pyrolysis chemical reaction. The nonlinear 3D IHC problems are solved using a nonlinear conjugate gradient method (CGM) based on three groups of measurement data including temperature and heat flux at back surface as well as the temperature at an interior plane. Demonstrative simulations are performed and results are presented.
where the thermal conductivity data \( k \) is temperature-dependent; volumetric specific volume \( C \) is calculated by combining the corresponding values of the fibers and matrix, depending on the fraction of the decomposed material [4]. The factor “2” in Eq. (4) is due to the fact that the measurement temperature on the back surface \((x = L)\), which is the mean value of fiber temperature and matrix temperature.

It must be pointed out that the term “solid part” in this paper is used to describe the material part in solid state which is a combination of fiber and matrix when the pyrolysis is in progress. However, it refers to the fiber only after the pyrolysis is completed.

Equation (4) is written based on the premise that the measurement temperature at an interior location is the average of the local solid and gas temperatures.

The pyrolysis is a rate-dependent process and the generated heat source term \( Q(x, y, z, t) \) in Eq. (1) is obtained by

\[
Q(x, y, z, t) = -\frac{\rho \Delta H}{1-x} \frac{dx}{dt}
\]

where the fraction \( \rho \) is evaluated based on the rate equation

\[
\frac{dx}{dt} = A(1-x)^{M/2} e^{Bx}
\]

where \( A \) is the frequency factor, \( B \) is activation energy, and \( M \) is the order of the decomposition reaction.

The convective heat exchange term in Eq. (1), \( G(x, y, z, t) \), is expressed as

\[
G(x, y, z, t) = \frac{h_{gas}(T_g - T)}{R_c^{2}(1-x)/2R_e} \text{H}(t - t_{pyro})
\]

where \( h_{gas} \) is computed based on 1D compressible gas flow simulation and \( \text{H}(t - t_{pyro}) \) is Heaviside function, which is zero before pyrolysis \( (t < t_{pyro}) \) and one after pyrolysis \( (t > t_{pyro}) \).

In the direct problem described above, the front-surface heat flux \( q_1(y, z, t) \) and the back-surface temperature \( Y_f(y, z, t) \) are considered to be known. The objective of the direct problem is to determine the transient temperature and heat flux distribution in the composite target.

The inverse problem associated with the above defined direct problem can be stated as follows. The heat flux \( q_1(y, z, t) \) at the front surface \((x = 0)\) is unknown and needs to be recovered. The temperature measurement on the back surface, \( Y_f(y, z, t) \), is used as the boundary condition at \( x = L \). The heat flux measurements on the back surface \( Y_d(y, z, t) \) and temperature measurements \( Y_f(y, z, t) \) at the interior plane of \( x = x_t \) are utilized as extra information required to recover the front-surface heat flux. The front-surface temperature is calculated as a by-product according to the temperature–heat flux relation defined by the classical Fourier’s law.

The CGM [8] is applied to solve the IHC problem. The inverse solution is obtained by minimizing the following functional (referred to as objective function)

\[
S[q_1(t)] = \int_{0}^{t_f} \left[ Y_d(t) - q[L(t); q_1(t)] \right]^2 dt + \int_{0}^{t_f} \left[ Y_f(t) - T[x_t; q_1(t)] \right]^2 dt
\]

Fig. 3 Gas flow models
where $t_f$ is the final simulation time, $q(L; t; q_1(t))$ is the estimated heat flux at the back surface, and $T(x_1; t; q_1(t))$ is the estimated average temperature at the interior position $x_1$.

The CGM mathematical formulation for the nonlinear inverse problems involving temperature-dependent thermal properties is similar to that in Ref. [14]. It is not described here for brevity.

2.2 1D Compressible Gas Flow. It is assumed that the gas flow produced by pyrolysis reaction is one-dimensional along the $x$-direction. The physical model of the 1D gas flow is depicted in Fig. 2. The black regions represent fibers, the gray regions denote matrix, and the white regions represent the gas flow channels. Each gas flow channel, together with its surrounding material, constitutes an element as the dash-line box shown in Fig. 2.

The 1D gas flow in the gas channel (white region in Fig. 2) is a compressible gas flow problem with area change, friction, heat, and mass addition. It is intractable since it is involved with many complicated factors, among which the mass addition is the trickiest one. Solution for such a gas flow problem has not been reported in literatures. To overcome this difficulty, the 1D gas flow with mass addition will be converted to a 1D gas flow without mass addition but with extra area change [15, 16]. This can be explained with the aid of Fig. 3.

Take an infinitesimal section $dx$ for consideration. The parameters appearing in Fig. 3 are as follows: $x$ is the coordinate variable, $p$ pressure, $T_g$ temperature, $\rho_g$ density, $V$ gas flow velocity along the $x$-direction, $A_c$ cross section area of the gas channel, $M_a$ Mach number, $\dot{m}$ mass flux of gas addition (units: kg/(m$^2$/s)), and $\delta q$ the heat addition per unit mass of gas (units: J/kg).

The continuity equation for the 1D gas flow with mass addition in Fig. 3(a) can be written as

$$\frac{d(\rho_g V)}{dx} = \frac{\rho_g V dA_c}{A_c} + \dot{m} \cdot \pi D(x)$$  \hspace{1cm} (11)

where $D(x)$ is the inner diameter of the gas flow channel. For the gas flow without mass addition in Fig. 3(b), the continuity equation is given by

$$\frac{d(\rho_g V)}{dx} = -\frac{\rho_g V A'_c}{A'_c}$$ \hspace{1cm} (12)

By comparing Eqs. (11) and (12), one can see that the gas flow with mass addition in Fig. 3(a) can be converted to a gas flow without mass addition shown in Fig. 3(b). The new cross section area $A'_c$ can be obtained by equating Eqs. (10) and (11).

<table>
<thead>
<tr>
<th>$T$ (K)</th>
<th>296.15</th>
<th>323.15</th>
<th>373.15</th>
<th>473.15</th>
<th>573.15</th>
<th>673.15</th>
<th>773.15</th>
<th>873.15</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$ [W/(m·K)]</td>
<td>0.802</td>
<td>0.86</td>
<td>0.955</td>
<td>0.974</td>
<td>0.768</td>
<td>0.429</td>
<td>0.584</td>
<td>0.68</td>
</tr>
</tbody>
</table>
\[
\frac{dA_c'}{A_c'} - \frac{dA_c}{A_c} - \frac{\dot{m} \cdot \pi D(x)dx}{\rho_c A_c V} = 0
\]  

(13)

where \(A_c'\) is the new cross section area after conversion; \(A_c\) is the cross section area before conversion

\[
A_c = \pi R_c^2 = \pi \cdot R_c^2
\]  

(14)

The mass flux \(\dot{m}\) of gas addition in Eq. (1) is computed based on a 3D porous structure using the local volume averaging method [17]

\[
\dot{m} = \frac{1}{2} \rho R_c^2 \frac{dx}{dt}
\]  

(15)

Based on the conversion described above, the 1D compressible gas flow in a composite material can be simulated by the gas flow without mass addition shown in Fig. 3(b). We can then summarize the continuity, momentum, and energy conservation equations for the gas flow problem in Fig. 3(b) as follows [16]:

\[
\frac{dp_g}{\rho_g} + \frac{dA_c'}{A_c'} + \frac{dV}{V} = 0
\]

(16)

\[
dp + \frac{1}{2} \rho V g f d\frac{dx}{D} + \rho g V dV = 0
\]

(17)

\[
\delta q = c_{pg} dT_{go}
\]

(18)

where \(f_c\) is the friction coefficient, which is defined as

\[
f_c = \frac{4 \tau_f / (1/2 \rho V^2)}{\frac{\tau_f}{\rho V}}
\]

with \(\tau_f\) being the shear stress due to wall friction, \(c_{pg}\) is the mass specific heat of gas at constant pressure, \(T_{go}\) is stagnation temperature (or referred to as total temperature), which is related to true temperature \(T_g\) by

\[
\frac{T_{go}}{T_g} = 1 + \frac{\gamma - 1}{2} M^2
\]

(19)

where \(\gamma = c_{pg}/c_{vg}\) is the ratio of specific heat.

Combining the governing equations (16)–(18), the ideal gas law

\[
\frac{dp}{\rho} - \frac{d\rho_g}{\rho g} - \frac{dT_g}{T_g} = 0
\]

(20)

and the Mach number equation

**Fig. 7** Recovered temperatures on the front surface
\begin{align}
\frac{dT_x}{T_x} + \frac{dM_x^2}{M_x^2} \frac{dV^2}{V^2} &= 0 \quad (21)
\end{align}

one can reach a final equation which is utilized to calculate the Mach number as a function of \( x \)

\begin{align}
\frac{dM_x}{dx} = \frac{M_a}{1 - M_a^2} \left[ 1 - \frac{1}{A_c^2} \int dM_x' \frac{\gamma f}{2D} \left( \frac{\gamma - 1}{2} M_x'^2 \right) + \frac{1 + \gamma M_a^2}{2c_{fg} T_x} \right] \quad (22)
\end{align}

After the gas flow velocity is determined by Eq. (22), the convective heat exchange between the pyrolyzed gas and the surrounding composite materials can be evaluated by the Reynolds’s analogy approach, in which the convective heat transfer coefficient can be calculated as [16]

\begin{align}
h_{gas} = \frac{1}{8} \rho_g V c_{fg} f_r
\end{align}

According to Eq. (18), the heat exchange between gas and the solid wall is calculated as

\begin{align}
\delta q &= c_{fg} \rho_g T_{go} \frac{h_{gas}(T - T_{go}) 2\pi R_c'}{\rho_g V (\pi R_c'^2)} \quad (24)
\end{align}

where \( R_c' \) is the radius of the gas flow channel after conversion. Substitution of Eq. (23) into Eq. (24) results in

\begin{align}
\frac{dT_{go}}{T - T_{go}} = f_r \frac{\delta q}{4R_c'} dx \quad (25)
\end{align}

Equation (25) is used to calculate the gas stagnation temperature \( T_{go} \), which, in turn, is applied to compute gas true temperature \( T_g \) using Eq. (19). Then, the convective heat exchange term \( G(y, z, t) \) can be estimated from Eq. (9).

3 Results and Discussion

3.1 Generation of Simulated Measurement Data. Instead of conducting actual experiment, the measurement data of temperature and heat flux are generated numerically by solving a direct problem with radiation and convection boundary conditions. Here, the “direct problem” is not exactly the same as that defined in Eqs. (1)–(6). Only after Eqs. (3) and (4) are replaced by radiation and convection boundary conditions, Eqs. (1)–(6) can be used for the generation of simulated measurement data. To account for the measurement error, one extra term is added to the simulated heat flux measurement data, \( Y_{q,exact}(y, z, t) \)

\begin{align}
Y_{q,exact}(y, z, t) = Y_{q,exact}(y, z, t) + \omega \delta_q
\end{align}

It is assumed that the temperature readings at back surface and interior locations contain no errors since temperature can be measured with much less uncertainty compared to the heat flux [18].

3.2 Simulation Parameters. A carbon fiber/epoxy composite is taken as the demonstrative material. The dimension of the 3D object is 3.0 \( \times \) 68.4 \( \times \) 68.4 mm. The laser heating flux at the front surface is assumed to be Gaussian in space and sinusoidal in time

\begin{align}
q_{laser}(y, z, t) = q_0^* \exp\{- (y^2 + z^2)/w^2\} \cdot (1 + \sin(2\pi ft)) \quad (27)
\end{align}

where \( q_0^* \) is the heat flux at the laser beam center (averaged over one period); \( f \) is the frequency of the laser heating flux. In this study, the following simulation parameters are used unless otherwise specified: \( q_0^* = 150 \text{ W/cm}^2, f = 3.0 \text{ Hz}, w = 7.6 \text{ mm} \), and the measurement random error in back-surface heat flux \( \delta_q = 5\% \cdot |Y_{q,exact}(t)|_{max} \).

The 3D finite difference mesh used is 53 \( \times \) 13 \( \times \) 13. The dense mesh in \( x \) direction (53) ensures the exact capturing of the pyrolysis progress. To measure both temperature and heat flux at the back surface, a fully populated temperature and heat flux sensor array should be attached to the surface. Another fully populated temperature sensor array should be inserted to an interior plane at \( x = x_1 \) to measure the temperature. In this study, the interior plane location is at \( x_1 = 0.2 \text{ mm} \). Our simulation shows that for low thermal conductivity materials, interior temperature measurement data are necessary to accurately recover the front-surface heating condition. The lower the thermal conductivity is, the closer the location \( x_1 \) should be moved toward the front surface. The temperatures and heat flux obtained from the direct analysis will be used as the measurement data for IHC analysis.

The pyrolysis gas is approximated as CO\(_2\) whose thermal properties can be found in standard thermophysics textbook. The

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig8.png}
\caption{2D contours of the temperatures at the front surface at the time of 4 s}
\end{figure}
density and specific heat of the carbon fiber are 1603 kg/m³ and 1267 J/(kg·K), respectively. The density and specific heat of the epoxy matrix are 1100 kg/m³ and 600 J/(kg·K), respectively. The thermal conductivity of carbon/epoxy composite is considered temperature-dependent, which is listed in Table 1.

3.3 Results of Direct Problem. Figure 4 shows the temperature transients at the laser spot center on the front surface of the composite heated by a laser beam with $q_0 = 150$ W/cm². For comparison, the result obtained by a pure heat conduction model, which does not consider the pyrolysis gas flow effect, is also shown. It can be seen that the two curves in Fig. 4 are identical before the onset of pyrolysis, at about 0.7 s. After that, the two curves diverge from each other. This is because pyrolysis reaction begins and the decomposing process gives off gaseous by-products that flow outward from the pyrolysis zone to the front surface. The outgassing flow has a cooling effect on the composite bulk heated by laser irradiation, as evidenced by the observation in Fig. 4 that the curve 2 is below curve 1 after $t = 0.7$ s (Fig. 4(a)) and the difference between curve 2 and curve 1 is negative (Fig. 4(b)). In addition, as seen in Fig. 4(b), the difference between the results with and without pyrolysis is also fluctuates after the pyrolysis begins. The difference becomes smaller and smaller as time proceeds, indicating that the convective heat transfer effect due to pyrolysis becomes weaker with time.

Figure 5 shows the temporal evolvement of the gas channel shape. It appears that the gas channel shape can be divided to two
sections. One section is flat (e.g., $x = 0$–1.3 mm for curve 7), which corresponds to the status in which the decomposed $x$ reaches its maximum value $x_{\text{max}}$. The other section is the gradually converging section (e.g., $x = 1.3$–1.9 mm for curve 7), which corresponds to the status in which $x < x_{\text{max}}$. It can be clearly seen that the pyrolysis front advances toward deeper location of the composite as time elapses.

Figure 6 presents the distribution of the convective heat transfer coefficient $h_{\text{gas}}$ along the $x$-direction. The convective heat transfer due to pyrolysis at $t = 2$ s is the strongest. It is also observed that the distribution of $h_{\text{gas}}$ for all times can be divided to two sections. The horizontal sections of the curves correspond to $x = x_{\text{max}}$, which means that the pyrolysis is completed in this region. The gradually increasing sections of the curves correspond to $x < x_{\text{max}}$, in which section drastic pyrolysis reaction is occurring. Besides, it is seen from Fig. 6 that after $t = 2$ s, the convection heat coefficient $h_{\text{gas}}$ decreases with time at any particular $x$. This is because that as the chemical reaction proceeds, the amount of the pyrolyzed gas becomes less.

### 3.4 Results of Inverse Problems

Figure 7 shows the recovered temperatures at the laser spot and at the radius of 13.4 mm (the 1/e radius $w = 7.6$ mm). The location of 13.4 mm is chosen in a random way for illustrative purpose. The “exact solutions” shown in Fig. 7 are obtained from the solution of the direct problem with the radiation boundary conditions. As can be seen in Fig. 7, the temperatures can be well recovered from the IHC
analysis. As can be seen from the difference between exact solution and inverse solution (Fig. 7(b)), the largest error seems occurring at the most drastic moment of pyrolysis (at about 0.8 s). This is due to the extreme nonlinearity caused by the compressible gas flow. The stronger the pyrolysis effect, the more difficult to recover the front-surface temperature using an inverse approach. The rms difference between the exact and inverse solutions is calculated over the entire front surface and entire simulation time length, which is 3.36 K for this case. The error in different stage of simulation can be examined by a rms value defined in a different time range.

Figure 8 compares the 2D distributions of the recovered temperatures at the front surface at the time of 4.0 s. On this scale, the temperatures over the entire front surface appear identical.

Figure 9 plots the contour distributions of the errors in the recovered temperatures from 1 s to 6 s. As shown in Figs. 9(a)–9(f), the errors of the inverse solutions at t = 1 s is the highest. The errors at other times are quite small, less than 2 K. The location of the maximum error is not fixed, varying from time to time. However, the distributions of the numerical errors seem to be symmetric with regard to the laser spot center.

Figure 10 presents the simulation results when \( q_0 \) is increased to 300 W/cm². The temperatures at the laser spot center on the front surface are shown in Fig. 10(a). The cooling effect can be clearly seen and the pyrolysis onset time is about 0.5 s, which is earlier than that (0.7 s) of the case \( q_0 = 150 \) W/cm². The most drastic convective cooling effect is present from 0.5 to 0.7 s, shorter than that for the case of \( q_0 = 150 \) W/cm². For example, the length of the horizontal section at \( t = 3 \) s (curve 3) in Fig. 6 is about 0.6 mm, while it is about 1.0 mm in Fig. 10(b). This indicates that increasing the laser heating flux can cause pyrolysis at deeper depths.

The inverse solutions for \( q_0 \) is increased to 300 W/cm², presented in Figs. 10(c)–10(f). Figures 10(c) and 10(d) show the recovered temperatures and the difference between the exact solution and recovered solution on the front surface at laser spot center. Comparing Fig. 10(d) and Fig. 7(b), we can see that the higher the heating flux \( (q_0) \), the larger the inverse error at the most drastic moment of pyrolysis. Figures 10(e) and 10(f) show the recovered temperatures and the difference between the exact solution and recovered solution at \( r = 13.4 \) mm. The rms error in the front-surface temperature is 7.69 K.

If the frequency of the front heating flux is high, it usually becomes more difficult to recover the periodic information (amplitude and phase) in the front-surface temperature based on the measurement data below the heating surface due to the damping and lagging effects of heat diffusion. The effect of the frequency \( f \) on the inverse solutions is examined in Fig. 11, which shows the...
recovered temperatures at the laser spot center \((r=0)\) and at the radius of 13.4 mm for \(f=5 \text{ Hz}\) and \(q_{\text{G}}^0=150 \text{ W/cm}^2\). It can be seen that the temperatures at these two points can be well recovered. The rms error in the front-surface temperature is 5.29 K.

### 4 Conclusions

A new numerical model is developed to simulate the 3D inverse heat transfer in a composite target with pyrolysis and outgassing effects. The gas flow channel size and gas addition velocity are determined by using the rate equation of decomposition chemical reaction. In the 1D compressible gas flow model, the gas addition in a laser-irradiated composite material is accounted for with extra reaction. In the 1D compressible gas flow model, the gas addition determined by using the rate equation of decomposition chemical reaction. In the 1D compressible gas flow model, the gas addition determined by using the rate equation of decomposition chemical reaction.

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Test Resource Management Office for Simulation, Training and Instrumentation’s Contract T&E/S&T Program through the U.S. Army Program Executive Office for Simulation, Training and Instrumentation’s Contract No. W900KK-08-C-0002. The authors would also like to express their gratitude to Dr. James L. Griggs for his valuable discussions.

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