Integrated Thermal Response Modeling System
For Hypersonic Entry Vehicles

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Extended Abstract
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Abstract
The Integrated Thermal Response Modeling System consists of a two-
dimensional implicit thermal response and ablation program (TITAN), a commercialized
finite-element thermal/mechanical analysis code (MARC), a high fidelity Navier-Stokes
equation solver (GIANTS), and a boundary layer engineering correlation program
(MEIT). This system is developed for fully coupled thermal response analysis of
hypersonic entry vehicles with ablating heat-shield materials. The simulations performed
by this integrated modeling system include flow field, fluid/solid interaction, shape
change, and heat-shield/structure material thermal response. Because of the severe
aerothermal heating environment and the unique features of ablating heat-shield
materials, none of the commercialized finite-element codes have the capability of
simulating ablating heat-shield materials under hyper-velocity entry conditions.
Therefore, TITAN was developed specifically for modeling ablating heat-shield. The
structural materials underneath the heat-shield experience relatively benign heat loads,
and are usually multi-dimensional and have complicated geometries. Thus. the
commercialized finite-element code can be adapted for the thermal response simulation of
structural materials. The approach taken in this work to perform full vehicle thermal
analysis is simulating the ablating heat-shield using the TITAN code, and simulating the
structural materials using MARC. The ablating heat-shield is treated as an outer boundary
condition of structure. The continuity conditions of temperature and heat flux are
imposed at the interface between TITAN and MARC. The aerothermal environments
with fluid/solid interaction are predicted by coupling TITAN, GIANTS. and MEIT. The
aerothermal environments and the thermal response solutions for both ablating heat-
shield and structure materials can be obtained simultaneously. Representative
computations, including a proposed blunt body earth entry vehicle, a slender body re-
entry vehicle, and an arc-jet test model are demonstrated. The results are presented and
discussed in detail.

Nomenclature
$B'$ = $m / \rho, u, C_{\text{s}}$, dimensionless mass blowing rate
$B_{1}$ = pre-exponential constant in Eq.(8), s$^{-1}$
$C_{t}$ = skin friction coefficient
C_H = Stanton number for heat transfer
C_M = Stanton number for mass transfer
c_p = specific heat, J/kg-K
E = internal energy, J/kg
E_a = activation energy in Eq.(8), J/kmol
F = view factor
h = enthalpy, J/kg
H_r = recovery enthalpy, J/kg
k = thermal conductivity, W/m-K
m = mass flow rate, kg/m²-s
P = pressure, N/m²
q = heat flux, W/m²
q_c = conductive heat flux, W/m²
q_R = radiative heat flux, W/m²
Q = heat source term, J/m³
R = universal gas constant, J/kmol-K
R_c = corner radius, cm
R_n = nose radius, cm
s = stream length, m
s = surface recession rate, m/s
t = time, sec
T = temperature, K
u = velocity, m/s
v_s = species diffusion velocity, m/s
v_n = surface normal velocity component, m/s
Z* = coefficient in Eq.(3), defined in Ref. 14
α = surface absorptance
ε = surface emissivity
Γ = volume fraction of resin
λ = blowing reduction parameter
θ = momentum boundary layer thickness, m
ρ = total density, kg/m³
σ = Stefan-Boltzmann constant, W/m²-K⁴
τ = stress, N/m²
Ψ = decomposition reaction order
subscripts
c = char
e = boundary-layer edge
g = pyrolysis gas
i = density component (A, B, and C)
j = surface species
m.n = index of computation cell
v = virgin
Introduction

Spacecraft heat-shields often use Thermal Protection System (TPS) materials which pyrolyze and ablate at high temperature for mass-efficient rejection of aerothermal heat load. Pyrolysis is an internal decomposition of the solid which releases gaseous species, whereas ablation is a combination of processes which consume heat-shield surface material. For design and sizing of ablating spacecraft TPS materials, it is imperative to have a reliable numerical procedure which can predict surface recession rate, in-depth pyrolysis, and internal temperature history. In addition to a numerical code, the thermal properties and the boundary conditions of heat-shield must be precisely defined to perform an accurate simulation. The schematic diagram of Thermal Protection System is shown in Figure 1. The front face of heat-shield is exposed to aerothermal heating generated by fluid/solid interactions. A high fidelity Computational Fluid Dynamics (CFD) code with appropriate surface thermal chemistry boundary conditions or an engineering code with semi-empirical correlations can be used to provide the aerothermal environments. The back face of heat-shield is attached to a structure. Thus, the structure must be included in the thermal response simulation to correctly predict the bond-line temperature history. The structure is usually with complicated geometries, but has relatively simple thermal response as compared with heat-shield. Hence, a commercialized finite-element material response code can easily be adapted for structural material thermal response simulation.

In the past, a number of ablating heat-shield simulation programs were developed. The Charring Material Thermal Response and Ablation Program (CMA) was developed by the Aerotherm Corporation in the 1960's. It solved the internal energy balance and decomposition equations coupled with the ablating surface energy balance condition to simulate the response of ablative heat-shields in hypersonic flows. The Fully Implicit Ablation and Thermal Response program 2 (FIAT) was developed by Chen and Milos at NASA Ames Research Center. The structure of FIAT is similar to that of One-dimensional Multi-Layer Implicit Thermal Response Simulation code, OMLITS 3. FIAT is numerically more stable, and solves much wider range of problems compared with CMA, and has been used for TPS sizing calculations in various NASA's space missions. However, the governing equations solved in both CMA and FIAT codes are one-dimensional. Thus, these two codes are not applicable for conditions in which a one-dimensional assumption is not true, such as the nose-tip of a sharp body re-entry vehicle.

The Ablation and Shape Change code 4 (ASCC) developed by the Aerotherm Corporation is an engineering code for fully coupled fluid/solid simulation with axisymmetric or planar geometry. Nonetheless, the effect of pyrolysis gas due to internal decomposition was not implemented in ASCC, and its thermal diffusion equation was solved using an old fashioned finite-difference scheme. It has been shown that the accuracy of ASCC thermal response prediction is poor for both steady state and transient conditions 5. The two-dimensional ablation code developed by Hogan et al at Sandia National Lab used the finite-control-volume method with unstructured grids 6. In this code, the mesh motion was modeled by assuming the mesh behaves as a linear elastic
solid. In addition to two-dimensional thermal diffusion equation, a two-dimensional linear elastic solid mechanics model was applied to predict the motion of interior nodes. The effect of pyrolysis gas was not considered in Hogan's work, and the interaction between solid and fluid was not discussed.

In order to support the development of Ultra-High Temperature Ceramics (UHTCs) at NASA Ames Research Center, and to demonstrate their potential to enable sharp leading edges for hypersonic flight, an integrated analysis tool, MARC/ASCC, was developed. Because of the unique structural, thermal, and chemical properties of UHTCs, the analysis requires full coupling of the flow environment and the material thermal response. Thus, this integrated tool consists of a graphical user interface, a finite-element thermal and stress analysis package, a flow environment simulation code, and a material property database. The graphical user interface is known as Mentat, the finite-element material response code is MARC, and the flow environment simulation program is based on the Momentum and Energy Integral Technique Procedure, MEIT, in the ABRES Shape Change Code. However, the integrated MARC/ASCC code is not capable of simulating ablating TPS materials.

Recently the Two-dimensional Implicit Thermal Response and Ablation (TITAN) Program was developed to perform high fidelity thermal response and shape change simulation for charring materials. The governing equations include energy conservation and a three-component decomposition model with a moving grid, and are discretized using a finite-volume approximation with general body fitted coordinates. The time accurate solution is achieved by the implicit time marching technique using Gauss-Siedel line relaxation with alternating sweeps.

A fully coupled fluid-solid simulation is required for an accurate prediction of shape change. This is because shape change can not be correctly determined without appropriate aerothermal heating, and aerothermal heating is very sensitive to the geometry of the solid surface. The Navier-Stokes solver, GIANTS, and the Momentum and Energy Integral Technique Procedure, MEIT, were successfully coupled with the TITAN code using a loosely coupled method for fluid/solid simulation.

The purpose of this work is to integrate the aerothermal environment code, ablating heat-shield simulation code, and structural material response code to perform full vehicle thermal response analysis. This system is built around the commercialized finite-element code, MARC. The TITAN, GIANTS, and MEIT codes are integrated with MARC through user supplied boundary condition subroutines. The ablating heat-shields are simulated using the TITAN code and the structural materials are simulated using MARC. This is because TITAN is a finite-volume code and thus is not as flexible as a finite-element code for solving complicated multi-dimensional objects. This integrated system can predict aerothermal heating, shape change, and heat-shield and structure thermal response simultaneously. To demonstrate the capability of this integrated material thermal response modeling system, the simulations of a proposed blunt body earth entry vehicle, a slender body re-entry vehicle, and an arc-jet test model are performed. The results will be presented and discussed in the final paper.
Integrated Thermal Response Modeling System

The flow chart for Integrated Thermal Response Modeling System is shown in Fig. 2. The four major components in this system are MARC, TITAN, GIANTS, and MEIT. The brief description of each code is listed in the following sections. The accuracy of codes has been previously studied\textsuperscript{47,71} and is not the focus of this work. This modeling system is integrated around the MARC code. The front end of MARC is known as Mental\textsuperscript{11}, which is a graphical user interface program. The material properties are provided from TPSX\textsuperscript{12}, which is the TPS material property database developed at NASA Ames Research Center. The Multi-Component Ablation Thermochemistry code\textsuperscript{13}, MAT, is used to generate the tables of normalized mass blowing rate.

MARC and TITAN are interfaced through the user provided heat flux boundary condition routine, FLUX. The continuity conditions of heat flux and temperature are imposed at the interface:

\[
q_{MARC} = -k \nabla T |_{TITAN}\]  \hspace{1cm} (1)
\[
T_{TITAN} = T_{MARC}\]  \hspace{1cm} (2)

At each time increment, the front-face heat flux boundary condition of MARC is updated using the temperature gradient calculated by TITAN (Eq. 1), and the back-face temperature boundary condition of TITAN is equal to the temperature computed by MARC (Eq. 2) at each interface point.

TITAN and flow environment codes, including GIANTS and MEIT, are interfaced using the convective boundary condition. The conditions at the ablating surface are determined by convective and radiative heating and by surface thermochemical interactions with the boundary layer gases. The surface energy balance equation employed is of the convective transfer coefficient type. This energy balance equation takes the following form\textsuperscript{14}:

\[
\rho_e u_e (H_e - h_{m}) + \rho_e u_e C_v \left[ \sum (Z^*_{m} - Z^*_{m}) h_f^n - B' h_w \right] + \dot{m}_h + \dot{m}_c h_c
\]
\[
+ \alpha_e q_{m} - F \sigma \varepsilon_a T_m^n - q_{c, w} = 0 \]  \hspace{1cm} (3)

The first term in Eq. 3 represents the sensible convective heat flux. The sum of the second, third, and fourth terms in Eq. 3 is defined as the total chemical energy at the surface. The \( Z^* \) terms represent transport of chemical energy associated with chemical reactions at the wall and in the boundary layer\textsuperscript{14}. The \( Z^* \) driving forces for diffusive mass transfer include the effects of unequal diffusion coefficients. The fifth and sixth terms are the radiative heat fluxes absorbed and re-radiated by the wall, respectively, and the last term, \( q_{c, w} \), represents the rate of conduction into material. Here \( B' \) is the normalized mass blowing rate. The tables of \( B' \) for charring materials can be generated using ACE\textsuperscript{15} or MAT\textsuperscript{13}.

The computation starts from the MARC code. At each time increment, MARC calls TITAN to compute the new heat flux boundary condition, and, at the same time TITAN obtains the back-face temperature boundary condition from MARC and also calls the flow environment code to update the front-face convective boundary condition if necessary. When the maximum local surface recession exceeds the predefined criterion since last surface convective heating was updated, a flow-field grid is generated based on the current body geometry, and then the flow simulation routine, GIANTS or MEIT, is
called to compute the aerothermal heating environment. Each call to the flow environment routine is a steady state calculation. In this work, the non-ablating cold wall heating is calculated by GIANTS using a 5-species air chemistry (N₂, O₂, NO, N, and O), and a blowing reduction parameter of 0.5 is used in TITAN to take into account the blockage due to mass blowing. As expected, GIANTS calculation is much more computationally intensive as than the thermal response computation. For a fully coupled high fidelity simulation, most of CPU time is consumed by the flow environment calculation. Thus, the CPU time required for simulation is primarily determined by the efficiency of the GIANTS code.

MARC
The structure material thermal response and thermal stress analysis are performed using the commercialized finite-element code, MARC. Heat transfer and mechanical analysis can be done separately or fully coupled. The energy conservation law is

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot \kappa \nabla T = Q$$

The boundary conditions include prescribed temperature, heat flux, and convective heat transfer coefficient to the environment. For transient analysis, the initial temperature has to be specified to start the calculation. To perform thermal stress analysis, the MARC program uses an instantaneous thermal expansion coefficient defined as:

$$\varepsilon^{th}_{ij} = \alpha \delta_{ij} dT$$

In most cases, the thermal expansion data is given with respect to a reference temperature T°, as:

$$\varepsilon^{th} = \bar{\alpha} (T - T°)$$

Hence, the conversion of the expansion data to the instantaneous thermal expansion coefficient becomes:

$$\alpha = \bar{\alpha} + \frac{d\bar{\alpha}}{dT} (T - T°)$$

TITAN
The ablating TPS material thermal response and shape change computation is performed using TITAN. The governing equations include energy conservation and three-component decomposition model. The surface energy balance condition (Eq. 3) is solved with a moving grid to calculate the shape change due to surface recession. The internal energy balance is a transient thermal conduction equation with additional pyrolysis terms.

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) - (h_v - h) \nabla \cdot m_v + m_v \cdot \nabla h_v + S \rho c_p \nabla T$$

The individual terms in Eq. 8 may be interpreted as follows: rate of storage of sensible energy, net rate of thermal conductive heat flux, pyrolysis energy-consumption rate, net
rate of energy convected by pyrolysis, and convection rate of sensible energy due to coordinate system movement.

A three-component decomposition model is used. The resin filler is presumed to consist of two components which decompose separately, while the reinforcing material is the third component which can decompose. The instantaneous density of the composite is given by:

\[
\rho = \Gamma (\rho_A + \rho_B) + (1 - \Gamma) \rho_C
\]

(9)

where A and B represent components of the resin, and C represents the reinforcing material. \( \Gamma \) is the volume fraction of resin and is an input quantity. Each of the three components can decompose following the relation:

\[
\frac{\partial \rho_i}{\partial t} = -B \exp\left(-\frac{E}{RT}\right) \rho_i \left(\frac{\rho_i - \rho_{ni}}{\rho_{vi}}\right)^n + \frac{\partial}{\partial \eta} \rho_i
\]

(10)

where \( \rho_i \) is the residual or terminal density of component i, and \( \rho_{ni} \) is the original density of component i (i = A, B, and C). The motion of pyrolysis gas is assumed to be one-dimensional (along \( \eta \) direction), and thus the mass flow rate of pyrolysis gas at the surface is calculated using the following approximation:

\[
\dot{m}_g = \frac{1}{A_w} \int_{\eta_0}^{\eta_1} \left(\frac{\partial \rho}{\partial \eta}\right) A_w d\eta
\]

(11)

Governing equations are discretized using a finite-volume approximation with a general body fitted coordinate system. The time accurate solution is achieved by the implicit time marching technique using Gauss-Siedel line relaxation with alternating sweeps. The computational grid is compressed during the course of computation to reflect the surface recession.

MEIT

The inviscid flow modeling in the MEIT code includes the prediction of the surface pressure distribution and the bow shock shape. The surface pressure ratio distribution is predicted by sophisticated semi-empirical correlations, each of which is specialized for specific regions of the body. The shock shape and shock standoff distance are predicted with an approximate integral solution of the continuity and momentum equations.

The solution method for viscous boundary layer employed is known as the Momentum/Energy Integral Technique (MEIT). The following three basic equations are solved simultaneously:

Integral Momentum Equation:
\[
\frac{1}{r^n \rho_n u_r^2} \frac{d}{ds} \left( r^n \rho_n u_r^2 \right) = \frac{C_i}{2} + \frac{\rho_n v_n u_{n,u}}{\rho_n u_r^2} + \frac{110}{\rho_n u_r^2} \frac{dp}{ds}
\]

Integral Energy Equation:

\[
\frac{1}{r^n \rho_n u_r (h_r - h_n)} \frac{d}{ds} \left( r^n \rho_n u_r (h_r - h_n) \phi \right) = \frac{\rho_n v_n (h_{r,n} - h_n)}{\rho_n u_r (h_r - h_n)} \]

Entrainment Relation:

\[
\rho_n u_r \phi = (2r)^n F \mu \text{Re}_\mu - 2^n \int_0^r r^n \rho_n v_n ds
\]

Here, \( n = 1 \) for axi-symmetric formulation and \( n = 0 \) for 2-D planar flow. The inviscid flow solution provides the boundary layer edge conditions, and the surface energy balance computations provide the wall boundary conditions for the solution of the boundary layer integral equations. The boundary layer edge thermodynamic state is determined by lookup on pressure and entropy in a real gas Mollier table. Pressure is known from the inviscid flow solution, and entropy is calculated from consideration of the bow shock shape and boundary layer mass entrainment. The integral equations are solved in two ways: 1.) series solutions near the stagnation point; 2.) finite difference numerical solutions away from the stagnation point.

Various influence coefficients are defined in MEIT. The influence coefficients are factors derived by comparing the convective heat transfer to what it would be along the ideal plate for the same boundary layer state. The factors are derived in principle by considering one nonlinear behavioral mechanism at a time. Care is required to formulate the influence coefficients with the proper bases so that when the integral equations are integrated, the experimental data or exact solutions are accurately reproduced. The detail discussion regarding the implementation of influence coefficients are listed in Ref4.

The heating in the free molecular flow environment can be solved in closed analytical form. Prediction of the physics in the transitional regime presents a formidable challenge. The solutions of direct Monte-Carlo simulations require large amount of time. The approach taken in MEIT to compute transitional heating is very simple and consists of combing the free molecular and continuum value using an appropriate bridging relation.

**GIANTS**

The correlations implemented in MEIT are good for the slender body vehicle only. Thus, the flow simulation over a blunt body has to be performed using the GIANTS code. The GIANTS code solves the time-dependent conservation equations of mass, momentum, and energy for chemical and thermal non-equilibrium flowfield. The species mass conservation equation is given by

\[
\frac{\partial \rho_j}{\partial t} + \nabla \cdot (\rho_j u_j) = \frac{\partial}{\partial x_j} (\rho_j v_j) + w_j
\]

the momentum conservation is written as
\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial}{\partial x_j} (\tau_{ij}) \quad (16)
\]
and the energy conservation as
\[
\frac{\partial}{\partial t} E + \frac{\partial}{\partial x_j} ((E + p)u_j) = -\frac{\partial}{\partial x_j} (q_i + q_v) - \frac{\partial}{\partial x_j} (u, \tau_{ij}) - \sum_h \frac{\partial}{\partial x_j} v_{ij} h_i
\]
\[
(17)
\]
The governing equations are discretized using finite-volume method. The numerical method that was used to solve these discretized equations is exactly the same as that used in the TITAN code. It's fully implicit and uses Gauss-Seidel line relaxation. This technique has been shown to yield steady-state results efficiently. A 5-species air chemistry with bifurcation diffusion model was implemented in this version of code.

**Results and Discussion**

Three test cases will be demonstrated in this work. The first case is a blunt body entry vehicle, the second one is a slender body re-entry vehicle, and the third one is a flat faced arc-jet model. Their temperature contours are shown in Figs 3 to 5, respectively. The detail of simulations will be discussed in the final paper.

**References**