MODELING OF ONE DIMENTIONAL ABLATION

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Abstract. The development of a one-dimensional (planar) material thermal response with ablation is presented. The mixture energy equation, under uniform heat conduction is solved with Fourier's law to model heat conduction, and the ideal gas law to model the state of the pyrolysis gases. Consequently, the temperature, profile is predicted for a decomposing ablator. The control volume finite element spatial discretization method (CVFEM), the Euler implicit time integrator, and a contracting grid scheme are used for the solution of the mixture energy equation. The mixture energy equation is solved using segregated Newton solvers, which allow for nonlinear iteration on the entire system of nodal equations that are discretized according to a residual formulation. The block Gauss-Seidel segregated solution procedure has been implemented to globally iterate on the system of governing equations resulting in a fully coupled solution.

Keywords: Thermal Response, Ablation, control volume.

Nomenclature

A	Area
Α	Area vector
h	Specific enthalpy
E	Energy content
m ["]	Mass flux
<i>m</i> ^{""}	Volumetric mass source term
$q^{"}$	Heat flux
q ["]	Heat flux vector

$\hat{M}_{ m s}$	Molecular weight Surface recession
s. S	Surface recession rate
(e)	Element
T	Temperature
t	Time
Z	Coordinate with respect to initial ablation front
Z	Nodal velocity

Greek symbols

Γ	Initial resin volume fraction
η	Landau coordinate
ξ	Local coordinate
ψ	Reaction order in Arrhenius relationship
ρ	Density

Subscripts

i	Composite component index
c	Char
cv	Control volume
S	Solid
V	Virgin plastic
g	Gas

Superscripts

n	Time level
V	Iteration level

1. Introduction

Ablation has been defined as self regulating heat and mass transfer process in which incident thermal energy is expended by sacrificial loss of material.

Charring ablators provide the most efficient TPS for aerospace applications. These are being processed by the method of synthetic assembly of resin binder and a refractory reinforcement in order to obtain certain special characteristics and properties. The char is a thermal insulation, the interior of which is cooled by volatile material percolating through it from decomposing polymer (Figure.1). A thick char provides an efficient insulation barrier, reradiates a large amount of incoming heat from the surface, and is a very efficient ablator. Very good char strength has been obtained with carbon phenolic TPS materials.



Figure 1.Heat transfer mechanism of charring ablators under hot flow

1.1 Literature Review

Aerotherm Corporation, one of NASA's contractors developed Charring Materials Ablation (CMA), and it has served as the industry standard for several decades. CMA is a one-dimensional material thermal response code with in-depth decomposition that solves the energy equation with pyrolysis gas effects. One of the primary physical assumptions that the developers, Moyer and Rindal [9], made was that for a given time step, the pyrolysis gas generated further in-depth than a given node was assumed to flow pass that node during the time step. In terms of numerics, CMA has a finite difference spatial discretization of the governing differential equations and the Euler implicit time integrator. Mover and Rindal implemented a translating grid scheme in which the grid is attached to the receding surface and the overall number of nodes in the domain is reduced as mass is removed at the ablating surface. Since the energy equation is nonlinear in both surface recession rate and temperature, a linearization method is necessary to find a solution. Moyer and Rindal accomplished this by lagging the thermo-physical properties and surface recession rate one time step for the interior node equations while they iteratively solve the surface energy balance to find the updated recession rate.

Recently J.L.Lin, C.S.Yang [5] presented experimental and numerical work under the aerodynamic heating of charring ablators. The experiment model is a stainless steel cone with an attached charring ablator, in which supersonic hot flow impinges and the numerical simulation is based on physical and mathematical models including one dimensional unsteady energy transport and mass conservation equations coupled with calculations of aerodynamic heating, thermal degradation, heat transfer of the ablating surface and the ablation model. The findings from the numerical calculations are time history of temperature distribution inside the charring material and the backup structure

1.2 Present work

The study is focused to obtain the temperature profile for the effective design of the back-up structure under the assumption of steady state conduction, in finite volume method considering the effect variations in material and thermo-physical properties.

2. Mathematical modeling

Under the assumptions that the pyrolysis gas is a single nonreactive entity, the solid and gas are in thermal equilibrium, and there is no in-depth energy source, then the solid and gas energy equations for a moving grid reduce to a mixture energy equation given by

$$\int_{cs} \frac{d}{dt} dA + \int_{cs} \phi \rho_g h_g v_g dA - \int_{cs} \rho h v_{cs} dA + \frac{d}{dt} \int_{cv} \rho e dV = 0....(1)$$

2.1. Boundary conditions

Arrays of boundary conditions for the mixture energy equation are studied and the most commonly used for engineering applications are convective aerodynamic heating and radiation. Assuming equal species diffusion coefficients and equal mass and heat transfer Stanton numbers, the aerodynamic heating/radiation boundary condition with ablative and pyrolysis gas flux energy terms is given by

$$q'' = \rho_e u_e C_{ho} \left(\frac{C_h}{C_{ho}} \right) (h_w - h_r) + \varepsilon \sigma \left(T_{bnd}^4 - T_{res}^4 \right) + m''_s h_w + m''_g h_w \dots (2)$$

where C_h/C_{ho} is an empirical Stanton number correction for mass

blowing and hot wall effects. The wall gas enthalpy (h_w) is defined as the enthalpy resulting from equilibrated reactions between ablation products, pyrolysis gases being injected into the boundary layer, and boundary layer gases from the surrounding environment.

2.2 Material Model

In order to complete the explanation of the governing equations and boundary conditions, it is important to understand the material model used to characterize the state of the solid/gas mixture. It is assumed that all the pores are interconnected, and therefore pyrolysis gases occupy all of the pore space and are free to flow through it. Consequently, the density of the solid/gas mixture is described by

$$\rho = \phi \rho_g + \rho_s \dots (3)$$

In terms of units Eq.3 can be expressed as

$$\left[\frac{mixture\,mass}{mixture\,vol}\right] = \left[\frac{pore\,vol}{mixture\,vol}\right] \left[\frac{gas\,mass}{pore\,vol}\right] + \left[\frac{solid\,mass}{mixture\,vol}\right] \dots \dots (4)$$

It is assumed that the thermodynamic state of the pyrolysis gases can be described by the perfect gas law, and that the solid and gas phases are in thermal equilibrium resulting in

$$P = \rho_g \frac{\hat{R}}{M_g(T_g)} T_g.....(5)$$

where

$$T_g = T_s = T$$

The solid material model adopted in this study is similar to [9, 13] solid bulk density is given by

$$\rho_s = \Gamma(\rho_A + \rho_B) + (1 - \Gamma)\rho_C \dots \dots (6)$$

The reaction is irreversible, and the pyrolysis gases are assumed to not react among them or with the remaining solid in the pore space. Taking the temporal derivative of Eq. (6) gives the solid decomposition rate in terms of component decomposition rates.

$$\frac{\partial \rho_s}{\partial t} = \Gamma \left(\frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_B}{\partial t} \right) + (1 - \Gamma) \frac{\partial \rho_C}{\partial t} \dots \dots (7)$$

It is assumed that the decomposition of each component can be described by an Arrhenius relationship of the form

which applies at a constant spatial location.

The intermediate solid is modeled as some interpolated state between virgin and char. This interpolated state is characterized by the extent of reaction (β), or degree of char, given by

$$\beta = \frac{\rho_v - \rho_s}{\rho_v - \rho_c} \dots \dots (9)$$

In a similar light CMA [9] defines imaginary virgin mass fraction

$$y_{v} = \frac{\rho_{v}}{\rho_{v} - \rho_{c}} \left(1 - \frac{\rho_{c}}{\rho_{s}} \right)$$

2.3. Property Model

Discussions of properties are required for the solution of governing equation therefore thermo-physical and thermodynamic properties which are input parameters are given in the following table.

Input parameter	Description
$C_{\nu_{\nu}}(T)$	Specific heat of virgin material Vs. Temp
$C_{v_c}(T)$	Specific heat of char material Vs. Temp
T _{ref}	Reference temp. for heat of formation
$\left(h_{f}^{o} ight)_{\!\scriptscriptstyle V}$	Virgin plastic heat of formation
$\left(h_{f}^{o} ight)_{c}$	Char heat of formation
$\left(h_{f}^{o} ight)_{g}$	Pyrolysis gas heat of formation
$k_v(T)$	Thermal conductivity of the virgin material Vs. Temp
$k_c(T)$	Thermal conductivity of the char material Vs. Temp
$\in_{c} (T)$	Emissivity of virgin material Vs.Temp
$\in_{v} (T)$	Emissivity of char material Vs. Temp
$h_g(T)$	Pyrolysis gas enthalpy Vs. Temp
$M_{g}(T)$	Pyrolysis gas molecular weight Vs. Temp
$\phi(eta)$	Porosity Vs. Extent of reaction
$\kappa(\beta)$	Permeability Vs. Extent of reaction
$\mu(T)$	Pyrolysis gas dynamic viscosity Vs. Extent of reaction

 Table 1: Thermo-physical and thermodynamic property input

 parameters

2.4 Specific Internal Energy and Gas Enthalpy Models

The specific internal energy of the mixture will take into account both the solid and gas phases. The solid specific internal energy and enthalpy can be found from

 $e_s(T) = h_s(T) = y_v e_v(T) + (1 - y_v) e_c(T)$(10)

where $e_v(T)$ and $e_c(T)$ are determined by parabolic interpolation in the virgin and char specific internal energy tables and also provide details regarding parabolic interpolation routine.

2.4.1Specific Internal Energy and Gas Enthalpy Table Generation

Through integration of the tabulated specific heat functions, specific internal energy tables can be generated for the virgin and char. The code requires an input reference temperature, Tref, that will serve as the "zero" datum for both the specific internal energy functions and the pyrolysis gas specific enthalpy table. It is important to note that although the pyrolysis gas specific enthalpy is a function of pressure and temperature, it is assumed that there is weak pressure dependence, and therefore the gas enthalpy is a function of temperature only.

$$h_g(T) = [h_g(T)]_{i/p} + (h_f^0)_g$$
.....(11)

so that the enthalpy at the reference temperature is consistent with the solid internal energy tables.

$$e(T_{k}) = h_{f}^{0} - \int_{T_{1}}^{T_{ref}} C_{v}(T) dT \text{ for } k = 1$$

= $e(T_{1}) + \left[\sum_{j=1}^{i-1} \frac{1}{2} \left[C_{v}(T_{j}) + C_{v}(T_{j-1}) \right] \left(T_{j} - T_{j-1} \right) \right] \text{ for } k = 2....n....(12)$

2.5. Domain Description and Discretization Method

Before discussing the discretization of the governing equations and their respective solution procedures, it is necessary to provide a description of the coordinate systems, grid motion scheme, and spatial discretization method. The method uses the following grid generation:

1. Automatic non-uniform grid generation with a geometric progression based on domain length, number of elements specified, and either first or last element thickness where

$$\frac{\Delta z_{j+1}}{\Delta z_j}$$

and

$$\Delta z_i = z_{i+1} - z_i$$

2.5.1 Spatial Discretization and Coordinate System

The control volume finite element method, which has been previously used for ablation problems [1, 15], associates a control volume with each node in the discretized domain. The method uses the co-ordinate system used in [15] to describe the surface recession with grid velocity.

3. Mixture Energy Equation

The mixture energy conservation equation

$$\int_{cs} q \cdot dA + \int_{cs} \phi \rho_g h_g v_g \cdot dA - \int_{cs} \rho h v_{cs} \cdot dA + \frac{d}{dt} \int_{cv} \rho e dV = 0$$

where the discretization of each term is discussed in the subsequent sections. For both the mixture energy and gas mass conservation equations, a consistent sign convention is adopted such that [Outflow terms] – [inflow terms] + [rate of change of content] = [source terms]

Therefore energy equation becomes

and the energy balance terms can be seen in figure.2 Section 2.3 presented the model for determining thermo-physical and thermodynamic properties of the gas, solid, and mixture that are necessary for the solution of the mixture energy equation.

While solving the mixture energy equation, nodal temperatures and the surface recession rate are treated as the dependent variables while nodal values of solid density, gas density, and gas velocity are constant.



Figure 2: Energy balance terms for the control volume surrounding node j

The linear system, for the five node domain, is of the form in which there is non linear dependence on surface recession rate

3.1. Conduction

Fourier's law is used to model the heat conducted at a control volume boundary and the heat conduction rate is given by

where $X = \frac{(X_{j+1} + X_j)}{2}$ and X is any quantity. The element representation of heat conduction is

In general, the heat conduction vector is a nonlinear function of temperature and recession rate since the thermal conductivity depends on temperature and Δz_j depends on the surface recession rate. Therefore an iterative solution procedure is necessary to solve for the time accurate nonlinearities. To aid in the iterative process, it is convenient to linearize the element conduction vector with a Taylor series expansion in iteration space treating the nodal temperatures and surface recession rate as the independent variables

Performing the required differentiation for planar geometry (A(z) = 1) gives

$$\frac{\partial \dot{Q}_{j}}{\partial s} = \frac{\bar{k}A}{\Delta z_{j}^{2}} \left(T_{j} - T_{j+1}\right) \frac{\partial \Delta z_{j}}{\partial s} \\
\frac{\partial \dot{Q}_{j+1}}{\partial s} = \frac{\bar{k}A}{\Delta z_{j}^{2}} \left(T_{j} - T_{j+1}\right) \frac{\partial \Delta z_{j}}{\partial s} \\
\frac{\partial \dot{Q}_{j}}{\partial T_{j}} = \frac{\bar{k}A}{\Delta z_{j}^{2}} \left[1 + \frac{\left(T_{j} - T_{j+1}\right)}{2\bar{k}} \left(\frac{\partial k}{\partial T}\right)_{j}\right] \\
\frac{\partial \dot{Q}_{j}}{\partial T_{j+1}} = \frac{\bar{k}A}{\Delta z_{j}^{2}} \left[-1 + \frac{\left(T_{j} - T_{j+1}\right)}{2\bar{k}} \left(\frac{\partial k}{\partial T}\right)_{j+1}\right] \\
\frac{\partial \dot{Q}_{j+1}}{\partial T_{j}} = \frac{\bar{k}A}{\Delta z_{j}^{2}} \left[-1 - \frac{\left(T_{j} - T_{j+1}\right)}{2\bar{k}} \left(\frac{\partial k}{\partial T}\right)_{j}\right] \\
\frac{\partial \dot{Q}_{j+1}}{\partial T_{j+1}} = \frac{\bar{k}A}{\Delta z_{j}^{2}} \left[1 - \frac{\left(T_{j} - T_{j+1}\right)}{2\bar{k}} \left(\frac{\partial k}{\partial T}\right)_{j+1}\right]$$
....(18)

where

$$\frac{\partial \Delta z_j}{\partial s} = \Delta t^{n+1} \left(\eta_{j+1} - \eta_j \right) = \Delta t^{n+1} \Delta \eta_j \dots \dots \dots (19)$$

3.2 Energy Content and Time Integration

The energy content for an element can be divided into terms corresponding to each of the two sub-control volumes within an element.

The internal energy per unit volume in Eq. (20) can be expressed by a Taylor series expansion in position about the element center

The elemental energy content vector can now be expressed as $\int_{-\infty}^{-\infty} dx \, dx$

where

$$(\rho e)_{\overline{z}_{j}} = \overline{\rho e} = \frac{1}{2} \Big[(\rho e)_{j} + (\rho e)_{j+1} \Big]$$

To aid in the integration process it is convenient to employ a local coordinate system in which the shape functions within an element are written as

$$N_{1}(\xi) = \frac{1}{2}(1-\xi)$$

$$N_{2}(\xi) = \frac{1}{2}(1-\xi) = 1-N_{1}(\xi)$$
 for -1<\xi<1.....(23)

the global coordinate z, and the local coordinate ξ , are related through

$$z = N_1(\xi) z_j + N_2(\xi) z_{j+1} = \overline{z}_j + \frac{\xi}{2} \Delta z_j \dots \dots (24)$$

and consequently the differential length is

$$dz = \frac{\Delta z_j}{2} d\xi$$

If a finite central difference is used to approximate $\begin{pmatrix} \partial(\rho e) \\ \partial z \end{pmatrix}$, the energy

capacitance terms can be rewritten in terms of local coordinates as $\begin{bmatrix} -\Delta z & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} z & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -\Delta z & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} z & 0 \\ 0 & 0 \end{bmatrix}$

Performing the integration for planar geometry $(A(\xi) = 1)$ gives

The result is simply a weighted average of nodal values where the weighting factor matrix is geometry dependent. The time rate of change of energy content according to an implicit time integrator can be expressed as $\int \left[\frac{1}{2k} - \frac{1}{2} \right]^{n+1} \left[\left[\frac{1}{2k} - \frac{1}{2} \right]^n \right]_{n+1} = \left[\frac{1}{2k} - \frac{1}{2} \right]^n$

$$\frac{d}{dt} \begin{bmatrix} E_j \\ E_{j+1} \end{bmatrix}^{n+1} = \left\{ \begin{bmatrix} E_j \\ E_{j+1} \end{bmatrix}^{n+1} - \begin{bmatrix} E_j \\ E_{j+1} \end{bmatrix}^n \right\} \frac{1}{\Delta t^{n+1}} \dots \dots \dots (27)$$

and linearizing in iteration space according to a Taylor series expansion gives

$$\frac{d}{dt}\begin{bmatrix} \mathbf{E}_{j} \\ \mathbf{E}_{j+1} \end{bmatrix}^{\nu+1} = \left\{ \begin{bmatrix} \mathbf{E}_{j} \\ \mathbf{E}_{j+1} \end{bmatrix}^{\nu} + \begin{bmatrix} \frac{\partial \mathbf{E}_{j}}{\partial s_{j}} & \frac{\partial \mathbf{E}_{j}}{\partial T_{j}} & \frac{\partial \mathbf{E}_{j}}{\partial T_{j+1}} \\ \frac{\partial \mathbf{E}_{j+1}}{\partial s_{j}} & \frac{\partial \mathbf{E}_{j+1}}{\partial T_{j}} & \frac{\partial \mathbf{E}_{j+1}}{\partial T_{j+1}} \end{bmatrix}^{\nu} \begin{bmatrix} \Delta s \\ \Delta T_{j} \\ \Delta T_{j+1} \end{bmatrix}^{\nu+1} - \begin{bmatrix} \mathbf{E}_{j} \\ \mathbf{E}_{j+1} \end{bmatrix}^{n} \right\} \frac{1}{\Delta t^{n+1}} \dots \dots \dots (28)$$

where the sensitivity matrix entries are

$$\frac{\partial \overline{E}_{j}}{\partial s_{j}} = A \frac{\partial \Delta z_{j}}{\partial s} \left[\frac{3}{8} (\rho e)_{j} + \frac{1}{8} (\rho e)_{j+1} \right]$$

$$\frac{\partial \overline{E}_{j+1}}{\partial s_{j}} = A \frac{\partial \Delta z_{j}}{\partial s} \left[\frac{1}{8} (\rho e)_{j} + \frac{3}{8} (\rho e)_{j+1} \right]$$

$$\frac{\partial \overline{E}_{j}}{\partial T_{j}} = \frac{3A\Delta z_{j}}{8} (\rho C_{v})_{j}$$

$$\frac{\partial \overline{E}_{j+1}}{\partial T_{j+1}} = \frac{A\Delta z_{j}}{8} (\rho C_{v})_{j+1}$$

$$\frac{\partial \overline{E}_{j+1}}{\partial T_{j+1}} = \frac{3A\Delta z_{j}}{8} (\rho C_{v})_{j+1}$$
(29)

The resulting linear system contributions for each jth element are

$$e(j) = e(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial E_{j}}{\partial s_{j}}$$

$$e(j+1) = e(j+1) + \frac{1}{\Delta t^{n+1}} \frac{\partial E_{j+1}}{\partial s_{j}}$$

$$b(j) = b(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial E_{j}}{\partial T_{j}}$$

$$c(j) = c(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial E_{j}}{\partial T_{j+1}}$$

$$d(j) = d(j) - \frac{1}{\Delta t^{n+1}} \left(E_{j}^{v} - E_{j}^{n} \right)$$

$$a(j+1) = a(j+1) + \frac{1}{\Delta t^{n+1}} \frac{\partial E_{j+1}}{\partial T_{j+1}}$$

$$d(j+1) = b(j+1) - \frac{1}{\Delta t^{n+1}} \left(E_{j+1}^{v} - E_{j+1}^{n} \right)$$
(30)

The resulting linear system contributions for each jth element are

$$e(j) = e(j) + \frac{\partial Q_{-j}}{\partial s}$$

$$e(j+1) = e(j+1) + \frac{\partial Q_{-j+1}}{\partial s}$$

$$b(j) = b(j) + \frac{\partial Q_{-j}}{\partial T_{-j}}$$

$$c(j) = c(j) + \frac{\partial Q_{-j}}{\partial T_{-j+1}}$$

$$d(j) = d(j) - Q_{-j}^{*}$$

$$a(j+1) = a(j+1) + \frac{\partial Q_{-j+1}}{\partial T_{-j}}$$

$$b(j+1) = b(j+1) + \frac{\partial Q_{-j+1}}{\partial T_{-j+1}}$$

3. RESULTS AND DISCUSSION

Assuming conduction and uniform heat flux distribution along the thickness will eliminate the convection and gas flux terms in the energy equation considering constant property, non-ablating, non-decomposing, one-dimensional, uniform density, planar slab with a specified constant heat flux on the front face and an adiabatic back face. The governing equation, parameters associated with this problem are:

$$\int_{cs}^{L} q \, .dA + \frac{d}{dt} \int_{cv} \rho e dV = 0.....(32)$$

Table 2. Conduction problem parameters

T = 3500K
-
$q = 18.8 \text{MW/m}^2$
$\rho = 1369 \text{ kg/m}^2$
$k = 4 W/m^2 K$
$C_v = 651.24 \text{ J/kg K}$

The problem here is a linear convergence problem which undergoes iterative process to obtain the temperature distribution in the ablator.



Figure.3. Temperature profile

4. Conclusions

The method gives the acceptable temperature variation, showing less gradient in the charring zone and a step gradient in the decomposing zone where the density gradient does exists prompting the heat transfer towards the virgin zone but the constant temperature in the region protects the backup structure from the heat transfer ensuring the safety of the system.

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