A NUMERICAL ANALYSIS OF THE TRANSIENT RESPONSE OF AN ABLATION SYSTEM INCLUDING EFFECTS OF THERMAL NON-EQUILIBRIUM, MASS TRANSFER AND CHEMICAL KINETICS

by Ronald Keith Clark

Thesis submitted to the Graduate Faculty of the Virginia Polytechnic Institute and State University in Candidacy for the degree of

DOCTOR OF PHILOSOPHY

in

Mechanical Engineering

May 1972

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APPROVED: 

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Blacksburg, Va.
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(ABSTRACT)

The differential equations governing the transient response of a
one-dimensional ablative thermal protection system undergoing stagnation
ablation are derived for the general case of thermal non-equilibrium
between the pyrolysis gases and the char layer and kinetically con-
trolled chemical reactions and mass transfer between the pyrolysis
gases and the char layer. The boundary conditions are written for
the particular case of stagnation heating with surface removal by
oxidation or sublimation and pyrolysis of the uncharred layer occurring
in a plane.

The governing equations and boundary conditions are solved
numerically using the modified implicit method (Crank-Nicolson method).
Numerical results are compared with exact solutions for a number of
simplified cases. The comparison is favorable in each instance.

Numerical results are presented for a typical ablation system
subjected to a square heat pulse. The effects of chemical reactions
and mass transfer are pronounced.
ACKNOWLEDGEMENTS

The author is grateful to Dr. Felix J. Pierce, Advisory Committee Chairman, for his suggestions and criticisms throughout this effort and to the entire committee for their review of this thesis.

The author is also indebted to the National Aeronautics and Space Administration for permission to use material obtained from research at the Langley Research Center in this thesis. Thanks are due many people at the Langley Research Center who made this effort possible. In particular the support of Mr. Robert T. Swann throughout the program is appreciated as is the encouragement received from Mr. Marvin B. Dow. The assistance of Mr. Claud M. Pittman and Mrs. Kay L. Brinkley was invaluable in completing the programming of the finite difference equations. And last but not least, the author appreciates the patience of his wife who must have heard the phrase "I think I've found the problem" 200 times.
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mass flow rate of pyrolysis gases (kg/m²·sec)

M₁ molecular weight of chemical species i (kg/mole)

Mₘ₀₂ molecular weight of O₂ (kg/mole)

Mₛ molecular weight of char layer (kg/mole)

ṁₕ rate of pyrolysis of uncharred material (kg/m²·sec)

ṁᵢ mass flow rate of chemical species i (kg/m²·sec)

ṁ₀₂ mass rate of diffusion of O₂ through the boundary layer to the char layer surface (kg/m²·sec)

ṁₛ mass rate of char removal (kg/m²·sec)

ṁᵣ effective rate of mass injection into the boundary layer (kg/m²·sec)

n order of chemical reaction

n unit vector normal to the surface

ṁᵢ₁ mass flux of chemical species i relative to a fixed coordinate system (kg/m²·sec)

Nₗₑ dimensionless parameter (k/ρCₐD), Lewis Number

Nₚᵣ dimensionless parameter (μCₚ/k), Prandtl Number

Nₛₑ dimensionless parameter (μ/ρD), Schmidt Number

P Laplace transform of T' defined by ∫₀^∞ e⁻ˢᵗ T'(X;t)dt or pressure (N/m²)

P₁ pyrolysis gas pressure at finite difference station 1 (N/m²)

Pₑ pressure at edge of boundary layer (N/m²)

P₀₂ partial pressure of O₂ (N/m²)

Pₜₗ₀ initial pressure at char layer surface (N/m²)

Pₛₜₗ₀ stagnation wall pressure (N/m²)

$q$ rate of energy transfer in pyrolysis gases by conduction (W/m²)
q''' rate of energy generated in pyrolysis gases by sources (W/m$^3$)
$q_{Aero}$ net aerodynamic heating rate to the surface (W/m$^2$)
$q_B$ net heating rate to the back surface of the insulation layer (W/m$^2$)
$q_C$ cold wall convective heating rate to the front surface (W/m$^2$)
$q_{C,net}$ net convective heating rate to the front surface (W/m$^2$)
$q_R$ radiant heating rate to the front surface (W/m$^2$)
$q_s$ rate of energy transfer in solid by conduction (W/m$^2$)
$q_s'''$ rate of energy generated in solid by sources (W/m$^2$)
$r(r)$ net rate of progress of $r^{th}$ chemical reaction (1/m$^3$-sec)
$Rad$ radius of curvature of surface (m)
$r_h$ net rate of progress of $r^{th}$ heterogenous chemical reaction (1/m$^3$-sec)
$R_{h_i}$ molar rate of production of chemical species $i$ by heterogeneous chemical reactions (moles/m$^3$-sec)
$R_{h_s}$ molar rate of production of solid by heterogeneous chemical reactions (moles/m$^3$-sec)
$r_{h_s}$ mass rate of production of solid by heterogeneous chemical reactions (kg/m$^3$-sec)
$R_i$ molar rate of production of chemical species $i$ by homogeneous chemical reactions (moles/m$^3$-sec)
$R_s$ molar rate of production of solid by homogeneous chemical reactions (moles/m$^3$-sec)
$r_s$ mass rate of production of solid by homogeneous chemical reactions (kg/m$^3$-sec)
$R_{T_i}$ net molar rate of production of chemical species $i$ (moles/m$^3$-sec)
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<td>$T_o$</td>
<td>initial temperature of pyrolysis gases (°K) or reservoir temperature (°K)</td>
</tr>
<tr>
<td>$T_s$</td>
<td>solid temperature (°K)</td>
</tr>
<tr>
<td>$\bar{T}_l$</td>
<td>maximum char surface temperature used when limiting temperature at that station (°K)</td>
</tr>
<tr>
<td>$u$</td>
<td>component of velocity vector (m/sec)</td>
</tr>
<tr>
<td>$\hat{U}$</td>
<td>internal energy per unit mass of pyrolysis gases (J/kg)</td>
</tr>
<tr>
<td>$V$</td>
<td>volume (m$^3$)</td>
</tr>
<tr>
<td>$\hat{V}$</td>
<td>volume of pyrolysis gases per unit mass (m$^3$/kg)</td>
</tr>
<tr>
<td>$v$</td>
<td>component of velocity vector (m/sec) or velocity of pyrolysis gases in char layer (m/sec)</td>
</tr>
<tr>
<td>$V_c$</td>
<td>velocity of finite difference station in moving coordinate system (m/sec)</td>
</tr>
</tbody>
</table>
\( v_0 \) superficial velocity of pyrolysis gases in char layer (m/sec)

\( v \) flow field velocity external of the boundary layer (m/sec)

\( x \) dimensionless moving coordinate attached to the char layer surface

\( x' \) dimensionless moving coordinate attached to the pyrolysis zone

\( x'' \) dimensionless coordinate attached to the uncharred layer-insulation layer interface

\( x_d \) moving coordinate attached to the char layer surface (m)

\( x'_d \) moving coordinate attached to the pyrolysis zone (m)

\( x''_d \) coordinate attached to the uncharred layer-insulation layer interface (m)

\( x_i \) mole fraction of chemical species \( i \)

\( x_{O_2} \) mole fraction of \( O_2 \)

\( y \) fixed coordinate (m)

\( z \) fixed coordinate (m)

**Greek letters:**

\( \alpha \) absorptivity of front surface

\( \alpha_c \) weighting factor for char material injected into boundary layer

\( \alpha_p \) weighting factor for pyrolysis gases injected into boundary layer

\( \alpha_1, \alpha_2, \alpha_3, \alpha_4 \) coefficients in linearized differential equation for solid temperature

\( \beta \) trigger for selecting blocking approximation; \( \beta = 0 \) for 2nd order approximation, \( \beta = 1 \) for linear approximation
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>$\beta_1, \beta_2, \beta_3$</td>
<td>coefficients in linearized differential equation for pyrolysis gas temperature</td>
</tr>
<tr>
<td>$\gamma_1, \gamma_2, \gamma_3, \gamma_4$</td>
<td>coefficients in linearized differential equation for pyrolysis gas pressure</td>
</tr>
<tr>
<td>$\bar{\sigma}$</td>
<td>unit tensor</td>
</tr>
<tr>
<td>$\Delta_1, \Delta_2, \Delta_3$</td>
<td>coefficients in linearized chemical species conservation equation</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>heat of reaction for heterogeneous chemical reaction</td>
</tr>
<tr>
<td>$\Delta H_c$</td>
<td>heat of combustion of char (J/mole)</td>
</tr>
<tr>
<td>$\Delta H_p$</td>
<td>heat of pyrolysis of uncharred material (J/kg)</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>increment in time (sec)</td>
</tr>
<tr>
<td>$\Delta T_{\text{surface}}$</td>
<td>change in temperature of char layer surface ($^\circ$K)</td>
</tr>
<tr>
<td>$\Delta x$</td>
<td>dimensionless distance between finite difference stations</td>
</tr>
<tr>
<td>$\Delta \rho$</td>
<td>difference in density of uncharred material and char layer at the pyrolysis zone (kg/m$^3$)</td>
</tr>
<tr>
<td>$\varepsilon_s$</td>
<td>emissivity of char surface</td>
</tr>
<tr>
<td>$\varepsilon''_s$</td>
<td>emissivity of back surface</td>
</tr>
<tr>
<td>$\eta$</td>
<td>char layer porosity</td>
</tr>
<tr>
<td>$\eta_I$</td>
<td>char layer porosity at pyrolysis zone</td>
</tr>
<tr>
<td>$\eta_o$</td>
<td>initial char layer porosity</td>
</tr>
<tr>
<td>$\bar{\eta}$</td>
<td>blocking coefficient used with linear ablation theory</td>
</tr>
<tr>
<td>$\theta_j$</td>
<td>fraction of surface sites occupied by molecules of chemical species $j$</td>
</tr>
<tr>
<td>$\theta_o$</td>
<td>fraction of surface sites which are void</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>ratio of char layer mass removed to mass of oxygen diffusing to the surface</td>
</tr>
<tr>
<td>$\mu$</td>
<td>viscosity of pyrolysis gases or boundary layer fluid (N - sec/m$^2$)</td>
</tr>
</tbody>
</table>
\( \mu_i \) chemical potential of chemical species \( i \) (J/kg)

\( \nu'_i \) coefficient of chemical species \( i \) appearing as a reactant in a stoichiometric representation of a chemical reaction (moles)

\( \nu''_i \) coefficient of chemical species \( i \) appearing as a product in a stoichiometric representation of a chemical reaction (moles)

\( \rho \) density of pyrolysis gases or boundary layer fluid (kg/m\(^3\))

\( \bar{\rho} \) normalized density of boundary layer fluid

\( \rho_{HS} \) density of heat sink at interface of uncharred layer and insulation layer (kg/m\(^3\))

\( \rho_{HSP} \) density of heat sink at back of insulation layer (kg/m\(^3\))

\( \rho_i \) density of chemical species \( i \) (kg/m\(^3\))

\( \rho_s \) density of solid (kg/m\(^3\))

\( \rho_{so} \) density of char layer at the front surface (kg/m\(^3\))

\( \rho_{\infty} \) flow field density external to the boundary layer (kg/m\(^3\))

\( \sigma \) Stefan-Boltzmann constant (W/m\(^2\)-sec-°K\(^4\))

\( \Pi \) viscous stress tensor (N/m\(^2\))

\( \tau_{xx} \) xx-element of the viscous stress tensor in moving coordinate system (N/m\(^2\))

\( \tau_{yy} \) yy-element of the viscous stress tensor in fixed coordinate system (N/m\(^2\))

Overlines

- normalized or averaged

^ per unit mass

\( \rightarrow \) vector

\( \Rightarrow \) tensor
Superscripts

' uncharred layer
" insulation layer
P at start of time step
P+ Δt at end of time step
P+ Δt/2 at middle of time step
r chemical reaction r

Subscripts

CO carbon monoxide
C_s solid carbon
e free stream
f forward direction
h heterogeneous chemical reaction
hom homogeneous chemical reaction
I pyrolysis zone
i chemical species i
I+J interface of uncharred layer and insulation layer
I+J+K back surface of insulation layer
N station N
New moving coordinate system
o initial value
Old initial fixed coordinate system
O_2 oxygen
r reverse direction
s  solid or stagnation point
w  wall
l  char layer surface
Space vehicles reentering the earth's atmosphere or entering other planetary environments are subjected to severe aerodynamic heating. Several methods of protecting the interior of the spacecraft have been proposed. Conditions resulting in high aerodynamic heating rates require use of ablation materials for thermal protection. The charring ablator thermal protection material (see schematic diagram, Fig. 1) has been found most effective as a thermal shielding material for a wide range of heating conditions. In Ref. 1 Swann discusses weights and efficiencies of various thermal protection systems for a range of heating conditions.

The favorable performance of the charring ablator is largely attributable to the tough char layer which forms on the surface of the material as it is heated. This char layer is capable of withstanding very high temperatures, and during reentry a significant amount of the total heat input at the surface is radiated to the environment by the high temperature char surface. Gases generated in the pyrolysis zone of the charring ablator percolate through the high temperature porous char layer to the surface. As these pyrolysis gases flow through the char layer, they absorb energy by increasing in temperature and undergoing chemical reactions.

The performance of ablative thermal protection systems has been the subject of extensive research over the past decade. Refs. 2, 3,
Figure 1.- Schematic diagram of charring ablator.
and 4 by Chapman, Dow and Tompkins, and Chapman and Dow are typical of the many reports presenting results of experimental evaluation of the ablative performance of thermal protection materials. The experimental programs whose results are reported in Refs. 2, 3 and 4 involved testing candidate thermal protection materials in arc-heated tunnels to compare their performance as thermal protection systems for reentry applications.

Many analytical reports have been devoted to developing theories of ablation. In Refs. 5, 6 and 7 Roberts considers the effects of mass transfer processes near the stagnation point on heat transfer to two-dimensional or axisymmetric bodies. Ref. 5 presents a simplified analysis of mass transfer cooling near the stagnation point for two dimensional or axisymmetric bodies, showing the reduction in heat transfer in terms of the properties of the cooling fluid. Ref. 6 presents a simplified analysis of the shielding mechanism which reduces the stagnation point heat transfer when ablation takes place at the surface. Ref. 7 presents a theoretical study of the shielding mechanism whereby the rates of heat transfer are reduced near the stagnation point of two-dimensional and three dimensional bodies when melting and vaporization occur simultaneously.

A large body of literature exists which describes the experimental and analytical effort directed toward studying the performance of ablative thermal protection systems including the interaction of the ablator with the boundary layer. In Ref. 8 Scala and Gilbert present
a theoretical analysis of the overall response of a char-forming plastic during hypersonic flight. The rate of pyrolysis of the plastic is calculated by means of a chemical kinetic equation. A mathematical description of the gas flow through the char is included. Hypersonic boundary layer mass transfer effects are also considered in the overall energy balance. Results are presented for the forward stagnation line of an unyawed cylinder in hypersonic flow undergoing quasi-steady ablation.

An analysis of the effects of environmental conditions on the performance of charring ablators is presented in Ref. 9 by Swann, Dow and Tompkins. Equations relating different environments which produce the same material response are derived for the case of surface removal by oxidation. The effects of environmental parameters on the thermal performance of ablators are examined.

In Ref. 10 Swann presents an analysis of the performance of char-forming ablators. It includes a derivation of the equations governing the response of charring ablators subject to char removal by diffusion controlled oxidation. Results are presented for the case of a constant enthalpy level and the effects of various material properties and environmental parameters are discussed.

A study of the effects of oxidation on the performance of charring ablators is presented in Ref. 11 by Dow and Swann. Char-forming ablation specimens were exposed to high energy gas streams of nitrogen and different oxygen concentrations. Surface removal data from these
tests were correlated in terms of a diffusion limited oxidation mechanism. An energy balance calculated for specimens exposed to 11.5 percent oxygen concentration showed that the heat input from combustion is a significant part of the total heat input.

Further attempts at defining the effects of environment and material properties on the performance of ablators are discussed by Clark in Ref. 12 and Swann, Brewer and Clark in Ref. 13.

Because of the many complex factors involved, the usefulness of developing computer simulation programs as a practical tool for solving ablation problems was obvious early in the previous decade. Early analyses of ablative thermal protection systems neglected or greatly simplified the complex processes and rate controlling mechanisms that occur in charring ablation systems. Ref. 14 by Swann and Pittman represents an early numerical treatment of an ablative thermal protection system. It presents a derivation in finite difference form of the energy transfer equations for a charring ablator system in which thermal equilibrium exists between the char layer and the pyrolysis gases. Removal of material at the surface by chemical and/or mechanical processes is achieved by modelling any of the following mechanisms:

1) ablation at a given temperature

2) material erosion as a given function of time

3) material erosion such that the char thickness is a given function of time.

Pyrolysis of the uncharred material occurs at a single given temperature, so that a well-defined interface exists between the char layer
and the uncharred layer. Reduction of aerodynamic heating at the surface resulting from injection of pyrolysis gases into the boundary layer is accounted for by using a second-degree approximation to the boundary layer solutions for air-to-air injection. The effect of chemical reactions involving the pyrolysis gases as they flow through the char layer is included by using an effective specific heat for the pyrolysis gases which is adjusted to account for endothermic and exothermic chemical processes. Ref. 14 presents some typical results from computer calculations and some comparisons with experimental results.

In Ref. 15 Kratsch, Hearne and McChesney present a sound effort at developing and experimentally verifying a theoretical model of a charring ablation thermal protection system. They present the coupled energy and mass transfer equations for a two-component resin-fabric composite with a complete description of the chemical processes involved. However, it invokes the assumption of thermal equilibrium between the char layer and pyrolysis gases. It also assumes steady state conditions exist. Experimental and computed results are presented for comparison.

Ref. 16 by Swann, Pittman and Smith presents what is perhaps the most widely employed numerical ablation analysis. Basically it represents a greatly improved version of the earlier analysis by Swann and Pittman (Ref. 14). The improvements include the following: (1) treatment of surface removal by chemical oxidation with consideration of rate controlled and diffusion controlled regimes; (2) pyrolysis
of the uncharred layer as an exponential function of temperature, and
(3) transformation of governing equations to a moving coordinate
system to accommodate changes in location of the surfaces of the abla-
tor. However, their analysis also invokes the assumption of thermal
equilibrium between the char layer and pyrolysis gases. Ref. 16 pre-
sents a comparison of computed results with exact solutions for
simplified cases. The agreement between the numerical and exact
solutions is good.

More recently strong interest has been directed toward the chemical
processes occurring within the char layer of an ablation system. The
experimental work by Clark which is reported in Refs. 17 and 18
demonstrates the intensity of these processes. This work also shows
that the pyrolysis gases and char layer are not always in thermal
equilibrium. Ref. 19 by Brewer, Stroud and Clark shows a thirty
percent variation in thermal protection requirements for a typical
reentry vehicle depending on whether the pyrolysis gases in the char
are in chemical equilibrium or frozen as they flow from the pyrolysis
zone to the surface.

This report presents an analysis of the transient response of a
one-dimensional ablative thermal protection system undergoing
stagnation ablation. The differential equations governing heat and
mass transfer are derived out for both the char layer and the
pyrolysis gases flowing through the char layer. These equations are
coupled through a convective heat transfer term which represents
energy transferred from the char layer to the pyrolysis gases. The
differential equation governing the pressure distribution in the char layer is formulated. Chemical rate equations describing the chemical reactions occurring in the char layer are formulated.

The boundary conditions are written for the particular case of stagnation heating with surface removal by oxidation and/or sublimation, and temperature dependent pyrolysis of the uncharred material occurring in a plane.

The governing equations and boundary conditions are solved numerically using a digital computer. Numerical solutions are obtained for a number of simple problems where exact solutions are available to test the integrity of various parts of the total program. Results are presented for a body subjected to stagnation heating with surface removal by oxidation and finite-rate chemistry occurring in the char layer to illustrate the form of results obtained using this tool. A discussion of the use of this program in design of thermal protection systems is included.
A charring ablator system can be described by three distinct layers as shown in Fig. 1. These layers are the char layer and the uncharred material, which make up the ablator, and the heat sink and substrate insulation which are behind the ablator. The char layer is exposed to aerodynamic and/or radiant heating at the front surface. The surface of the char layer may also interact with the external boundary layer resulting in erosion of the char layer by chemical reactions and/or mechanical means. The region separating the char layer and the uncharred material is labeled the pyrolysis zone and is assumed to be a plane. The uncharred material undergoes pyrolysis at this interface at a rate given by an empirical Arrhenius type relation producing gaseous pyrolysis products and a porous char layer. The gaseous products absorb energy and undergo chemical reactions as they flow through the porous char layer to the front surface where they are injected into the boundary layer. From this discussion it is seen to be necessary to consider the three layers separately in deriving the differential equations which govern the behavior of an ablative system.

The char layer consists of two phases – the porous solid residue or char and the gaseous pyrolysis products, or pyrolysis gases, flowing through the porous residue. The porous residue experiences heat conduction and mass and heat transfer from interaction with the flow of
pyrolysis products. The pyrolysis products flowing through the porous residue undergo chemical reactions in addition to interacting with the solid. The uncharred layer and the substrate insulation experience heat conduction only.

**Char Layer Equations**

The char layer requires two differential equations for conservation of energy - one for the char and one for the pyrolysis gases. Mass transfer processes affecting the char must be considered to obtain an equation for variation of the char porosity. The pyrolysis gases also require differential equations for conservation of chemical species, total mass and momentum, and chemical reaction rate equations.

**Char temperature differential equation.**—The energy conservation equation for the char is obtained by considering a control volume $V$ within the char layer. The char occupies a fraction of this volume equal to $(1 - \eta)$ where $\eta$ is the char layer porosity. The energy conservation equation applied to the solid phase of the char layer states that the rate of change of energy contained in the solid phase of the char within the control volume $V$ equals the sum of the net ratio of energy transfer into the solid phase by conduction heat transfer, convection to the pyrolysis gases, mass transfer from the pyrolysis gases to the solid resulting from homogeneous chemical reactions and heterogeneous chemical reactions (reactions occurring on the solid surface), heats of reaction given up by the solid in heterogeneous chemical reactions involving the pyrolysis gases and
the solid, radiation of energy to the solid and energy produced within the solid by any internal source.

The total energy contained in the solid phase of the char within a unit volume of the char layer is equal to the product of the theoretical solid density, enthalpy and solid phase volume fraction which is \((1 - \eta)\). The terms of the char energy equation may be written as follows:

Non-stationary volume term

\[ \int_V \frac{\partial}{\partial t} [(1 - \eta) \rho_s H_s] \, dV \]

Conduction heat transfer term

\[ - \int_S \mathbf{q}_s \cdot \mathbf{n} \, dS \]

Convection to the pyrolysis gases

\[ - \int_V H_A (T_s - T) \, dV \]

where the volumetric heat transfer coefficient for convective energy transfer from the char to the pyrolysis gases is given by Bland in Ref. 20 as

\[ H_A = \frac{K_v}{N_{Pr}} \sum \frac{\rho_i C_{pi}}{M_i} \]

(2-1)
Mass transfer from the pyrolysis gases to the solid resulting from homogeneous chemical reactions

\[ f_v \eta r_s \hat{H}(T)_s \ dV \]

Mass transfer from the pyrolysis gases to the solid resulting from heterogeneous chemical reactions

\[ f_v \eta r_{hs} \hat{H}_s \ dV \]

Heats of reaction given up by the solid in heterogeneous chemical reactions

\[- f_v \eta \sum_r r_h(r) \Delta H(r) \ dV \]

Radiation of energy to the solid

\[ f_v (1 - \eta)(A - \varepsilon) \ dV \]

Energy produced within the solid by any internal source

\[ f_v (1 - \eta) q'''_s \ dV \]

Combining these terms in equation form gives
\[ \int_V \frac{\partial}{\partial t} \left[ (1 - \eta) \rho_s \hat{H}_s \right] \, dV = -\int_S \frac{\hat{q}_s}{\hat{n}} \cdot \hat{n} \, dS - \int_V H_A (T_s - T) \, dV \]

\[ + \int_V \eta \, r_s \hat{H}(T_s) \, dV + \int_V \eta \, r_h \hat{H}_s \, dV - \int_V \eta \sum_r^{(r)} \Delta H^{(r)} \, dV \]

\[ + \int_V (1 - \eta)(A - \epsilon) \, dV + \int_V (1 - \eta) q_s''' \, dV \]  

(2-2)

which is a statement of conservation of thermal and chemical energy for the portion of a control volume in the char layer occupied by solid. The energy term associated with stresses has not been included since that term is negligible with respect to other terms. The use of enthalpy in this equation is consistent with its nearly universal usage as a measure of the energy content of solids; however, implicit with its use is the assumption that enthalpy and internal energy are equal. This assumption is valid for incompressible solids.

The term associated with the heats of reaction for heterogeneous chemical reactions is obtained by assuming that the heat of reaction for each reaction is supplied by the char. As an example, consider the \( r^{th} \) heterogeneous chemical reaction which is the oxidation of solid carbon to form carbon monoxide. The stoichiometric equation representing this reaction is

\[ O_2 + 2C_s \rightarrow 2CO \]  

(2-3)

and the heat supplied to the reaction is just the difference in enthalpy of the products and the reactants, or in equation form
\[ \Delta H^{(r)} = 2H(T_s)C_0 - H(T)O_2 - H(T_s)C_s \]  

(2-4)

Applying Gauss's Theorem to the surface integral to obtain a volume integral results in the following equation

\[ \int_V \left\{ \frac{\partial}{\partial t} \left[ (1 - \eta) \rho_s \hat{H}_s \right] + \hat{V} \cdot \hat{q}_s + H_A (T_s - T) - \eta \rho_s \hat{H}(T_s) - \eta \rho_{hs} \hat{H}_s \right\} \, dV = 0. \]  

(2-5)

This equation is true for any volume \( V \); therefore, the integral can vanish only if the integrand vanishes everywhere. Thus, the differential form of the char energy equation is

\[ \frac{\partial}{\partial t} \left[ (1 - \eta) \rho_s \hat{H}_s \right] + \hat{V} \cdot \hat{q}_s + H_A (T_s - T) - \eta \rho_s \hat{H}(T_s) - \eta \rho_{hs} \hat{H}_s \]

\[ + \eta \sum_r r_h^{(r)} \Delta H^{(r)} - (1 - \eta)(A - \varepsilon) - (1 - \eta) q''' \]  

(2-6)

The non-stationary term is expanded to obtain

\[ \frac{\partial}{\partial t} \left[ (1 - \eta) \rho_s \hat{H}_s \right] = (1 - \eta) \rho_s \frac{\partial \hat{H}_s}{\partial t} + (1 - \eta) \hat{H}_s \frac{\partial \rho_s}{\partial t} - \rho_s \hat{H}_s \frac{\partial \eta}{\partial t}. \]  

(2-7)

But the theoretical density of the char is constant; therefore,

\[ \frac{\partial}{\partial t} \left[ (1 - \eta) \rho_s \hat{H}_s \right] = (1 - \eta) \rho_s \frac{\partial \hat{H}_s}{\partial t} - \rho_s \hat{H}_s \frac{\partial \eta}{\partial t}. \]  

(2-8)
The char layer energy equation now takes the form

$$
(1 - \eta)\rho_s \frac{\partial H_s}{\partial t} = - \nabla \cdot q_s - H_A(T_s - T) + n r_s \dot{H}(T) + \eta r_s H_s \\
- \eta \sum_r r^{(r)} \Delta H^{(4)} + (1 - \eta)(A - \varepsilon) + (1 - \eta)q_{s''} + \rho_s \dot{H}_s \frac{\partial \eta}{\partial t}.
$$

(2-9)

It is more convenient to work with temperature than enthalpy. The char enthalpy may be written as

$$
\hat{H}_s = \int_0^{T_s} C_p \hat{d}T_s + \hat{H}_{s0}.
$$

(2-10)

The time rate of change of char enthalpy is obtained by differentiating Eq. 2-10,

$$
\frac{\partial \hat{H}_s}{\partial t} = \frac{2}{C_p} \int_0^{T_s} \frac{\partial C_p}{\partial T_s} dT_s + \frac{2}{\partial \hat{H}_{s0}}.
$$

(2-11)

The derivative of the integral appearing here is obtained by applying the Leibnitz Rule for differentiation under the integral sign as in Hildebrand (Ref. 21). Thus Eq. 2-11 becomes

$$
\frac{\partial \hat{H}_s}{\partial t} = \int_0^{T_s} \frac{\partial C_p}{\partial T_s} dT_s + C_p \frac{\partial T_s}{\partial T_s} + \frac{\partial \hat{H}_{s0}}{\partial T_s}.
$$

(2-12)
but $C_{ps}$ is not a function of time and $H_s$ is constant so

$$\frac{\partial H_s}{\partial t} = \frac{C_{ps}}{\partial t} \frac{\partial T_s}{\partial t}. \quad (2-13)$$

Combining Eq. 2-13 and Fourier's conduction equation,

$$q_s = -k_s \nabla T_s, \quad (2-14)$$

with Eq. 2-9 gives the differential equation for conservation of energy in the char layer as

$$(1 - \eta) \rho_s C_{ps} \frac{\partial T_s}{\partial t} = \nabla \cdot (k_s \nabla T_s) - H_s (T_s - T) + \eta r_s \hat{H}(T)_s$$

$$+ \eta r_{hs} \hat{H}_s - \eta \sum_r r_{hr} \Delta H(r) + (1 - \eta)(A - \varepsilon)$$

$$+ (1 - \eta) q_s''' + \frac{\rho_s \hat{H}_s}{\partial \hat{H}_s} \frac{\partial \eta}{\partial t}. \quad (2-15)$$

The specific quantities $C_{ps}, H_s(T), \Delta H_j$ and $H_s$ and the chemical production terms $r_s$ and $r_{hs}$ may be expressed in terms of the respective mole quantities and Eq. 2-15 becomes

$$(1 - \eta) \frac{\rho_s C_{ps}}{M_s} \frac{\partial T_s}{\partial t} = \nabla \cdot (k_s \nabla T_s) - H_s (T_s - T) + \eta R_s \hat{H}(T)_s$$

$$+ \eta R_{hs} H_s - \eta \sum_r r_{hr} \Delta H(r) + (1 - \eta)(A - \varepsilon)$$

$$+ (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \frac{\partial \eta}{\partial t}. \quad (2-16)$$
Char porosity differential equation. - The porosity differential equation results from consideration of mass transfer between the char and the pyrolysis gases. Mass transfer between these two phases results from two sources. One source is the solid material formed by homogeneous chemical reactions in the pyrolysis gases. This solid material is deposited from the gas phase to the solid phase. The other source is the solid material formed or consumed by heterogeneous chemical reactions which occur at the char-gas interface.

The rate of formation of solid material by homogeneous chemical reactions in the pyrolysis gases is determined from the appropriate chemical reaction rate equations to be \( R_s \) (moles solid per unit volume of gas per unit time). The product of the char porosity (void fraction of the char layer), the molecular weight of the solid, and the rate of formation of solid gives the rate of material deposited in mass units per unit volume of char layer. Or, in equation form

\[
\text{Mass Rate of Deposition} = \eta \frac{M_s R_s}{\rho_s}.
\] (2-17)

This deposit occupies a volume equal to \( \frac{1}{\rho_s} \) volume units per unit mass and this volume represents a decrease in the porosity of the char layer. Thus the time rate of change of char porosity due to homogeneous chemical reactions is

\[
\frac{\partial \eta}{\partial t}_{\text{hom}} = - \eta \frac{M_s R_s}{\rho_s}.
\] (2-18)
Similarly, the rate of formation of solid by heterogeneous chemical reactions, $R_{hs}$, is determined from the appropriate chemical reaction rate equations. Thus the time rate of change of char porosity due to heterogeneous chemical reactions is

$$\left(\frac{\partial n}{\partial t}\right)_h = -\eta \frac{M_s}{\rho_s} R_{hs} .$$

(2-19)

Summing Eqs. 2-18 and 2-19 gives the time rate of change of char layer porosity as

$$\frac{\partial n}{\partial t} = -\frac{\eta}{\rho_s} \left(\frac{M_s}{\rho_s} (R_{hs} + R_s) \right).$$

(2-20)

**Pyrolysis gas energy differential equation.** - The energy conservation equation applied to the fluid phase of the char layer states that the time rate of change of internal and kinetic energy contained in the pyrolysis gases within the control volume $V$ equals the sum of the net rates of convection of internal and kinetic energy transferred into the pyrolysis gases due to the mass average velocity, conduction of energy in the pyrolysis gases, radiation of energy to the pyrolysis gases, work done on the pyrolysis gases by external forces, work done on the pyrolysis gases by pressure forces, work done on the pyrolysis gases by viscous forces, energy transfer to the pyrolysis gases by convection from the char, energy loss by the pyrolysis gases due to mass transfer and energy gained by the pyrolysis gases due to
heterogeneous chemical reactions. The terms of the pyrolysis gas energy equation may be written as follows:

Non-stationary volume term

\[ \int_V \frac{\partial}{\partial t} \left[ \eta \rho \left( \hat{w} + \frac{1}{2} v^2 \right) \right] \, dV \]

Convection by mass average velocity

\[-\int_S \left( \hat{w} + \frac{1}{2} v^2 \right) \rho v_o \cdot \hat{n} \, dS \]

where \( v \) is the velocity of the pyrolysis gases in the char layer and \( v_o \) is the superficial velocity (volume rate of flow through a unit cross-sectional area of the char plus pyrolysis gases).

Conduction term

\[-\int_S q \cdot \hat{n} \, dS \]

Radiation term

\[ \int_V \eta (A' - \varepsilon') \, dV \]

Work by external forces

\[ \int_V \eta \sum_i \hat{n}_i \cdot \hat{g}_i \, dV \]
where $\hat{n}_1$ is a mass flux vector equal to the sum of the mass flux due to mass average velocity and the mass flux due to diffusion, or in equation form

$$\hat{n}_1 = \rho_1 \hat{v} + \hat{j}_1.$$  (2-21)

Work by pressure forces

$$- \int_S P \hat{v}_o \cdot \hat{n} \, dS$$

Work by viscous forces

$$\int_S [\bar{T} \cdot \hat{v}_o] \cdot \hat{n} \, dS$$

Convection from the char

$$\int_V H_A (T_s - T) \, dV$$

Energy loss by mass transfer resulting from homogeneous chemical reactions

$$- \int_V \eta \, r_s \hat{H(T)}_s \, dV$$

Energy loss by mass transfer resulting from heterogeneous chemical reactions
Energy gain resulting from heterogeneous chemical reactions

$$\int_V \eta \sum_r \Delta H(r) \, dV$$

Combining these terms in equation form gives

$$\int_V \frac{\partial}{\partial t} [\eta (\hat{U} + \frac{1}{2} \hat{v}^2)] \, dV =$$

$$- \int_S (\hat{U} + \frac{1}{2} \hat{v}^2) \rho \hat{v} \cdot \hat{n} \, dS - \int_S q \cdot \hat{n} \, dS$$

$$+ \int_V \eta (A' - e') \, dV + \int_V \eta \sum_i \hat{n}_i \cdot \hat{g}_i \, dV$$

$$- \int_S \hat{p} \hat{v} \cdot \hat{n} \, dS + \int_S (\hat{\tau} \cdot \hat{v}_o) \cdot \hat{n} \, dS$$

$$+ \int_V H_A (T_s - T) \, dV - \int_V \eta \sum_r \hat{H}(r) \, dV$$

$$- \int_V \eta \sum_r \hat{H}_s \, dV + \int_V \sum_r \Delta H(r) \, dV . \quad (2-22)$$

Applying Gauss' Theorem to convert the surface integrals to volume integrals gives
This equation is true for any volume \( V \); therefore, the integral can vanish only if the integrand vanishes everywhere. Thus the differential form of the pyrolysis gas internal and kinetic energy equation is

\[
\frac{\partial}{\partial t} \left[ \eta \rho (\hat{U} + \frac{1}{2} \nu^2) \right] + \hat{\nabla} \cdot \left[ (\hat{U} + \frac{1}{2} \nu^2) \rho \hat{v}_o \right] + \hat{\nabla} \cdot q
- \eta (A' - \epsilon') - \eta \sum_{i} \hat{n}_i \cdot \hat{g}_i + \hat{\nabla} \cdot \rho \hat{v}_o
- \hat{\nabla} \cdot \left[ \tau \cdot \hat{v}_o \right] - H_A (T_s - T) + \eta r_s \hat{H}(T)_s + \eta r_{hs} \hat{H}_s
- \eta \sum_{r} r^{(r)} \Delta H^{(r)} = 0 ,
\]

This equation can be simplified by subtracting from it the equation of mechanical energy. The equation of mechanical energy for
a fluid flowing through porous media results from taking the scalar product of the fluid velocity with the equation of motion. The equation of motion for a fluid flowing through porous media states that the time rate of change of momentum contained in the pyrolysis gas within the control volume $V$ equals the sum of the net rates of momentum increase resulting from momentum convection by mass average velocity, pressure force per unit volume of pyrolysis gases, viscous transfer per unit volume of pyrolysis gases and gravitational force per unit volume of pyrolysis gases. In equation form

$$V \frac{\partial}{\partial t} (\eta \rho \vec{v}) \ dV = - \int_S (\rho \vec{v}) \vec{v}_o \cdot \vec{n} \ dS - \int_S \eta \ P \ \vec{\xi} \cdot \vec{n} \ dS$$

$$+ \int_S \eta \ \vec{\tau} \cdot \vec{n} \ dS + \int_V \eta \rho \vec{g} \ dV . \quad (2-25)$$

Gauss's theorem may be applied to Eq. 2-25 to convert the surface integrals to volume integrals giving

$$\int_V \{ \frac{\partial}{\partial t} (\eta \rho \vec{v}) + \vec{v} \cdot \rho \vec{v} \vec{v}_o + \vec{\tau} \eta \ P$$

$$- \vec{v} \cdot \vec{\tau} - \eta \rho \vec{g} \} \ dV = 0 . \quad (2-26)$$

This equation is true for any volume $V$; therefore, the integral can vanish only if the quantity in brackets vanishes everywhere. Thus the
differential form of the equation of motion for flow through porous media is

\[ \frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot \rho \vec{v} \vec{v}_0 + \nabla \cdot \nabla P = 0 \]  

Forming the scalar product of the pyrolysis gas velocity with Eq. 2-27 gives the equation of mechanical energy for the pyrolysis gases as

\[ \frac{1}{2} \frac{\partial}{\partial t} (\rho \vec{v}^2) + \frac{1}{2} \eta \vec{v}^2 \frac{\partial \rho}{\partial t} + \frac{1}{2} \rho \vec{v}^2 \frac{\partial \eta}{\partial t} + \frac{1}{2} \vec{v} \cdot \rho \vec{v}^2 \vec{v}_0 + \frac{1}{2} \mu \vec{v} \vec{v}_0 + \nabla \cdot \nabla P \vec{v}_0 \]
\[ - \eta \vec{v} 
abla \cdot \vec{v} - \vec{v} \cdot \nabla \cdot [\vec{v} \vec{v}_0] + \eta \nabla : \vec{v} = 0 \]  

Equation 2-28 is subtracted from Eq. 2-24 to obtain the thermal energy equation of the pyrolysis gases as
Equation 2-29 can be simplified somewhat by expressing the internal energy in terms of the enthalpy and the state variables pressure and density and by making use of the mass conservation equation. The internal energy-enthalpy relation

\[ U = H - \frac{P}{\rho} \]  

yields

\[ \frac{DU}{Dt} = \frac{DH}{Dt} - \frac{1}{\rho} \frac{DP}{Dt} + \frac{P}{\rho^2} \frac{DP}{Dt} \]  

**Chemical species continuity equation.** The chemical species continuity equation applied to the pyrolysis gases flowing through the char layer states that the time rate of change of mass of some species within the control volume \( V \) equals the sum of the net rate of mass of that chemical species transferred into the control volume.
by the mass average velocity and mass diffusion and the net rate of formation of that chemical species by chemical processes. Writing this equation in integral form gives

\[ \int_V \frac{\partial}{\partial t} (\eta \rho_i) \, dV = -\int_S \rho_i \vec{v}_o \cdot \vec{n} \, dS \]

\[ + \int_V \eta \, r_{T_i} \, dV - \int_S \eta \, \vec{j}_i \cdot \vec{n} \, dS \]  \hspace{0.5cm} (2-32)

Applying Gauss's Theorem to convert the surface integrals to volume integrals gives

\[ \int_V \left[ \frac{\partial}{\partial t} (\eta \rho_i) + \nabla \cdot (\rho_i \vec{v}_o) - \eta r_{T_i} + \nabla \cdot (\eta \vec{j}_i) \right] \, dV = 0 \]  \hspace{0.5cm} (2-33)

which yields the chemical species conservation equation

\[ \frac{\partial}{\partial t} (\eta \rho_i) + \nabla \cdot (\rho_i \vec{v}_o) + \nabla \cdot (\eta \vec{j}_i) - \eta r_{T_i} = 0 \]  \hspace{0.5cm} (2-34)

**Total mass conservation equation.** - The total mass conservation equation is obtained by summing the chemical species conservation equation over all species. Thus

\[ \frac{\partial}{\partial t} (\eta \rho) + \nabla \cdot (\rho \vec{v}_o) - \eta \sum_{i} r_{T_i} = 0 \]  \hspace{0.5cm} (2-35)
Equations 2-29, 2-31 and 2-35 are combined to give the pyrolysis gas energy equation in terms of enthalpy as

\[ \eta \rho \frac{DH}{Dt} = \eta \frac{DP}{Dt} + P \frac{DH}{Dt} - \eta (H - \frac{1}{2} v^2) \sum r_{T_1} \]

\[ + \eta \tau : \hat{\nabla} v + \eta \sum_{i} j_i \cdot g_i - \hat{\nabla} \cdot \hat{q} + \eta (A' - \varepsilon') \]

\[ + H_A (T_s - T) - \eta r_s \hat{H}(T_s) - \eta r_{hs} \hat{H}_s \]

\[ + \eta \sum_{r} r_h^{(r)} \Delta H^{(r)} \]

(2-36)

It is more convenient to work with the pyrolysis gas energy equation written in terms of \( \hat{C} \) rather than \( \hat{H} \). The desired form of the pyrolysis gas energy equation is obtained by combining Eq. 2-36 with the Gibbs equation written in terms of \( \hat{H} \) and the First Law of Thermodynamics.

The Gibbs equation for a system in equilibrium as written by Hatsopoulos and Keenan (Ref. 22) is

\[ d\hat{H} = T d\hat{S} + \hat{V} dP + \sum \mu_i d(\rho_i / \rho) \]

(2-37)

It will now be assumed that, although the pyrolysis gases are not in true equilibrium, there exists within small mass elements a state of local equilibrium for which a bulk gas temperature can be defined and for which the local entropy \( \hat{S} \) is a well-defined function of the
various parameters which are necessary to define the macroscopic state of the system completely. With this assumption Eq. 2-37 becomes valid for a mass element followed along its center of motion, thus

\[
\frac{DH}{Dt} = T \left( \frac{DS}{Dt} + \frac{\hat{V}}{DT} + \sum_i \frac{\hat{\mu}_i}{D} \frac{D}{Dt} (\rho_i/\rho) \right). \tag{2-38}
\]

Equation 2-38 can be made more useful by expressing entropy in terms of \( P, \hat{V} \) and \( T \). Assuming the system is composed of a mixture of thermally perfect gases the entropy may be expressed as a function of \( P, T \), and \( \frac{\rho_i}{\rho} \), or

\[
\hat{S} = S(P, T, \rho_i/\rho) \tag{2-39}
\]

which yields

\[
d\hat{S} = \left( \frac{\partial \hat{S}}{\partial P} \right)_{T, \rho_i/\rho} dP + \left( \frac{\partial \hat{S}}{\partial T} \right)_{P, \rho_i/\rho} dT + \sum_i \left( \frac{\partial \hat{S}}{\partial \rho_i/\rho} \right)_{P, T} d(\rho_i/\rho). \tag{2-40}
\]

Writing Eq. 2-37 in terms of specific heat

\[
d\hat{S} = \frac{C}{T} \hat{S} dT - \frac{\hat{V}}{T} dP - \frac{1}{T} \sum_i \hat{\mu}_i d(\rho_i/\rho). \tag{2-41}
\]
Equating the coefficients for \( dT \) in Eqs. 2-40 and 2-41 gives

\[
(\frac{\partial S}{\partial T})_{P, \rho_i/\rho} = \frac{C_p}{T}. \tag{2-42}
\]

The coefficient of \( dP \) in Eq. 2-40 is replaced by its equivalent from the Maxwell relation

\[
(\frac{\partial S}{\partial P})_{T, \rho_i/\rho} = -\left(\frac{\partial V}{\partial T}\right)_{P, \rho_i/\rho}. \tag{2-43}
\]

Equations 2-40, 2-42 and 2-43 are combined to give a differential entropy expression in terms of \( P, V \) and \( T \).

\[
dS = \frac{C_p}{T} dT - \left(\frac{\partial V}{\partial T}\right)_{P, \rho_i/\rho} dT + \sum_i \left(\frac{\partial S}{\partial \rho_i/\rho}\right)_{P, T} d(\rho_i/\rho). \tag{2-44}
\]

This equation may be written for a mass element followed along its center of motion as

\[
\frac{dS}{dt} = \frac{C_p}{T} \frac{dP}{dt} - \left(\frac{\partial V}{\partial T}\right)_{P, \rho_i/\rho} \frac{DP}{dt} + \sum_i \left(\frac{\partial S}{\partial \rho_i/\rho}\right)_{P, T} \frac{D}{dt} \left(\frac{\rho_i}{\rho}\right). \tag{2-45}
\]

Equation 2-45 may be combined with Eq. 2-38 to give

\[
\frac{dH}{dt} = C_p \frac{dT}{dt} + V \frac{dP}{dt} - T \left(\frac{\partial V}{\partial T}\right)_{P, \rho_i/\rho} \frac{DP}{dt} + \sum_i \left[\mu_i + T \left(\frac{\partial S}{\partial \rho_i/\rho}\right)_{P, T}\right] \frac{D}{dt} \left(\frac{\rho_i}{\rho}\right). \tag{2-46}
\]
The summation term in this equation can be reduced by considering the relation between partial properties. The entropy of a system is written as

\[ \hat{S} = \sum_i \left( \frac{\rho_i}{\rho} \right) \hat{S}_i. \] (2-47)

From Eq. 2-47 we have that

\[ d\hat{S} = \sum_i \frac{\rho_i}{\rho} d\hat{S}_i + \sum_i \hat{S}_i d\left( \frac{\rho_i}{\rho} \right). \] (2-48)

Since entropy of a pure substance may be expressed as a function of \( P \) and \( T \), Eq. 2-48 written for a constant pressure and temperature process is

\[ d\hat{S} = \sum_i \hat{S}_i d\left( \frac{\rho_i}{\rho} \right). \] (2-49)

Thus

\[ \left( \frac{\partial \hat{S}}{\partial \rho_i/\rho} \right)_{P,T} = \hat{S}_i. \] (2-50)

The partial specific Gibbs function is defined as

\[ \hat{\mu}_i = \left( \frac{\partial G}{\partial \hat{M}_i} \right)_{P,T}. \] (2-51)
But

\[ G = H - TS \]  \hspace{1cm} (2-52)

or

\[ G = \sum M_i (\dot{H}_i - \dot{S}_i) \]  \hspace{1cm} (2-53)

Equation 2-53 is combined with Eq. 2-51 to give the partial specific Gibbs function as

\[ \dot{\mu}_i = \dot{H}_i - T \dot{S}_i \]  \hspace{1cm} (2-54)

Equations 2-50 and 2-54 are combined with Eq. 2-46 to satisfy the First Law of Thermodynamics applied to an element of mass near equilibrium followed along its center of motion. In equation form

\[ \frac{D\dot{H}}{Dt} = \frac{C}{p} \frac{D\dot{T}}{Dt} + \dot{V} \frac{DP}{Dt} - T \left( \frac{3\dot{V}}{\dot{T}} \right)_p \rho_1 / \rho \frac{DP}{Dt} \]

\[ + \sum_i \dot{H}_i \frac{D}{Dt} (\rho_1 / \rho) \]  \hspace{1cm} (2-55)

Equation 2-55 is combined with Eq. 2-36 to give the pyrolysis gas energy equation in terms of \( \dot{C}_p \) as
The derivative of $\frac{\rho_i}{\rho}$ can be expanded and combined with the chemical species and total mass continuity equations (Eqs. 2-34 and 2-35) to give

$$\frac{D}{Dt} \left( \frac{\rho_i}{\rho} \right) = \frac{1}{\rho} \frac{D \rho_i}{Dt} - \frac{1}{\eta \rho} \nabla \cdot \mathbf{j}_i - \frac{\rho_i}{\rho^2} \frac{D}{Dt} \mathbf{j}_i .$$  (2-57)

Equation 2-57 is combined with Eq. 2-56 and the specific quantities $\hat{C}_p$, $\hat{H}$, $\hat{H}_i$, and $\hat{H}_s(T)$ and the chemical production terms $r_i$, $r_{hs}$, and $r_s$ are written in terms of their respective mole quantities to give the pyrolysis gas energy equation in terms of mole quantities as
Pyrolysis gas pressure differential equation.- The basic law governing the velocity of fluids flowing through porous media is the phenomenological law of Darcy which states that the rate of flow through porous media is directly proportional to the pressure gradient causing flow. Darcy's law written in equation form as in Scheidegger (Ref. 23) is

\[ \vec{v} = -\frac{K}{\mu} \vec{\nabla} p \]  

or

\[ \vec{v} = -\frac{K}{\mu n} \vec{\nabla} p . \]
Equation 2-59 may be combined with the total mass conservation equation to give

\[
\frac{\partial}{\partial t} (\eta \rho) - \vec{\nabla} \cdot \left( \frac{\partial K}{\mu} \vec{\nabla} \vec{P} \right) - \eta \sum_i R_{T_i} M_i = 0. \tag{2-61}
\]

The equation of state for the pyrolysis gases,

\[
P = \rho \frac{RT}{u} \tag{2-62}
\]

and the identity

\[
P \frac{\partial}{\partial \vec{P}} \vec{P} = \frac{1}{2} \vec{\nabla} \vec{P}^2 \tag{2-63}
\]

are used in Eq. 2-61 to give the differential equation for pyrolysis gas pressure as

\[
\vec{\nabla} \cdot \vec{\nabla} \vec{P}^2 + \frac{\mu T}{K} \vec{\nabla} \left( \frac{K}{\mu T} \right) \cdot \vec{\nabla} \vec{P}^2
\]

\[
- \frac{2\mu R T}{K M} \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_i R_{T_i} M_i \right] = 0. \tag{2-64}
\]

**Chemical reaction rate equations.**—The rate of chemical reactions occurring within the char layer must be computed using an appropriate chemistry model. The model considered here treats homogeneous and heterogeneous reactions. The rate of removal of chemical species by
homogeneous reactions is governed by the Law of Mass Action which states that the rate of removal of a chemical species is proportional to the product of the concentrations of the reacting species where each and every chemical species concentration is raised to a power equal to its stoichiometric coefficient. In equation form, the Law of Mass Action as written by Clarke and McChesney (Ref. 24) for a one-step chemical reaction described by the following stoichiometric relation

\[ \Sigma v'_i A_i + \Sigma v''_i A_i \]  

is

\[ \text{reaction rate} = k \prod_{i} [A_i]^{v'_i} \]  

(2-66)

where the reaction rate constant \( k \) is considered to be independent of the concentration of chemical species and dependent on temperature. The reaction rate constant is given by

\[ k = A T^S \exp\left(-\frac{B}{T}\right) \]  

(2-67)

where \( A \) and \( B \) are the frequency factor and activation energy for the reaction.

Simultaneous forward and reverse chemical reactions are represented by
The rate of forward reaction for the chemical reaction represented by the \( r \)\textsuperscript{th} equation is

\[
\text{rate of forward reaction} = k_f^{(r)} \prod_{\text{i}} [A_i]^\nu_{\text{i}}^{(r)'}
\]  

(2-69)

and the rate of reverse reaction is

\[
\text{rate of reverse reaction} = k_r^{(r)} \prod_{\text{i}} [A_i]^\nu_{\text{i}}^{(r)''}
\]  

(2-70)

Thus the net rate of progress of the \( r \)\textsuperscript{th} reaction in the forward direction is given by

\[
r^{(r)} = k_f^{(r)} \prod_{\text{i}} [A_i]^\nu_{\text{i}}^{(r)'} - k_r^{(r)} \prod_{\text{i}} [A_i]^\nu_{\text{i}}^{(r)''}
\]  

(2-71)

Now this reaction yields a predetermined number of moles of chemical species \( \text{i} \) as indicated by the coefficients in the stoichiometric
representation of the chemical reaction. Therefore, the molar rate of production of chemical species \( i \) is given by

\[
R_i = \sum_r \left[ v_i(r)^{\prime} - v_i(r)^{\prime\prime} \right] \{ k_i(r) \Pi_i [A_i] \}^\prime \frac{v_i(r)^{\prime}}{v_i(r)^{\prime\prime}} - k_i(r) \Pi_i [A_i] \} \frac{v_i(r)^{\prime}}{v_i(r)^{\prime\prime}}. \tag{2-72}
\]

Equations 2-69 and 2-70 are based on the Law of Mass Action and are general expressions for the forward and reverse reaction rates of some chemical reaction occurring in a gaseous system. Most frequently, the chemical kinetics data for a particular reaction are based on empirical curve fits to experimental data. Such chemical kinetics data are usually presented with a rate law which best describes the particular chemical process.

The theory describing heterogeneous chemical reactions or reactions occurring at the gas-solid interface is somewhat more complicated than for homogeneous chemical reactions. It was assumed by Laidler (Ref. 25) that there are four steps involved in the interaction of the gas molecules with the solid phase. These steps are: (1) The reacting molecules diffuse to the solid surface. (2) The molecules are adsorbed on the surface. (3) The molecules undergo chemical reactions giving gaseous and/or solid products. (4) The gaseous product molecules diffuse from the surface. The usual treatment of surface reactions is based on a concept due to Langmuir and Hinshelwood.
which is discussed in Emmett (Ref. 26). The Langmuir-Hinshelwood mechanism assumes that the reactants are in adsorptive equilibrium with the solid surface. The reaction then involves the adsorbed molecules. Quantitative treatment of the reactions by this mechanism, therefore, involves obtaining an expression, using the adsorption isotherm, for the concentration of the reactant molecules on the surface. Thus, expressing the rate of reaction in terms of these surface concentrations, the rate of reaction can be expressed in terms of the concentrations of the gaseous reactants.

Following the development of Alekseyev (Ref. 27), the Law of Surface Action for the heterogeneous reaction

\[ \sum_{j} v_j' A_j \rightarrow \sum_{j} v_j'' A_j \]  

(2-73)

states that the rate of the process is proportional to the product of the portions of the surface occupied by reacting species raised to powers equal to the corresponding stoichiometric coefficients. In equation form

\[ \text{reaction rate} = k \prod_{j} \left( \theta_j^0 \right)^{v_j'} \left( \theta_j^o \right)^{v_j''} \]  

(2-74)

where the reaction rate constant is given by an equation of the form

\[ k = A \exp \left(-\frac{B}{T}\right) \]  

(2-75)
Simultaneous forward and reverse heterogeneous chemical reactions are represented by

\[
\begin{align*}
\sum_{j} k_{f}^{(r)} v_{j}^{(r)} A_{j} & + \sum_{j} k_{r}^{(r)} v_{j}^{(r)"} A_{j} \\
\end{align*}
\]  

(2-77)

where \( r = 1, 2, \ldots, m \) independent reactions. The rate of the forward reaction for the chemical reaction represented by the \( r^{th} \) equation is

\[
\text{rate of forward reaction} = k_{f}^{(r)} \prod_{j} \theta_{j} v_{j}^{(r)'} \theta_{o}^{n(r)}
\]  

(2-78)

and the rate of the reverse reaction is

\[
\text{rate of reverse reaction} = k_{r}^{(r)} \prod_{j} \theta_{j} v_{j}^{(r)"} \theta_{o}^{n(r)}
\]  

(2-79)

Thus the net rate of the \( r^{th} \) reaction is given by

\[
r_{h}^{(r)} = \left\{ k_{f}^{(r)} \prod_{j} \theta_{j} v_{j}^{(r)'} - k_{r}^{(r)} \prod_{j} \theta_{j} v_{j}^{(r)"} \right\} \theta_{o}^{n(r)} A_{s}
\]  

(2-80)

and the molar rate of production of chemical species \( j \) resulting from the set of reactions (Eq. 2-77) is
\[ R_{h_j} = \sum_r [v_j^{(r)}'' - v_j^{(r)}'] \left\{ k_f^{(r)} \prod_j \theta_j^{(r)} \right\} A_s \theta_o^n(r) \]  

(2-81)

where the factor \( A_s \) is the surface area per volume and is included to give rate of production per volume for heterogeneous chemical reactions occurring in porous media.

There is very little chemical kinetics data available for reactions and conditions of interest in the field of ablation. When data are available it is presented with a rate law which best describes the particular chemical reaction.

Uncharred Material and Substrate Insulation Equations

The single energy transfer mechanism occurring in the uncharred material and substrate insulation is heat transfer by conduction. Thus the differential equation governing the thermal behavior of these regions is the conduction equation given by

\[ \mathbf{\bar{v}} \cdot k'_s \mathbf{\bar{v}} T'_s = \rho'_s \hat{C}' p_s \frac{\partial T'_s}{\partial t} \]  

(2-82)

and

\[ \mathbf{\bar{v}} \cdot k''_s \mathbf{\bar{v}} T''_s = \rho''_s \hat{C}'' p_s \frac{\partial T''_s}{\partial t} , \]  

(2-83)

respectively.
CHAPTER III

BOUNDARY CONDITIONS AND INITIAL CONDITIONS

This analysis refers to the stagnation point of a body, hence the governing equations derived in Chapter II are reduced to one dimension in space. The equations to be solved are:

Char Layer Equations.

Char temperature

\[
(1 - \eta) \frac{\rho_s C_p}{M_s} \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial y} \left( k_s \frac{\partial T_s}{\partial y} \right) - H_A (T_s - T) \\
+ \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \Sigma \frac{H_s}{R_h} (r) \Delta H(r) + (1 - \eta) (A - \varepsilon) \\
+ (1 - \eta) \rho_s + \frac{\rho_s H_s}{M_s} \frac{\partial \eta}{\partial t}
\]  

(3-1)

Char porosity

\[
\frac{\partial \eta}{\partial t} = - \eta \frac{M_s}{\rho_s} (R_{hs} + R_s)
\]

(3-2)

Pyrolysis gas temperature

\[
\eta \Sigma \frac{\rho_i C_{pi}}{M_i} \left( \frac{\partial T}{\partial t} + v \frac{\partial T}{\partial y} \right) = -\eta \left( \frac{\partial}{\partial T} \frac{\partial \rho}{\partial T} \right) p_0 x_i \left( \frac{\partial P}{\partial t} \right) + v \frac{\partial P}{\partial y} - \eta \Sigma H_i R_i T_i + \eta \Sigma H_i \frac{\partial J_i}{\partial t} + P \frac{\partial \eta}{\partial t} + P v \frac{\partial \eta}{\partial y}
\]
\[ + \frac{1}{2} \eta v^2 \sum_i R_{ti} M_i + \eta \frac{\partial}{\partial y} \frac{\partial v}{\partial y} + \eta \sum_i \frac{J_i g_i}{M_i} - \frac{\partial}{\partial y} q_y \]

\[ + \eta (A' - \epsilon') + H_A (T_s - T) - \eta R_s H(T)_s - \eta R_{hs} H_s \]

\[ + \eta \sum_r \frac{r_h}{r} \Delta H(r) \quad (3-3) \]

Chemical species continuity equation

\[ \frac{\partial}{\partial t} (\eta \rho_i) + \frac{\partial}{\partial y} (\rho_i v_o) + \frac{\partial}{\partial y} \eta l_i - \eta r_{ti} = 0 \quad (3-4) \]

Total mass conservation equation

\[ \frac{\partial}{\partial t} (\eta \rho) + \frac{\partial}{\partial y} (\rho v_o) - \eta \sum \frac{r_{ti}}{M_i} = 0 \quad (3-5) \]

Pressure of pyrolysis gas

\[ \frac{3 \rho^2}{\partial y^2} + \frac{\mu T}{\kappa} \frac{\partial}{\partial y} \left( \frac{\kappa M}{\mu T} \right) \frac{3 \rho^2}{\partial y} - \frac{2 \mu R_s}{\kappa M} \left[ \frac{\partial}{\partial t} (\eta \rho) \right] \]

\[ - \eta \sum \frac{R_s}{M_i} = 0 \quad (3-6) \]

Uncharred Layer and Substrate Insulation Equations.

Uncharred layer temperature

\[ \frac{\partial}{\partial y} \left( k'_s \frac{\partial T'}{\partial y} \right) = \rho'_s \frac{C'_s}{p'_s} \frac{\partial T'}{\partial t} \quad (3-7) \]
Substrate insulation temperature

\[ \frac{\partial}{\partial y} \left( k'' \frac{\partial T''}{\partial y} \right) = \rho'' c'' \frac{\partial T''}{\partial t}. \]  

(3-8)

It is convenient to treat the equations for char temperature, uncharred layer temperature and substrate insulation temperature as a set of coupled equations. That is, the char temperature equations are related to the uncharred layer temperature equation through the boundary condition at the char-uncharred interface. The equations for the uncharred layer and the insulation layer are similarly related. From this point forward, reference to the solid temperature will mean the temperature of the particular layer of interest.

Solid Temperature Equations

Two conditions must be specified at the front surface of the char layer. The first condition is an expression for the rate of material removal or the surface temperature and the second is an energy balance.

Surface removal by oxidation.—There are two regimes of surface removal by oxidation. The first regime is the rate controlled regime. The rate of surface removal by oxidation is rate controlled when conditions of temperature and pressure are low enough that the rate of oxygen consumption in the chemical process does not exceed the rate of oxygen diffusion through the boundary layer to the surface. As the surface temperature and pressure increase, the rate of surface removal
goes through a transition from the rate controlled regime to a diffusion controlled regime. In the diffusion controlled regime, surface removal by oxidation depends on the rate of oxygen diffusion to the surface. Nolan and Scala (Ref. 28) express the rate of surface removal by oxidation in the rate controlled regime in terms of chemical kinetics, writing the mass loss rate as

\[ \dot{m}_s = k \left( P_{02} \right)_w^n \]  

(3-9)

where the exponent \( n \) is the order of the reaction. The specific reaction rate is obtained from

\[ k = A_s \exp\left(-\frac{B_s}{T_s} \right). \]  

(3-10)

The oxygen partial pressure at the wall may be written in terms of the mass fraction of oxygen as follows:

\[ \left( P_{02} \right)_w = \left( x_{02} \right)_w P_e \]  

(3-11)

\[ P_w = P_e \]  

(3-12)

\[ \left( x_{02} \right)_w = C_w \frac{\bar{M}_w}{M_{02}}. \]  

(3-13)

Therefore,
Equations 3-9, 3-10, and 3-14 are combined to give the rate of surface removal by rate controlled oxidation as

\[
\dot{m}_s = A_s \exp\left(-\frac{B_s}{T_{s1}}\right) \left(\frac{C_w \bar{M}_w}{M_{O_2}} \frac{P_e}{P_{e0}}\right)^n.
\]  

(3-15)

In subsonic and supersonic flow, the stagnation pressure is given by the solution of the inviscid flow problem. The stagnation pressure in hypersonic flow is approximated in Truitt (Ref. 29) by

\[
P_{w,s} = \frac{11}{12} \rho_e v_e^2.
\]  

(3-16)

In Ref. 30 Chapman relates the heating rate and enthalpy to the free stream conditions by

\[
q_c \propto \sqrt{\frac{\rho_e}{\text{Rad}}} v_e^3.
\]  

(3-17)

and

\[
\hat{H}_e \propto v_e^2.
\]  

(3-18)

Thus the wall pressure is approximated by
\[ P_{w,s} = 5.693 \times 10^6 \text{ Rad} \left( \frac{q_c}{H_e} \right)^2. \] (3-19)

In the current problem,

\[ P_w = P_{w,s} \] (3-20)

thus

\[ P_w = 5.693 \times 10^6 \text{ Rad} \left( \frac{q_c}{H_e} \right)^2. \] (3-21)

In the diffusion controlled regime, surface removal by oxidation depends on the rate of oxygen diffusion to the surface as expressed in the following equation

\[ \dot{m}_s = \lambda \dot{n}_0. \] (3-22)

where \( \lambda \) is the ratio of the mass of char layer removed by oxidation to the mass of oxygen diffusing to the surface.

In Ref. 10 Swann presents an analysis of oxidation of carbon surfaces near the stagnation region of a body in a nonreacting mixture of two gases having the same specific heats. Following Swann's development, the boundary layer equation for conservation of oxygen is

\[ \bar{\rho} u \frac{\partial C}{\partial z} + \bar{\rho} v \frac{\partial C}{\partial y} = \frac{\partial}{\partial y} \left( \bar{\rho} u \frac{\partial C}{\partial y} \right) \] (3-23)
and the boundary layer energy equation is

\[
\bar{\rho} u \frac{\partial \hat{H}}{\partial z} + \bar{\rho} v \frac{\partial \hat{H}}{\partial y} = \frac{\partial}{\partial y} \left[ \frac{\mu}{N_{Pr}} \frac{\partial \hat{H}}{\partial y} + \frac{\mu}{2} \left( 1 - \frac{1}{N_{Pr}} \right) \frac{\partial u^2}{\partial y} \right].
\]  

Equations 3-21 and 3-22 are formally similar if \( N_{Pr} = 1 \) or if \( \frac{\partial u^2}{\partial y} \) is small relative to \( \frac{\partial H}{\partial y} \), which is valid at stagnation regions. Also, the boundary conditions for these two equations are identical, that is

\[
\begin{align*}
C &= C_w \quad \text{at } y = 0 \\
\hat{H} &= \hat{H}_w
\end{align*} \quad (3-25)
\]

and

\[
\begin{align*}
C &= C_e \quad \text{at } y = \infty . \\
\hat{H} &= \hat{H}_e
\end{align*} \quad (3-26)
\]

Nondimensionalizing Eqs. 3-23 and 3-24 with
Therefore, the solutions of the oxygen conservation equation and the energy conservation equation are formally similar. If the solution of the boundary layer energy equation is

\[ \Phi = F_1(\zeta, y, N_{Pr}) \]  

then the solution of the oxygen conservation equation is

\[ \Phi = F_1(\zeta, y, N_{Sc}) \]
The rate of oxygen transfer to the surface by diffusion may be expressed as

\[ \dot{m}(O_2) = (C_e - C_w) \left( \frac{\mu}{N_{Sc}} \frac{\partial C}{\partial y} \right)_w \]  

(3-31)

and the rate of energy transfer to the surface may be expressed as

\[ q = (H_e - H_w) \left( \frac{\mu}{N_{Pr}} \frac{\partial H}{\partial y} \right)_w. \]  

(3-32)

Fay and Riddell (Ref. 31) show that the rate of energy transfer to the surface may be expressed as

\[ q_{c,\text{net}} = 0.76 N_{Pr}^{-0.6} (\rho_w \mu_w)^{0.1} (\rho_s \mu_s)^{0.4} (H_e - H_w) \sqrt{\frac{du_e}{dz}}. \]  

(3-33)

Therefore, the rate of oxygen diffusion to the surface is

\[ m_{O_2} = 0.76 N_{Sc}^{-0.6} (\rho_w \mu_w)^{0.1} (\rho_s \mu_s)^{0.4} (C_e - C_w) \sqrt{\frac{du_e}{dz}}. \]  

(3-34)

Equations 3-33 and 3-34 are combined to give the rate of oxygen diffusion to the surface in terms of the energy transfer rate as

\[ \dot{m}_{O_2} = \frac{N_{Sc}^{-0.6} (C_e - C_w)}{N_{Pr}^{-0.6} (H_e - H_w)} q_{c,\text{net}}. \]  

(3-35)
The rate of surface removal by oxidation in terms of energy transfer rate is obtained upon combining Eqs. 3-22 and 3-36. Thus,

$$\dot{m}_s = \frac{C_e - C_w}{H_e - H_w} \lambda N^{0.6} Le q_{c,net}.$$  \hspace{1cm} (3-37)

Equation 3-15 written for a reaction of order 1 is combined with Eq. 3-37 to give an equation for the rate of surface removal which does not contain the oxygen concentration at the wall. Thus,

$$\dot{m}_s = \frac{k P \tilde{M}_e}{H_e - H_w} \left( \frac{M_0}{k P \tilde{M}_e} \right) \frac{C_e - C_w}{H_e - H_w} + \frac{M_0}{\lambda N^{0.6} Le q_{c,net}}$$  \hspace{1cm} (3-38)

where

$$k = A_s \exp \left( - \frac{B_s}{T_{s1}} \right).$$  \hspace{1cm} (3-39)

**Front surface energy balance.** - The second condition to be specified at the front surface is a surface energy balance. Energy transfer to the surface results from convective and radiative heating and combustion heating in the case of surface removal by oxidation. This energy is accommodated by blocking due to mass injection into the boundary layer, reradiation from the
surface, conduction to the interior, and sublimation of the char layer when the surface temperature reaches the sublimation temperature of the char material.

Figure 2 from Swann, Pittman and Smith (Ref. 16) shows the effect of mass injection into the boundary layer on energy transfer to the surface. The exact solution is from the boundary layer solution by Roberts (Ref. 6) for air-to-air injection. The linear approximation is

$$q_{c, net} = q_c (1 - \frac{H_w}{H_e}) \left[ 1 - \frac{\dot{m}_T H_e}{q_c} \right] \quad (3-40)$$

where

$$\dot{m}_T = \alpha c \dot{m}_s + \alpha p \dot{m}_1 \quad (3-41)$$

and $\bar{\eta} = 0.6$. The second-order approximation, which was obtained by fitting a curve through points at $\dot{m}_T H_e/q_c = 0, 1.0,$ and $2.5$ is

$$q_{c, net} = q_c (1 - \frac{H_w}{H_e}) \left[ 1 - 0.724 \frac{\dot{m}_T H_e}{q_c} - 0.13 \left( \frac{\dot{m}_T H_e}{q_c} \right)^2 \right] \quad (3-42)$$

Figure 2 shows the linear approximation to be good for values of $\dot{m}_T H_e/q_c \leq 1$. The second-order approximation is good for $\dot{m}_T H_e/q_c < 2.25$. In Ref. 16 Swann, Pittman and Smith specify a minimum value of
Figure 2.- Blocking effectiveness for a laminar boundary layer with air-to-air injection.
\[
q_{c,\text{net}} = \frac{q_c}{(1 - H_w/H_e)} \quad \text{of} \quad 0.04 \quad \text{at} \quad \frac{\dot{m}_T H_e}{q_c} = 2.25, \quad \text{where the second order curve departs the exact curve.}
\]

Writing the surface energy balance in equation form (Ref. 16)

\[
q_c \quad (1 - H_w/H_e) \quad \{ 1 - (1 - \beta) \quad [0.724 \quad \frac{\dot{m}_T H_e}{q_c} ^{0.724} \]
\]

\[
\text{Cold Wall Convective Heating Rate} \quad \text{Hot-wall correction} \quad \text{Aerodynamic}
\]

\[
-0.13 \quad (\frac{\dot{m}_T H_e}{q_c})^2 \quad - \beta \quad \frac{\dot{m}_T H_e}{q_c} \quad + \quad \alpha \quad q_R
\]

\[
\text{Blocking} \quad \text{Radiative Heating Rate}
\]

\[
\text{Heating} \quad \text{Reradiation}
\]

\[
+ [1 - S(T_{s_L} - \bar{T}_L)] \quad \dot{m}_s \quad \Delta H_c = \sigma \quad \varepsilon_s \quad T_{s_L}^4
\]

\[
\text{Combustion Heating Rate} \quad \text{Reradiation}
\]

\[
- \frac{\partial T_s}{\partial y} \quad + \quad S(T_{s_L} - \bar{T}_L) \quad \dot{m}_s \quad H_c
\]

\[
\text{Conduction} \quad \text{Heat of Sublimation to Interior of Char}
\]

where

\[
(3-43)
\]
\[ \beta = 1 \text{ when } \hat{m}_T \hat{H}_e / q_c \leq 1.0 \]

\[ \beta = 0 \text{ when } \hat{m}_T \hat{H}_e / q_c > 1.0 \]

\[ S(T_{s1} - \bar{T}_1) \text{ is a step function defined by} \]

\[ S(T_{s1} - \bar{T}_1) = 1 \text{ when } T_{s1} = \bar{T}_1 \]

\[ S(T_{s1} - \bar{T}_1) = 0 \text{ when } T_{s1} < \bar{T}_1. \]

When the surface temperature is less than the sublimation temperature, Eq. 3-43 is solved for the temperature gradient at the surface \( \frac{\partial T_s}{\partial y} \) which is used as a boundary condition for solving the char temperature equation.

When the temperature of the char layer surface equals the sublimation temperature of the char material, the specified sublimation temperature of the material is used as a boundary condition and Eq. 3-43 is used to compute the rate of surface removal by sublimation.

**Pyrolysis zone energy balance.**- The second boundary condition to be specified for the char temperature equation is at the interface of the char layer and the uncharred layer. This equation is just an expression of conservation of energy at the interface energy conducted from the char layer to the interface is accommodated by pyrolysis reactions and conduction into the uncharred layer. In equation form
Also, the temperature of the char layer equals the temperature of the uncharred layer at their interface.

$$T_s = T'_u.$$  \hspace{1cm} (3-45)

**Rate of pyrolysis of uncharred material.** The pyrolysis rate at the interface is given by an Arrhenius equation as follows:

$$\dot m_g = A' \exp \left( \frac{-B'}{T'_u} \right).$$  \hspace{1cm} (3-46)

It is sometimes desirable to limit the temperature at the pyrolysis zone to some value $T'_u$. When such a restriction is used Eqs. 3-44 and 3-46 are employed as described until the pyrolysis zone temperature reaches $T'_u$, then Eq. 3-44 is used to determine the rate of pyrolysis of the uncharred layer and the boundary condition for $T_s$ at the pyrolysis zone becomes $T_{sI} = \overline{T}_u$.

**Energy balance at the uncharred material-insulation interface.** The boundary condition at the interface of the char layer and the uncharred layer also satisfies one of the requirements of the uncharred temperature equation for boundary conditions. The other boundary condition for the uncharred temperature equations results from an expression of conservation of energy at the interface of the uncharred
layer and the insulation layer—energy conducted from the uncharred layer to the surface is accommodated by energy conduction into the insulation and by increasing the temperature of the heat sink at the interface. In equation form

\[ -\left( k' \frac{\partial T'_s}{\partial y} \right) I + J = -\left( k'' \frac{\partial T''_s}{\partial y} \right) I + J + \rho_{Hs} \hat{C}_{phs} l_{Hs} \left( \frac{\partial T''_s}{\partial t} \right) I + J \]  

(3-47)

Also the temperatures of the two layers are equal at their interface. Thus

\[ T'_s I + J = T''_s I + J \]  

(3-48)

**Back surface energy balance.**—Equation 3-47 satisfies one of the requirements of the insulation temperature equation for boundary conditions. The other boundary condition for the insulation temperature equation results from an energy balance at the back surface—energy transfer to the back surface (conduction through the insulation plus energy transfer to the surface from the surroundings) is accommodated by energy radiation to the surroundings and by increasing the temperature of the heat sink at the back surface. In equation form

\[ -\left( k'' \frac{\partial T''_s}{\partial y} \right) I + J + K + q_B = \sigma \varepsilon'' T''_s^4 \]

\[ + \rho_{HSP} \hat{C}_{phsp} l_{HSP} \left( \frac{\partial T''_s}{\partial t} \right) I + J + K \]  

(3-49)
The effect of an adiabatic surface is achieved by setting the rate of energy transfer to the surface from the surroundings equal to the rate of energy radiated by the surface to the surroundings. Thus, for an adiabatic back surface

\[ q_B = \sigma \varepsilon_s T_s^4 \]  

(3-50)

Initial conditions. - Initially, the complete system is at a specified temperature; thus the initial condition for the solid phase temperature is

\[ T_s(y,t) = T_s(y) \text{ at } t = 0 \]  

(3-51)

Char Porosity Equation

A single boundary condition is required for solution of the char layer porosity equation. The condition used in this analysis is a specified porosity of the char layer at the pyrolysis interface. The initial condition for the char layer porosity is

\[ \eta(y,t) = \eta_0(y) \text{ at } t = 0. \]  

(3-52)

Pyrolysis Gas Temperature Equation

The pyrolysis gas temperature equation requires a single boundary
condition. The condition employed is that the pyrolysis gas
temperature is equal to the solid phase temperature at the pyrolysis
zone. The initial condition for the pyrolysis gas temperature is

\[ T(y,t) = T(y) \text{ at } t = 0. \] (3-53)

**Pyrolysis Gas Pressure Equation**

The pyrolysis gas pressure distribution equation requires two
boundary conditions.

**Specified pressure at the front surface.** - The first boundary
condition is that the pressure is specified at the surface,

\[ P_1 = P_w. \] (3-54)

**Specified pressure gradient at the pyrolysis zone.** - The second is
that the pressure gradient is specified at the interface. In developing
the governing differential equation for pyrolysis gas pressure in
Chapter II, Darcy's law was used to determine the superficial velocity
of the pyrolysis gases in the char layer. In equation form, Darcy's
law for a one-dimensional system is
Equation 3-55 is multiplied by $\rho$ and the equation of state is used to give

$$v_o = -\frac{K}{\mu} \frac{\partial P}{\partial y}$$  \hspace{1cm} (3-55)

$$\rho v_o = -\frac{KM}{\mu R_u T} P \frac{\partial P}{\partial y}.$$  \hspace{1cm} (3-56)

Equation 3-56 is applied at the pyrolysis zone and use is made of the equation

$$(\rho v_o)_l = -\dot{m}_g$$  \hspace{1cm} (3-57)

to obtain

$$\left(\frac{\partial P}{\partial y}\right)_l = R_u \left(\frac{1}{KMP}\right)_l \dot{m}_g.$$  \hspace{1cm} (3-58)

But

$$\frac{\partial P}{\partial y} = \frac{1}{2P} \frac{\partial^2 P}{\partial y^2}$$  \hspace{1cm} (3-59)

therefore

$$\left(\frac{\partial P^2}{\partial y}\right)_l = 2 R_u \left(\frac{1}{KMP}\right)_l \dot{m}_g.$$  \hspace{1cm} (3-60)
Initial conditions. - The initial condition for the pyrolysis gas pressure is

\[ P(y,t) = P_{w,o} \text{ at } t = 0. \quad (3-61) \]

Total Mass Conservation Equation

The mass conservation equation is solved for the product \(\rho v_o\), or the local mass flow rate. It requires a single boundary condition. The boundary condition used is that the mass flow rate is known at the pyrolysis interface, or in equation form

\[ (\rho v_o)_I = -\dot{m}_g. \quad (3-62) \]

The initial condition for the mass flow rate is

\[ (\rho v_o)_y, t = \dot{m}_g(y) \text{ at } t = 0. \quad (3-63) \]

Chemical Species Conservation Equation

The chemical species continuity equation is solved for the local mass flow rate of each chemical species. It requires a single boundary condition. The boundary condition is obtained from the molar composition of the pyrolysis gases which is specified at the pyrolysis interface and the total pyrolysis gas flow rate at that point. This
boundary condition is expressed in equation form as

$$\left( \rho_1 v \right)_I = - \left( \frac{x_1}{\eta M} \right)_I M_m g_i. \quad (3-64)$$

The initial condition for the species continuity equation is

$$\left( \rho_1 v \right)_{y,t} = \left( \rho_1 v \right)_{y,0} \text{ at } t = 0. \quad (3-65)$$
CHAPTER IV

TRANSFORMATION AND LINEARIZATION OF EQUATIONS AND BOUNDARY CONDITIONS

The governing equations and boundary conditions presented to this point are for a physical system with boundaries which move relative to each other and relative to a fixed coordinate system. In maintaining a fixed number of stations in layers of varying thickness when obtaining a numerical solution to an equation it is necessary to interpolate after each iteration as the location of the stations change. Each such operation introduces a small error. This problem can be eliminated by transforming to a moving coordinate system in which the locations of the stations remain fixed and the coordinate system moves to accommodate changes in the location of the boundaries. The transformations presented by Swann, Pittman and Smith in Ref. 16 will be employed here.

The location of the system boundaries with the new coordinate system is shown in Fig. 3. The finite char layer of thickness \( L_0 \) at time \( t = 0 \) is required for obtaining a numerical solution to the governing equations.

The equations and boundary conditions for the char layer are transformed to a coordinate system with the origin attached to the front surface. The dimensional moving coordinate system with the origin attached to the front surface results from the following transformation
Figure 3.- Location of system boundaries and coordinates.
where the integral represents the total surface recession at some time \( t \). Equation 4-1 is nondimensionalized by the char layer thickness \( \ell \) to give the transformed dimensionless coordinate for the char layer as

\[
x_d = y - \int_0^t \frac{\dot{m}_s}{\rho_s \rho_o} \, dt
\]

\[
x = \frac{y - \int_0^t \frac{\dot{m}_s}{\rho_s \rho_o} \, dt}{\ell}
\]

Note that the new coordinate system for the char layer is attached to the char layer surface and extends to the pyrolysis zone. The coordinates of the front surface and pyrolysis zone are constant at \( x = 0 \) and \( x = 1 \) respectively.

Similarly, the governing equations and boundary conditions for the uncharred layer are transformed to a moving coordinate system with the origin attached to the pyrolysis zone. The dimensional moving coordinate system with the origin attached to the pyrolysis zone results from the following transformation

\[
x_d' = y - \ell_o - \int_0^t \frac{\dot{m}_s}{\Delta \rho} \, dt
\]

where \( \ell_o \) is the finite char thickness at time \( t = 0 \) and the integral represents the thickness of uncharred material which has been degraded at some time \( t \). Equation 4-3 is nondimensionalized by the uncharred material thickness \( \ell' \) to give the transformed dimensionless coordinate for the uncharred layer as
Note that the new coordinate system for the uncharred layer is attached to the pyrolysis zone and extends to the uncharred material - insulation layer interface. The coordinates of the uncharred layer boundaries are $x' = 0$ and $x' = 1$.

The boundaries of the insulation layer are fixed so the new coordinate system is stationary with the origin at the boundary between the uncharred layer and the insulation. The new coordinate system for the insulation layer results from transforming the initial system by an amount equal to the total initial thickness of the char layer and the uncharred layer and nondimensionalizing the result by the thickness of the insulation layer. In equation form

$$x'' = \frac{y - (l_0' + \xi')}{\xi''}.$$  

(4-5)

The coordinates of the insulation boundaries are $x'' = 0$ and $x'' = 1$.

Char Layer Equations

Equation 4-2 is used to transform the governing equations for the char layer. The following derivative expressions are obtained:

$$\left( \frac{\partial}{\partial t} \right)_{\text{Old}} = \left( \frac{\partial}{\partial t} \right)_{\text{New}} + \left[ \frac{\partial x}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial x}{\partial \xi} \frac{\partial \xi}{\partial t} + \frac{\partial x}{\partial t} \right] \frac{\partial}{\partial x}$$  

(4-6)

but
\[
\frac{\partial x}{\partial y} = \frac{1}{\lambda} \\
\frac{\partial x}{\partial \lambda} = -x/\lambda \\
\frac{\partial x}{\partial t} = -\frac{1}{\lambda} \frac{\dot{m}_s}{\rho_{s_0}} \\
\begin{cases}
\dot{\lambda} = \lambda_0 + \int_0^t [\dot{m}_g/\Delta \rho - \dot{m}_s/\rho_{s_0}] \, dt \\
\dot{\lambda} = \dot{m}_g/\Delta \rho - \dot{m}_s/\rho_{s_0} 
\end{cases}
\]

(4-7)

Therefore

\[
\frac{\partial}{\partial t} \left( \frac{\partial}{\partial t} \right)_{\text{Old}} = \left( \frac{\partial}{\partial t} \right)_{\text{New}} - v_c \frac{\partial}{\partial x} \\
\] (4-8)

where

\[
v_c = \frac{1}{\lambda} \left[ \frac{\dot{m}_s}{\rho_{s_0}} + x(\dot{m}_g/\Delta \rho - \dot{m}_s/\rho_{s_0}) \right].
\] (4-9)

Also

\[
\frac{\partial}{\partial y} = \frac{\partial x}{\partial y} \frac{\partial}{\partial x}
\] (4-10)

or
\[
\frac{\partial}{\partial y} = \frac{1}{\lambda} \frac{\partial}{\partial x} \quad (4-11)
\]
and
\[
\frac{\partial^2}{\partial y^2} = \frac{1}{\lambda^2} \frac{\partial^2}{\partial x^2} \quad (4-12)
\]

**Char temperature equation.** Using these derivative expressions, the char temperature equation becomes

\[
(1 - \eta) \frac{\rho_s C_p s}{M_s} \left[ \frac{\partial T_s}{\partial t} - V_c \frac{\partial T_s}{\partial x} \right] = \frac{k_s}{\lambda^2} \frac{\partial^2 T_s}{\partial x^2} + \frac{1}{\lambda^2} \frac{\partial k_s}{\partial x} \frac{\partial T_s}{\partial x} - H_A (T_s - T) + \eta \frac{R_s}{H(T)_s} H(T)_s + \eta \frac{R_s}{H_h_s} H_h_s - \eta \sum_r (r) \Delta H^{(r)} + (1 - \eta) (A - \epsilon)
\]

\[
+ (1 - \eta) q'''' + \frac{\rho_s H_s}{M_s} \left( \frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial x} \right). \quad (4-13)
\]

This equation can be written as

\[
\frac{\partial^2 T_s}{\partial x^2} + \alpha_1 \frac{\partial T_s}{\partial x} + \alpha_2 T_s + \alpha_3 + \alpha_4 \frac{\partial T_s}{\partial t} = 0 \quad (4-14)
\]

where
\[
\alpha_1 = \frac{1}{k_s} \left[ \frac{\partial k_s}{\partial x} + \rho_s \frac{\partial}{\partial x} \left( 1 - \eta \right) \frac{C_{ps}}{M_s} v_c \right] 
\] (4-15)

\[
\alpha_2 = -\frac{H_A}{k_s} \frac{\partial^2}{\partial x^2} 
\] (4-16)

\[
\alpha_3 = \frac{\partial^2}{k_s} \left[ H_A T + \eta R_s H(T) + \eta R_h S_h - \eta \sum_r \Delta H_r + (1 - \eta)(A - \varepsilon) 
\right.
\]

\[
+ (1 - \eta)q_s''' + \frac{\rho_s H_s}{M_s} \left( \frac{\partial\eta}{\partial t} - v_c \frac{\partial\eta}{\partial x} \right) - \eta \sum_j R_j \Delta H_j \]
\] (4-17)

\[
\alpha_4 = -\left(1 - \eta\right) \frac{\partial^2}{k_s} \frac{C_{ps}}{M_s} = \frac{\rho_s}{M_s} 
\] (4-18)

The form of Eq. 4-12 is convenient for obtaining a solution by numerical methods. In obtaining a numerical solution to Eq. 4-12 the \( \alpha' \)s are considered to be independent of \( T_s \), thus Eq. 4-12 becomes linear.

Char porosity equation.- The transformed char layer porosity equation is

\[
\frac{\partial \eta}{\partial t} - v_c \frac{\partial \eta}{\partial x} + \eta \frac{M_s}{\rho_s} (R_{hs} + R_r) = 0 
\] (4-19)

or, writing it in the linear form,

\[
\frac{\partial \eta}{\partial x} + \varepsilon_1 \eta + \varepsilon_2 + \varepsilon_3 \frac{\partial \eta}{\partial t} = 0 
\] (4-20)
where

\[ \varepsilon_1 = -\frac{\frac{M_s}{\rho_s}}{2} \left( \frac{R_{hs} + R_s}{V_c} \right) \] (4-21)

\[ \varepsilon_2 = 0 \] (4-22)

\[ \varepsilon_3 = 1/V_c \] (4-23)

**Pyrolysis gas temperature equation.** - The transformed pyrolysis gas temperature equation is

\[
\eta \sum_{i} \frac{\rho_i C_p_i}{M_i} \left[ \frac{\partial T}{\partial t} + \frac{(v/\ell - v_c)}{\ell} \frac{\partial T}{\partial x} \right] = -\eta \left( \frac{\partial \ln \rho}{\partial \ln T} \right) P, x, i \left[ \frac{\partial P}{\partial t} \right] + \frac{1}{\ell} \eta v^2 \sum_{i} H_{i} R_{T_i} T_i + \frac{1}{2} \eta v^2 \sum_{i} H_{i} R_{T_i} M_i
\]

\[
+ (v/\ell - v_c) \frac{\partial T}{\partial x} - \eta \sum_{i} H_{i} R_{T_i} T_i + \frac{1}{2} \eta v^2 \sum_{i} H_{i} R_{T_i} M_i
\]

\[
+ \frac{\eta}{\lambda^3} \frac{\partial^2 T}{\partial x^2} + \eta \sum_{i} \left( \frac{J_i}{M_i} \right) - \frac{1}{\lambda^2} \frac{\partial^2 q_x}{\partial x^2}
\]

\[
+ \eta \left( A' - \varepsilon' \right) + H_A (T_s - T) - R_s H(T) s - R_{hs} H_s
\]

\[
+ \eta \sum_{r} H_r \Delta H_r. \tag{4-24}
\]

Since
\[ \rho = \frac{P}{R_u T} \]  
\[ \left( \frac{\partial \ln \rho}{\partial \ln T} \right)_{P, X_i} = -1. \]  
(4-25)  
(4-26)

Also

\[ \frac{\partial P}{\partial t} = \sum_i \frac{\rho_i}{M_i} R_u \frac{\partial T}{\partial t} + R_u T \frac{\partial}{\partial t} \sum_i \frac{\rho_i}{M_i} \]  
(4-27)

and

\[ \frac{\partial P}{\partial x} = \sum_i \frac{\rho_i}{M_i} R_u \frac{\partial T}{\partial x} + R_u T \frac{\partial}{\partial x} \sum_i \frac{\rho_i}{M_i}. \]  
(4-28)

Therefore Eq. 4-24 can be written as

\[ \eta \left( \frac{v}{\ell} - V_c \right) \left[ \sum_i \frac{\rho_i}{M_i} \frac{C_p}{T} - R_u \sum_i \frac{\rho_i}{M_i} \right] \frac{\partial T}{\partial x} + \left( H_A \right. \]
\[ - \eta R_u \left[ \frac{\partial}{\partial t} \left( \frac{\partial T}{\partial t} - V_c \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial t} \left( \sum_i \frac{\rho_i}{M_i} \right) \right] + \left( v \frac{v}{\ell} - V_c \right) \frac{\partial}{\partial x} \left( \sum_i \frac{\rho_i}{M_i} \right) \right) \]
\[ + \eta \sum_i H_i R_{i,1} \]
\[ - \frac{1}{\ell} \sum_i H_i \frac{\partial}{\partial x} J_i - \eta \frac{V_c}{2} \sum_i R_{i,1} M_i - \frac{\tau_{xx}}{\ell^3} \frac{\partial v}{\partial x} \]
\[ - \eta \sum_i \frac{J_i}{M_i} g_i + \frac{1}{\ell^2} \frac{\partial}{\partial x} q_x - \eta \left( A' - \epsilon' \right) - H_{As} \]
\[ + \eta R_s H(T)_s + \eta R_h H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + \eta \left( \sum_i \frac{\rho_i C_{pi}}{M_i} \right) \]

\[- R_u \sum \frac{\rho_i}{M_i} \frac{\partial \theta}{\partial t} = 0 \quad (4-29)\]

or, in the linear form,

\[ \frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 \quad (4-30) \]

where

\[ \beta_1 = \left\{ \begin{array}{l}
H_A - \eta R_u \left[ \frac{\rho}{M} \left( \frac{\partial n}{\partial t} - \frac{\partial n}{\partial x} \right) + \frac{\partial}{\partial t} \left( \sum_i \frac{\rho_i}{M_i} \right) \right] \\
+ \left( \frac{v}{\kappa} - v_c \right) \frac{\partial}{\partial x} \left( \sum_i \frac{\rho_i}{M_i} \right) \right\} / D1 \quad (4-31) \]

\[ D1 = \eta \left( \frac{v}{\kappa} - v_c \right) \left[ \sum \frac{\rho_i C_{pi}}{M_i} - R_u \sum \frac{\rho_i}{M_i} \right] \quad (4-32) \]

\[ \beta_2 = \left[ \eta \sum_i H_i R_{T1} - \frac{1}{\kappa} \sum_i H_i \frac{\partial}{\partial x} J_1 - \eta \frac{v^2}{2} \sum_i R_{T1} M_i \right] \]

\[ - \frac{\tau_{xx}}{\kappa^3} \frac{\partial v}{\partial x} - \eta \sum_i \frac{J_1 g_i}{M_i} + \frac{1}{\kappa} \frac{\partial}{\partial x} q_x \]

\[ - \eta (A' - \epsilon') - H_AT_s + \eta R_s H(T)_s + \eta R_h H_s \]

\[- \eta \sum_r r_h^{(r)} \Delta H^{(r)} \right\} / D1 \quad (4-33) \]
\[ \beta_3 = \eta \left( \sum_{i} \frac{\rho_i C_{pi}}{M_i} - R_u \sum_{i} \frac{\rho_i}{M_i} \right) / Dl \] (4-34)

**Chemical species continuity equation.** The transformed chemical species continuity equation is

\[ \frac{\partial}{\partial t} (n_1 \rho_1) - V_c \frac{\partial}{\partial x} (n_1 \rho_1) + \frac{1}{\lambda} \frac{\partial}{\partial x} (\rho_1 v_o) + \frac{1}{\lambda} \frac{\partial}{\partial x} n_{ij} - \eta R_{T_i} M_i = 0 \] (4-35)

This equation is combined with the identities

\[ \dot{m}_1 = -n_1 v \] (4-36)

and

\[ v_o = n_1 v \] (4-37)

to obtain

\[ \eta \left( \frac{V_c}{v} - \frac{1}{\lambda} \right) \frac{\partial}{\partial x} \dot{m}_1 + \left( \frac{V_c}{v} - \frac{1}{\lambda} \right) \frac{\partial n_1}{\partial x} - \frac{n_1}{v} \frac{\partial v}{\partial x} + \frac{1}{v} \frac{\partial n_1}{\partial t} \left[ \dot{m}_1 + \frac{1}{\lambda} \frac{\partial n_{ij}}{\partial x} - \eta R_{T_i} M_i + \eta \frac{\partial n_{ij}}{\partial t} \right] = 0 \] (4-38)

or, in linear form,

\[ \frac{\partial \dot{m}_1}{\partial x} + \Delta_1 \dot{m}_1 + \Delta_2 \dot{m}_1 + \Delta_3 \frac{\partial \dot{m}_1}{\partial t} = 0 \] (4-39)
where

$$\Delta_{1i} = \frac{1}{\eta} \eta \frac{\partial \eta}{\partial x} + \left[ \frac{\eta R_T M_i}{R_i} - \eta \frac{V_c}{V} \frac{\partial V}{\partial x} - \frac{\partial \eta}{\partial t} \right] / D_2 \tag{4-40}$$

$$D_2 = \eta(V_c - \frac{V}{\lambda}) \tag{4-41}$$

$$\Delta_{2i} = \nu \left( \frac{1}{\lambda} \frac{\partial \eta x}{\partial x} - \eta \frac{\partial \rho}{\partial t} \right) / D_2 \tag{4-42}$$

$$\Delta_{3i} = 0 \tag{4-43}$$

**Total mass conservation equation.**—The transformed total mass conservation equation is

$$\frac{\partial}{\partial t} (\eta \rho) - V_c \frac{\partial}{\partial x} (\eta \rho) + \frac{1}{\lambda} \frac{\partial}{\partial x} (\rho V_o) - \eta \sum_{i=1}^{N} R_T M_i = 0 \tag{4-44}$$

This equation is combined with the identity

$$\dot{\rho} = - \rho V_o \tag{4-45}$$

to obtain

$$\frac{\partial}{\partial x} \dot{\rho} = \lambda \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_{i=1}^{N} R_T M_i \right. $$

$$- V_c \left( \eta \frac{\partial \rho}{\partial x} + \rho \frac{\partial \eta}{\partial x} \right) \right] \tag{4-46}$$
It is convenient to integrate this equation numerically rather than use finite difference methods, hence, it is not expressed in the linear form. The solution to this equation is used with the total density obtained from the equation of state to determine the mass average velocity of the pyrolysis gases.

**Pyrolysis gas pressure equation.** - The transformed pyrolysis gas pressure equation is

\[
\frac{\partial^2 P}{\partial x^2} + \frac{\mu T}{KM} \frac{\partial}{\partial x} \left( \frac{KM}{\mu T} \right) \frac{\partial p}{\partial x} - 2 \frac{\mu R}{KM} \left[ \frac{\partial p}{\partial t} (\eta \rho) \right. \\
- V_c \frac{\partial}{\partial x} (\eta \rho) - \eta \sum_i R_{Ti} M_i \left]
\right. = 0.
\] (4-47)

This equation is combined with the equation of state to give

\[
\frac{\partial^2 P}{\partial x^2} + \frac{1}{K} \left[ \frac{T}{\bar{M}} \frac{\partial}{\partial x} \left( \frac{KM}{\mu T} \right) + \frac{\eta V_c}{P} \right] \frac{\partial p}{\partial x} \\
- \frac{2\mu}{\bar{M}KP} \left[ \eta \left( \frac{\partial \bar{M}}{\partial t} - \frac{\bar{M}}{T} \frac{\partial T}{\partial t} \right) + \bar{M} \left( \frac{\partial \eta}{\partial t} \right) \\
- V_c \frac{\partial \eta}{\partial t} \right] \eta \left( \frac{\partial \bar{M}}{\partial x} - V_c \frac{\partial \bar{M}}{\partial x} \right) \right) P^2 \\
+ \frac{2\mu \eta}{KP} \sum_i R_{Ti} M_i - \frac{\mu \eta}{KP} \frac{\partial P^2}{\partial t} = 0
\] (4-48)

or, in the linear form,
\[
\frac{\partial^2 p}{\partial x^2} + \gamma_1 \frac{\partial p}{\partial x} + \gamma_2 \frac{\partial^2 p}{\partial t^2} + \gamma_3 + \gamma_4 \frac{\partial p}{\partial t} = 0 \quad (4-49)
\]

where

\[
\gamma_1 = \frac{\mu}{K} \left[ \frac{T}{\bar{M}} \frac{\partial}{\partial x} \left( \frac{K\bar{M}}{\mu T} \right) + \frac{\eta}{P} \right] \quad (4-50)
\]

\[
\gamma_2 = -\frac{2\mu}{MKP} \left[ \eta \left( \frac{\partial \bar{M}}{\partial t} - \frac{\bar{M}}{T} \frac{\partial T}{\partial t} \right) \right. \]

\[+ \left. \bar{M} \left( \frac{\partial n}{\partial t} - \frac{v}{c} \frac{\partial n}{\partial x} \right) + \eta \left( \frac{\bar{M}}{T} \frac{\partial T}{\partial x} - \frac{v}{c} \frac{\partial \bar{M}}{\partial x} \right) \right] \quad (4-51)
\]

\[
\gamma_3 = \frac{2\mu n}{K P} \sum_{i} \bar{R}_{T_i} M_i \quad (4-52)
\]

\[
\gamma_4 = -\frac{\mu n}{KP} \quad (4-53)
\]

**Uncharred Layer Equation**

Equation 4-4 is used to transform the governing energy equation for the uncharred layer. The following derivative expressions are obtained:

\[
\left( \frac{\partial}{\partial t} \right)_{\text{old}} = \left( \frac{\partial}{\partial t} \right)_{\text{new}} + \left[ \frac{\partial}{\partial y} \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \frac{\partial}{\partial t} + \frac{\partial}{\partial t} \right] \frac{\partial}{\partial x} \quad (4-54)
\]

but
\[
\frac{\partial x'}{\partial y} = \frac{1}{\xi'} \]
\[
\frac{\partial x'}{\partial \xi'} = -\frac{x'}{\xi'}
\]
\[
\frac{\partial x'}{\partial t} = -\frac{1}{\xi'} \frac{\dot{m}}{\Delta \rho} \]
\[
\xi' = \xi'_0 - \int_0^t \frac{\dot{m}}{\Delta \rho} dt
\]
\[
\frac{\partial \xi'}{\partial t} = -\frac{\dot{m}}{\Delta \rho}.
\]

Therefore
\[
\left(\frac{\partial}{\partial t}\right)_{old} = \left(\frac{\partial}{\partial t}\right)_{new} \frac{\dot{m}}{\Delta \rho} \left(\frac{x' - 1}{\xi'}\right) \frac{\partial}{\partial x'}.
\]

Also
\[
\frac{\partial}{\partial y} = \frac{\partial x'}{\partial y} \frac{\partial}{\partial x'}
\]

or
\[
\frac{\partial}{\partial y} = \frac{1}{\xi'} \frac{\partial}{\partial x'}.
\]
These equations are employed to obtain the transformed energy equation for the uncharred layer as

\[
\frac{\partial^2}{\partial y^2} = \frac{1}{\lambda'^2} \frac{\partial^2}{\partial x'^2}.
\]  

(4-59)

where the superscript on \( T_s \) is omitted. The linear form of this equation is

\[
\frac{\partial^2 T_s}{\partial x'^2} + \alpha'_1 \frac{\partial T_s}{\partial x'} + \alpha'_2 T_s + \alpha'_3 + \alpha'_4 \frac{\partial T_s}{\partial t} = 0
\]

(4-61)

where

\[
\alpha'_1 = \frac{1}{k' s} \left[ \frac{\partial k'}{\partial x'} + \frac{\lambda' \rho' C'_s \hat{m}}{\Delta \rho} (1 - x') \right]
\]

(4-62)

\[
\alpha'_2 = 0
\]

(4-63)

\[
\alpha'_3 = 0
\]

(4-64)
\[ \alpha_4' = \frac{-\rho_s' C_p's l_x'^2 / k_s'}{10.4 s_p s} \quad (4-65) \]

**Insulation Layer Equation**

Equation 4-5 is used to transform the governing energy equation for the insulation layer. The following derivative expressions are obtained:

\[
\left( \frac{\partial}{\partial t} \right)_{\text{Old}} = \left( \frac{\partial}{\partial t} \right)_{\text{New}} \quad (4-66)
\]

\[
\frac{\partial}{\partial y} = \frac{\partial x''}{\partial y} \frac{\partial}{\partial x''}
\]

\[
= \frac{1}{x''} \frac{\partial}{\partial x''}
\]

\[
\frac{\partial^2}{\partial y^2} = \frac{1}{x''^2} \frac{\partial^2}{\partial x''^2}
\]

The insulation layer temperature equation becomes

\[
\frac{k''}{x''^2} \frac{\partial^2 T_s}{\partial x''^2} + \frac{1}{x''^2} \frac{\partial k''}{\partial x''} \frac{\partial T_s}{\partial x''} - \rho'' S \frac{C''}{P_s} \frac{\partial T_s}{\partial t} = 0 \quad (4-67)
\]

or

\[
\frac{\partial^2 T_s}{\partial x''^2} + \alpha_1'' \frac{\partial T_s}{\partial x''} + \alpha_2'' T_s + \alpha_3'' + \alpha_4'' \frac{\partial T_s}{\partial t} = 0 \quad (4-68)
\]
where

\[ \alpha_1'' = \frac{1}{k_s} \frac{\partial k_s''}{\partial x''} \quad (4-69) \]

\[ \alpha_2'' = 0 \quad (4-70) \]

\[ \alpha_3'' = 0 \quad (4-71) \]

\[ \alpha_4'' = -\frac{\rho_s' a'' e'' \ell''^2}{k_s} \quad (4-72) \]

**Boundary Conditions**

The transformed boundary conditions are as follows:

**Rate of surface removal by oxidation**

\[ \dot{m}_s = k_{p_e} C_{e} \frac{\dot{M}_w}{M_0} + k_{p_e} (H_e - H_w) \]

\[ M_0 + \frac{k_{p_e} (H_e - H_w)}{\lambda N_{_0.6}^0} \]q_{c,net}\]

**Energy balance at the front surface**

\[ q_c (1 - H_w/H_e) \left\{ 1 - (1 - \beta) \left[ 0.724 \frac{\dot{H}_e}{q_c} - 0.13 \left( \frac{\dot{H}_e}{q_c} \right)^2 \right] - \beta \frac{\dot{H}_e}{q_c} \right\} = \alpha_R + \left[ 1 - S(T_{s_1} - \bar{T}_1) \right] \dot{m}_s \Delta H_c \]

\[ = \sigma \varepsilon_s T_{s_1}^4 - \frac{k_s}{\ell} \frac{\partial T}{\partial x} + s(T_{s_1} - \bar{T}_1) \dot{m}_s H_c \quad (4-74) \]
Energy balance at the pyrolysis zone

\[- \left( \frac{k_s}{\Delta x} \frac{\partial T_s}{\partial x} \right)_{x=1} = \dot{m}_g \Delta H_p - \left( \frac{k'_s}{\Delta x'} \frac{\partial T_s}{\partial x'} \right)_{x'=0} \]  

(4-75)

Rate of pyrolysis of uncharred material

\[\dot{m}_g = A' \exp \left( \frac{-B'/T_s}{x=1} \right) \]  

(4-76)

Energy balance at the interface of the uncharred layer and the insulation layer

\[- \left( \frac{k'_s}{\Delta x'} \frac{\partial T_s}{\partial x'} \right)_{x'=1} = - \left( \frac{k''_s}{\Delta x''} \frac{\partial T_s}{\partial x''} \right)_{x''=0} + \rho_{HS} \frac{C_{p,HS}}{\Delta x''} \frac{\partial T_s}{\partial t} \]  

x' = 1

(4-77)

Energy balance at the back surface of the insulation layer

\[- \left( \frac{k''_s}{\Delta x''} \frac{\partial T_s}{\partial x''} \right)_{x''=1} = \sigma \varepsilon'' \frac{T_s}{\Delta x''} \frac{4}{4} - q_B + \rho_{HSP} \frac{C_{p,HSP}}{\Delta x''} \frac{\partial T_s}{\partial t} \]  

x'' = 1

(4-78)

Specified char porosity at the pyrolysis zone

\[\eta_x = 1 = \eta_o \]  

(4-79)

Specified temperature of pyrolysis gas at the pyrolysis interface

\[T_x = 1 = T_{Sx} \]  

(4-80)
Specified pressure at the front surface

\[ P_x = 0 = P_w \]  \hspace{1cm} \text{(4-81)}

Specified pressure gradient at the pyrolysis interface

\[ \left( \frac{\partial}{\partial x} P^2 \right) x = 1 = 2 \ell R_\mu \left( \frac{\mu T}{Kn} \right) x = 1 \dot{m}_g \]  \hspace{1cm} \text{(4-82)}

Specified mass flow rate at the pyrolysis interface

\[ (\dot{m}) x = 1 = \dot{m}_g \]  \hspace{1cm} \text{(4-83)}

Specified chemical species mass flow rate at the pyrolysis interface

\[ (\rho_1 v) x = 1 = \left( \frac{x_1}{\eta M} \right) x = 1 M_i \dot{m}_g \]  \hspace{1cm} \text{(4-84)}
CHAPTER V

FINITE DIFFERENCE EQUATIONS

The system of equations derived in Chapter II of this paper includes six partial differential equations with variable coefficients thus it is necessary to solve them numerically. The procedure employed to solve all equations except the total mass conservation equation involves deriving the governing differential equations in finite difference form and solving the resulting sets of algebraic equations by iteration. The total mass conservation equation is solved by numerical integration from the char layer - uncharred layer interface.

Figure 4 shows the locations of the finite-difference stations and the boundary conditions at each boundary. The distances between stations in the char layer, the uncharred layer, and the insulation layer are

\[ \Delta x = \frac{1}{I - 1} \]
\[ \Delta x' = \frac{1}{J} \]
\[ \Delta x'' = \frac{1}{K} \]  \hspace{1cm} (5-1)

The station coordinates are
Figure 4.— Location of finite difference stations.
for the char layer,

\[ x' = (N - I)\Delta x' \]  \hspace{1cm} (5-3)

for the uncharred layer, and

\[ x'' = (N - I - J)\Delta x'' \]  \hspace{1cm} (5-4)

for the insulation layer.

**Solid Phase Temperature Equations**

The differential equation for the char temperature is

\[
\frac{\partial^2 T_s}{\partial x^2} + \alpha_1 \frac{\partial T_s}{\partial x} + \alpha_2 T_s + \alpha_3 + \alpha_4 \frac{\partial T_s}{\partial t} = 0.
\]  \hspace{1cm} (5-5)

**Interior stations of the char layer.** At interior stations the partial derivatives are replaced by central difference approximations. The central difference approximations of the partial derivative are obtained from Taylor series expansions at the station \( N \) evaluated at \( N + 1 \) and \( N - 1 \). Thus

\[ T_s(N + 1) = T_s(N) + \left( \frac{\partial T_s}{\partial x} \right)_N \Delta x + \left( \frac{\partial^2 T_s}{\partial x^2} \right)_N \frac{\Delta x^2}{2!} \]
\[
\frac{\partial^3 T_s}{\partial x^3} \left( \frac{\Delta x}{3!} \right) N + \ldots \quad (5-6)
\]
\[
T_s(N - 1) = T_s(N) - \left( \frac{\partial T_s}{\partial x} \right)_N \Delta x + \left( \frac{\partial^2 T_s}{\partial x^2} \right)_N \left( \frac{\Delta x^2}{2!} \right)
\]
\[
- \left( \frac{\partial^3 T_s}{\partial x^3} \right)_N \left( \frac{\Delta x^3}{3!} \right) + \ldots \quad (5-7)
\]

Subtracting Eq. 5-7 from Eq. 5-6 gives

\[
\left( \frac{\partial T_s}{\partial x} \right)_N = \frac{T_s(N + 1) - T_s(N - 1)}{2\Delta x} - \left( \frac{\partial^3 T_s}{\partial x^3} \right)_N \left( \frac{\Delta x^2}{12} \right) \quad (5-8)
\]

Therefore the equation

\[
\left( \frac{\partial T_s}{\partial x} \right)_N = \frac{T_s(N + 1) - T_s(N - 1)}{2\Delta x} \quad (5-9)
\]

is accurate to terms of the order \( \Delta x^2 \). Similarly, adding Eqs. 5-6 and 5-7 gives

\[
\left( \frac{\partial^2 T_s}{\partial x^2} \right)_N = \frac{T_s(N + 1) - 2T_s(N) + T_s(N - 1)}{\Delta x^2} \quad (5-10)
\]

which is accurate to terms of the order \( \Delta x^2 \).

Equations 5-9 and 5-10 are used in Eq. 5-5 to obtain
\[ \frac{1}{\Delta x^2} \left[ T_s(N+1) - 2T_s(N) + T_s(N-1) \right] + \frac{\alpha_1(N)}{2\Delta x} \left[ T_s(N+1) - T_s(N-1) \right] + \alpha_2(N) T_s(N) + \alpha_3(N) + \alpha_4(N) \left( \frac{\partial T_s}{\partial t} \right)_N = 0 \]  

(5-11)

The finite difference approximation of the last term to the left in Eq. 5-11 is obtained from Taylor series expansions at time \( P + \Delta t/2 \) evaluated at time \( P \) and \( P + \Delta t \). Thus

\[
\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^P = \left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^P + \Delta t/2 - \frac{\Delta t}{2} \left[ \frac{\partial}{\partial t} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^P + \Delta t/2 + \frac{\Delta t^2}{4} \left[ \frac{\partial^2}{\partial t^2} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^P + \Delta t/2 \]  

(5-12)

\[
\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^P + \Delta t = \left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^P + \Delta t/2 + \frac{\Delta t}{2} \left[ \frac{\partial}{\partial t} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^P + \Delta t/2 + \frac{\Delta t^2}{4} \left[ \frac{\partial^2}{\partial t^2} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^P + \Delta t/2 \]  

(5-13)

Solving these two equations for \( \left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^P + \Delta t/2 \),

\[
\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^P + \Delta t/2 = \frac{1}{2} \left[ \alpha_4^P \frac{\partial T_s}{\partial t}^P + \alpha_4^P + \Delta t \frac{\partial T_s}{\partial t}^P + \Delta t \right] \]  

(5-14)

which is accurate to terms of the order \( \Delta t^2 \). Now
and \( \alpha_4 \frac{\partial T_s}{\partial t} \) and \( \alpha_4 \frac{\partial T_s}{\partial t} + \Delta t \) are obtained from the explicit and implicit formulations of Eq. 5-11, that is

\[
\begin{align*}
\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)_N &= \frac{1}{2} \left[ T_s(N + 1)_P^P - 2 T_s(N)_P^P + T_s(N - 1)_P^P \right] \\
&- \frac{\alpha_1(N)}{2 \Delta x} \left[ T_s(N + 1)_P^P - T_s(N - 1)_P^P \right] - \alpha_2(N)_P^P T_s(N)_P^P \\
&- \alpha_3(N)_P^P 
\end{align*}
\] (5-17)

\[
\begin{align*}
\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)_N &= \frac{1}{2} \left[ T_s(N + 1)_P^P + \Delta t - 2 T_s(N)_P^P + \Delta t + T_s(N - 1)_P^P + \Delta t \right] \\
&- \frac{\alpha_1(N)}{2 \Delta x} \left[ T_s(N + 1)_P^P + \Delta t - T_s(N - 1)_P^P + \Delta t \right] - \alpha_2(N)_P^P + \Delta t T_s(N)_P^P + \Delta t \\
&- \alpha_3(N)_P^P + \Delta t 
\end{align*}
\] (5-18)

Therefore, the modified implicit finite difference equation for \( T_s \) at interior stations is
\[
\begin{aligned}
[\alpha_4(N)^P + \alpha_4(N)^P + \Delta t] & \left( \frac{T_s(N)^P + \Delta t - T_s(N)^P}{\Delta t} \right) + \frac{1}{\Delta x^2} [T_s(N + 1)^P - 2 T_s(N)^P + T_s(N - 1)^P] \\
& - 2 T_s(N)^P + T_s(N - 1)^P \right] + \frac{\alpha_1(N)^P}{2\Delta x} [T_s(N + 1)^P - T_s(N - 1)^P] \\
+ \alpha_2(N)^P T_s(N)^P + \alpha_3(N)^P + \frac{1}{\Delta x^2} [T_s(N + 1)^P + \Delta t - 2 T_s(N)^P + \Delta t] \\
+ T_s(N - 1)^P + \Delta t] + \frac{\alpha_1(N)^P + \Delta t}{2\Delta x} [T_s(N + 1)^P + \Delta t - T_s(N - 1)^P + \Delta t] \\
+ \alpha_2(N)^P + \Delta t T_s(N)^P + \Delta t + \alpha_3(N)^P + \Delta t = 0 \quad (5-19)
\end{aligned}
\]

or

\[
A_s(N) T_s(N - 1)^P + \Delta t + B_s(N) T_s(N)^P + \Delta t + C_s(N) T_s(N + 1)^P + \Delta t
\]

\[
= D_s(N) \quad (5-20)
\]

where

\[
A_s(N) = \frac{1}{\Delta x^2} - \alpha_1(N)^P + \Delta t / 2\Delta x \quad (5-21)
\]

\[
B_s(N) = \alpha_2(N)^P + \Delta t - 2 / \Delta x^2 + \frac{1}{\Delta t} [\alpha_4(N)^P + \alpha_4(N)^P + \Delta t] \quad (5-22)
\]

\[
C_s(N) = \frac{1}{\Delta x^2} + \alpha_1(N)^P + \Delta t / 2\Delta x \quad (5-23)
\]
\[
D_s(N) = -\alpha_3(N)^P - \alpha_3(N)^P + \Delta t \left[ -\frac{1}{\Delta x^2} + \frac{\alpha_1(N)^P}{2\Delta x} \right] T_s(N - 1)
\]

\[
- \left\{ \alpha_2(N)^P - \frac{2}{\Delta x^2} - \frac{1}{\Delta t} \left[ \alpha_4(N)^P + \alpha_4(N)^P + \Delta t \right] \right\} T_s(N)^P
\]

\[
- \left[ -\frac{1}{\Delta x^2} + \frac{\alpha_1(N)^P}{2\Delta x} \right] T_s(N + 1)^P .
\]

(5-24)

**Interior stations of the uncharred layer.** -- The modified implicit finite difference equation at interior stations of the uncharred layer is obtained by analogy from Eq. 5-19. The resulting equation is

\[
A_s'(N) T_s(N - 1)^P + \Delta t + B_s'(N) T_s(N)^P + \Delta t + C_s' T_s(N + 1)^P + \Delta t
\]

\[
= D_s'(N)
\]

(5-25)

where

\[
A_s'(N) = \frac{1}{\Delta x^2} - \frac{\alpha_1(N)^P + \Delta t}{2\Delta x'}
\]

(5-26)

\[
B_s'(N) = \frac{\alpha_2(N)^P + \Delta t}{\Delta x'^2} - \frac{2}{\Delta x'^2} + \frac{1}{\Delta t} \left[ \alpha_4(N)^P + \alpha_4(N)^P + \Delta t \right]
\]

(5-27)

\[
C_s'(N) = \frac{1}{\Delta x^2} + \frac{\alpha_1(N)}{2\Delta x'}
\]

(5-28)
\[ D_s'(N) = -\alpha_3'(N)P - \alpha_3'(N)P + \Delta t - \left[ \frac{1}{\Delta x'^2} - \frac{\alpha_1'(N)P}{2\Delta x''} \right] T_s'(N - 1)P \]

\[ - \{\alpha_2'(N)P - \frac{2}{\Delta x'^2} - \frac{1}{\Delta t} [\alpha_4'(N)P + \alpha_4'(N)P + \Delta t] \} T_s'(N)P \]

\[ - \left[ \frac{1}{\Delta x'^2} + \frac{\alpha_1'(N)P}{2\Delta x''} \right] T_s'(N + 1)P \]

(5-29)

**Interior stations of the insulation.** - The modified implicit finite difference equation at interior stations of the insulation layer is similarly obtained as

\[ A''(N) T_s'(N - 1)P + \Delta t + B''(N) T_s'(N)P + \Delta t + C''(N) T_s'(N + 1)P + \Delta t \]

\[ = D''(N) \]

(5-30)

where

\[ A''(N) = \frac{1}{\Delta x''^2} - \frac{\alpha_1''(N)P + \Delta t}{2\Delta x''} \]

(5-31)

\[ B''(N) = \alpha_2''(N)P + \Delta t - \frac{2}{\Delta x''^2} + \frac{1}{\Delta t} [\alpha_4''(N)P + \alpha_4''(N)P + \Delta t] \]

(5-32)

\[ C''(N) = \frac{1}{\Delta x''^2} + \frac{\alpha_1''(N)P + \Delta t}{2\Delta x''} \]

(5-33)

\[ D''(N) = -\alpha_3''(N)P - \alpha_3''(N)P + \Delta t - \left[ \frac{1}{\Delta x''^2} - \frac{\alpha_1''(N)P}{2\Delta x''} \right] T_s'(N - 1)P \]
Boundary stations.— Boundary conditions other than a parameter being specified at a point are employed by combining the governing differential equation and the equation expressing the boundary condition to obtain a differential equation which is valid only at the boundary. The solution of this equation satisfies both the boundary condition and the governing differential equation.

At the front surface (N = 1).— The front surface boundary condition is

\[
- \frac{1}{2} \left( k \frac{\partial T_s}{\partial x} \right)_{N = 1} = q_{c, \text{net}} - \sigma \varepsilon T_{s1}^4.
\]

The second order derivative term in Eq. 5-5 is written as

\[
\frac{\partial^2 T_s}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right).
\]

The derivative of the temperature gradient is obtained from Taylor series expansions at the station \( N = 1 \) evaluated at \( N = 2, N = 3, \) and \( N = 4. \) Thus
\[
\left( \frac{\partial T_s}{\partial x} \right)_{N=2} = \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + \Delta x \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^2}{2} \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^3}{6} \left[ \frac{\partial^3}{\partial x^3} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^4}{24} \left[ \frac{\partial^4}{\partial x^4} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \cdots \quad (5-37)
\]

\[
\left( \frac{\partial T_s}{\partial x} \right)_{N=3} = \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + \Delta x \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \Delta x^2 \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^3}{3} \left[ \frac{\partial^3}{\partial x^3} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^4}{24} \left[ \frac{\partial^4}{\partial x^4} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \cdots \quad (5-38)
\]

\[
\left( \frac{\partial T_s}{\partial x} \right)_{N=4} = \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + \Delta x \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^2}{2} \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^3}{3} \left[ \frac{\partial^3}{\partial x^3} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^4}{24} \left[ \frac{\partial^4}{\partial x^4} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \cdots \quad (5-39)
\]

Solving for \( \left[ \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} \)

\[
\left[ \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} = \frac{1}{6 \Delta x} \left[ -11 \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + 18 \left( \frac{\partial T_s}{\partial x} \right)_{N=2} - 9 \left( \frac{\partial T_s}{\partial x} \right)_{N=3} + 2 \left( \frac{\partial T_s}{\partial x} \right)_{N=4} \right] \quad (5-40)
\]

which is accurate to terms of the order \( \Delta x^3 \). Therefore,
\[
\left(\frac{\partial^2 T_s}{\partial x^2}\right)_{N=1} = \frac{1}{6\Delta x} \left[ -11 \left(\frac{\partial T_s}{\partial x}\right)_{N=1} + 18 \left(\frac{\partial T_s}{\partial x}\right)_{N=2} - 9 \left(\frac{\partial T_s}{\partial x}\right)_{N=3} + 2 \left(\frac{\partial T_s}{\partial x}\right)_{N=4} \right], \quad (5-41)
\]

Combining Eq. 5-41 with Eq. 5-5 written for station \(N = 1\) gives

\[
[\alpha_1(N) - \frac{11}{6\Delta x}] \left(\frac{\partial T_s}{\partial x}\right)_{N=1} + \frac{3}{\Delta x} \left(\frac{\partial T_s}{\partial x}\right)_{N=2} - \frac{3}{2\Delta x} \left(\frac{\partial T_s}{\partial x}\right)_{N=3} + \frac{1}{3\Delta x} \left(\frac{\partial T_s}{\partial x}\right)_{N=4} + \alpha_2(1) T_s(1) + \alpha_3(1) + \alpha_4(1) \left(\frac{\partial T_s}{\partial t}\right)_{N=1} = 0, \quad (5-42)
\]

The temperature gradient at station \(N = 1\) is given by Eq. 5-35. The temperature gradients of neighboring stations are approximated by central difference expressions. The resulting finite difference equation is

\[
\left\{ \left[\alpha_1(1) - \frac{11}{6\Delta x} \right] \frac{2}{k_s(1)} \sigma \varepsilon_s T_s(1)^3 - \frac{3}{2\Delta x^2} + \alpha_2(1) \right\} T_s(1)
+ \frac{3}{4\Delta x^2} T_s(2) + \left(\frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2}\right) T_s(3) - \frac{3}{4\Delta x^2} T_s(4)
+ \frac{1}{6\Delta x^2} T_s(5) + \alpha_3(1) - \frac{q_{\text{net}}}{k_s(1)} \left[\alpha_1(1) - \frac{11}{6\Delta x} \right]
+ \alpha_4(1) \left(\frac{\partial T_s}{\partial t}\right)_{N=1} = 0, \quad (5-43)
\]
Following the procedure used to obtain the modified implicit finite difference equation for interior stations, the analogous equation for the station at the front surface becomes

\[
\begin{align*}
\{(\alpha_1(1)^p + \Delta t - \frac{11}{6\Delta x} \frac{\varepsilon P + \Delta t}{k_s(1)^p + \Delta t} \sigma \varepsilon_s [T_s(1)^p + \Delta t]^3 - \frac{3}{2\Delta x^2} \\
+ \alpha_2(1)^p + \Delta t + \frac{1}{\Delta t} [\alpha_4(1)^p + \alpha_4(1)^p + \Delta t] T_s(1)^p + \Delta t \\
+ \frac{3}{4\Delta x^2} T_s(2)^p + \Delta t + \left( \frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2} \right) T_s(3)^p + \Delta t - \frac{3}{4\Delta x^2} T_s(4)^p + \Delta t \\
+ \frac{1}{6\Delta x^2} T_s(5)^p + \Delta t = - \alpha_3(1)^p - \alpha_3(1)^p + \Delta t + [\alpha_1(1)^p + \Delta t] \\
- \frac{11}{6\Delta x} q_{c,\text{net}} P + \Delta t = \varepsilon P + \Delta t + [\alpha_1(1)^p - \frac{11}{6\Delta x} q_{c,\text{net}} P + \frac{\varepsilon P}{k_s(1)^p} \\
- \{(\alpha_1(1)^p - \frac{11}{6\Delta x} \frac{\varepsilon P + \Delta t}{k_s(1)^p + \Delta t} \sigma \varepsilon_s [T_s(1)^p]^3 - \frac{3}{2\Delta x^2} \\
+ \alpha_2(1)^p - \frac{1}{\Delta t} [\alpha_4(1)^p + \alpha_4(1)^p + \Delta t] T_s(1)^p \\
- \frac{3}{4\Delta x^2} T_s(2)^p - \left( \frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2} \right) T_s(3)^p + 3/4\Delta x^2 T_s(4)^p \\
- \frac{1}{6\Delta x^2} T_s(5)^p \}
\end{align*}
\]

or

\[\text{(5-44)}\]
\[ B_{1s} T_s(1)^P + \Delta t + C_{1s} T_s(2)^P + \Delta t + G_{1s} T_s(3)^P + \Delta t \]
\[ + H_{1s} T_s(4)^P + \Delta t + I_{1s} T_s(5)^P + \Delta t = D_{1s} \quad (5-45) \]

where

\[ B_{1s} = [\alpha_1(1)^P + \Delta t - \frac{11}{6\Delta x}] \frac{\xi^P + \Delta t}{k_s(1)^P + \Delta t} \sigma \varepsilon_s[T_s(1)^P + \Delta t]^3 \]
\[ - \frac{3}{2\Delta x^2} + \alpha_2(1)^P + \Delta t + \frac{1}{\Delta t} [\alpha_4(1)^P + \alpha_4(1)^P + \Delta t] \quad (5-46) \]

\[ G_{1s} = \frac{3}{8\Delta x^2} \quad (5-47) \]

\[ G_{1s} = \frac{3}{4\Delta x^2} - \frac{1}{12\Delta x^2} \quad (5-48) \]

\[ H_{1s} = -\frac{3}{8\Delta x^2} \quad (5-49) \]

\[ I_{1s} = \frac{1}{12\Delta x^2} \quad (5-50) \]

\[ D_{1s} = -\alpha_3(1)^P - \alpha_3(1)^P + \Delta t + [\alpha_1(1)^P + \Delta t - \frac{11}{6\Delta x}] q_{c,net} \frac{\xi^P + \Delta t}{k_s(1)^P + \Delta t} \]
\[ + [\alpha_1(1)^P - \frac{11}{6\Delta x}] q_{c,net} \frac{\xi^P}{k_s(1)^P} - [\alpha_1(1)^P \]
\[ - \frac{11}{6\Delta x} \frac{\xi^P}{k_s(1)^P} \sigma \varepsilon_s[T_s(1)^P]^3 - \frac{3}{2\Delta x^2} + \alpha_2(1)^P \]
\[- \frac{1}{\Delta t} \left[ \alpha_4(1)^P + \alpha_4(1)^P + \Delta t \right] T_s(1)^P - \frac{3}{4\Delta x} T_s(2)^P \]

\[- \left( \frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2} \right) T_s(3)^P + \frac{3}{4\Delta x^2} T_s(4)^P \]

\[- \frac{1}{6\Delta x^2} T_s(5)^P \quad (5-51) \]

At the pyrolysis zone (N = 1). - The boundary condition at the pyrolysis zone is

\[- \frac{1}{\ell} \left( k_s \frac{\partial T_s}{\partial x} \right) \bigg|_{N = 1} = \frac{m}{\ell} \Delta H_p - \frac{1}{\ell} \left( k_s \frac{\partial T_s}{\partial x} \right) \bigg|_{N = 1} \quad (5-52) \]

The second order derivative in the governing equation for char layer temperature is approximated by a four-point backward difference expression analogous to Eq. 5-41. Thus

\[
\left( \frac{\partial^2 T_s}{\partial x^2} \right) \bigg|_{N = 1} = \frac{1}{6\Delta x} \left[ \left( \frac{\partial T_s}{\partial x} \right) \bigg|_{N = 1} - 18 \left( \frac{\partial T_s}{\partial x} \right) \bigg|_{N = 1} - \frac{9}{\Delta x} \left( \frac{\partial T_s}{\partial x} \right) \bigg|_{N = 1 - 2} - 2 \left( \frac{\partial T_s}{\partial x} \right) \bigg|_{N = 1 - 3} \right] \quad (5-53) \]

Using this equation in the governing equation for char layer temperature and solving for the char layer temperature gradient at the pyrolysis zone gives
The analogous expression for the uncharred layer temperature gradient is

\[
\left( \frac{\partial T_s}{\partial x} \right)_{N = 1} = \frac{6}{11} \left[ 3 \left( \frac{\partial T_s}{\partial x} \right)_{N = I - 1} - \frac{3}{2} \left( \frac{\partial T_s}{\partial x} \right)_{N = I - 2} + \frac{1}{3} \left( \frac{\partial T_s}{\partial x} \right)_{N = I - 3} - \alpha_1(I) \Delta x \left( \frac{\partial T_s}{\partial x} \right)_{N = I} - \alpha_2(I) \Delta x T_s(I) - \alpha_3(I) \Delta x \right]
\]

\[
- \alpha_4(I) \Delta x \frac{\partial T_s}{\partial t}
\]

\[N = I \quad \text{.} \quad (5-54)\]

Combining Eqs. 5-52, 5-54, and 5-55 gives

\[
\left( \frac{\partial T_s}{\partial x} \right) = \frac{\Delta x k_s(I) \alpha_4(I)}{\frac{\Delta x'}{2} + \frac{k_s'(I)\alpha_4'(I)}{2} \frac{k_s(I) \alpha_4(I)}{2}} \left[ \frac{k_s(I)}{2} \left( \frac{\partial T_s}{\partial x} \right)_{N = I - 1} \right]
\]

\[-\frac{3}{2} \left( \frac{\partial T_s}{\partial x} \right)_{N = I - 2} + \frac{1}{3} \left( \frac{\partial T_s}{\partial x} \right)_{N = I - 3} - \alpha_1(I) \Delta x \left( \frac{\partial T_s}{\partial x} \right)_{N = I} - \alpha_2(I) \Delta x T_s(I) \]

\[N = I \quad \text{.} \quad (5-55)\]
\[- \alpha_3(I) \Delta x' \right] + \frac{11}{6} \hat{m} g \Delta H_p - \frac{k_s(I)}{\xi} \left[ \frac{3}{\Delta x} \frac{\partial T_s}{\partial x} \right]_{N = I + 1} - \frac{3}{2} \frac{\partial T_s}{\partial x} \right]_{N = I + 2} \\
+ \frac{1}{3} \left[ \frac{\partial T_s}{\partial x} \right]_{N = I + 3} + \alpha_1'(I) \Delta x' \frac{\partial T_s}{\partial x'} \right]_{I} + \alpha_2'(I) \Delta x' T_s(I) \\
+ \alpha_3'(I) \Delta x' \right) \right\} \\
(5-56)

which is valid at the pyrolysis zone.

Approximating the temperature gradient of the char layer and the uncharred layer by four-point backward difference and forward difference expressions, respectively, and using central difference approximations for the temperature gradients at interior stations gives

\[
\left( \frac{\partial T_s}{\partial t} \right)_{N = I} = \frac{k_s(I) \alpha_4'(I) \Delta x}{\xi} \left\{ \frac{k_s(I)}{\xi} \left[ - \frac{1}{6 \Delta x} T_s(I - 4) \\
+ \left( \frac{3}{4 \Delta x} \frac{\alpha_1'(I)}{3} \right) T_s(I - 3) - \left( \frac{4}{3 \Delta x} \frac{\alpha_1(I)}{2} \right) T_s(I - 2) \\
- \left( \frac{3}{4 \Delta x} - 3 \alpha_1(I) \right) T_s(I - 1) \right\} + \left[ \frac{k_s(I)}{\xi} \left( \frac{3}{2 \Delta x} - \frac{11}{6} \alpha_1(I) \right) \\
- \alpha_2(I) \Delta x \right] + \frac{k_s'(I)}{\xi'} \left( \frac{3}{2 \Delta x} + \frac{11}{6} \alpha_1'(I) - \alpha_2'(I) \Delta x' \right) \right\} T_s(I) \\
+ \frac{11}{6} \hat{m} g \Delta H_p - \frac{k_s(I) \alpha_3'(I) \Delta x}{\xi} - \frac{k_s'(I) \alpha_3'(I) \Delta x'}{\xi'} \\
- \frac{k_s'(I)}{\xi'} \left[ \left( \frac{3}{4 \Delta x'} + 3 \alpha_1'(I) \right) T_s(I + 1) + \left( \frac{4}{3 \Delta x'} - \frac{3 \alpha_1'(I)}{2} \right) T_s(I + 2) \\
- \left( \frac{3}{4 \Delta x'} - \frac{\alpha_1'(I)}{3} \right) T_s(I + 3) + \frac{1}{6 \Delta x'} T_s(I + 4) \right\} \right\} \right\} \right\} \\
(5-57)
The modified implicit finite difference equation results from taking an average of Eq. 5-57 written in explicit form and in implicit form. The result is

\[ ZI_s T_s(I - 4)P + \Delta t + YI_s T_s(I - 3)P + \Delta t + XI_s T_s(I - 2)P + \Delta t \]

\[ + AI_s T_s(I - 1)P + \Delta t + BI_s T_s(I)P + \Delta t \]

\[ + CI_s T_s(I + 1)P + \Delta t + EI_s T_s(I + 2)P + \Delta t \]

\[ + FI_s T_s(I + 3)P + \Delta t + GI_s T_s(I + 4)P + \Delta t \]

\[ = DI_s \] (5-58)

where

\[ ZI_s = \frac{-k_s(I)P + \Delta t/(12 \Delta x \xi P + \Delta t)}{k_s(I)P + \Delta t \alpha_4(I)P + \Delta t \Delta x + k'_s(I)P + \Delta t \alpha'_4(I)P + \Delta t \Delta x'} \] (5-59)

\[ YI_s = \frac{k_s(I)P + \Delta t \left[ \frac{3}{4\Delta x} + \frac{\alpha_1(x)P + \Delta t}{3} \right]}{2} \frac{1}{\xi P + \Delta t} \] (5-60)
$$s = 2$$

$$AI_s = \frac{k_s(I)^P + \Delta t \left[\frac{4}{3 \Delta x} + \frac{3 \alpha_1(x)}{2} \right] P + \Delta t}{k_s(I)^P + \Delta t + k_s'(I)^P + \Delta t_{\Delta x}} / \mu^P + \Delta t$$

$$XI_s = \frac{[k_s(I)^P + \Delta t \alpha_4(I)^P + \Delta t_{\Delta x} + k_s'(I)^P + \Delta t \alpha_4'(I)^P + \Delta t_{\Delta x}']}{2 \left[\mu^P + \Delta t + \mu_{\Delta x}^P + \Delta t\right]}$$

$$EI_s = \frac{[k_s(I)^P + \Delta t \alpha_4(I)^P + \Delta t_{\Delta x} + k_s'(I)^P + \Delta t \alpha_4'(I)^P + \Delta t_{\Delta x}']}{2 \left[\mu^P + \Delta t + \mu_{\Delta x}^P + \Delta t\right]}$$

$$AI_s = \frac{k_s(I)^P + \Delta t \left[\frac{3}{4 \Delta x} - 3 \alpha_1(I)^P + \Delta t\right]}{2 \left[\mu^P + \Delta t + \mu_{\Delta x}^P + \Delta t\right]}$$

$$CI_s = \frac{-k_s'(I)^P + \Delta t \left[\frac{4}{3 \Delta x'} + 3 \alpha_1'(I)^P + \Delta t\right]}{2 \left[\mu_{\Delta x}^P + \Delta t\right]}$$
\[
FI_s = \frac{k'_s(I)P + \Delta t \left[ \frac{3}{4\Delta x^3} - \frac{1}{3} \alpha'_1(I)P + \Delta t \right]}{\Delta t} / P + \Delta t
\]

\[
GI_s = - \frac{k'_s(I)P + \Delta t / (12 \Delta x^2 \Delta t P + \Delta t)}{\left[ \frac{k'_s(I)P + \Delta t \alpha'_4(I)P + \Delta t \Delta x}{\Delta t} \right] + \frac{k'_s(I)P + \Delta t \alpha'_4(I)P + \Delta t \Delta x'}{\Delta t}}
\]

\[
DI_s = \frac{1}{2\left[ \frac{k'_s(I)P + \Delta t \alpha'_4(I)P + \Delta t \Delta x}{\Delta t} \right] + \frac{k'_s(I)P + \Delta t \alpha'_4(I)P + \Delta t \Delta x'}{\Delta t}}}
\]

\[
+ \frac{k'_s(I)P + \Delta t \alpha'_3(I)P + \Delta t \Delta x'}{\Delta t} / P + \Delta t}
\]

\[
+ \left[ \frac{k'_s(I)P \alpha'_4(I)P \Delta x}{\Delta t^2} + \frac{k'_s(I)P \alpha'_4(I)P \Delta x'}{\Delta t^2} \right]
\]

\[
+ \frac{1}{2\left[ \frac{k'_s(I)P \alpha'_3(I)P \Delta x}{\Delta t^2} + \frac{k'_s(I)P \alpha'_3(I)P \Delta x'}{\Delta t^2} \right]}
\]

\[
\frac{k'_s(I)P / \Delta t}{\left[ \frac{k'_s(I)P \alpha'_4(I)P \Delta x}{\Delta t^2} + \frac{k'_s(I)P \alpha'_4(I)P \Delta x'}{\Delta t^2} \right]}
\]

\[
\left[ - \frac{1}{6\Delta x} T_s(I - 4)P \right]
\]
\[
\left\{ \frac{k_s(I)^p}{\xi(I)^p} \right\} \left( \begin{array}{c} \frac{3}{2\Delta x} \\
\end{array} \right)
\]

At the uncharred material - insulation interface (\(N = I + J\)).

The boundary condition at the interface of the uncharred material and the insulation is
This equation is combined with the uncharred material temperature equation and the insulation temperature equation following the procedure used for the pyrolysis zone equations. The resulting modified implicit finite difference equation is

\[ Z_p \Delta T_s (I + J - 4)P + \Delta t + Y_p \Delta T_s (I + J - 3)P + \Delta t \]

\[ + X_p \Delta T_s (I + J - 2)P + \Delta t + A_p \Delta T_s (I + J - 1)P + \Delta t \]

\[ + B_p \Delta T_s (I + J)P + \Delta t + C_p \Delta T_s (I + J + 1)P + \Delta t \]

\[ + E_p \Delta T_s (I + J + 2)P + \Delta t + F_p \Delta T_s (I + J + 3)P + \Delta t \]

\[ + G_p \Delta T_s (I + J + 4)P + \Delta t = D_p \]

(5-70)

where

\[ Z_p = \frac{k'_s(I+J)^P+\Delta t/(12 \Delta' \Delta P+\Delta t)}{\left[ k'_s(I+J)^P+\Delta t a'_4(I+J)^P+\Delta t \Delta x' \right] + \frac{k''(I+J)^P+\Delta t a''(I+J)^P+\Delta t \Delta x''}{\Delta P+\Delta t} - \rho_{HS} C_{PHS} \Delta T_s^P \]

(5-71)
\[ YP_s = \frac{k'_s(I+J)P+\Delta t/\ell',P+\Delta t}{\ell',P+\Delta t} \left[ \frac{3}{4\Delta x'} + \frac{\alpha'_1(I+J)^P+\Delta t}{3} \right] + \frac{k''(I+J)^P+\Delta t\Delta x''}{\ell'',P+\Delta t} - \rho_{HS} \frac{\hat{c}_p}{\ell_{HS}} \]

\[ XP_s = \frac{-k'_s(I+J)^P+\Delta t/\ell',P+\Delta t}{\ell',P+\Delta t} \left[ \frac{4}{3\Delta x'} + \frac{\frac{3}{2} \alpha'_1(I+J)^P+\Delta t}{\ell'} \right] + \frac{k''(I+J)^P+\Delta t\Delta x''}{\ell'',P+\Delta t} - \rho_{HS} \frac{\hat{c}_p}{\ell_{HS}} \]

\[ AP_s = \frac{-k'_s(I+J)^P+\Delta t/\ell',P+\Delta t}{\ell',P+\Delta t} \left[ \frac{3}{4\Delta x'} - \frac{3\alpha'_1(I+J)^P+\Delta t}{\ell'} \right] + \frac{k''(I+J)^P+\Delta t\Delta x''}{\ell'',P+\Delta t} - \rho_{HS} \frac{\hat{c}_p}{\ell_{HS}} \]

\[ BP_s = \frac{1}{2} \left[ \frac{k'_s(I+J)^P+\Delta t\alpha'_4(I+J)^P+\Delta t\Delta x'}{\ell',P+\Delta t} + \frac{k''(I+J)^P+\Delta t\alpha''_4(I+J)^P+\Delta t\Delta x''}{\ell'',P+\Delta t} - \rho_{HS} \frac{\hat{c}_p}{\ell_{HS}} \right] \]

\[ \left\{ \begin{array}{l}
\frac{k'_s(I+J)^P+\Delta t}{\ell',P+\Delta t} \left[ \frac{\alpha'_4(I+J)^P+\Delta t - \frac{11}{6} \alpha'_1(I+J)^P+\Delta t \Delta x'}{2} \right] \\
\frac{k''(I+J)^P+\Delta t}{\ell'',P+\Delta t} \left[ \frac{\alpha''_4(I+J)^P+\Delta t - \frac{11}{6} \alpha'_1(I+J)^P+\Delta t \Delta x''}{2} \right] - \frac{1}{\Delta t}
\end{array} \right\} (5-75) \]
\[
\left\{- \frac{1}{6\Delta x^t} T_s (I + J - 4)^p + \left[ \frac{3}{4\Delta x^t} + \frac{1}{3} \alpha_1^p (I + J)^p \right] T_s (I + J - 3)^p \\
- \left[ \frac{4}{3\Delta x^t} + \frac{3}{2} \alpha_1^p (I + J)^p \right] T_s (I + J - 2)^p - \left[ \frac{3}{4\Delta x^t} - 3 \alpha_1^p (I + J)^p \right] T_s (I + J - 1)^p \right\}
\]

\[
+ \frac{1}{2} \left[ \frac{k_s^{''}(I+J)^p \alpha_4^p (I+J)^p \Delta x^t}{\xi^p} + \frac{k_s^{''}(I+J)^p \alpha_4^p (I+J)^p \Delta x^t}{\xi^p} - \rho_{HS} \frac{\hat{C}_{HS} \xi_{HS}}{P} \right]
\]

\[
\left\{ \frac{k_s^{''}(I+J)^p}{\xi^p} \left[ \frac{3}{2\Delta x^t} - \frac{11}{6} \alpha_1^p (I+J)^p - \alpha_2^p (I+J)^p \Delta x^t \right] + \frac{k_s^{''}(I+J)^p}{\xi^p} \left[ \frac{3}{2\Delta x^t} \\
+ \frac{11}{6} \alpha_1^p (I+J)^p - \alpha_2^p (I+J)^p \Delta x^t \right] \right\} + \frac{1}{\Delta t} \right] T_s (I+J)^p
\]

\[
+ \frac{k_s^{''}(I+J)^p}{\xi^p} \frac{k_s^{''}(I+J)^p}{\xi^p} \left[ \frac{k_s^{''}(I+J)^p \Delta x^t}{\xi^p} + \frac{k_s^{''}(I+J)^p \Delta x^t}{\xi^p} - \rho_{HS} \frac{\hat{C}_{HS} \xi_{HS}}{P} \right]
\]

\[
\left\{ \frac{3}{4\Delta x^t} + 3 \alpha_1^p (I+J)^p \right\} T_s (I+J+1)^p + \left[ \frac{4}{3\Delta x^t} - \frac{3}{2} \alpha_1^p (I+J)^p \right] T_s (I+J+2)^p \\
- \left[ \frac{3}{4\Delta x^t} - \frac{1}{3} \alpha_1^p (I+J)^p \right] T_s (I+J+3)^p + \frac{1}{6\Delta x^t} T_s (I+J+4)^p \right\}.
\]

(5–80)

At the back surface \( N = I + J + K \). The back surface boundary condition is

\[
- \frac{1}{\xi^p} \left( k_s^{''} \frac{\partial T_s}{\partial x^t} \right)_{N = I + J + K} = \sigma \epsilon^{''}_s T_s (I + J + K)^4
\]

\[
- q_B + \rho_{HS} \frac{\hat{C}_{HS} \xi_{HS}}{P} \frac{\partial T_s}{\partial t} \left( \frac{\partial T_s}{\partial x^t} \right)_{N = I + J + K}.
\]

(5–81)
This equation is combined with the insulation temperature equation following the procedure used for the front surface boundary condition and char layer temperature equation. The resulting modified implicit finite difference equation is

\[ ZZ_s \frac{T_s (I + J + K - 4)P + \Delta t + YZ_s T_s (I + J + K - 3)P + \Delta t}{12 Ax^2 V} + XZ_s T_s (I + J + K - 2)P + \Delta t + AZ_s T_s (I + J + K - 1)P + \Delta t \]

\[ + BZ_s T_s (I + J + K)P + \Delta t = DZ_s \]  

(5-82)

where

\[ ZZ_s = \frac{k''(I+J+K)^P}{s(I+J+K)(12 Ax^2 V)} \]

(5-83)

\[ YZ_s = -4.5 ZZ_s \]  

(5-84)

\[ XZ_s = 8 ZZ_s \]  

(5-85)

\[ AZ_s = - YZ_s \]  

(5-86)

\[ BZ_s = [6a''(I+J+K)^P + \Delta t^2 - 9] ZZ_s - \frac{1}{\Delta t} \]
\[
\sigma \varepsilon'' \left[ T_s (I+J+K) \right]^{P+\Delta t} \left[ \alpha''_1 (I+J+K) \right]^{P+\Delta t} + \frac{11}{6 \Delta x''} \right] \\
2 \left\{ \rho_{HSP} \hat{C}_{P} \lambda_{HSP} \left[ \alpha''_1 (I+J+K) \right]^{P+\Delta t} + \frac{11}{6 \Delta x''} \right\} - \frac{\alpha''_1 (I+J+K) \epsilon''_{k_s} (I+J+K) \epsilon'' \Delta t}{\lambda''} \\
\right\} \\
(5-87) 
\]

\[
DZ_s = - \frac{\alpha''_1 (I+J+K) \epsilon + 11/6 \Delta x''}{2 \left\{ \rho_{HSP} \hat{C}_{P} \lambda_{HSP} \left[ \alpha''_1 (I+J+K) \right]^{P+\Delta t} + \frac{11}{6 \Delta x''} \right\} - \frac{\alpha''_1 (I+J+K) \epsilon_{k_s}'' (I+J+K) \epsilon'' \Delta t}{\lambda''} \\
\left\{ \frac{P^{P+\Delta t}}{q_B} + \frac{\alpha''_3 (I+J+K) k''_s (I+J+K) \epsilon'' \Delta t}{\alpha''_1 (I+J+K) \epsilon + 11/6 \Delta x''} + \frac{k''_s (I+J+K) \epsilon'' \Delta t}{\alpha''_1 (I+J+K) \epsilon + 11/6 \Delta x''} \right\} \\
\left\{ \frac{1}{6 \Delta x''^2} T_s (I+J+K) P - \frac{3}{4 \Delta x''^2} T_s (I+J+K-3) P + \frac{4}{3 \Delta x''^2} T_s (I+J+K-2) P \\
+ \frac{3}{4 \Delta x''^2} T_s (I+J+K-1) P - \left[ \frac{3}{2 \Delta x''^2} - \alpha''_2 (I+J+K) P \right] T_s (I+J+K) P \right\} \\
- \sigma \varepsilon'' \left[ T_s (I+J+K) \right]^{P+\Delta t} + \frac{1}{\Delta t} T_s (I+J+K) P \right) \\
(5-88) 
\]
Char Layer Porosity Equation

The differential equation for the char layer porosity is

$$\frac{\partial n}{\partial x} + \varepsilon_1 \eta + \varepsilon_2 + \varepsilon_3 \frac{\partial n}{\partial t} = 0 \quad (5-89)$$

The second term in this equation may be much less than 1. Therefore, to assure that the finite difference form of this equation is suitable for obtaining a numerical solution, the first order partial derivative is replaced by a forward difference approximation.

The forward difference approximation of the derivative is obtained from Taylor series expansions at the station \(N\) evaluated at \(N + 1\) and \(N + 2\). Thus

$$\eta(N + 1) = \eta(N) + \left(\frac{\partial \eta}{\partial x}\right)_N \Delta x + \left(\frac{\partial^2 \eta}{\partial x^2}\right)_N \frac{\Delta x^2}{2} + \left(\frac{\partial^3 \eta}{\partial x^3}\right)_N \frac{\Delta x^3}{6} + \cdots \quad (5-90)$$

$$\eta(N + 2) = \eta(N) + 2 \left(\frac{\partial \eta}{\partial x}\right)_N \Delta x + 2 \left(\frac{\partial^2 \eta}{\partial x^2}\right)_N \Delta x^2 + \frac{4}{3} \left(\frac{\partial^3 \eta}{\partial x^3}\right)_N \Delta x^3 + \cdots \quad (5-91)$$

Eliminating the second order derivative from this pair of equations and solving for the first order derivative gives:

$$\left(\frac{\partial \eta}{\partial x}\right)_N = \left[-3\eta(N) + 4\eta(N + 1) - \eta(N + 2)\right]/2\Delta x \quad (5-92)$$

which is accurate to terms of the order \(\Delta x^2\).
Combining Eqs. 5-89 and 5-92 gives

\[
[\varepsilon_1(N) - \frac{3}{2\Delta x} \eta(N) + \frac{2}{\Delta x} \eta(N+1) - \frac{1}{2\Delta x} \eta(N+2)]
+ \varepsilon_2(N) + \varepsilon_3(N) \left( \frac{\partial \eta}{\partial t} \right)_N = 0
\]  

(5-93)

which yields the following modified implicit finite difference equation.

\[
B(N) \eta(N)^P + \Delta t + C(N) \eta(N+1)^P + \Delta t + E(N) \eta(N+2)^P + \Delta t
= D(N)
\]  

(5-94)

where

\[
B(N) = \frac{1}{2\Delta t} \left[ \varepsilon_3(N)^P + \varepsilon_3(N)^P + \Delta t \right]
+ \frac{1}{2} \left[ \varepsilon_1(N)^P + \Delta t - \frac{3}{2\Delta x} \right]
\]  

(5-95)

\[
C(N) = \frac{1}{\Delta x}
\]  

(5-96)

\[
E(N) = -\frac{1}{4\Delta x}
\]  

(5-97)
\[ D(N) = -\frac{1}{2} \left[ \varepsilon_2(N)^P + \varepsilon_2(N)^P + \Delta t \right] \]

\[-\frac{1}{2} \{ \varepsilon_1(N)^P - \frac{3}{2}\Delta x - \frac{1}{\Delta t} [\varepsilon_3(N)^P + \varepsilon_3(N)^P + \Delta t ]\} \eta(N)^P \]

\[-\frac{1}{\Delta x} \eta(N+1)^P + \frac{1}{4\Delta x} \eta(N+2)^P. \quad (5-98)\]

Equation 5-93 is valid at all stations from \( N = 1 \) to \( N = I - 2 \). At \( N = I - 1 \) the third term in Eq. 5-93 would contain \( \eta(I + 1) \) which is not defined. The finite difference equation for station \( I - 1 \) is obtained in a manner identical to that used to obtain Eq. 5-93 except that the first order derivative is approximated by a two-point forward difference equation. Thus:

\[ \left( \frac{\partial n}{\partial x} \right)_{N = I - 1} = \frac{\eta(I) - \eta(I - 1)}{\Delta x} \quad (5-99)\]

which is accurate to terms of the order \( \Delta x \). The resulting modified implicit finite difference equation for station \( I - 1 \) is

\[ B(I - 1)\eta(I - 1)^P + \Delta t + C(I - 1)\eta(I)^P + \Delta t = D(I - 1) \quad (5-100)\]

where
112

\[ B(I - 1) = \frac{1}{\Delta t} [\varepsilon_3(I - 1)^P + \varepsilon_3(I - 1)^{P+\Delta t}] + \varepsilon_1(I - 1)^{P+\Delta t} - \frac{1}{\Delta x} \]

(5-101)

\[ C(I - 1) = \frac{1}{\Delta x} \]

(5-102)

\[ D(I - 1) = - [\varepsilon_2(I - 1)^P + \varepsilon_2(I - 1)^P] - \varepsilon_1(I - 1)^P - \frac{1}{\Delta x} \]

\[ - \frac{1}{\Delta t} [\varepsilon_3(I - 1)^P + \varepsilon_3(I - 1)^P + \Delta t])\eta(I - 1)^P \]

\[ - \frac{1}{\Delta x} \eta(I)^P \]

(5-103)

The single boundary condition for char layer porosity equation is

\[ \eta(I) = \eta_I \]

(5-104)

This identity is used instead of a finite difference equation at station I.

Pyrolysis Gas Temperature Equation

The differential equation for the pyrolysis gas temperature is

\[ \frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 \]

(5-105)

The single boundary condition for this equation is
\[ T(I) = T_s(I) \quad (5-106) \]

The forms of the pyrolysis gas temperature equation and its boundary conditions are identical to the char layer porosity equation and boundary condition; therefore, the modified implicit finite difference equation for pyrolysis gas temperature is of the same form as the equations for char layer porosity. Thus for \( 1 \leq N \leq I - 2 \)

\[
B(N) \left(T(N)^P + \Delta t\right) + C(N) \left(T(N + 1)^P + \Delta t\right) + E(N) \left(T(N + 2)^P + \Delta t\right) = D(N) \quad (5-107)
\]

where

\[
B(N) = \frac{1}{2\Delta t} \left[ \beta_3(N)^P + \beta_3(N)^P + \Delta t \right] + \frac{1}{2} \left[ \beta_1(N)^P + \Delta t - \frac{3}{2\Delta x} \right] \quad (5-108)
\]

\[
C(N) = \frac{1}{\Delta x} \quad (5-109)
\]

\[
E(N) = -\frac{1}{4\Delta x} \quad (5-110)
\]

\[
D(N) = -\frac{1}{2} \left[ \beta_2(N)^P + \beta_2(N)^P + \Delta t \right] - \frac{1}{2} \left( \beta_1(N)^P - \frac{3}{2\Delta x} \right)
- \frac{1}{\Delta t} \left[ \beta_3(N)^P + \beta_3(N)^P + \Delta t \right] T(N)^P - \frac{1}{\Delta x} T(N + 1)^P + \frac{1}{4\Delta x} T(N + 2)^P \quad (5-111)
\]
and, for \( N = I - 1 \),

\[
B(I - 1) \ T(I - 1)^P + \Delta t + C(I - 1) \ T(I)^P + \Delta t = D(I - 1)
\]  

(5-112)

where

\[
B(I - 1) = \frac{1}{\Delta t} \ [\beta_3(I - 1)^P + \beta_3(I - 1)^P + \Delta t] + \beta_1(I - 1)^P + \Delta t - \frac{1}{\Delta x}
\]

(5-113)

\[
C(I - 1) = \frac{1}{\Delta x}
\]

(5-114)

\[
D(I - 1) = - [\beta_2(I - 1)^P + \beta_2(I - 1)^P + \Delta t] - \beta_1(I - 1)^P - \frac{1}{\Delta x} - \frac{1}{\Delta t} \ [\beta_3(I - 1)^P + \beta_3(I - 1)^P + \Delta t]] \ T(I - 1)^P - \frac{1}{\Delta x} \ T(I)^P
\]

(5-115)

The equation applied at \( N = I \) is

\[
T(I) = T_s(I)
\]

(5-116)
Pyrolysis Gas Pressure Equation

The differential equation for the pyrolysis gas pressure is

\[
\frac{\partial^2 P}{\partial x^2} + \gamma_1 \frac{\partial P}{\partial x} + \gamma_2 P^2 + \gamma_3 + \gamma_4 \frac{\partial P}{\partial t} = 0. \tag{5-117}
\]

**Interior stations.**—The form of this equation is identical to that of the solid phase temperature equation; hence at interior stations the modified implicit finite difference equations for the pyrolysis gas pressure are written from the finite difference equations for the solid phase temperature as

\[
A_p(N) P^2(N - 1) + \Delta t + B_p(N) P^2(N) + \Delta t
\]

\[+ C_p(N) P^2(N + 1) + \Delta t = D_p(N) \tag{5-118}
\]

where

\[
A_p(N) = \frac{1}{\Delta x^2} - \frac{\gamma_1(N) P + \Delta t}{2\Delta x} \tag{5-119}
\]

\[
B_p(N) = \gamma_2(N) P + \Delta t - \frac{2}{\Delta x^2} + \frac{1}{\Delta t} \left[ \gamma_4(N) P + \gamma_4(N) P + \Delta t \right] \tag{5-120}
\]

\[
C_p(N) = \frac{1}{\Delta x^2} + \frac{\gamma_1(N) P + \Delta t}{2\Delta x} \tag{5-121}
\]
\[ D_p(N) = -\gamma_3(N)^p - \gamma_3(N)^p + \Delta t \left[ \frac{1}{\Delta x^2} - \frac{\gamma_1(N)^p}{2\Delta x} \right] p^2(N - 1)^p \]

\[- \{\gamma_2(N)^p - \frac{2}{\Delta x^2} - \frac{1}{\Delta t} [\gamma_4(N)^p + \gamma_4(N)^p + \Delta t]\} p^2(N)^p \]

\[- \left[ \frac{1}{\Delta x^2} + \frac{\gamma_1(N)^p}{2\Delta x} \right] p^2(N + 1)^p \]  \hspace{1cm} (5-122)

**Front surface boundary condition (N = 1).** - The boundary condition for pressure at the front surface is

\[ P(1) = P_w \]  \hspace{1cm} (5-123)

or

\[ P^2(1) = P_w^2 \]  \hspace{1cm} (5-124)

which is used instead of a finite difference equation at station 1.

**Pyrolysis zone boundary condition (N = I).** - The second boundary condition for the pressure equation is the specified pressure gradient at the pyrolysis zone -

\[ \left( \frac{\partial p^2}{\partial x} \right)_N = 2 R_u \ell \left( \frac{\mu T}{\kappa M} \right)_N = \dot{m}_g \]  \hspace{1cm} (5-125)

The second order derivative of Eq. 5-117 is written as the first derivative of the gradient of \( p^2 \),
The derivative of the gradient of $P^2$ is then approximated by a four-point backward difference expression obtained from Taylor series expansions at the station $N = I$ evaluated at $N = I - 1$, $N = I - 2$, and $N = I - 3$. Thus

\[
\frac{\partial^2 P^2}{\partial x^2} = \frac{\partial}{\partial x} \left[ \frac{\partial P}{\partial x} \right]. \tag{5-126}
\]

Combining Eq. 5-127 with Eq. 5-117 written for station $N = I$ gives

\[
\left[ \frac{11}{6\Delta x} + \gamma_1(I) \right] \frac{\partial P^2}{\partial x} = \frac{3}{\Delta x} \frac{\partial P^2}{\partial x} - \frac{3}{2\Delta x} \frac{\partial P^2}{\partial x} + \gamma_2(I) P^2(I) + \gamma_3(I)
\]

\[
+ \gamma_4(I) \frac{\partial P^2}{\partial t} = 0. \tag{5-128}
\]

In Eq. 5-128 the gradient of $P^2$ at the pyrolysis zone is replaced with Eq. 5-125 and the gradients at neighboring stations are approximated by central difference expressions yielding
The modified implicit finite difference equation for pressure at the pyrolysis zone is obtained from Eq. 5-129 using the procedure previously outlined. Writing the equation,\

\[
\frac{1}{2} \frac{F}{\Delta x^2} P^2 (I - 4) - \frac{3}{4} \frac{F}{\Delta x^2} P^2 (I - 3) + \frac{4}{3} \frac{F}{\Delta x^2} P^2 (I - 2)
\]

\[
+ \frac{3}{4} \frac{F}{\Delta x^2} P^2 (I - 1) + \left[ \gamma_2 (I) - \frac{3}{2} \frac{F}{\Delta x^2} \right] P^2 (I) + \gamma_3 (I)
\]

\[
+ \left[ \frac{11}{6} \frac{F}{\Delta x} + \gamma_1 (I) \right] R u \left( \frac{\mu T}{k M} \right) N = I
\]

\[
+ \gamma_4 (I) \left( \frac{\partial P^2}{\partial t} \right)_N = 0
\]

(5-129)
\[ PZ = \frac{3}{3\Delta x^2} \]  

(5-133)

\[ AP = -PY \]  

(5-134)

\[ BP = \frac{1}{2\Delta t} \left[ \gamma_4(I)^P + \gamma_4(I)^P + \Delta t \right] + \frac{1}{2} \left[ \gamma_2(I)^P + \Delta t \right] \]

\[ - \frac{3}{2\Delta x^2} \]  

(5-135)

\[ DP = -\frac{1}{2} \left[ \gamma_3(I)^P + \gamma_3(I)^P + \Delta t \right] - \left[ \frac{11}{6\Delta x} \right. \]

\[ + \gamma_1(I)^P \right] R_u \mu^P \hat{m}^P \left( \frac{\mu T}{K_M} \right)^P \]

\[ N = I \]

\[ - \left[ \frac{11}{6\Delta x} + \gamma_1(I)^{P+\Delta t} \right] R_u \mu^{P+\Delta t} \hat{m}^{P+\Delta t} \left( \frac{\mu T}{K_M} \right)^{P+\Delta t} \]

\[ N = I \]

\[ - \frac{1}{12\Delta x^2} P^2(I - 4)^P + \frac{3}{8\Delta x^2} P^2(I - 3)^P - \frac{3}{3\Delta x^2} P^2(I - 2)^P \]

\[ - \frac{3}{8\Delta x^2} P^2(I - 1)^P - \frac{1}{2} \left\{ \gamma_2(I)^P - \frac{3}{2\Delta x^2} \right. \frac{1}{\Delta t} \left[ \gamma_4(I)^P \right. \]

\[ + \gamma_4(I)^P + \Delta t \} P^2(I)^P \right. \]  

(5-136)

**Chemical Species Conservation Equation**

The differential equation for conservation of chemical species is

\[ \frac{\partial}{\partial x} \hat{m}_1 + \Delta_1 \hat{m}_1 + \Delta_2 \hat{m}_2 + \Delta_3 \frac{\partial \hat{m}_1}{\partial t} = 0. \]  

(5-137)
The single boundary condition for this equation is

\[ \frac{\hat{m}_i}{N = I} = -M_i \left( \frac{\chi_i}{\eta M} \right) \hat{m}_g. \]  

(5-138)

This equation and its boundary condition are of the same form as the first order equations and boundary conditions handled previously. Therefore the modified implicit finite difference equation for conservation of chemical species is written directly as

\[ B_1(N) \hat{n}_1(N)^P + \Delta t + C_1(N) \hat{n}_1(N + 1)^P + \Delta t \]

\[ + E_1(N) \hat{n}_1(N + 2)^P + \Delta t = D_1(N) \]  

(5-139)

for \( 1 \leq N \leq I - 2 \)

where

\[ B_1(N) = \frac{1}{2\Delta t} \left[ \Delta_{1_1}^+ (N)^P + \Delta_{1_1}^- (N)^P + \Delta t \right] \]

\[ + \frac{1}{2} \left[ \Delta_{1_1}^+ (N)^P + \Delta t - \frac{3}{2\Delta x} \right] \]  

(5-140)

\[ C_1(N) = \frac{1}{\Delta x} \]  

(5-141)

\[ E_1(N) = -\frac{1}{4\Delta x} \]  

(5-142)
\[ D_1(N) = -\frac{1}{2} \left[ \Delta_{2_1}^2(N) + \Delta_{2_1}^2(N) + \Delta t \right] \]

\[ -\frac{1}{2} \left( \Delta_{1_1}^1(N)^P - \frac{3}{2\Delta x} \Delta t \left[ \Delta_{3_1}^3(N)^P \right. \right. \]

\[ + \Delta_{3_1}^3(N)^P + \Delta t \left] \right) \hat{m}_1(N)^P - \frac{1}{\Delta x} \hat{m}_1(N + 1)^P \]

\[ + \frac{1}{4\Delta x} \hat{m}_1(N + 2)^P \]  \hspace{1cm} (5-143)

and, for \( N = I - 1 \),

\[ B_1(I - 1)\hat{m}_1(I - 1)^P + \Delta t + C_1(I - 1)\hat{m}_1(I)^P + \Delta t = D_1(I - 1) \] \hspace{1cm} (5-144)

where

\[ B_1(I - 1) = \frac{1}{\Delta t} \left[ \Delta_{3_1}^3(I - 1)^P + \Delta_{3_1}^3(I - 1)^P + \Delta t \right] \]

\[ + \Delta_{1_1}^1(I - 1)^P + \Delta t - \frac{1}{\Delta x} \] \hspace{1cm} (5-145)

\[ C_1(I - 1) = \frac{1}{\Delta x} \] \hspace{1cm} (5-146)

\[ D_1(I - 1) = -\Delta_{2_1}^2(I - 1)^P - \Delta_{2_1}^2(I - 1)^P + \Delta t - \Delta_{1_1}^1(I - 1)^P \]

\[ - \frac{1}{\Delta x} - \frac{1}{\Delta t} \left[ \Delta_{3_1}^3(I - 1)^P + \Delta_{3_1}^3(I - 1)^P \right] m_1(I - 1)^P - \frac{1}{\Delta x} m_1(I)^P \] \hspace{1cm} (5-147)
and, for $N = I$, 

$$
\hat{\Phi}_I(N) = -M_I \left( \frac{\chi_1}{\eta M} \right) \hat{\Phi}_g.
$$

(5-148)
CHAPTER VI

SOLUTION OF EQUATIONS

The equations formulated to this point are solved on a digital computer. The linearized finite difference equations for solid temperature and pyrolysis gas pressure are solved using the method suggested by L. H. Thomas of the Watson Scientific Computing Laboratory. Thomas' method is presented in Bruce, Peaceman and Rachford (Ref. 32).

Consider the finite difference equations for the solid temperature -

At the front surface of the char layer (N = 1):

\[ B_1 s \Delta t s_1 p + A t + C_1 s \Delta t s_2 p + C_1 s \Delta t s_3 p + H_1 s \Delta t s_4 p + I_1 s \Delta t s_5 p + \Delta t = D_1 s \] (6-1)

Within the char layer (1 < N < I):

\[ A_s(N) \Delta t s(N - 1)p + A t + B_s(N) \Delta t s(N)p + A t + C_s(N) \Delta t s(N + 1)p + \Delta t = D_s(N) \] (6-2)

At the pyrolysis zone (N = I):
\[
Z_{I_s} T_s(I - 4)^p + \Delta t + Y_{I_s} T_s(I - 3)^p + \Delta t + X_{I_s} T_s(I - 2)^p + \Delta t
+ A_{s(I)} T_s(I - 1)^p + \Delta t + B_{s(I)} T_s(I)^p + \Delta t + C_{s(I)} T_s(I + 1)^p + \Delta t
+ E_{I_s} T_s(I + 2)^p + \Delta t + F_{I_s} T_s(I + 3)^p + \Delta t + G_{I_s} T_s(I + 4)^p + \Delta t
= D_s(I) \tag{6-3}
\]

Within the uncharred material \((I < N < I + J)\):

\[
A_{s(N)} T_s(N - 1)^p + \Delta t + B_{s(N)} T_s(N)^p + \Delta t + C_{s(N)} T_s(N + 1)^p + \Delta t = D_s(N) \tag{6-4}
\]

At the uncharred layer-insulation layer interface \((N = I + J)\):

\[
Z_{P_s} T_s(I + J - 4)^p + \Delta t + Y_{P_s} T_s(I + J - 3)^p + \Delta t + X_{P_s} T_s(I + J - 2)^p + \Delta t
+ A_{P_s} T_s(I + J - 1)^p + \Delta t + B_{P_s} T_s(I + J)^p + \Delta t
+ C_{P_s} T_s(I + J + 1)^p + \Delta t + E_{P_s} T_s(I + J + 2)^p + \Delta t
+ F_{P_s} T_s(I + J + 3)^p + \Delta t + G_{P_s} T_s(I + J + 4)^p + \Delta t
= D_s(I + J) \tag{6-5}
\]
Within the insulation layer \((I + J < N < I + J + K)\):

\[
A_s(N) T_s(N - 1)^P + \Delta t + B_s(N) T_s(N)^P + \Delta t + C_s(N) T_s(N + 1)^P + \Delta t = D_s(N)
\]

\((6-6)\)

At the back surface of the insulation \((N = I + J + K)\):

\[
Z Z_s T_s(I + J + K - 4)^P + \Delta t + Y Z_s T_s(I + J + K - 3)^P + \Delta t + X Z_s T_s(I + J + K - 2)^P + \Delta t + A Z_s T_s(I + J + K - 1)^P + \Delta t
\]

\[
+ B Z_s T_s(I + J + K)^P + \Delta t = D_z s
\]

\((6-7)\)

Equation 6-1 is combined with Eq. 6-2 written for stations 2, 3, and 4 to obtain an equation relating \(T_s(1)\) and \(T_s(2)\) which is valid at station 1. Also Eq. 6-7 is combined with Eq. 6-6 written for stations \((I + J + K - 4), (I + J + K - 3),\) and \((I + J + K - 2)\) to obtain an equation relating \(T_s(I + J + K - 1)\) and \(T_s(I + J + K)\) which is valid at station \((I + J + K)\). Similarly, the interface equations are combined with equations for neighboring stations to obtain equations relating the interface temperature to the temperature at the two adjacent stations. The resulting set of equations is tri-diagonal and may be written as
Thomas' method for solving Eq. 6-8 is equivalent to Gaussian elimination, but it avoids the error growth associated with the back solution of the elimination method and it minimizes the storage requirements for machine calculations. Ref. 30 summarizes the method as follows: For the set of Eqs. 6-8

let

\begin{align}
W(1) &= B_s(1) \\
W(N) &= B_s(N) - A_s(N) B(N-1) \quad 2 \leq N \leq I + J + K \\
B(N) &= C_s(N) / W(N) \quad 1 \leq N \leq I + J + K - 1
\end{align}

\begin{align}
&\begin{cases}
B_s(1) T_s(1)^P + \Delta t + C_s(1) T_s(2)^P + \Delta t = D_s(1) \quad N = 1 \\
A_s(N) T_s(N-1)^P + \Delta t + B_s(N) T_s(N)^P + \Delta t + C_s(N) T_s(N+1)^P + \Delta t = D_s(N) \quad 1 < N < I + J + K \\
A_s(I + J + K) T_s(I + J + K - 1)^P + \Delta t + B_s(I + J + K) T_s(I + K + K)^P + \Delta t = D_s(I + J + K) \quad N = I + J + K
\end{cases}
\end{align}
The solution is

\[ T_s(I + J + K)P + \Delta t = G(I + J + K) \]  
\[ T_s(N)P + \Delta t = G(N) - B(N) T_s(N + 1)P + \Delta t \quad 1 \leq N \leq I + J + K - 1. \]  

The finite difference equations for the pyrolysis gas pressure within the char layer are of the same form as those for the solid temperature, hence they are solved in the same manner.

The finite difference equations for the pyrolysis gas temperature, conservation of chemical species, and char layer porosity differ from the solid temperature and gas pressure equations in that the equations at internal stations are not symmetric with respect to the diagonal elements. Treatment of the set of equations for the pyrolysis gas temperature is shown as an example.

The set of finite difference equations for the pyrolysis gas temperature is

\[ \begin{align*}
B(N) T(N)^P + \Delta t + C(N) T(N + 1)^P + \Delta t + E(N) T(N + 2)^P + \Delta t &= D(N) \\
1 \leq N \leq I - 2 \\
B(I - 1) T(I - 1)^P + \Delta t + C(I - 1) T(I)^P + \Delta t &= D(I - 1) \\
T(I)^P + \Delta t &= T_s(I)^P + \Delta t.
\end{align*} \]  

\[ (6-12) \]
Since each equation relates the temperature at a station to the temperature at forward stations the solution to this set of equations is obtained directly by working from the pyrolysis zone toward the front surface. Thus

\[
\begin{align*}
T(I)^P + \Delta t &= T_s(I)^P + \Delta t \\
T(I - 1)^P + \Delta t &= [D(I - 1) - C(I - 1) T(I)^P + \Delta t]/B(I - 1) \quad (6-13) \\
T(N)^P + \Delta t &= [D(N) - C(N) T(N + 1)^P + \Delta t] - E(N) T(N + 2)^P + \Delta t]/B(N) \quad 1 \leq N \leq I - 2.
\end{align*}
\]

The differential equation for conservation of mass is solved by numerical integration from the pyrolysis zone, where the mass flow rate of pyrolysis gases is known, to the front surface of the char layer. The transformed mass conservation equation is written in integral form as

\[
\int_a^b \frac{3}{a} (m) \ dx = \ell \int_a^b \left[ \frac{3}{dt} (\eta \rho) - \eta \sum_i R_T M_i \right. - V_c \frac{3}{dx} (\eta \rho) \left. \right] dx. \quad (6-14)
\]

The term on the left side of this equation is integrated immediately to obtain

\[
\hat{\dot{n}} = \hat{n}_a + \ell \int_a^b \left[ \frac{3}{dt} (\eta \rho) - \eta \sum_i R_T M_i - V_c \frac{3}{dx} (\eta \rho) \right] dx. \quad (6-15)
\]
If the lower limit of integration is station \( N \) and the upper limit is the pyrolysis zone \( (N = I) \), Eq. 6-14 becomes

\[
\dot{m}(N) = \dot{m}(I) - \ell \int_{x(N)}^{I} \left[ \frac{\partial}{\partial t} (\eta\rho) - \eta \sum_{i} \frac{R_i}{T_i} M_i \right] \, dx
\]

\[
+ \int_{x(N)}^{I} v_{c} \frac{\partial}{\partial x} (\eta\rho) \, dx. \tag{6-16}
\]

Equation (4-9) for \( v_{c} \) is used in the second integral in Eq. 6-16 and the result is integrated by parts to obtain

\[
\dot{m}(N) = \dot{m}(I) - \ell \int_{x(N)}^{I} \left[ \frac{\partial}{\partial t} (\eta\rho) - \eta \sum_{i} \frac{R_i}{T_i} M_i \right] \, dx
\]

\[
+ v_{c} (I) \eta(I) \rho(I) - v_{c}(N) \eta(N) \rho(N)
\]

\[
- (\dot{\rho}_{g}/\Delta \rho - \dot{\rho}_{s}/\rho_{s}) \int_{x(N)}^{I} \eta \rho \, dx. \tag{6-17}
\]

These sets of equations were programmed for solution by a digital computer. As these equations are quasi-linear it is necessary to iterate to obtain a solution. A total of nine homogeneous and heterogeneous chemical reactions involving 12 gaseous species plus solid carbon were considered.

Table 1 shows the chemical reactions, kinetics data, and rate laws included in the program. Table 2 gives a set of thermophysical properties data for a typical ablation material (low density phenolic-
nylon) which was input to this program. Data for viscosity and thermal conductivity of the gaseous species were obtained from Svehla (Ref. 33). The viscosity and thermal conductivity of the pyrolysis gas mixture are computed using the method presented by Brokaw in Ref. 34. Specific heat and enthalpy data for the gaseous species and enthalpy data for the char layer (solid carbon) were obtained from McBride and Bauer (Refs. 35 and 36).

Appendix A presents a general flow chart of the program. Appendix B gives program usage instructions including definitions of the input terminology. The program Fortran 600 statements are presented in Appendix C. Appendix D defines the program terminology.
Table 1.- Chemical Reactions Involving Pyrolysis Gases and Char (Pike, Ref. 37).

(General reaction: \( aA + bB + \ldots + nN + oO + \ldots \))

\[
k = A \exp \left(\frac{-B}{T}\right)
\]

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Type</th>
<th>Rate law</th>
<th>Frequency factor, A</th>
<th>Activation energy, B</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. ( \text{CH}_4 + \frac{1}{2} \text{C}_2\text{H}_6 + \frac{1}{2} \text{H}_2 )</td>
<td>Homogeneous</td>
<td>( k \exp \left(\frac{7.6 \times 10^{14}}{80} \right) )</td>
<td>7.6 ( \times 10^{14} )</td>
<td>4.775 ( \times 10^{4} )</td>
</tr>
<tr>
<td>2. ( \text{C}_2\text{H}_6 + \text{C}_2\text{H}_4 + \text{H}_2 )</td>
<td>Homogeneous</td>
<td>( k \exp \left(\frac{3.14 \times 10^{15}}{80} \right) )</td>
<td>3.14 ( \times 10^{15} )</td>
<td>3.019 ( \times 10^{4} )</td>
</tr>
<tr>
<td>3. ( \text{C}_2\text{H}_4 + \text{C}_2\text{H}_2 + \text{H}_2 )</td>
<td>Homogeneous</td>
<td>( k \exp \left(\frac{2.57 \times 10^{8}}{80} \right) )</td>
<td>2.57 ( \times 10^{8} )</td>
<td>1.157 ( \times 10^{5} )</td>
</tr>
<tr>
<td>4. ( \text{C}_2\text{H}_2 + 2\text{C} + \text{H}_2 )</td>
<td>Homogeneous</td>
<td>( k \exp \left(\frac{2.14 \times 10^{10}}{80} \right) )</td>
<td>2.14 ( \times 10^{10} )</td>
<td>2.009 ( \times 10^{4} )</td>
</tr>
<tr>
<td>5. ( \text{C}_6\text{H}_6 + 6\text{C} + 3\text{H}_2 )</td>
<td>Homogeneous</td>
<td>( k \exp \left(\frac{1.4 \times 10^{11}}{80} \right) )</td>
<td>1.4 ( \times 10^{11} )</td>
<td>2.622 ( \times 10^{4} )</td>
</tr>
<tr>
<td>6. ( \text{C} + \text{CO}_2 + 2\text{CO} )</td>
<td>Heterogeneous</td>
<td>( k \exp \left(\frac{1.2 \times 10^{12}}{80} \right) )</td>
<td>1.2 ( \times 10^{12} )</td>
<td>4.282 ( \times 10^{4} )</td>
</tr>
<tr>
<td>7. ( \text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2 )</td>
<td>Heterogeneous</td>
<td>( k \exp \left(\frac{9.26 \times 10^{3}}{80} \right) )</td>
<td>9.26 ( \times 10^{3} )</td>
<td>3.524 ( \times 10^{4} )</td>
</tr>
<tr>
<td>8. ( \text{NH}_3 + \frac{1}{2} \text{N}_2 + 1.5\text{H}_2 )</td>
<td>Homogeneous</td>
<td>( k \exp \left(\frac{2.86 \times 10^{6}}{80} \right) )</td>
<td>2.86 ( \times 10^{6} )</td>
<td>3.055 ( \times 10^{4} )</td>
</tr>
<tr>
<td>9. ( \text{NH}_3 + \text{C} \rightarrow \text{HCN} + \text{H}_2 )</td>
<td>Heterogeneous</td>
<td>( k \exp \left(\frac{8.78 \times 10^{6}}{80} \right) )</td>
<td>8.78 ( \times 10^{6} )</td>
<td>3.885 ( \times 10^{4} )</td>
</tr>
</tbody>
</table>
Table 2.- Thermophysical Properties of Low-Density Phenolic-Nylon Ablation Material (Dow and Bush, Ref. 38).

<table>
<thead>
<tr>
<th>Char</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Oxidation kinetics (first order)</strong></td>
<td></td>
</tr>
<tr>
<td>Specific reaction rate constant, $\text{kg/m}^2\text{-sec-atm}$</td>
<td>$4.90\times10^{10}$</td>
</tr>
<tr>
<td>Activation energy, $\text{°K}$</td>
<td>$4.25\times10^4$</td>
</tr>
<tr>
<td><strong>Mass of char removed per mass of oxygen reaching the surface</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.75</td>
</tr>
<tr>
<td><strong>Heat of combustion, J/kg</strong></td>
<td>$1.20\times10^7$</td>
</tr>
<tr>
<td><strong>Heat of sublimation, J/kg</strong></td>
<td>$5.00\times10^7$</td>
</tr>
<tr>
<td><strong>Surface emissivity</strong></td>
<td>0.80</td>
</tr>
<tr>
<td><strong>Theoretical density, kg/m$^3$</strong></td>
<td>$1.43\times10^3$</td>
</tr>
<tr>
<td><strong>Porosity at pyrolysis zone</strong></td>
<td>0.85</td>
</tr>
<tr>
<td><strong>Proportionality constant in equation for gas char heat transfer coefficient, 1/m</strong></td>
<td>$1.00\times10^3$</td>
</tr>
<tr>
<td><strong>Permeability, $\text{m}^2$</strong></td>
<td>$1.00\times10^{-9}$</td>
</tr>
<tr>
<td><strong>Thermal conductivity, W/m-$\text{°K}$, at temperature of</strong></td>
<td></td>
</tr>
<tr>
<td>$278\text{°K}$</td>
<td>0.16</td>
</tr>
<tr>
<td>$833\text{°K}$</td>
<td>0.16</td>
</tr>
<tr>
<td>$1110\text{°K}$</td>
<td>0.50</td>
</tr>
<tr>
<td>$1390\text{°K}$</td>
<td>1.22</td>
</tr>
<tr>
<td>$1670\text{°K}$</td>
<td>1.87</td>
</tr>
<tr>
<td>$1940\text{°K}$</td>
<td>2.65</td>
</tr>
<tr>
<td>$2220\text{°K}$</td>
<td>3.74</td>
</tr>
<tr>
<td>$2500\text{°K}$</td>
<td>4.75</td>
</tr>
<tr>
<td>$2780\text{°K}$</td>
<td>6.24</td>
</tr>
<tr>
<td>$3050\text{°K}$</td>
<td>7.66</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Uncharred Material</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pyrolysis kinetics</strong></td>
<td></td>
</tr>
<tr>
<td>Specific reaction rate constant, $\text{kg/m}^2\text{-sec-atm}$</td>
<td>$7.74\times10^6$</td>
</tr>
<tr>
<td>Activation energy, $\text{°K}$</td>
<td>$1.289\times10^4$</td>
</tr>
<tr>
<td><strong>Effective heat of pyrolysis, J/kg</strong></td>
<td>$1.28\times10^6$</td>
</tr>
<tr>
<td><strong>Specific heat, J/kg-$\text{°K}$, at temperature of</strong></td>
<td></td>
</tr>
<tr>
<td>$311\text{°K}$</td>
<td>$1.51\times10^3$</td>
</tr>
<tr>
<td>$367\text{°K}$</td>
<td>$1.80\times10^3$</td>
</tr>
<tr>
<td>$423\text{°K}$</td>
<td>$2.07\times10^3$</td>
</tr>
<tr>
<td>$478\text{°K}$</td>
<td>$2.24\times10^3$</td>
</tr>
<tr>
<td>$533\text{°K}$</td>
<td>$2.28\times10^3$</td>
</tr>
<tr>
<td>$589\text{°K}$</td>
<td>$2.28\times10^3$</td>
</tr>
<tr>
<td><strong>Thermal conductivity, W/m-$\text{°K}$, at temperature of</strong></td>
<td></td>
</tr>
<tr>
<td>$300\text{°K}$</td>
<td>0.080</td>
</tr>
<tr>
<td>$390\text{°K}$</td>
<td>0.084</td>
</tr>
<tr>
<td>$500\text{°K}$</td>
<td>0.088</td>
</tr>
<tr>
<td>$610\text{°K}$</td>
<td>0.092</td>
</tr>
<tr>
<td>$710\text{°K}$</td>
<td>0.094</td>
</tr>
<tr>
<td>Chemical Species</td>
<td>Mole Fraction</td>
</tr>
<tr>
<td>------------------</td>
<td>--------------</td>
</tr>
<tr>
<td>CH₄</td>
<td>0.0</td>
</tr>
<tr>
<td>H₂</td>
<td>0.294</td>
</tr>
<tr>
<td>C₂H₄</td>
<td>0.0</td>
</tr>
<tr>
<td>C₂H₂</td>
<td>0.0</td>
</tr>
<tr>
<td>CO</td>
<td>0.59</td>
</tr>
<tr>
<td>H₂O</td>
<td>0.0</td>
</tr>
<tr>
<td>NH₃</td>
<td>0.0</td>
</tr>
<tr>
<td>N₂</td>
<td>0.009</td>
</tr>
<tr>
<td>CO₂</td>
<td>0.0</td>
</tr>
<tr>
<td>HCN</td>
<td>0.0</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>0.0</td>
</tr>
<tr>
<td>C₆H₆</td>
<td>0.107</td>
</tr>
</tbody>
</table>
The developments presented in Chapters IV and V represent the usual approach to obtaining numerical solutions to differential equations of engineering and physics. However, the system of algebraic equations resulting from that procedure were found to be unstable for certain conditions. This problem was overcome by including a graded finite difference spacing in the char layer and the uncharred layer and by rewriting the char layer equation (Eq. 4-12) to include the complete term, $H_A(T_s - T)$, in the "$a_3$" term. The graded finite difference spacing was used to reduce the spacing in regions of large gradients (near the front surface of the char layer and in the uncharred layer, near the pyrolysis zone). Numerical solutions have been compared with exact solutions for a number of simplified cases. The results of these comparisons are presented in the following sections.

Comparison of Numerical Results With Exact Solutions

The set of equations whose solution is presented here is too complex to obtain an exact solution for a general case to check the accuracy of the numerical analysis. However, exact solutions have been obtained for a number of simplified problems to serve as a check of results obtained using the finite difference equations.
The exact solutions employed here are for the following problems

(1) The Laplace equation for $P^2$.

(2) Flow of a constant property, incompressible fluid through an isothermal slab.

(3) Heat sink case (flat plate subjected to surface heating).

(4) Quasi-steady ablation case.

Laplace equation for $P^2$.—The differential equation governing the pyrolysis gas pressure in the char layer is given by Eq. 4-47

$$\frac{\partial^2 P^2}{\partial x^2} + \gamma_1 \frac{\partial P^2}{\partial x} + \gamma_2 P^2 + \gamma_3 + \gamma_4 \frac{\partial P^2}{\partial t} = 0 .$$

where the coefficients are not constant. The boundary and initial conditions imposed on $P^2$ are

$$P^2_{x=0} = P^2_w$$

$$\left( \frac{\partial P^2}{\partial x} \right)_{x=1} = 2 \ell R u \left( \frac{\mu T}{\kappa M} \right)_{x=1}^{\frac{1}{m}}$$

Equation 7-1 written for the idealized case of flow of a constant property, incompressible fluid through an isothermal slab with the fluid and slab in thermal equilibrium reduces to the Laplace equation,

$$\nabla^2 P^2 = 0.$$
The solution of the Laplace equation subject to Eq. 7-2 is

\[ P = \left[ \frac{2\mu \ell R T \dot{m}}{kM} x + p_w^2 \right]^{1/2} \]  

(7-3)

Results obtained from Eq. 7-3 were compared with the results from the numerical analysis for this idealized case. These results are shown in Fig. 5a and 5b for \( P_w = 0.01 \) and \( P_w = 0.1 \) Atm, respectively. Note that the error is less than 0.02% for each set of results.

Flow of a constant property incompressible fluid through an isothermal slab. The differential equation governing the pyrolysis gas temperature is given by Eq. 4-30

\[ \frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial \epsilon} = 0 \]  

(7-4)

where the coefficients are not constant. The boundary and initial conditions imposed on \( T \) are

\[
\begin{align*}
T(1,t) &= T_s \\
T(x,0) &= T_s \\
T(1,t) &= T_s \\
T(x,0) &= T_s \\
\end{align*}
\]

(7-5)

The governing energy equation for the idealized case of a constant property incompressible fluid flowing from a reservoir of specified temperature through an isothermal slab (Fig. 6) is
Figure 5a.- Comparison of results for numerical and exact solutions to the Laplace equation for $P^2$ with $P_w = 0.01$ ATM.

$\dot{m}_g = 0.05 \text{ kg/m}^2 \text{ sec}$

$\mu = 2.75 \times 10^{-5} \text{ N-sec/m}^2$

$T = 750^\circ \text{ K}$

$K = 2.0 \times 10^{-10} \text{ m}^2$

$l = 0.01 \text{ m}$
Figure 5b.— Comparison of results for numerical and exact solutions to the Laplace equation for $P^2$ with $P_w = 0.1$ ATM.

$m_g = 0.05 \text{ kg/m}^2\text{-sec}$
$\mu = 2.75 \times 10^{-5} \text{ N-sec/m}^2$
$T = 750^0 \text{ K}$
$K = 2.0 \times 10^{-10} \text{ m}^2$
$l = 0.01 \text{ m}$
Figure 6.— Flow of constant property incompressible fluid through an isothermal slab.
\[
\frac{\partial T'}{\partial x'} + AT' + \frac{\partial T'}{\partial t} = 0
\] (7-6)

where

\[
T' = \frac{T - T_s}{T_0 - T_s}
\]

\[
x' = x/\nu
\]

\[
A = \frac{H_A}{\eta \rho C_p}
\]

and the boundary and initial conditions for \(T'\) are

\[
T'(0,t) = 1.0 \text{ for } t > 0
\]

\[
T'(x',0) = 0.
\] (7-8)

To solve this set of equations the Laplace transform of \(T\) defined by

\[
P = \int_0^\infty e^{-st} T'(x',t) \, dt
\] (7-9)

is introduced. Equations 7-6 and 7-8 become
The solution to Eq. 7-10 is

$$P = \exp (- Ax') \frac{1}{S} \exp (- Sx').$$  

(7-11)

Performing the reverse transformation of Eq. 7-11 gives the solution to Eq. 7-6 and 7-8 as

$$T'(x', t) = \exp(- Ax') S(t - x')$$  

(7-12)

where

$$S(t - x') = \begin{cases} 
0 & \text{when } 0 < t < x' \\
1 & \text{when } t > x'.
\end{cases}$$  

(7-13)

This is just the mathematical expression for a traveling wave of diminishing strength.

This idealized case was solved with $A = 1.0$ and $\lambda/v = 1.0$ using the finite difference equations. These numerical results are compared with the exact solution obtained from Eqs. 7-12 and 7-13 in
Figs. 7a and 7b for dimensionless finite difference spacings of 0.001 and 0.01. The comparison with the transient results is favorable for the fine spacing, but, as expected, the ability to indicate a step change decreases with increased grid spacing. The steady profile solutions differ by less than 0.02% for each case.

**Heat sink case.**—The exact solution for the temperature response of a flat plate subjected to a constant surface heating is (Carslaw and Jaeger, Ref. 39)

\[
T_s = T_{s0} + \frac{q(\ell + \ell')}{k_s} \left\{ \frac{k_s t}{\rho_s \hat{C}_p (\ell + \ell')^2} + \frac{1}{2} (1 - x)^2 - \frac{1}{6} \right\} - 2 \sum_{n=1}^{\infty} \left( \frac{-1}{n^2} \right) \cos \left[ n\pi(1 - x) \right] \exp \left[ -\frac{n^2 \pi^2}{\rho_s \hat{C}_p (\ell + \ell')^2} \right].
\]  

(7-14)

This equation was used to determine the transient response of a flat plate using the heating rate and material properties listed in Table 3. Solutions were obtained for the same problem using the finite-difference equations.

Figure 8 shows a comparison between the numerical results and the exact solution for time steps of 0.01 and 0.1 second. It can be seen that the error at \( t = 2.0 \) second is less than 2.0% for the large time step of 0.1 second.
Figure 7a.— Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with $\Delta X = .001$. 
Figure 7b.— Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with $\Delta X = .01$. 
Table 3.— Inputs Used in Exact Solution to Heat Sink Case.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q$</td>
<td>$1 \times 10^6$ W/m$^2$</td>
</tr>
<tr>
<td>$\ell$</td>
<td>0.01 m</td>
</tr>
<tr>
<td>$\ell'$</td>
<td>0.01 m</td>
</tr>
<tr>
<td>$k_s$</td>
<td>0.624 W/m$^2$-$^\circ$K</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>2140 kg/m$^3$</td>
</tr>
<tr>
<td>$\hat{C}_{p_s}$</td>
<td>715.16 J/kg-$^\circ$K</td>
</tr>
<tr>
<td>$T_{s_0}$</td>
<td>300$^\circ$ K</td>
</tr>
</tbody>
</table>
Figure 8.- Comparison of numerical results with the exact solution for the heat sink problem.
Quasi-steady ablation case.- A quasi-steady-state ablating system is one in which the pyrolysis interface and the front surface recede at the same rate, that is it maintains a constant char thickness. If in addition the pyrolysis gases are inert, incompressible, and in local thermal equilibrium with the char layer, material properties of the system are uniform and independent of temperature, there are no energy sources, viscous dissipation or diffusion and conditions exist such that no energy is transferred into the uncharred layer, an exact solution to the governing mathematical equations can be obtained.

The equation governing the char layer temperature is (Eq. 4-11)

\[
(1 - \eta) \frac{\rho_s C_p}{M_s} \left[ \frac{\partial T_s}{\partial t} - V_c \frac{\partial T_s}{\partial x} \right] - \frac{k_s}{\ell^2} \frac{\partial^2 T_s}{\partial x^2} + \frac{1}{\ell^2} \frac{\partial k_s}{\partial x} \frac{\partial T_s}{\partial x} - H_A(T_s - T) + \eta R_s H(T_s)
\]

\[+ \eta R_s H(T_s) - \eta \sum_r \rho_h h_r^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \varepsilon)\]

\[+ (1 - \eta) q_s'' + \frac{\rho_s H_s}{M_s} \left( \frac{\partial h}{\partial x} - V_c \frac{\partial h}{\partial x} \right) \]

The equation governing the pyrolysis gas temperature is (Eq. 4-27)

\[\eta (v/l - V_c) \left[ \sum_i \frac{\rho_i C_{pi}}{M_{pi}} - R_u \sum_i \frac{\rho_i/M_i}{M_{pi}} \right] \frac{\partial T}{\partial x} - H_A(T_s - T)\]

\[- \eta R_u \left[ \frac{\partial h}{\partial t} - V_c \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial t} \left( \sum_i \frac{\rho_i/M_i}{M_{pi}} \right) + (v/l)\]
\[- V_c \frac{\partial}{\partial x} \left( \sum_{i} \frac{\rho_i}{M_i} \right) \] 

\[- \frac{2}{\eta} \sum_{i} R_{ti} \frac{M_i}{T_i} - \frac{1}{\varrho^2} \frac{\partial}{\partial x} \right) \frac{\partial \varrho}{\partial x} - \eta \sum_{i} \frac{J_{i g_i}}{M_i} + \frac{1}{\varrho^2} \frac{\partial}{\partial x} q_x \]

\[- \eta(A' - e') + \eta R_s H(T)_s + \eta R_{h_s} H_s \]

\[- \sum_{r h} r(r) \Delta H(r) + \eta \left( \sum_{r h} \frac{\rho_i C_p}{M_i} - R_u \sum_{i} \rho_i / M_i \right) \frac{\partial T}{\partial t} = 0. \tag{7-16} \]

With quasi-steady-state ablation, \( \lambda, \dot{\rho}_g, \) and \( \dot{\rho}_s \) are constant and

\[
\frac{\dot{\rho}_g}{\Delta \rho} = \frac{\dot{\rho}_s}{\rho_s} \]

\[
\frac{\partial T_s}{\partial t} = 0 \]

\[
\frac{\partial T_s}{\partial t} = 0. \tag{7-17} \]

Using Eq. 7-17 with the assumptions of no chemical reactions, incompressible pyrolysis gases, constant material properties, and no energy sources, viscous dissipation, or diffusion, Eq. 7-15 and 7-16 reduce to

\[
\frac{\partial^2 T_s}{\partial x^2} + \frac{\varrho}{k_s C_p} \dot{\rho}_s \frac{\partial T_s}{\partial x} - \frac{\varrho}{k_s} H_s(T_s - T) = 0 \tag{7-18} \]
\[ \eta (v/\ell - \dot{m}_s/\rho_{s_0}) \left[ \rho C_p - R_u \sum \rho_i/M_i \right] \frac{\partial^2 T_s}{\partial x^2} - H_A (T_s - T) = 0. \]  

(7-19)

Equations 7-18 and 7-19 are combined to eliminate the term, \( H_A (T_s - T) \), thus

\[ \frac{\partial^2 T_s}{\partial x^2} + \frac{\dot{q}}{k_s} \left[ \frac{\partial^2 T_s}{\partial x^2} - \eta (v - \dot{m}_s/\rho_{s_0}) (\rho C_p \frac{\partial T_s}{\partial x} - R_u \sum (\rho_i/M_i) \frac{\partial T_s}{\partial x}) \right] = 0. \]  

(7-20)

Invoking the assumption of local thermal equilibrium between the pyrolysis gases and char layer \( (T = T_s \text{ and } \frac{\partial T_s}{\partial x} = \frac{\partial T_s}{\partial x}) \) gives

\[ \frac{\partial^2 T_s}{\partial x^2} + D \frac{\partial T_s}{\partial x} = 0 \]  

(7-21)

where

\[ D = \frac{\dot{q}}{k_s} \left[ \frac{\dot{m}_s}{\rho_{s_0}} \frac{C_p}{C_s} + \left( \frac{\dot{m}_g}{\rho_{s_0}} + \eta \frac{\rho\dot{m}_s}{\rho_{s_0}} \right) \left( \frac{C_p}{C_s} \frac{R_u}{N} \right) \right]. \]  

(7-22)

The solution of Eq. 7-21 is

\[ T_s = C_1 + C_2 \exp (-Dx). \]  

(7-23)

The integration constants are determined from the boundary conditions:
The mass loss rates $\dot{m}_s$ and $\dot{m}_g$ and the char layer thickness $\ell$ are obtained from this equation with the following equations

$$\frac{\dot{m}_g}{\Delta \rho} = \frac{\dot{m}_s}{\rho_s}$$

$$\left( \frac{\partial T_s}{\partial x} \right)_{x=0} = \frac{q}{k_s} \left( \dot{m}_s H_C - q_{aero} \right)$$

$$\left( \frac{\partial T_s}{\partial x} \right)_{x=1} = - \frac{\dot{m}_g \Delta H_p}{k_s} q_{aero}$$

where energy transfer into the uncharred layer is neglected. Thus

$$\dot{m}_s = \frac{\rho_{s,g} q_{aero}}{\Delta \rho}$$

$$\dot{m}_s = \frac{q_{aero}}{H_C + \Delta H_p + D' (\bar{T}_1 - \bar{T}_I)}$$

$$\dot{m}_g = \frac{q_{aero}}{H_C + \Delta H_p + D' (\bar{T}_1 - \bar{T}_I)}$$

$$\ell = \frac{k_s}{q_{aero} D'} \left[ H_C + \Delta H_p + D' (\bar{T}_1 - \bar{T}_I) \right] \ln \left[ \frac{\Delta H_p + D' (\bar{T}_1 - \bar{T}_I)}{\Delta H_p} \right]$$
where

\[ D' = \hat{C}_p + \left( \hat{C}_p - \frac{R_u}{M} \right) \left( \frac{\Delta \rho + \eta \rho}{\rho_{so}} \right) \]  

(7-28)

The inputs used to obtain an exact solution to a quasi-steady-state ablation problem are listed in Table 4.

Numerical solutions were obtained using the finite difference equations. The assumption of incompressibility was satisfied by specifying the pyrolysis gas density to be constant. In an attempt to satisfy the assumption of local thermal equilibrium between the pyrolysis gases and the char layer a very large value was used for the proportionality constant appearing in the equation for \( H_A \), the convective heat transfer coefficient,

\[ H_A = \frac{K_h v}{N_{Pr}} \sum \frac{\rho_i C_p_i}{M_i} \]  

(7-29)

Calculations were made using a value for \( K_h \) of \( 5 \times 10^5 \) 1/m yet a temperature difference of \( 1.5^\circ \)K exists between the char layer and the pyrolysis gases at the front surface. These results are compared with the exact solution in Table 5. Note that the char thickness and mass loss rates are within 2% of the exact solution.

An additional set of calculations was made in which the pyrolysis gas temperature was set equal to the char layer temperature and the term, \( H_A(T_s - T) \), appearing in the char layer equation was replaced using the following equation
### Table 4.- Inputs Used in Exact Solution to Quasi-Steady-State Ablation Case.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q_{aero}$</td>
<td>$0.8 \times 10^5$ W/m$^2$</td>
</tr>
<tr>
<td>$k_s$</td>
<td>$0.624$ W/m$^2$ K</td>
</tr>
<tr>
<td>$\rho_{so}$</td>
<td>$320.$ kg/m$^3$</td>
</tr>
<tr>
<td>$\Delta \rho$</td>
<td>$320.$ kg/m$^3$</td>
</tr>
<tr>
<td>$\hat{C}_{ps}$</td>
<td>$2090.$ J/kg K</td>
</tr>
<tr>
<td>$\hat{C}_{ps}$</td>
<td>$2090.$ J/kg K</td>
</tr>
<tr>
<td>$\overline{T}_I$</td>
<td>$2222.$ K</td>
</tr>
<tr>
<td>$\overline{T}_I$</td>
<td>$556.$ K</td>
</tr>
<tr>
<td>$\Delta H_P$</td>
<td>$2.324 \times 10^6$ J/kg</td>
</tr>
<tr>
<td>$H_C$</td>
<td>$2.324 \times 10^6$ J/kg</td>
</tr>
<tr>
<td>$M$</td>
<td>$0.029$ kg/g-mole K</td>
</tr>
</tbody>
</table>
Table 5.—Comparison of the Exact Solution and the Numerical Solution Obtained with $K_h = 5 \times 10^5$ l/m for a Quasi-Steady State Condition.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Numerical Solution</th>
<th>Exact Solution</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{m}_s$, kg/m$^2$sec</td>
<td>$7.304 \times 10^{-2}$</td>
<td>$7.185 \times 10^{-2}$</td>
<td>1.66</td>
</tr>
<tr>
<td>$\dot{m}_g$, kg/m$^2$sec</td>
<td>$7.301 \times 10^{-2}$</td>
<td>$7.185 \times 10^{-2}$</td>
<td>1.61</td>
</tr>
<tr>
<td>$\lambda$, m</td>
<td>$2.924 \times 10^{-3}$</td>
<td>$2.973 \times 10^{-3}$</td>
<td>-1.65</td>
</tr>
</tbody>
</table>
Thus the assumption of local thermal equilibrium between the pyrolysis gases and the char layer was satisfied. Results from this set of calculations shown in Fig. 9 are within 1% of the exact solution. Note that the system reached a quasi-steady-state condition after only 30 sec. The near discontinuity in the surface removal rate curve illustrates the three regimes of mass removal at the surface. The initial segment of the curve represents that portion of time when oxidation of the char layer was governed by the exponential rate equation. The second portion of lesser slope represents the time period when the rate of oxidation of the char was governed by the rate of diffusion of oxygen through the boundary layer. The final portion of the curve represents the time during which the char layer was subliming.
Figure 9.- Numerical results for $\dot{m}_s$, $\dot{m}_g$, $l$, surface temperature, and pyrolysis temperature for a case run to quasi-steady-state condition.
CHAPTER VIII

RESULTS AND DISCUSSION

The analysis of heat transfer and ablation mechanisms present in ablative thermal protection systems during entry is of major importance in the design of heat shields for aerospace applications. The role that ablation analysis plays in the total program of heat shield design is shown in Fig. 10. The first stage of the program involves defining the entry environment. This definition is obtained from trajectory analysis experts. Once the environment is defined a heat shield material can be selected - the material may be one of a family of existing materials or it may be necessary to develop a new material which possesses characteristics required for a particular trajectory. Thermo-physical property data are then obtained. The definition of the environment and the material characterization are then used in a computer program to determine the response of the material to entry conditions. Because of uncertainties in the material characterization and simplifying assumptions made in the analysis, it is necessary to have checks on the results. Initially, the material is subjected to simulated entry conditions in our ground test facilities. Later the material may be flight-tested. There frequently is feedback from the analysis and ground test phases to the materials development phase to obtain improved materials. It is sometimes necessary to adjust the property data which typically contains many uncertainties to obtain good agreement between numerical and experimental data. Once the
Figure 10. - The role of ablation analysis in the design of thermal protection systems for aerospace applications.
computed results are found to be satisfactory the analysis is used to
determine the amount of ablation material required for the mission.

Results from a typical computer calculation for an ablation system
subjected to a square heat pulse are presented in Figs. 11-13 as an
illustration of the type of data available from this analysis. The
heating rate, enthalpy, and pressure histories for this calculation
are given in Table 6. The ablation system properties considered in
this calculation are those given in Table 2. Figure 11 shows time
histories of surface removal rate, pyrolysis rate, char thickness,
char surface temperature, and pyrolysis gas temperature at the surface
for this calculation. Of particular interest in Fig. 11 is the
short time during which the mode of performance is highly transient.
After 100 seconds the temperature and mass transfer rates are changing
much slower than initially. The spike in $\dot{m}_g$ occurring at 10 sec
corresponds to the rapid increase in system temperature at initiation
of heating. The sharp drop in $\dot{m}_g$ results from the growth of the char
layer which insulates the pyrolysis zone and the blocking effect of the
pyrolysis gases which reduces the rate of heat transfer to the char
surface. The substantial difference in temperature of the char and
pyrolysis gases at times less than 50 sec results from two factors —1) Because of the thin char layer at early times, the fluid mechanical
time is very small as is the energy transfer per mass of pyrolysis gas;
and 2) For very low surface pressures, the reduction in gas temperature
Table 6.- Trajectory Data Used in Making Calculation for a Typical Ablation System.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q_c$, W/m², at time, sec</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>$2.162 \times 10^3$</td>
</tr>
<tr>
<td>10</td>
<td>$8.0 \times 10^5$</td>
</tr>
<tr>
<td>1000</td>
<td>$8.0 \times 10^5$</td>
</tr>
<tr>
<td>$P_w$, N/m², at time, sec</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>$1.0 \times 10^{-6}$</td>
</tr>
<tr>
<td>9</td>
<td>$1.0 \times 10^{-4}$</td>
</tr>
<tr>
<td>29</td>
<td>$9.0 \times 10^{-4}$</td>
</tr>
<tr>
<td>39</td>
<td>$1.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>1000</td>
<td>$1.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>$H_e$, J/kg</td>
<td>$3.1 \times 10^5$</td>
</tr>
<tr>
<td>$C_e$</td>
<td>0.23</td>
</tr>
</tbody>
</table>
Figure 11.- Typical time histories of $\dot{m}_s$, $\dot{m}_g$, $l$, surface temperature, and pyrolysis gas temperature at the surface for an ablation system subjected to a square heat pulse.
associated with expansion of the pyrolysis gas flowing through the char layer is appreciable. The rate controlled and diffusion controlled regimes of surface oxidation are obvious in Fig. 11. The initial steep slope (highly temperature dependent) is associated with the rate controlled oxidation regime. The $\dot{m}_s$ curve undergoes an orderly transition on the much flatter region which corresponds to the diffusion controlled oxidation regime.

Figures 12 and 13 show profiles of pyrolysis gas temperature, molecular weight, mass flow rate, and pressure and char layer temperature and porosity at times of 50 and 500 sec, respectively, for the case whose data are presented in Fig. 11. Note that $x = 0$ is the char layer surface and $x = 1$ is the pyrolysis zone. Of particular interest in Fig. 12 is the greater temperature difference between the char layer and pyrolysis gas near the pyrolysis zone. The difference in temperature is greater in this region because of the larger gradient in char layer temperature. As the pyrolysis gas temperature increases to about 1200° K the chemical reactions and mass transfer processes within the system become significant. The decrease in molecular weight results from a breaking down of larger molecular weight species and loss of carbon through deposition of solid carbon in the porous char layer. The rate of carbon deposition is reflected in the reduced local mass flow rate ($\dot{m}$). The net carbon deposited is indicated by the porosity profile.

The profiles in Fig. 13 are of the same form as those in Fig. 12. Because of the larger char layer thickness at 500 sec the pyrolysis gas temperature is nearer the char layer temperature in the region near the surface.
Figure 12.- Profiles of pyrolysis gas temperature, char layer temperature, pyrolysis gas molecular weight, char porosity, local mass flow rate, and pyrolysis gas pressure at a time of 50 sec for the case represented in Fig. 11.

Char thickness $= 5.46 \times 10^{-3}$ m

$P_w = 1.013 \times 10^4$ N/m$^2$

$m_g = 3.54 \times 10^{-2}$ kg/m$^2$-sec

$M = 2.573 \times 10^{-2}$ kg/g-mole

$T_{s1} - T_{sI} = 1102^0$ K

$P - P_w$
Figure 13.- Profiles of pyrolysis gas temperature, char layer temperature, pyrolysis gas molecular weight, char porosity, local mass flow rate, and pyrolysis gas pressure at a time of 500 sec for the case represented in Fig. 11.
CHAPTER IX

SUMMARY

The differential equations governing the transient response of a one-dimensional ablative thermal protection system undergoing stagnation ablation have been derived for the general case of thermal non-equilibrium between the pyrolysis gases and the char layer and kinetically controlled chemical reactions and mass transfer between the pyrolysis gases and the char layer. The boundary conditions have been written for the particular case of stagnation heating with surface removal by oxidation or sublimation and pyrolysis of the uncharred layer occurring in a plane.

The governing equations and boundary conditions have been solved numerically using the modified implicit method (Crank-Nicolson method). Exact solutions were obtained for a number of simplified problems. Numerical results compared favorably with exact results in every instance.

Numerical results were presented for a typical ablation system subjected to a square heat pulse. The effects of chemical reactions and mass transfer are pronounced.
REFERENCES


APPENDIX A

GENERAL FLOW CHART

START
Read Data
Initialize Program Constants
Write Input Data And Initial Conditions
Check Iteration Count, Max Count

1

2

Less Than Max

Reduce Time Step

Calculate Pyrolysis Rate
Calculate Surface Heating and Pressure
Calculate Surface Removal Rate
Determine Property Data For Char Layer and Pyrolysis Gases
Continue
Transfer To Subroutine VISC: Determine Viscosity And Prandtl Number
Continue

Transfer To Subroutine PDE2:
Calculate Tri-diagonal Matrix Coefficients
And Solve Matrix For T

3

Calculate New Thickness Values
For Char and Uncharred Layers

Check Solutions

No

Go To 1

Yes

Print Results

Less Than Min.

Check Thickness Uncharred Layer

Stop

Greater Than Min.

Check Time

Greater Than Max.

Less Than Max.

Replace Old Parameters With New Values

Stop

Greater Than 1

Check Iteration Count

Equal 1

Go To 2

Increase Time Step

Go To 2
This program calculates the transient response of a one-dimensional ablative thermal protection system subjected to stagnation heating. It treats thermal non-equilibrium between the pyrolysis gases and the char layer, mass transfer between the fluid and solid phases, and a total of nine chemical reactions involving twelve gaseous species plus solid carbon. Surface removal by oxidation or sublimation and pyrolysis of the uncharred material occurring in a plane are considered. It considers a single layer of ablation material backed up by a single layer of insulation material with heat sinks between the ablation material and the insulation and behind the insulation. A maximum of 50 stations each may be considered for the char layer and the uncharred layer of the ablation material and a maximum of 10 stations may be considered for the insulation.

INPUT

FORTRAN IV NAMELIST with the names PERM, PIKUP, and LIST is used to load the input data. PERM contains physical constants, program constants and tables of thermodynamic and chemical kinetics data which are considered to be permanent inputs. PIKUP contains initial solutions plus selected program constants and material properties. These data are changed when beginning a computer calculation at some time other
than 0. seconds. LIST contains those data and system parameters which are most frequently changed from one calculation to another. The following list contains the input variables with the dimensions used in the program. The NAMELIST name containing each variable is indicated in its description. The size of an array is limited to the dimensions stated.

<table>
<thead>
<tr>
<th>FORTRAN VARIABLE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC</td>
<td>Specific reaction rate constant for first order oxidation of char layer (LIST).</td>
</tr>
<tr>
<td>ACEF(12)</td>
<td>Specific reaction rate constant for forward chemical reaction (PERM).</td>
</tr>
<tr>
<td>ACER(12)</td>
<td>Specific reaction rate constant for reverse chemical reaction (PERM).</td>
</tr>
<tr>
<td>AEXP</td>
<td>Specific reaction rate constant for pyrolysis of uncharred material (LIST).</td>
</tr>
<tr>
<td>ALFC</td>
<td>Weight factor for transpiration effectiveness of mass removal by oxidation or sublimation (LIST).</td>
</tr>
<tr>
<td>ALFP</td>
<td>Weight factor for transpiration effectiveness of pyrolysis gases (LIST).</td>
</tr>
<tr>
<td>ALPHA</td>
<td>Absorptivity of char surface (LIST).</td>
</tr>
<tr>
<td>BC</td>
<td>Activation temperature for first order oxidation of char layer (LIST).</td>
</tr>
<tr>
<td>BCEF(12)</td>
<td>Activation temperature for forward chemical reaction (PERM).</td>
</tr>
<tr>
<td>BCER(12)</td>
<td>Activation temperature for reverse chemical reaction (PERM).</td>
</tr>
<tr>
<td>BEXP</td>
<td>Activation temperature for pyrolysis of uncharred material (LIST).</td>
</tr>
<tr>
<td>CE</td>
<td>Mass fraction of oxygen at edge of boundary layer (LIST).</td>
</tr>
</tbody>
</table>
CPKT(40,12) Table of gaseous species heat capacity versus temperature (PERM).

CPPPV Constant heat capacity of insulation layer (LIST).

CPPT(40) Table of uncharred material heat capacity versus temperature (LIST).

CPSV Constant heat capacity of char layer (LIST).

CRNI Crank-Nicolson factor, 1/2 for modified implicit solutions (PERM).

DHC Heat of combustion of char layer (LIST).

DHP Heat of pyrolysis of uncharred material (LIST).

DIFER Convergence criteria for solid temperature equation (PERM).

DRHO Difference in density of uncharred material and density of char layer at the pyrolysis zone (LIST).

DT Time increment (PIKUP).

DX Distance between finite difference stations in char layer in region of course grid spacing (PERM).

DX1 Distance between finite difference stations in char layer in region of fine grid spacing (PERM).

DXP Distance between finite difference stations in uncharred layer in region of course grid spacing (PERM).

DXP1 Distance between finite difference stations in uncharred layer in region of fine grid spacing (PERM).

DXPP Distance between finite difference stations in insulation layer (PERM).

EPSP Emissivity of radiating heat sink surface behind insulation layer (LIST).

EPSS Emissivity of char surface (LIST).

ETA(50) Porosity of char layer (PIKUP).

HC Heat of sublimation of char layer (LIST).

HE Enthalpy of free stream (LIST).
HKT(40,13)  Table of gaseous species enthalpy versus temperature (PERM).
HSTT(40)  Table of char layer enthalpy versus temperature (PERM).
HTSK  Value of \(\rho C_p,\&\) for heat sink at uncharred layer insulation layer interface (LIST).
HTSKP  Value of \(\rho C_p,\&\) for heat sink behind insulation layer (LIST).
I  Number of finite difference stations in char layer (PERM).
IL  Thickness of insulation layer (LIST).
IOPTI  Trigger for selecting method of computing pyrolysis rate (LIST).
IOPTP  Trigger for selecting method of determining wall pressure (LIST).
IOPT1  Trigger for selecting method of computing surface removal by sublimation (LIST).
IZ  Total number of finite difference stations in char layer, uncharred layer and insulation layer (PERM).
ITR  Maximum iteration count (LIST).
JK  Number of finite difference stations in uncharred layer (PERM).
KPPI  Thermal conductivity of uncharred layer at pyrolysis zone (PIKUP).
KPPV  Constant thermal conductivity of insulation layer (LIST).
KPT(40)  Table of uncharred material thermal conductivity versus temperature (LIST).
KSPI  Thermal conductivity of char layer at pyrolysis zone (PIKUP).
KSP1  Thermal conductivity of char layer at surface (PIKUP).
KST(40)  Table of char layer thermal conductivity versus temperature (LIST).
KT  Number of gaseous species considered (PERM).
KUPT(40,12)  Table of gaseous species thermal conductivity versus temperature (PERM).
L  Initial thickness of char layer (PIKUP).
LAM Ratio of mass char layer removed to free stream oxygen consumed in first order oxidation of char (LIST).
LP  Initial thickness of uncharred layer (PIKUP).
LPMIN  Minimum thickness of uncharred layer (PERM).
M(13)  Molecular weight of chemical species (PERM).
MCPP Order of interpolation in CPPT (LIST).
MFK(50,12)  Initial mole fraction of gaseous species (PIKUP).
MFKI(12) Mole fraction of gaseous species at pyrolysis zone (LIST).
MGDOT Initial rate of pyrolysis of uncharred layer (PIKUP).
MKP Order of interpolation in KPT (LIST).
MKS Order of interpolation in KST (LIST).
MNO Order of interpolation in HSTT, HKT, CPKT, MUKT and KUPT (PERM).
MQC Order of interpolation in QCTAB (LIST).
MSDOT Initial rate of surface removal (PIKUP).
MSQPT Order of interpolation in SQPT (LIST).
MUKT(40,12)  Table of gaseous species viscosity versus temperature (PERM).
NCPP Number of entries in KPT (LIST).
NKS Number of entries in KST (LIST).
NNO Number of entries in HSTT, HKT, CPKT, MUKT and KUPT (PERM).
NQC Number of entries in QCTAB (LIST).
NRCT Number of chemical reactions considered (PERM).
NSQPT Number of entries in SQPT (LIST).
P  Initial pyrolysis gas pressure (PIKUP).
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMV</td>
<td>Constant permeability of char layer (LIST).</td>
</tr>
<tr>
<td>PRNTFRQ</td>
<td>Time interval for printing output (PIKUP).</td>
</tr>
<tr>
<td>PROPC</td>
<td>Proportionality constant in expression for $H_A$ (LIST).</td>
</tr>
<tr>
<td>PTIME</td>
<td>Time at start of calculation (PIKUP).</td>
</tr>
<tr>
<td>QCTAB(40)</td>
<td>Table of cold wall heating rate versus time (LIST).</td>
</tr>
<tr>
<td>QRS</td>
<td>Radiant heat transfer at surface (LIST).</td>
</tr>
<tr>
<td>RAD</td>
<td>Vehicle nose radius for hypersonic velocities (LIST).</td>
</tr>
<tr>
<td>RHOPPV</td>
<td>Constant density of insulation layer (LIST).</td>
</tr>
<tr>
<td>RHOST</td>
<td>Theoretical density of char layer (LIST).</td>
</tr>
<tr>
<td>RU</td>
<td>Universal gas constant (PERM).</td>
</tr>
<tr>
<td>SGMA</td>
<td>Stephan-Boltzmann constant (PERM).</td>
</tr>
<tr>
<td>SQPT(40)</td>
<td>Table of square root of wall pressure versus time (LIST).</td>
</tr>
<tr>
<td>T</td>
<td>Initial pyrolysis gas temperature (PIKUP).</td>
</tr>
<tr>
<td>T1BAR</td>
<td>Sublimation temperature of char layer (LIST).</td>
</tr>
<tr>
<td>TCPP(40)</td>
<td>Temperature table for CPPT (LIST).</td>
</tr>
<tr>
<td>TEMP (40)</td>
<td>Temperature table for HSTT, HKT, CPKT, MKT and KUPT (PERM).</td>
</tr>
<tr>
<td>TIBAR</td>
<td>Maximum temperature of pyrolysis zone (LIST).</td>
</tr>
<tr>
<td>TIME</td>
<td>Time at start of calculation (PIKUP).</td>
</tr>
<tr>
<td>TIMET(40)</td>
<td>Time table for QCTAB (LIST).</td>
</tr>
<tr>
<td>TKP(40)</td>
<td>Temperature table for KPT (LIST).</td>
</tr>
<tr>
<td>TKS(40)</td>
<td>Temperature table for KST (LIST).</td>
</tr>
<tr>
<td>TMPRESS(40)</td>
<td>Time table for SQPT (LIST).</td>
</tr>
<tr>
<td>TRAB</td>
<td>Trigger for selecting blocking approximation (LIST).</td>
</tr>
<tr>
<td>TREF</td>
<td>Transpiration effectiveness (LIST).</td>
</tr>
<tr>
<td>TS</td>
<td>Initial char layer temperature (PIKUP).</td>
</tr>
</tbody>
</table>
OUTPUT

The computed results are available in tabular form. The following tabular data are printed at time intervals determined by the input PRNTFRQ.

1. Time, sec.
2. Current time increment, sec.
3. Number of iterations required to obtain solution.
4. Temperature of char layer surface, K.
5. Temperature of pyrolysis gases leaving char layer, K.
6. Ratio of energy conducted into char layer to cold wall heating rate.
7. Surface removal rate, kg/m$^2$-sec.
8. Rate of pyrolysis of uncharred layer, kg/m$^2$-sec.
9. Pyrolysis gas mass injection rate at surface, kg/m$^2$-sec.
10. Char layer thickness, m.
11. Uncharred layer thickness, m.
12. Temperature at each station of char layer, uncharred layer and insulation layer, K.
13. Porosity of char layer at each station.
14. Pyrolysis gas temperature at each station, K.
15. Pyrolysis gas pressure at each station, N/m$^2$.
16. Mole fraction of gaseous species at each station.
17. Average molecular weight of pyrolysis gas at each station, kg/m$^m$-mole.
18. Mass flow rate of pyrolysis gases at each station, kg/m$^2$-sec.
APPENDIX C

PROGRAM IN FORTRAN 600 STATEMENTS
PROGRAM ABLATE(INPUT, OUTPUT, TAPE5=INPUT, TAPE2=OJTPJT)

A NUMERICAL SOLUTION OF THE DIFFERENTIAL EQUATIONS GOVERNING THE
TRANSIENT RESPONSE OF A ONE-DIMENSIONAL ABLATION SYSTEM INCLUDING
EFFECTS OF THERMAL NON-EQUILIBRIUM, MASS TRANSFER, AND CHEMICAL
REACTIONS.

REFERENCE— CLARK, RONALD K.— A NUMERICAL ANALYSIS OF THE TRANSIENT RESPONSE OF AN ABLATION SYSTEM INCLUDING EFFECTS OF THERMAL NON-EQUILIBRIUM, MASS TRANSFER, AND CHEMICAL KINETICS.

DOCTOR OF PHILOSOPHY DISSERTATION, VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY, BLACKSBURG, VA. 1972.

PRIMARY INPUTS

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DHC</td>
<td>Heat of Combustion of Char Layer</td>
</tr>
<tr>
<td>DHP</td>
<td>Heat of Pyrolysis</td>
</tr>
<tr>
<td>DRHO</td>
<td>Density Change Across Pyrolysis Interface</td>
</tr>
<tr>
<td>DT</td>
<td>Time Increment</td>
</tr>
<tr>
<td>EPSP</td>
<td>Back Surface Emissivity</td>
</tr>
<tr>
<td>EPSS</td>
<td>Char Surface Emissivity</td>
</tr>
<tr>
<td>H0C</td>
<td>Heat of Sublimation of Char Layer</td>
</tr>
<tr>
<td>HE</td>
<td>Enthalpy of Free Stream</td>
</tr>
<tr>
<td>HTSK</td>
<td>Value of Thermal Capacity of Heat Sink at Back of Uncarved Material</td>
</tr>
<tr>
<td>HTSKP</td>
<td>Value of Thermal Capacity of Heat Sink at Back of Insulation Layer</td>
</tr>
<tr>
<td>IOPT1</td>
<td>Trigger for Selecting Method of Computing Pyrolysis Rate. (IOPT1=0 no restriction on temperature of pyrolysis zone—pyrolysis rate computed using Arrhenius type rate equation, IOPT1=1 temperature of pyrolysis zone limited to TIBAR—pyrolysis rate computed using energy balance when TS(I)=TIBAR)</td>
</tr>
<tr>
<td>IOPT1</td>
<td>Trigger for Selecting Mode of Behavior of Surface Temperature During Sublimation. (IOPT1=0 no restriction on surface temperature, IOPT1=1 surface temperature limited to TIBAR)</td>
</tr>
</tbody>
</table>
IUPTP triggers for selecting method of computing wall pressure. (IUPTP=1 use table lookup, IUPTP=0 compute wall pressure from hypersonic flow theory)

- KT: number of gaseous species considered
- LOP: initial thickness of uncharred layer
- NRCT: number of chemical reactions considered
- OCTAB: table of cold wall convective heating rate vs time
- QRS: radiant heating rate
- RAD: radius of body
- KHOST: theoretical density of char material
- SQPT: table of wall pressure vs time
- TIBAR: maximum temperature of pyrolysis zone used with
- TIBBAR: sublimation temperature of char layer

Chemical species identification:
1. CH4
2. H2
3. C2H4
4. C2H2
5. CO
6. H2O
7. NH3
8. N2
9. CO2
10. HCN
11. C2H6
12. C6H6
13. C (solid)

For double subscripted quantities—first subscript refers to reaction, station, or temperature and second subscript refers to chemical species.

Dimension:
11, KSPI, KPPI, PRNTFRQ
NAMELIST /LIST/ PROPC, ALFC, ALFP, ALPHA, DHC, ITR, QRS, EPSS, EPSN, HC, RHO
1ST, RAD, TIBAR, DIP, LAM, CE, AC, BC, HE, TREF, TRAB, MFKI, AEXP, BEXP, IL, CPPPV
2, KPPV, RHOPPV, HTSK, HTSKP, CPSV, PMV, KPT, TKP, MKS, NKS, KST, CPPT, TCPP, MCP
3, NCPP, MKP, TIMET, QCTAB, MQC, NQC, TMPRES, SQPT, MSQPT, NSQPT, TKS, NKP, IOP
4, T, IOPTI, TIBAR, IOPTP, DRHO

C READ INPUT DATA
READ (5, PERM)
READ (5, PIKUP)
READ (5, LIST)

C INITIALIZE PROGRAM CONSTANTS
KTT = KT + 1
KM = KT - 2
IM = I - 1
IN = I + 1
IN2 = I + 2
IP = I + JK
IOD = IP - 1
ID = IP - 2
NITC = 0
NITA = 0
MS = M (13)
AINT1(I) = 0
AINT3(I) = 0
IP1 = IP + 1
IZ1 = IZ - 1
NIT = 0
NITG = 0
ICHCOM = 0
NTIME = 0

C CONVET INPUT DATA TO PROPER UNITS (SYSTEM INTERNATIONAL)

C DATA FOR HEAT CAPACITY OF CHAR LAYER- SOLID CARBON- ARE INPUT
C IN UNITS OF JOULES/KILOGRAM (.012 KILOGRAM/G-10LE)
C DATA FOR HEAT CAPACITY AND ENTHALPY ARE INPUT WITH ENERGY IN
C UNITS OF THERMOCHEMICAL CALORIE (4.184 J/CAL)
C DATA FOR VISCOSITY OF GASEUUS SPECIES ARE INPUT IN UNITS OF
POISES (0.0000001 NEWTON-SECOND/METER SQ PER POISE)

CPSV=.012*CPSV
DO 1 K=1,NRCT
BCEF(K)=4.184*9CEF(K)
ACER(K)=0.
1 BGER(K)=4.184*8CER(K)
DO 2 N=1,NNO
HSTT(N)=HSTT(N)*4.184
DO 2 K=1,KT
MUKT(N,K)=MUKT(N,K)*1.E-7
KUPT(N,K)=KUPT(N,K)*4.184E-4
IF (K.GT.KM) GO TO 2
CPKT(N,K)=4.184*CPKT(N,K)
HKT(N,K)=4.184*HKT(N,K)
2 CONTINUE
DO 3 N=1,NNO
C WRITE INPUT DATA
3 HKT(N,13)=4.184*HKT(N,13)
WRITE (2,PERM)
WRITE (2,PIKJP)
WRITE (2,LIST)
C INITIALIZE ALL PARAMETERS
KS(1)=KSP1
KS(I)=KSP1
KP(I)=KSP1
MGDOTP=MGDOT
MSDOTP=MSDOT
LPP=L
LPPP=LP
QPNET=SGMA*EPS*TS(IZ)**4
DO 6 N=1,I
DETADX(N)=0.
DRODX(NJ)=0.
AMDOT(N)=MGDOT
PP(N)=P(N)
RHD(N) = 0.
RHS(N) = 0.
RS(N) = 0.
RUM(N) = 0.
DO 4 KI = 1, <T
RHOK(N,KI) = P(N) * M(KI) * MFK(N,KI) / (RJ * T(N))
ROM(N) = RJM(N) + RHOK(N,KI) / M(KI)
RHOKP(N,KI) = RHOK(N,KI)
DHJ(N,KI) = 0.
K(N,KI) = 0.
RHR(N,KI) = 0.
4 RHQ(N) = RHQ(N) + RHOK(N,KI)
PRHM(N) = PROM(N)
V(N) = -MGDOTP / (RHO(N) * ETA(N))
KOPM(N) = P(N) * 2. / (RJ * T(N))
DO 5 K = 1, KT
5 PMGDOT(N,K) = -RHOK(N,K) * V(N)
DVDX(N) = 0.
6 PRHD(N) = RHO(N)
DO 7 N = 1, IP
TSP(N) = TS(N)
PTS(N) = 300.
IF (N .GT. I) GO TO 7
PT(N) = 300.
AP(N) = 0.
TP(N) = T(N)
ETA(N) = .85
7 CONTINUE
DO 8 N = IP, IZ
PTS(N) = 300.
TSP(N) = TS(N)
8 CONTINUE


\[ \frac{1}{212}(0.20) + \frac{1}{213}(1.0) + 214 \]

\( \text{GO TO 12} \)

\( \text{BEGIN ITERATION} \)

\( \text{CONTINUE} \)

\( \text{IF (NIT.GE.40)) GO TO 12} \)

\( \text{ESTIMATE SOLUTION AT NEXT TIME STEP} \)

\( \text{DO 11 N=1,IL} \)

\( \text{TS(N)} = \text{TS(N)} + \text{YT}(N) \times \text{DT} \)

\( \text{IF (N.GT.IL) GO TO 11} \)

\( \text{RHU(N)} = \text{RHU(N)} + \text{YRH}(N) \times \text{DT} \)

\( \text{T(N)} = \text{T(N)} + \text{YT}(N) \times \text{JT} \)

\( \text{P(N)} = \text{P(N)} + \text{YP}(N) \times \text{DT} \)

\( \text{ETA(N)} = \text{ETA(N)} + \text{YETA}(N) \times \text{DT} \)

\( \text{DO 10 K=1,KT} \)

\( \text{RHUK(N,K)} = \text{RHUK(N,K)} + \text{YRHUK(N,K)} \times \text{DT} \)

\( \text{CONTINUE} \)

\( \text{NIT=NIT+1} \)

\( \text{RHOSO=RHOST*(1.-ETA(1))} \)

\( \text{Determine heating at back surface} \)

\( \text{QNET=SGMA*EPSSP*TS(1L)**4} \)

\( \text{CHECK ITERATION COUNT— REDUCE TIME STEP IF MAX ITER EXCEEDED} \)

\( \text{IF (NIT.LT.10)) GO TO 15} \)

\( \text{TIME=TIME-\text{DT}} \)

\( \text{MGDOT=MGDOTP} \)

\( \text{DO 14 N=1,IL} \)

\( \text{IF (N.GT.IL) GO TO 14} \)

\( \text{DO 13 K=1,KT} \)

\( \text{RHUK(N,K)} = \text{RHUKP(N,K)} \)

\( \text{T(N)} = \text{TP}(N) \)

\( \text{RHU(N)} = \text{PRHIC(N)} \)

\( \text{P(N)} = \text{PP}(N) \)

\( \text{ETA(N)} = \text{ETAP}(N) \)

\( \text{TS(N)} = \text{TS}(N) \)

\( \text{HBKKN2=PHBFKN2} \)

\( \text{HBKKN2=PHBFK12} \)
L=LPP
LP=LPPP
DT=.75*DT
GO TO 109
CONTINUE
C
COMPUTE MASS RATE OF PURULYSIS GAS GENERATED AT INTERFACE
C
CALCULATE PYROLYSIS RATE
C
CHECK IOPTI= IOPTI=1 AND TS(I)=TIBAR USE EQ 3-42 FOR MGDOT
C
IOPTI=0 USE EQ 3-44 FOR MGDOT
IF (NIT.GT.1) GO TO 20
SP=1.0
IF (TS(I).LE.(TI3AR-6.)) GO TO 16
SP=(TIBAR-TS(I))/6.
IF (SP.LT.0.) SP=0.
CONTINUE
IF ((MGDOT.GT.1.E-5).AND.(NITA.EQ.1)) GO TO 17
NITP=0
IF (MGDOT.GT.1.E-3) NITP=1
IF ((NITP.EQ.1).AND.(NITA.EQ.0)) DT=.0525
1 CONTINUE
TIME=TIME+DT
GO TO 19
18 MGDOT=AEXP*EXP(-BEXP/TS(I))
19 CONTINUE
IF (MGDOT.GT.0.) GO TO 21
MGDOT=0.
IF (IOPTI.EQ.0) GO TO 21
TS(I)=TS(I)-1.E-4
20 CONTINUE
IF (IOPTI.EQ.0) GO TO 18
AMGDOT=AEXP*EXP(-BEXP/TS(I))
BMGDOT=(-KS(I)*((11.*TS(I)-18.*TS(I+1)+9.*TS(I-2)-2.*TS(I-3)))/(6.*DX)
2L)-KP(I)*((11.*TS(I)-18.*TS(I+1)+9.*TS(I+2)-2.*TS(I+3)))/(6.*EXP1*L)
2P))/DHP
MGDOT=SP*MGDOT+(1.-SP)*BMDOT

CONTINUE

MGDOT=.675*MGDOTP+.125*MGDOT

IF (NIT.EQ.1) GO TO 22

GO TO 26

CONTINUE

IF (NITC.EQ.0) GO TO 23

AMDOT(1)=AMDOT(1)*MGDOT/MGDOTP

CONTINUE

C DETERMINE SURFACE HEATING AND PRESSURE

CALL FTLJP (TIME,QC,MQC,NQC,TIMET,QCTAB)

IF (IOPTP.EQ.1) GO TO 24

PWP=5.69306E6*RAD*(0C/HE)**2

GO TO 25

CONTINUE

CALL FTLJP (TIME,PW,MSOPT,NSOPT,TMPRES,SPPT)

PW=P**2

PWP=1.013E5*PW

CONTINUE

P(1)=PWP

CONTINUE

AMDOT(1)=MGDOT

DO 27 N=1,NNJ

HKTV(N)=HKT(N,8)

CALL FTLUP (TS(1),HBRKN2,MNO,NNO,TEMP,HKT V)

DO 28 N=1,NNO

HKTV(N)=HKT(N,13)

CALL FTLUP (TS(1),HBRK02,MNO,NNO,TEMP,HKT V)

Hw=.790795*HBRKN2+.209205*HBRK02

C CALCULATE SURFACE REMOVAL RATE

C CHECK IOPT1= IOPT1=1 AND TS(1)=T1BAR USE EQ 3-41 FOR MSDOT

C IOPT1=0 USE EQ 3-36 FOR MSDOT

IF (NIT.GT.1) GO TO 29

S=1.

IF (TS(1).LE.(T1BAR-22.)) GO TO 29
S = (T1BAR - TS(1)) / 22.
IF (S .LT. 0.) S = 0.

29 CONTINUE
KA = AG * EXP(-BC / TS(1))
AMSDOT = KA * PW * CE * 0.901 / (1. + KA * PW * (HE - HW) / (0.032 * LAM * QCT))
BMSD = QCT + ALPHA * QCT - SIGMA * EPS * TS(1)**4 - 1000ND / HC
MSDOT = S * AMSDOT + (1. - S) * BMSD
IF (MSDOT .GT. 0.) GO TO 30
MSDOT = 0.
IF (IOPT .EQ. 0) GO TO 30
TS(1) = TS(1) - 1. * E-4
30 CONTINUE
MSDOT = 0.875 * MSDOTP + 0.125 * MSDOT
MPDOT = ALFC * MSDOT + ALFP * AMDOT(1)

C CALCULATE NET AERODYNAMIC HEATING RATE TO SURFACE: EQ. 3-40
QFAC = HE * MPDOT / (QC * 0.029)
IF (QFAC .GT. 2.25) GO TO 31
QCT = HE / (QC * 0.029) * MPDOT - 13 * (HE * MPDOT / (QC * 0.029))**2
GO TO 32
31 QCT = QC * (1. - HW / HE) * (1. - TREF * TRAB * MPDOT * HE / (QC * 0.029) - (1. - TRA3) * (0.724 * HE / (QC * 0.029) * MPDOT - 13 * (HE * MPDOT / (QC * 0.029))**2))
GO TO 32
32 CONTINUE
Q = QCT + ALPHA * QCT + S * MSDOT * DHC - (1. - S) * MSDOT * HC
Dx = DX1
C DETERMINE PROPERTY DATA FOR CHAR LAYER AND PYROLYSIS GASES
IF (T(20) .GT. 1000.) ICHCOM = 1
X = -Dx
IF (NIT .GT. 1) GO TO 37
DO 34 N = 5, I, 5
J = N
IF (N .EQ. 5) J = 1
NSTEP = J
IF (T(J) .LT. 299.) GO TO 33
C CALL SUBROUTINE VISC TO COMPUTE VISCOSITY AND PRANDTL NUMBER DF
A 317
A 318
A 319
A 320
A 321
A 322
A 323
A 324
A 325
A 326
A 327
A 328
A 329
A 330
A 331
A 332
A 333
A 334
A 335
A 336
A 337
A 338
A 339
A 340
A 341
A 342
A 343
A 344
A 345
A 346
A 347
A 348
A 349
A 350
A 351
C  
PYROLYSIS GASES
CALL VISC
CONTINUE
CONTINUE
DO 35 N=2,9
ANJ=(N-1)/9.*
MU(N)=MU(1)+ANJ*(MU(10)-MU(1))
35  
PR(N)=PR(1)+ANJ*(PR(10)-PR(1))
DO 36 N=15,1,-5
KON=4
APR=(PR(N)-PR(N-5))/5.*
AMU=(MU(N)-MU(N-5))/5.*
DO 36 J=1,4
PR(N-KON)=PR(N-5)+J*APR
MU(N-KON)=MU(N-5)+J*AMU
36  
KON=KON-1
PMU=MU(1)
CONTINUE
DO 53 N=1,1
CALL FTLJP (T(N),HK(N,13),MNO,NNO,TEMP,HKT)
AVGMF(N)=0.
DO 38 K=1,KT
AVGMF(N)=AVGMF(N)+MFK(N,K)*M(K)
38  
CONTINUE
IF (N.EQ.21) DDX=DX
X=X+DDX
VC(N)=(MSDOT/RHOSO+X*(MGDOT/DRHO-MSDOT/RHOSO))/L
IF (NITC.EQ.0) GO TO 39
IF (ABS(TS(N)-PTS(N))*.LT.5.) GO TO 40
PTS(N)=TS(N)
39  
CONTINUE
CALL FTLJP (TS(N),HS(N),MNO,NNO,TEMP,HST)
IF (NITC.GT.0) GO TO 40
AVGMFP(N)=AVGMF(N)
PM(N)=PMV
CPS(N)=CPSV
40 CONTINUE
CALL FTLUP (TS(N),KS(N),MKS,NKS,TKS,KST)
C NEGLECT HEAT CONDUCTION IN FLUID
NSTEP=N
IF (ICHCOM.EQ.0) GO TO 41
C CALL SUBROUTINE CHCOM TO DETERMINE CHEMICAL REACTION RATES OF
C EACH SPECIES
CALL CHCOM (TIME)
41 CONTINUE
IF (NITC.EQ.0) GO TO 42
IF (ABS(T(N)-PT(N)).LT.5.1) GO TO 50
PT(N)=T(N)
IF (T(N).LT.300.) GO TO 43
42 CONTINUE
43 CONTINUE
CALL FTLUP (T(N),HST(N),MNO,NNO,TEMP,HSTT)
DO 45 K=1,KM
DO 44 J=1,NNO
CPKTV(J)=CPKT(J,K)
HKTV(J)=HKT(J,K)
44 CONTINUE
45 CONTINUE
CALL FTLJP (T(N),HK(N,K),MNO,NNO,TEMP,HKTV)
CALL FTLUP (T(N),CPK(N,K),MNO,NNO,TEMP,CPKTV)
CALL FTLUP (TS(N),DHK(N,K),MNO,NNO,TEMP,HKTV)
46 CONTINUE
NITS=0
CONTINUE
IF (T(N).GT.15.) GO TO 47
CPK(N,11)=(2.882035E00+2.*5.16099E.--03*T(N)+3.*3.971480E06*T(N)**2
1-4.*3.708198E-09*T(N)**3 + 5.*8.949908E-13*T(N)**4)*RU
CPK(N,12)=(3.511186E-01+2.*1.876996E-02*T(N)-3.*2.649369E-06*T(N)*
1*2-4.*1.877262E-09*T(N)**3+5.*6.077093E-13*T(N)**4)*RU
HK(N,11)=(2.882035E00*T(N)+5.160995E-03*T(N)**2+3.971480E-06*T(N)*
1*3-3.708198E-09*T(N)**4+8.949908E-13*T(N)**5)*RU-1.157984E04
47 CONTINUE
HK(N,12) = (3.511186E-01*T(N)+1.876996E-02*T(N)**2-2.649069E-05*T(N)**3+1.877262E-09*T(N)**4+6.077093E-13*T(N)**5)*RJ+1.143849E04  
GO TO 43  
GO TO 48  
CPK(N,11) = (1.430804E00+2.*9.444913E-03*T(N)-3.*2.348033E-06*T(N)**2+4.*2.968006E-10*T(N)**3+5.*2.515503E-14*T(N)**4)*RU  
CPK(N,12) = (4.619871E00+2.*1.440481E-02*T(N)-3.*3.748451E-06*T(N)**2+4.*4.894085E-10*T(N)**3+5.*2.515503E-14*T(N)**4)*RU  
HK(N,11) = (1.430804E00*T(N)+9.444913E-03*T(N)**2-2.348033E-06*T(N)**3-2.968006E-10*T(N)**4-1.489961E-14*T(N)**5)*RU+1.143849E04  
HK(N,12) = (4.619871E00*T(N)+1.440481E-02*T(N)**2-3.748451E-06*T(N)**3+4.894085E-10*T(N)**4-2.515503E-14*T(N)**5)*RU+1.157984E04  
CONTINUE  
IF (NITS.EQ.1) GO TO 49  
TSAVE = T(N)  
CPK(N,11) = CPK(N,11)  
CPK(N,12) = CPK(N,12)  
HK(N,11) = HK(N,11)  
HK(N,12) = HK(N,12)  
T(N) = TS(N)  
NITS = NITS+1  
GO TO 46  
T(N) = TSAVE  
DHK(N,11) = HK(N,11)  
DHK(N,12) = HK(N,12)  
HK(N,11) = HSA11  
HK(N,12) = HSA12  
CPK(N,11) = CPSA11  
CPK(N,12) = CPSA12  
DHJ(N,6) = 2.*DHK(N,5)-HK(N,9)-HS(N)  
DHJ(N,7) = DHK(N,5)+DHK(N,2)-HK(N,6)-HS(N)  
DHJ(N,9) = DHK(N,10)+DHK(N,2)-HK(N,7)-HS(N)  
CONTINUE  
HRJSUM(N) = 0.  
HRJSUM(N) = 0.  
RM(N) = 0.
ROCPM(N)=0.
ROHM(N)=0.
DO 51 K=1,KT
RM(N)=RM(N)+R(N,K)*M(K)
DO 52 K=1,KT
HRJSUM(N)=HRJSUM(N)+RHR(N,K)*DHJ(N,K)
HRSUM(N)=HRSUM(N)+R(N,K)*HK(N,K)
ROHM(N)=ROHM(N)+RHJK(N,K)*HK(N,K)*M(K)
ROCPM(N)=ROCPM(N)+RHJK(N,K)*CPK(N,K)/M(K)
CONTINUE
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CALL FTLUP (TS(N),KP(N),MKP,NKP,TKP,PT)
CALL FTLJP (TS(N),CPP(N),MCPP,NCPP,TCPP,CPPT)
RHUP(N)=576.
57 CONTINUE
IF (NITC.GT.0) GO TO 60
DO 58 N=1,I
HA(N)=PROP*C*ROCPM(N)*V(N)/PR(N)
58 CONTINUE
DO 59 N=IP,IL
KPP(N)=KPPV
CPPP(N)=CPPPV
RHOPP(N)=RHOPPV
59 CONTINUE
KPPP1P=KPP(IP)
58 CONTINUE
DU 58 N=1,I
HA(N)=PROPC*ROCPM(N)*V(N)/PR(N)
58 CONTINUE
DO 59 N=IP,IL
KPP(N)=KPPV
CPPP(N)=CPPPV
RHOPP(N)=RHOPPV
59 CONTINUE
KPPP1P=KPP(IP)
KPPP1P=KPPV
CPPP1P=CPPPV
RHOPP1P=RHOPPV
60 CONTINUE
DKSDX(1)=(-11.*KS(1)+18.*KS(2)-9.*KS(3)+2.*KS(4))/(6.*DX1)
DKSDX(I)=(11.*KS(I)-18.*KS(IM)+9.*KS(I-2)-2.*KS(I-3))/(6.*DX)
DKSDX(IP)=(11.*KS(IP)-18.*KS(IP1)+9.*KS(IP-2)-2.*KS(IP-3))/(6.*DX)
60 CONTINUE
DO 62 N=2,IM
IF (N.EQ.20) GO TO 61
DKSDX(N)=(KSIN+1)-KS(N-1))/DX
62 CONTINUE
DKSDX(20)=(DX1**2*KS(21)+(DX1**2-DX1**2)*KS(20)-DX**2*KS(19))/(DX1**2)
1DX*(DX1+DX)
61 CONTINUE
DKPDX(I)=(11.*KP(I)+18.*KP(IN)-9.*KP(IN2)+2.*KP(I+4))/(6.*DXP1)
DKPDX(IP)=(11.*KP(IP)+18.*KP(IP1)-9.*KP(IP2)+2.*KP(IP+4))/(6.*DXP1)
62 CONTINUE
IF (N.EQ.(I+20)) GO TO 63

DKPDX(N) = (KP(N+1) - KP(N-1)) / (2.*DXP)

GO TO 64

63 DKPDX(I+20) = (DXP1**2*KP(I+21)*DXP2*KP(I+20) - DXP**2*KP(I+19)) / (DXP1*DXP*(DXP1+DXP))

DDX = DXP

CONTINUE

C SOLUTION OF PARTIAL DIFFERENTIAL EQUATION FOR CHAR LAYER

C CALCULATE COEFFICIENTS IN DIFFERENTIAL EQ FOR SOLID TEMPERATURE

DO 66 N=1,I

ATS(N) = TS(N)

ALPHA1(N) = (DKSDX(N) + L**2*(1. - ETA(N)) * CPS(N) * RHOST / MS * VC(N)) / KS(N)

ALPHA2(N) = 0.

ALPHA3(N) = L**2 / KS(N) * (HA(N) *(TP(N) - TSP(N)) * ETA(N) *(HST(V) * RHost(V) * WS(V) + RHost(V) * HRJSUM(N)) + RHOST * HS(N) / MS*(1. - ETA(N) - ETAP(N)) / DT - VC(N) / DE)

ALPHA4(N) = -(1. - ETA(N)) * L**2 * RHOST * CPS(N) / (MS * KS(N))

IF (NITC.NE.0) GO TO 65

ALPHAP1(N) = ALPHA1(N)

ALPHAP2(N) = ALPHA2(N)

ALPHAP3(N) = ALPHA3(N)

ALPHAP4(N) = ALPHA4(N)

CONTINUE

ALPHAP3(N) = CRNI * ALPHA3(N) + (1. - CRNI) * ALPHAP3(N)

ALPHAP4(N) = CRNI * ALPHA4(N) + (1. - CRNI) * ALPHAP4(N)

CONTINUE

IF (NITC.NE.0) GO TO 67

ALPHIP1 = ALPHA1(I)

ALPHIP2 = ALPHA2(I)

ALPHIP3 = ALPHA3(I)

ALPHIP4 = ALPHA4(I)

CONTINUE

ALPHII = ALPHA1(I)
ALPHI2=ALPHA2(I)
ALPHI3=ALPHA3(I)
ALPHI4=ALPHA4(I)
DDX=DXP
XP=0.
DO 68 N=I,IP
IF (N.EQ.(I+20)) DDX=DXP
ATS(N)=TS(N)
ALPHA1(N)=(DK*DX(N)+LP*RHOP(N)*CPP(N)*MGDOT*(1.-XP)/DRHO)/KP(N)
XP=XP+DDX
ALPHA2(N)=0.
ALPHA3(N)=0.
ALPHA4(N)=-RHOP(N)*CPP(N)*LP**2/KP(N)
ALPHB3(N)=0.
IF (NITC.NE.0) GO TO 68
ALPHP1(N)=ALPHA1(N)
ALPHP2(N)=ALPHA2(N)
ALPHP3(N)=ALPHA3(N)
ALPHP4(N)=ALPHA4(N)
68 ALPHB4(N)=CRNI*ALPHA4(N)+(1.-CRNI)*ALPHP4(N)
IF (NITC.NE.0) GO TO 69
GAMMPI1=ALPHA1(I)
GAMMPI2=ALPHA2(I)
GAMMPI3=ALPHA3(I)
GAMMPI4=ALPHA4(I)
GAMMIPP1=ALPHA1(IP)
GAMMIPP2=ALPHA2(IP)
GAMMIPP3=ALPHA3(IP)
GAMMIPP4=ALPHA4(IP)
69 CONTINUE
GAMM11=ALPHA1(I)
GAMM12=ALPHA2(I)
GAMM13=ALPHA3(I)
GAMM14=ALPHA4(I)
GAMIP1 = ALPHA1(IP)
GAMIP2 = ALPHA2(IP)
GAMIP3 = ALPHA3(IP)
GAMIP4 = ALPHA4(IP)
DO 71 N = IP, IL
ATS(N) = TS(N)
ALPHA1(N) = 0.
ALPHA2(N) = 0.
ALPHA3(N) = 0.
ALPHA4(N) = -RHOPP(N)*CPPP(N)*IL**2/KPP(N)
IF (NITC .NE. J) GO TO 70
ALPHAP1(N) = ALPHA1(N)
ALPHAP2(N) = ALPHA2(N)
ALPHAP3(N) = ALPHA3(N)
ALPHAP4(N) = ALPHA4(N)
ALPHBP3(N) = 0.
70 CONTINUE
71 ALPHB4(N) = CRNI*ALPHA4(N) + (1. - CRNI)*ALPHAP4(N)
IF (NITC .NE. 0) GO TO 72
KAP1P1 = ALPHA1(IP)
KAP1P2 = ALPHA2(IP)
KAP1P3 = ALPHA3(IP)
KAP1P4 = ALPHA4(IP)
CONTINUE
72 KAP1P1 = ALPHA1(IF)
KAP1P2 = ALPHA2(IP)
KAP1P3 = ALPHA3(IP)
KAP1P4 = ALPHA4(IP)
CALL SUBROUTINE PDE1 TO SOLVE FOR TS
CALL PDE1 (TS, CRNI)
C CALCULATE COEFFICIENTS IN DIFFERENTIAL EQ FOR P
DDX = DX1
DO 74 N = 1, I
AP(N) = P(N)
IF (N .NE. 1) GO TO 74
PAL2(N) = 2.*MJ(N)*ETA(N)*L**2/(PM(N)*HO(N)*RU*T(N))*AVGMF(N)*(T(N)
1.-TP(N))/(DT*T(N))=AVGMF(N)*VC(N)*DT*(X(N)*F(T(V))+V.*8) M8RDX(V).•.(AV
2GMF(N)-AVGMPF(N)/DT)
PAL3(N)=2.*MJ(N)*ETA(N)*P(N)*RM(N)*L**2/(PM(N)*RHO(N))
PAL4(N)=-MU(N)*ETA(N)*AVGMF(N)*L**2/(PM(N)*RHO(N)*R(U)*T(N))
IF (N.EQ.1) GO TO 74
IF (N.EQ.X) GO TO 73
PAL1(N)=4U(N)*ETA(N)*T(N)/(PM(N)*AVGMF(N))*PM(N+1)*AVGMF(N+1)/(MU
1(N+1)*ETA(N+1)*T(N+1)-PM(N-1)*AVGMF(N-1)/(MU(N-1)*ETA(N-1)*T(N-1)
2))/(2.*DDX)+MU(N)*ETA(N)*AVGMF(N)*L**2/(PM(N)*RHO(N)*R(U)*T(N))
GO TO 74
73 CONTINUE
PAL1(20)=MU(20)*ETA(20)*T(20)/(PM(23)*AVGMF(20))*(PM(21)*AVGMF(21)/(MU
1(21)*ETA(21)*T(21))-0X1**2*PM(21)*AV
202)/(MU(20)*ETA(20)*T(20)-DX**2*PM(21)*AVGMF(19)/(MU(19)*ETA(19)*T(19)));
3/(UX1*DX*DX1+MU(21)*ETA(20)*AVGMF(20)*L**2/(PM(20)*RHO(20)*T
4(20)*R(U))*VC(20)
74 CONTINUE
PAL1(I)=MU(I)*ETA(I)*T(I)/(PM(I)*AVGMF(I))*(11.*PM(I)*AVGMF(I)/(MU
1(I)*ETA(I)*T(I))-18.*PM(I)*AVGMF(I)/(MU(IM)*ETA(IM)*T(IM)))+9.*PM
2(I-2)*AVGMF(I-2)/(MU(I-2)*ETA(I-2)*T(I-2))-2.*PM(I-3)*AVGMF(I-3)/(I
3*MU(I-3)*ETA(I-3)*T(I-3)))*16*DX)+MU(I)*ETA(I)*AVGMF(I)*L**2*VC(I)
4/(PM(I)*RHO(I)*R(U)*T(I))
DO 76 N=2,1
IF (N.TC.GT.0) GO TO 75
PAP1(N)=0.
PAP2(N)=0.
PAP3(N)=0.
PAP4(N)=0.
75 PAP3(N)=CRNI*PAL3(N)+1.-CRNI)*PAP3(N)
PAP4(N)=CRNI*PAL4(N)+1.-CRNI)*PAP4(N)
CALL SUBROUTINE PDP TO SOLVE FOR P
CALL PDP(CRNI,DT,L,DX,DX1,MGD,MDT,MDTP,LPP,IM,R40,P,MU,T,TP,R(U)
CALL CALCULATE LOCAL PYROLYSIS GAS DENSIT
DO 77 N=1,I
   RHO(N)=P(N)*AVGMF(N)/(RU*T(N))
77 CONTINUE
   DRODX(1)=(-11.*RHO(1)+18.*RHO(2)-9.*RHO(3)+2.*RHO(4))/(5.*DX1)
   DDX=DX1
   DO 79 N=2,I
      IF (N.EQ.20) GO TO 78
      DRODX(N)=(RHO(N+1)-RHO(N-1))/(2.*DDX)
      GO TO 79
78 DDX=DX
   DRODX(N)=(DX1**2*RHO(N+1)+(DX**2-DX1**2)*RHC(N)-DX**2*RHO(N-1))/(D
1*DX*(DX1+DX))
79 CONTINUE
   DRODX(I)=(11.*RHO(I)-18.*RHO(I-1)+9.*RHO(I-2)-2.*RHO(I-3))/(6.*DX)
C CHECK PYROLYSIS RATE- IF LESS THAN MIN NEGLECT THERMAL NON-
C EQUILIBRIUM OF PYROLYSIS GASES AN) CHAR LAYER AND CHEMICAL
C REACTIONS
   IF (NITP.GT.0) GO TO 81
   DO 80 N=1,I
      ETA(N)=ETA(I)
      T(N)=T(N)
      AT(N)=T(N)
      AMDOT(N)=AVGDJ
      V(N)=-MGDOT/(RHO(N)*ETA(N))
      DO 80 K=1,KT
         RHOK(K,N)=FK(N,K)*RHO(N)*M(K)/AVGMF(N)
80 CONTINUE
   GO TO 101
81 CONTINUE
C CALCULATE LOCAL MASS FLOW RATE OF PYROLYSIS GASES
   AINT1(IM)=DX/2.*(ETA(I)*RHO(I)+ETA(IM)*RHO(IM))
   AINT3(IM)=DX/2.*(ETA(I)*((RHO(I)-PRH(I))/DT-R*M(I))+RHO(I)*ETA(I)
1-ETAP(I))/DT+ETA(IM)*((RHO(IM)-PRH(IM))/DT-R*M(IM))+RHO(IM)*ETA(I
2*M-ETAP(IM))/DT)
   KUN=I-2
DDX = DX
DO 83 N = 3, I
IF (KON .EQ. 0.19) GO TO 82
    AINT1(KON) = AINT1(KON+2) + DDX/3.*((ETA(KON+2)*RHO(KON+2)) + 4.*ETA(KON+1))
    AINT1(KON+1) = ETA(KON+1) + ETA(KON)*RHO(KON)
    AINT3(KON) = AINT3(KON+2) + DDX/3.*((ETA(KON+2)*(RHO(KON+2) - PRHO(KON+2)) +
        (4.*ETA(KON+2) - ETAP(KON+2))/DT + 4.*ETA(KON+1))
    AINT1(KON+1) = AINT1(KON+1) + ETA(KON+1) + ETA(KON)*RHO(KON+1)
    AINT3(KON+1) = AINT3(KON+1) + ETA(KON+1) + ETA(KON)*RHO(KON+1)
    KON = KON - 1
    DO 84 N = 1, I
    AMDOT(N) = MGDOT + L*(VC(I)*ETA(I)*RHO(I)-VCIN)*ETA(N)*RHO(N) -
        L*AINT3(N) - (MGDOT/RHO-MSD(T)/RHO(N))*AIN1(N)
    KON = KON - 1
    DO 85 N = 1, I
    V(N) = AMDOT(N)/(RHO(N)*ETA(N))
    CONTINUE
    DO 86 N = 1, I
    DVDX(N) = L*(VC(N)-V(N)/L)*((DRONX(N)/RHO(N) + ETA(I)*RHO(N))/ETA(N)) -
        (1(RHO(N)-PRHO(N))/DT)*ETA(N)*ETA(N)*ETA(N)*RHO(N)/RHO(N)
    DO 91 K = 1, KT
    NRHOK(K) = 0.
    DO 87 N = 1, I
    IF (((MFK(N,K).GT.1.E-5).OR.(R(N,K).GT.1.E-5)) NRHOK(K) = 1
    CONTINUE
    IF (NRHOK(K).EQ.0) GO TO 91
ARH(I) = M(K)*MFK(I,K)*MGDOT/(AVGMF(I)*ETA(I))

C CALCULATE COEFFICIENTS IN SPECIES CONTINUITY EQ

DO 89 N=1,I
  ARIH(N) = PAMGDT(N,K)
  DEN = ETA(N)*(V(N) - V(C)/L)
  DEL1(N,K) = CETAOX(N)/ETA(N) - ETA(N)*V(N)**2/(V(N)**2 + ETA(N)ETAP)
  DEL2(N,K) = V(N)*ETA(N)*((1.*RHOK(N,K) - RHC(N,K))/DT - R(N,K)*M(K))/DEN
  DEL3(N) = 0.
  IF (NITA.GT.0) GO TO 88
  DEPI(N,K) = DEL1(N,K)
  DEP2(N,K) = DEL2(N,K)
  DEP3(N) = DEL3(N)
  88 DEB2(N,K) = CRNI*CEL2(N,K) + (1. - CRNI)*DEP2(N,K)
  DEB3(N) = CRNI*DEP3(N) + (1. - CRNI)*DEP3(N)
  AL1(N) = DEL1(N,K)
  AP1(N) = DEP1(N,K)
  AB2(N) = DEB2(N,K)
  89 CONTINUE

C COMPUTE GAS DENSITY THROUGH CHAR LAYER

C CALL SUBROUTINE POE2 TO SOLVE FOR THE LOCAL MASS FLOW OF

C SPECIES

CALL POE2 (AL1, AB2, AB3, AP1, BRH, ARH, CRNI, DX, DX1, DT, I)
DO 90 N=1,I
  IF (ARH(N)*LT.1.E-100) ARH(N) = 1.E-100
  RHOK(N,K) = .875*RHC(N,K) - .125*ARH(N)/V(N)
  90 CONTINUE

91 CONTINUE
DO 92 N=1,I
  ROM(N) = 0.
  DO 92 K=1,KT
  ROM(N) = ROM(N) + RHOK(N,K)/M(K)
  92 DO 93 N=1,I

DO 93 K=1,KT
MFK(N,K)=RHOK(N,K)/(ROM(N)*M(K))

CALCULATE COEFFICIENTS IN PYROLYSIS GAS TEMPERATURE DIFFERENTIAL EQUATION
DO 95 N=1,I
AT(N)=T(N)
DEN=ETA(N)*(V(N)/L-VC(N))*((ROCPM(N)-RHO(N)*RU/AVGMF(N))
BETA1(N)=(HA(N)*TP(N)/T(N)-ETA(N)*RU*(((ROM(N)-PRM(N))/DT+(V(N)/L-
1VC(N))*(DRODA(N)/AVGMF(N)-RHO(N)*RM(N)*HRJ2(N))/AVGMF(N)))*DEN
BETA2(N)=(ETA(N)*(HRSUM(N)-V(N)**2/2.*RM(N)+RS(N)*HST(N)-RHS(N)*HS1(N))
BETA3(N)=ETA(N)*(ROCPM(N)-RHO(N)*RU/AVGMF(N))/DEN
IF (NITA.GT.J) GO TO 94
BETPI(N)=BETA1(N)
BETP2(N)=BETA2(N)
BETP3(N)=BETA3(N)
CONTINUE
BETB2(N)=CRNI*BETA2(N)+(1.-CRNI)*BETP2(N)
BETB3(N)=CRNI*BETA3(N)+(1.-CRNI)*BETP3(N)
CONTINUE
T(I)=TS(I)
CALL SUBROUTINE PDE2 TO SOLVE FOR T
CALL PDE2 (BETA1,BETB2,BETB3,BETP1,T,P,T,CRNI,DX,DX1,DT,TI)
DO 96 N=1,I
CALCULATE COEFFICIENTS IN POROSITY DIFFERENTIAL EQUATION
T(N)=.875*TP(N)+.125*T(N)
DO 98 N=1,I
EPSA1(N)=-MS*(RHS(N)+RS(N))/(RHST*VC(N))
EPSA2(N)=0.
EPSA3(N)=-1./VC(N)
IF (NITA.NE.D) GO TO 97
EPSP1(N)=EPSA1(N)
EPSP3(N)=EPSA3(N)
CONTINUE
EPS83(N)=CRNI*EPSA3(N)+(1.-CRNI)*EPS3(N)
CONTINUE

CALL SUBROUTINE PDE2 TO SOLVE FOR ETA
CALL PDE2 (EPSA1,EPSB2,EPSB3,EPSPI,ETAP,ETA,CRNI,DX,DXL,DT,I)

DETADX(1)=(-1.1.*ETA(1)+18.*ETA(2)-9.*ETA(3)+2.*ETA(4))/(6.*DX1)

DDX=DX
DO 100 N=2,IM
IF (N.EQ.20) GO TO 99
DETADX(N)=(ETA(N+1)-ETA(N-1))/(2.*DX)
GO TO 100

DETADX(20)=(DX1**2*ETA(21)-(DX1**2-1.*ETA(20)-DX**2*ETA(19)))/(A*DX1*DX)

DO 100 N=2,IM
DETADX(N)=(ETA(N+1)-ETA(N-1))/(2.*DX)
NITA=1
CONTINUE
NITC=1
CALCULATE NEW THICKNESS VALUES FOR CHARRED AND UNCHARRED LAYERS

OLP=(MGDOTP/D*U10+4.*(CRNI*MGDOT+(1.-CRNI)*MGDOTP)/DRHO+MGOOT/DRHO)*D116.
OLP=LPPP-OLP
IF (LP.LT.LPMIN) GO TO 110
L=LPPP+OL
CHECK SOLUTIONS- IF NO CHECK ITERATE AGAIN
DO 102 N=1,II
IF (ABS((TS(N)-ATS(N))/TS(N)).GT.DIFER) GO TO 12
IF (N.GT.I) GO TO 102
IF (ABS((P(N)-AP(N))/P(N)).GT.DIFER) GO TO 12
IF (ABS((T(N)-AT(N))/T(N)).GT.DIFER) GO TO 12
CONTINUE

PART=2.*DIFER*TS(1)
NITG=0
IF (ABS(TS(1)-TSP(1)) .GT. PART) NITS = 1
IF (ABS(TIME-PTIME-PRTFRQ) .LE. DT/2.) GO TO 103
IF ((TIME-PTIME-PRTFRQ) .GT. 0.) GO TO 103
GO TO 105
103  CONTINUE
ORAT=QC/QC
PRINT RESULTS
WRITE (2,112) TIME, DT, NIT, TS(1), T(1), ORAT, MSDOT, MDOT, AMDOT(1), L, L
WRITE (2,118)
WRITE (2,120) (TS(N), N=1,1Z)
WRITE (2,113)
WRITE (2,120) (ETA(N), N=1,1)
WRITE (2,117)
WRITE (2,120) (T(N), N=1,1)
WRITE (2,119)
WRITE (2,120) (P(N), N=1,1)
WRITE (2,114)
DO 104 K=1,KT
WRITE (2,111) SPECIES(K)
WRITE (2,122) (MFK(N,K), N=1,1)
104  CONTINUE
WRITE (2,115)
WRITE (2,120) (AVGF(N), N=1,1)
WRITE (2,116)
WRITE (2,120) (AMDCT(N), N=1,1)
PTIME=PTIME+10.
105  CONTINUE
C IF SOLUTIONS CHECK RETAIN CURRENT VALUES OF PARAMETERS
DO 108 N=1,IZ
YTS(N)=(TS(N)-TSP(N))/DT
IF (N.GT.1) GO TO 107
YETA(N)=(ETA(N)-ETAP(N))/DT
YRH(N)=(RH(N)-PRH(N))/DT
YP(N)=(P(N)-PP(N))/DT
PAP1(N) = PAL1(N)
PAP2(N) = PAL2(N)
PAP3(N) = PAL3(N)
PAP4(N) = PAL4(N)
PROM(N) = ROM(N)
PRHO(N) = RHO(N)
AVGMFP(N) = AVGMF(N)
PP(N) = P(N)
EPSP1(N) = EPSA1(N)
EPSP3(N) = EPSA3(N)
BETP1(N) = BETA1(N)
BETP2(N) = BETA2(N)
BETP3(N) = BETA3(N)
YT(N) = (T(N) - TP(N))/DT
DEP3(N) = DEL3(N)
DO 106 K = 1, KT
DEP1(N,K) = DEL1(N,K)
DEP2(N,K) = DEL2(N,K)
YRHOK(N,K) = (RHOK(N,K) - RHUKP(N,K))/DT
PAMGDOOT(N,K) = -RHOK(N,K)*V(N)
106
RHOKP(N,K) = RHOK(N,K)
HA(N) = ABS(PHOPC*RGCPM(N)*V(N)/P(N))
TP(N) = T(N)
ETAP(N) = ETA(N)
107 CONTINUE
ALPHP1(N) = ALPHA1(N)
ALPHP2(N) = ALPHA2(N)
ALPHP3(N) = ALPHA3(N)
ALPH4(N) = ALPHA4(N)
TSP(N) = TS(N)
MSDOTP = MSDOT
ALPHIP1 = ALPHI1
ALPHIP2 = ALPHI2
ALPHIP3 = ALPHI3
ALPHIP4 = ALPHI4
GAMMIP1=GAMMI1
GAMMIP2=GAMMI2
GAMMIP3=GAMMI3
GAMMIP4=GAMMI4
GAMIPP1=GAMIP1
GAMIPP2=GAMIP2
GAMIPP3=GAMIP3
GAMIPP4=GAMIP4
KAPIPP1=KAPIP1
KAPIPP2=KAPIP2
KAPIPP3=KAPIP3
KAPIPP4=KAPIP4
QPNET=QNET
PHBRKN2=HBRKN2
PHBRK02=H3PK02
QPT=Q
KSPI=KS(I)
KSPI2=KS(I1)
KPI1=KP(I)
KPI1P=KP(IP)
LPP=L
LPPP=LP
MGDOTP=MGDOT

C CHECK ITERATION COUNT- INCREASE TIME STEP IF ITERATION= 1
IF (NIT.GT.1) GO TO 109
IF (NTIME.LT.5) GO TO 109
DT=1.5*DT
IF (DT.GT.10) DT=10.
NTIME=0
109 NIT=0
NTIME=NTIME+1
GO TO 9
110 CONTINUE
WRITE (2,121) LP
STOP
111 FORMAT (50X, A10)
113 FORMAT (2X, 1HCHAR LAYER POROSITY)
114 FORMAT (2X, 2HMOLE FRACTION GASEOUS SPECIES)
115 FORMAT (2X, 4H AVERAGE MOLECULAR WEIGHT PYROLYSIS GASES)
116 FORMAT (2X, 3H CALORICAL MASS FLOW RATE OF PYROLYSIS GASES)
117 FORMAT (/2X, 17H FLUID TEMPERATURE)
118 FORMAT (/2X, 17H SOLID TEMPERATURE)
119 FORMAT (2X, 8H PRESSURE)
120 FORMAT (2X, 5E25.15)
121 FORMAT (20X, 36H MINIMUM THICKNESS VIRGIN MATERIAL = ,E20.10)
END
SUBROUTINE VISC
CALCULATION OF FLUID VISCOSITY AND PRANDTL NUMBER AT LOCAL TEMPERATURE (REF. BROKAW NASA TR-R-81)

DIMENSION MUK(12), KGK(12)
COMM /DELIKE/ PSI(12,12), PHI(12,12), DUMMY(1032)
COMM ACER(12), BCEF(12), BDER(12), CKNI, KUPT(40,12), KUPTV(40), M(13), MFK(50,12), MNC, NNO, MU(50), MUKT(40,12), MUKTV(40), PR(50), R(50,12), RHO(50), RHOK(50,12), RHOKP(50,12), T(50), TEMP(4), NRCT, KT, RUS
REAL MU, MUK, M, KUPT, MUKTV, MUKT, KUPTV, G, KGK
N=NSTEP
DO 2 K=1, KT
IF (MFK(N,K).LT.1.E-5) GO TO 2
DO 1 J=1, NNO
MUKTV(J)=MUKT(J,K)
KUPTV(J)=KUPT(J,K)
1 CONTINUE
CALL FTLUP (T(N), MUK(K), MNO, NNO, TEMP, MUKTV)
CALL FTLJP (T(N), KGK(K), MNO, NNO, TEMP, KUPTV)
IF (T(N).GE.300.) GO TO 2
MUK(K)=MUKTV(1)
KGK(K)=KUPTV(1)
2 CONTINUE
DO 4 K=1, KT
DO 4 J=1, KT
IF (K.EQ.J) GO TO 4
IF (MFK(N,K).LT.1.E-5) GO TO 3
PHI(K,J)=(1.*SQRT(MUK(K)/MUK(J)))*SQRT((SQRT(M(J)/M(K)))*2/(2.*SQR IT(2.)*SQRT(1.*M(K)/M(J))))
PSI(K,J)=PHI(K,J)*(1.*2.41*(M(K)-M(J))*(M(K)-.142*M(J))/(M(K)+M(J))**2)
Goto 4
3 CONTINUE
PHI(K,J)=0.
PSI(K,J)=0.
4 CONTINUE
MU(N) = 0.

1. IF (MFK(N,1).LT.1.E-5) GO TO 5
   A = 1. + PHI(1,2) * RHOK(N,2) * M(1)/(RHOK(N,1) * M(2)) + PHI(1,3) * RHOK(N,3) * M(1)/(RHOK(N,1) * M(3)) + PHI(1,4) * RHOK(N,4) * M(1)/(RHOK(N,1) * M(4)) + PHI(1,5) * RHOK(N,5) * M(1)/(RHOK(N,1) * M(5)) + PHI(1,6) * RHOK(N,6) * M(1)/(RHOK(N,1) * M(6)) + PHI(1,7) * RHOK(N,7) * M(1)/(RHOK(N,1) * M(7)) + PHI(1,8) * RHOK(N,8) * M(1)/(RHOK(N,1) * M(8)) + PHI(1,9) * RHOK(N,9) * M(1)/(RHOK(N,1) * M(9)) + PHI(1,10) * RHOK(N,10) * M(1)/(RHOK(N,1) * M(10)) + PHI(1,11) * RHOK(N,11) * M(1)/(RHOK(N,1) * M(11)) + PHI(1,12) * RHOK(N,12) * M(1)/(RHOK(N,1) * M(12)) + A.

2. CONTINUE

5. IF (MFK(N,2).LT.1.E-5) GO TO 6

6. CONTINUE

7. IF (MFK(N,3).LT.1.E-5) GO TO 7

7. CONTINUE

8. IF (MFK(N,4).LT.1.E-5) GO TO 8.

A = PHI(4,5) * RHOK(N,5) * M(4) / (RHOK(N,4) * M(5)) + PHI(4,6) * RHOK(N,6) * M(4) / (RHOK(N,4) * M(6))


CONTINUE

IF (MKF(N,5) .LT. 1.E-5) GO TO 9

CONTINUE

IF (MKF(N,6) .LT. 1.E-5) GO TO 10

CONTINUE

IF (MKF(N,7) .LT. 1.E-5) GO TO 11
(1) \( (\text{RHOK}(N, 7) \cdot M(2)) + \text{PHI}(7, 3) \cdot \text{RHOK}(N, 3) \cdot M(7) ) / (\text{RHOK}(N, 7) \cdot M(3)) + \text{PHI}(7, 4) \cdot \text{RHOK}(N, 4) \cdot M(7) ) / (\text{RHOK}(N, 7) \cdot M(4)) + \text{PHI}(7, 5) \cdot \text{RHOK}(N, 5) \cdot M(7) ) / (\text{RHOK}(N, 7) \cdot M(5)) + \text{PHI}(7, 6) \cdot \text{RHOK}(N, 6) \cdot M(7) ) / (\text{RHOK}(N, 7) \cdot M(6))

\[ \text{MU}(N) = \text{MUK}(7) / (\text{PHI}(7, 8) \cdot \text{RHOK}(N, 8) \cdot M(7) ) / (\text{RHOK}(N, 8) \cdot M(8)) + \text{PHI}(7, 9) \cdot \text{RHOK}(N, 9) \cdot M(7) ) / (\text{RHOK}(N, 9) \cdot M(9)) + \text{PHI}(7, 10) \cdot \text{RHOK}(N, 10) \cdot M(7) ) / (\text{RHOK}(N, 10) \cdot M(10)) + \text{PHI}(7, 11) \cdot \text{RHOK}(N, 11) \cdot M(7) ) / (\text{RHOK}(N, 11) \cdot M(11)) + \text{PHI}(7, 12) \cdot \text{RHOK}(N, 12) \cdot M(7) ) / (\text{RHOK}(N, 12) \cdot M(12)) + \text{A} + \text{MU}(N) \]

\[ \text{CONTINUE} \]

\[ \text{IF} (\text{MFK}(N, 8) < 1.0 \cdot 10^{-5}) \text{ GO TO 12} \]

\[ A = 1.0 + \text{PHI}(8, 1) \cdot \text{RHOK}(N, 1) \cdot M(8) ) / (\text{RHOK}(N, 1) \cdot M(1)) + \text{PHI}(8, 2) \cdot \text{RHOK}(N, 2) \cdot M(8) ) / (\text{RHOK}(N, 2) \cdot M(2)) + \text{PHI}(8, 3) \cdot \text{RHOK}(N, 3) \cdot M(8) ) / (\text{RHOK}(N, 3) \cdot M(3)) + \text{PHI}(8, 4) \cdot \text{RHOK}(N, 4) \cdot M(8) ) / (\text{RHOK}(N, 4) \cdot M(4)) + \text{PHI}(8, 5) \cdot \text{RHOK}(N, 5) \cdot M(8) ) / (\text{RHOK}(N, 5) \cdot M(5)) + \text{PHI}(8, 6) \cdot \text{RHOK}(N, 6) \cdot M(8) ) / (\text{RHOK}(N, 6) \cdot M(6))

\[ \text{MU}(N) = \text{MUK}(8) / (\text{PHI}(8, 7) \cdot \text{RHOK}(N, 7) \cdot M(8) ) / (\text{RHOK}(N, 8) \cdot M(7)) + \text{PHI}(8, 9) \cdot \text{RHOK}(N, 9) \cdot M(8) ) / (\text{RHOK}(N, 10) \cdot M(8)) + \text{PHI}(8, 10) \cdot \text{RHOK}(N, 11) \cdot M(8) ) / (\text{RHOK}(N, 11) \cdot M(11)) + \text{PHI}(8, 12) \cdot \text{RHOK}(N, 12) \cdot M(8) ) / (\text{RHOK}(N, 12) \cdot M(12)) + \text{A} + \text{MU}(N) \]

\[ \text{CONTINUE} \]

\[ \text{IF} (\text{MFK}(N, 9) < 1.0 \cdot 10^{-5}) \text{ GO TO 13} \]

\[ A = 1.0 + \text{PHI}(9, 1) \cdot \text{RHOK}(N, 1) \cdot M(9) ) / (\text{RHOK}(N, 1) \cdot M(1)) + \text{PHI}(9, 2) \cdot \text{RHOK}(N, 2) \cdot M(9) ) / (\text{RHOK}(N, 2) \cdot M(2)) + \text{PHI}(9, 3) \cdot \text{RHOK}(N, 3) \cdot M(9) ) / (\text{RHOK}(N, 3) \cdot M(3)) + \text{PHI}(9, 4) \cdot \text{RHOK}(N, 4) \cdot M(9) ) / (\text{RHOK}(N, 4) \cdot M(4)) + \text{PHI}(9, 5) \cdot \text{RHOK}(N, 5) \cdot M(9) ) / (\text{RHOK}(N, 5) \cdot M(5)) + \text{PHI}(9, 6) \cdot \text{RHOK}(N, 6) \cdot M(9) ) / (\text{RHOK}(N, 6) \cdot M(6))

\[ \text{MU}(N) = \text{MUK}(9) / (\text{PHI}(9, 7) \cdot \text{RHOK}(N, 7) \cdot M(9) ) / (\text{RHOK}(N, 9) \cdot M(7)) + \text{PHI}(9, 8) \cdot \text{RHOK}(N, 9) \cdot M(9) ) / (\text{RHOK}(N, 10) \cdot M(9)) + \text{PHI}(9, 10) \cdot \text{RHOK}(N, 11) \cdot M(9) ) / (\text{RHOK}(N, 11) \cdot M(11)) + \text{PHI}(9, 12) \cdot \text{RHOK}(N, 12) \cdot M(9) ) / (\text{RHOK}(N, 12) \cdot M(12)) + \text{A} + \text{MU}(N) \]

\[ \text{CONTINUE} \]

\[ \text{IF} (\text{MFK}(N, 10) < 1.0 \cdot 10^{-5}) \text{ GO TO 14} \]

\[ A = 1.0 + \text{PHI}(10, 1) \cdot \text{RHOK}(N, 1) \cdot M(10) ) / (\text{RHOK}(N, 1) \cdot M(1)) + \text{PHI}(10, 2) \cdot \text{RHOK}(N, 2) \cdot M(10) ) / (\text{RHOK}(N, 2) \cdot M(2)) + \text{PHI}(10, 3) \cdot \text{RHOK}(N, 3) \cdot M(10) ) / (\text{RHOK}(N, 3) \cdot M(3)) + \text{PHI}(10, 4) \cdot \text{RHOK}(N, 4) \cdot M(10) ) / (\text{RHOK}(N, 4) \cdot M(4)) + \text{PHI}(10, 5) \cdot \text{RHOK}(N, 5) \cdot M(10) ) / (\text{RHOK}(N, 5) \cdot M(5)) + \text{PHI}(10, 6) \cdot \text{RHOK}(N, 6) \cdot M(10) ) / (\text{RHOK}(N, 6) \cdot M(6))

\[ \text{MU}(N) = \text{MUK}(10) / (\text{PHI}(10, 7) \cdot \text{RHOK}(N, 7) \cdot M(10) ) / (\text{RHOK}(N, 10) \cdot M(7)) + \text{PHI}(10, 8) \cdot \text{RHOK}(N, 8) \cdot M(10) ) / (\text{RHOK}(N, 10) \cdot M(8)) + \text{PHI}(10, 9) \cdot \text{RHOK}(N, 9) \cdot M(10) ) / (\text{RHOK}(N, 10) \cdot M(9)) + \text{PHI}(10, 10) \cdot \text{RHOK}(N, 10) \cdot M(10) ) / (\text{RHOK}(N, 10) \cdot M(10)) + \text{A} + \text{MU}(N) \]
$2 \Omega K(N,10) \cdot M(9) \cdot \Phi I(10,11) \cdot \Omega H O K(N,11) \cdot M(11)/(\Omega H O K(N,10) \cdot M(11)) \cdot \Phi I(10,12) \cdot \Omega H O K(N,12) \cdot M(11)/(\Omega H O K(N,10) \cdot M(12)) + A) \cdot \Omega M(U(N))$

CONTINUE

IF (MFK(N,11) .LT. 1.E -5) GO TO 15

$A = 1. \cdot \Phi I(11,1) \cdot \Omega H O K(N,1) \cdot M(11)/(\Omega H O K(N,11) \cdot M(1)) + \Phi I(11,2) \cdot \Omega H O K(N,12) \cdot M(11)/(\Omega H O K(N,11) \cdot M(2)) + \Phi I(11,3) \cdot \Omega H O K(N,3) \cdot M(11)/(\Omega H O K(N,11) \cdot M(3)) + \Phi I(11,4) \cdot \Omega H O K(N,4) \cdot M(11)/(\Omega H O K(N,11) \cdot M(4)) + \Phi I(11,5) \cdot \Omega H O K(N,5) \cdot M(11)/(\Omega H O K(N,11) \cdot M(5)) + \Phi I(11,6) \cdot \Omega H O K(N,6) \cdot M(11)/(\Omega H O K(N,11) \cdot M(6))$

$\Omega M(U(N)) = \Omega M(U(N))/(\Phi I(11,7) \cdot \Omega H O K(N,7) \cdot M(11)/(\Omega H O K(N,11) \cdot M(7)) + \Phi I(11,8) \cdot \Omega H O K(N,8) \cdot M(11)/(\Omega H O K(N,11) \cdot M(8)) + \Phi I(11,9) \cdot \Omega H O K(N,9) \cdot M(11)/(\Omega H O K(N,11) \cdot M(9)) + \Phi I(11,10) \cdot \Omega H O K(N,10) \cdot M(11)/(\Omega H O K(N,11) \cdot M(10)) + \Phi I(11,11) \cdot \Omega H O K(N,11) \cdot M(11)/(\Omega H O K(N,11) \cdot M(11)) + \Phi I(11,12) \cdot \Omega H O K(N,12) \cdot M(11)/(\Omega H O K(N,11) \cdot M(12)) + A) \cdot \Omega M(U(N))$

CONTINUE

IF (MFK(N,12) .LT. 1.E -5) GO TO 16

$A = 1. \cdot \Phi I(12,1) \cdot \Omega H O K(N,1) \cdot M(12)/(\Omega H O K(N,12) \cdot M(1)) + \Phi I(12,2) \cdot \Omega H O K(N,12) \cdot M(12)/(\Omega H O K(N,12) \cdot M(2)) + \Phi I(12,3) \cdot \Omega H O K(N,3) \cdot M(12)/(\Omega H O K(N,12) \cdot M(3)) + \Phi I(12,4) \cdot \Omega H O K(N,4) \cdot M(12)/(\Omega H O K(N,12) \cdot M(4)) + \Phi I(12,5) \cdot \Omega H O K(N,5) \cdot M(12)/(\Omega H O K(N,12) \cdot M(5)) + \Phi I(12,6) \cdot \Omega H O K(N,6) \cdot M(12)/(\Omega H O K(N,12) \cdot M(6))$

$\Omega M(U(N)) = \Omega M(U(N))/(\Phi I(12,7) \cdot \Omega H O K(N,7) \cdot M(12)/(\Omega H O K(N,12) \cdot M(7)) + \Phi I(12,8) \cdot \Omega H O K(N,8) \cdot M(12)/(\Omega H O K(N,12) \cdot M(8)) + \Phi I(12,9) \cdot \Omega H O K(N,9) \cdot M(12)/(\Omega H O K(N,12) \cdot M(9)) + \Phi I(12,10) \cdot \Omega H O K(N,10) \cdot M(12)/(\Omega H O K(N,12) \cdot M(10)) + \Phi I(12,11) \cdot \Omega H O K(N,11) \cdot M(12)/(\Omega H O K(N,12) \cdot M(11)) + A) \cdot \Omega M(U(N))$

CONTINUE

$K G = 0.$

IF (MFK(N,1) .LT. 1.E -5) GO TO 17

$A = 1. \cdot \Phi I(1,2) \cdot \Omega H O K(N,2) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,3) \cdot \Omega H O K(N,3) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,4) \cdot \Omega H O K(N,4) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,5) \cdot \Omega H O K(N,5) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,6) \cdot \Omega H O K(N,6) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1))$

$K G = K G(K) + (\Phi I(1,1) \cdot \Omega H O K(N,1) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,8) \cdot \Omega H O K(N,8) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,9) \cdot \Omega H O K(N,9) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,10) \cdot \Omega H O K(N,10) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,11) \cdot \Omega H O K(N,11) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1)) + \Phi I(1,12) \cdot \Omega H O K(N,12) \cdot M(1)/(\Omega H O K(N,1) \cdot M(1))$
CONTINUE

IF (MFK(N,2).LT.1.E-5) GO TO 18

A=(1.+PSI(2,1)*RHOK(N,1)*M(2)/(RHOK(N,2)*M(1)))+PSI(2,3)*RHOK(N,3)*
1M(2)/(RHOK(N,2)*M(3))+PSI(2,4)*RHOK(N,4)*M(2)/(RHOK(N,2)*M(4))+PSI
2(2,5)*RHOK(N,5)*M(2)/(RHOK(N,2)*M(5))+PSI(2,6)*RHOK(N,6)*M(2)/(RHOK
3K(N,2)*M(6)))

KG=KGK(2)/(PSI(2,7)*RHOK(N,7)*M(2)/(RHOK(N,2)*M(7)))+PSI(2,8)*RHOK(4N,8)*M(2)/(RHOK(N,2)*M(8))+PSI(2,9)*RHOK(N,9)*M(2)/(RHOK(N,2)*M(9))
2+PSI(2,10)*RHOK(N,10)*M(2)/(RHOK(N,2)*M(10))+PSI(2,11)*RHOK(N,11)+
3*M(2)/(RHOK(N,2)*M(11))+PSI(2,12)*RHOK(N,12)*M(2)/(RHOK(N,2)*M(12))
4)+AI+KG

CONTINUE

IF (MFK(N,3).LT.1.E-5) GO TO 19

A=(1.+PSI(3,1)*RHOK(N,1)*M(3)/(RHOK(N,3)*M(1)))+PSI(3,2)*RHOK(N,2)*
1M(3)/(RHOK(N,3)*M(4))+PSI(3,4)*RHOK(N,4)*M(3)/(RHOK(N,3)*M(4))+PSI
2(3,5)*RHOK(N,5)*M(3)/(RHOK(N,3)*M(5))+PSI(3,6)*RHOK(N,6)*M(3)/(RHOK
3K(N,3)*M(6)))

KG=KGK(3)/(PSI(3,7)*RHOK(N,7)*M(3)/(RHOK(N,3)*M(7)))+PSI(3,8)*RHOK(1N,8)*M(3)/(RHOK(N,3)*M(8))+PSI(3,9)*RHOK(N,9)*M(3)/(RHOK(N,3)*M(9))
2+PSI(3,10)*RHOK(N,10)*M(3)/(RHOK(N,3)*M(10))+PSI(3,11)*RHOK(N,11)+
3*M(3)/(RHOK(N,3)*M(11))+PSI(3,12)*RHOK(N,12)*M(3)/(RHOK(N,3)*M(12))
4)+AI+KG

CONTINUE

IF (MFK(N,4).LT.1.E-5) GO TO 20

A=(1.+PSI(4,1)*RHOK(N,1)*M(4)/(RHOK(N,4)*M(1)))+PSI(4,2)*RHOK(N,2)*
1M(4)/(RHOK(N,4)*M(2))+PSI(4,3)*RHOK(N,3)*M(4)/(RHOK(N,4)*M(3))+PSI
2(4,5)*RHOK(N,5)*M(4)/(RHOK(N,4)*M(5))+PSI(4,6)*RHOK(N,6)*M(4)/(RHOK
3K(N,4)*M(6)))

KG=KGK(4)/(PSI(4,7)*RHOK(N,7)*M(4)/(RHOK(N,4)*M(7)))+PSI(4,8)*RHOK(1N,8)*M(4)/(RHOK(N,4)*M(8))+PSI(4,9)*RHOK(N,9)*M(4)/(RHOK(N,4)*M(9))
2+PSI(4,10)*RHOK(N,10)*M(4)/(RHOK(N,4)*M(10))+PSI(4,11)*RHOK(N,11)+
3*M(4)/(RHOK(N,4)*M(11))+PSI(4,12)*RHOK(N,12)*M(4)/(RHOK(N,4)*M(12))
4)+AI+KG

CONTINUE
IF (MFK(N,5) .LT. 1.E-5) GO TO 21
A=(1.+PSI(5,1)*RHOK(N,1)*M(5)/(RHOK(N,5)*M(1)) + PSI(5,2)*RHOK(N,2) * M(5)/(RHOK(N,5)*M(2)) + PSI(5,3)*RHOK(N,3)*M(5)/(RHOK(N,5)*M(3)) + PSI(5,4)*RHOK(N,4)*M(5)/(RHOK(N,5)*M(4)) + PSI(5,5)*RHOK(N,5)*M(5)/(RHOK(N,5)*M(5)) + A) + KG
CONTINUE

IF (MFK(N,6) .LT. 1.E-5) GO TO 22
A=(1.+PSI(6,1)*RHOK(N,1)*M(6)/(RHOK(N,6)*M(1)) + PSI(6,2)*RHOK(N,2) * M(6)/(RHOK(N,6)*M(2)) + PSI(6,3)*RHOK(N,3)*M(6)/(RHOK(N,6)*M(3)) + PSI(6,4)*RHOK(N,4)*M(6)/(RHOK(N,6)*M(4)) + PSI(6,5)*RHOK(N,5)*M(6)/(RHOK(N,6)*M(5)) + A) + KG
CONTINUE

IF (MFK(N,7) .LT. 1.E-5) GO TO 23
A=(1.+PSI(7,1)*RHOK(N,1)*M(7)/(RHOK(N,7)*M(1)) + PSI(7,2)*RHOK(N,2) * M(7)/(RHOK(N,7)*M(2)) + PSI(7,3)*RHOK(N,3)*M(7)/(RHOK(N,7)*M(3)) + PSI(7,4)*RHOK(N,4)*M(7)/(RHOK(N,7)*M(4)) + PSI(7,5)*RHOK(N,5)*M(7)/(RHOK(N,7)*M(5)) + A) + KG
CONTINUE
24)*RHOK(N,4)*M(8)/(RHOK(N,3)*M(4))+PSI(8,5)*RHOK(N,5)*M(8)/(RHOK(N, N,3,8)*M(5))+PSI(8,6)*RHOK(N,7)*M(8)/(RHOK(N,8)*M(6)))
KG=KGK(8)/(1+PSI(8,7)*RHOK(N,7)*M(8)/(RHOK(N,8)*M(7))+PSI(8,9)*RHO
1K(N,9)*M(8)/(RHCK(N,8)*M(9))+PSI(8,10)*RHOK(N,10)*M(8)/(RHOK(N,8)* M(10))+PSI(8,11)*RHOK(N,11)*M(8)/(RHOK(N,12)*M(11))+PSI(8,12)*RHOK( 3N,12)*M(8)/(RHOK(N,8)*M(12))+A)+KG

CONTINUE
IF (MFK(N,5).LT.1.E-5) GO TO 25
A=APSI(9,1)*RHOK(N,1)*M(9)/(RHOK(N,9)*M(1))+PSI(9,2)*RHOK(N,2)*M(9) 1/(RHOK(N,9)*M(2))+PSI(9,3)*RHOK(N,3)*M(9)/(RHOK(N,9)*M(3))+PSI(9, 24)*RHOK(N,4)*M(9)/(RHOK(N,9)*M(4))+PSI(9,5)*RHOK(N,5)*M(9)/(RHOK(N,3,9)*M(5))+PSI(9,6)*RHOK(N,6)*M(9)/(RHOK(N,9)*M(6)))
KG=KGK(9)/(1+PSI(9,7)*RHOK(N,7)*M(9)/(RHOK(N,9)*M(7))+PSI(9,8)*RHO
1K(N,8)*M(9)/(RHCK(N,9)*M(8))+PSI(9,10)*RHOK(N,10)*M(9)/(RHOK(N,9)* M(10))+PSI(9,12)*RHOK(N,12)*M(9)/(RHOK(N,9)*M(12))+A)+KG

CONTINUE
IF (MFK(N,10).LT.1.E-5) GO TO 26
A=APSI(10,1)*RHOK(N,1)*M(10)/(RHOK(N,10)*M(1))+PSI(10,2)*RHOK(N,2) 1*M(10)/(RHOK(N,10)*M(2))+PSI(10,3)*RHOK(N,3)*M(10)/(RHOK(N,10)*M(3) 2))+PSI(10,4)*RHOK(N,4)*M(10)/(RHOK(N,10)*M(4))+PSI(10,5)*RHOK(N,5) 3*M(10)/(RHOK(N,11)*M(5))+PSI(10,6)*RHOK(N,6)*M(10)/(RHOK(N,10)*M(6 4)))
KG=KGK(10)/(1+PSI(10,7)*RHOK(N,7)*M(10)/(RHOK(N,10)*M(7))+PSI(10, 18)*RHOK(N,8)*M(10)/(RHOK(N,10)*M(8))+PSI(10,11)*RHOK(N,9)*M(11)/( RH 20K(N,10)*M(9))+PSI(10,12)*RHOK(N,11)*M(10)/(RHOK(N,10)*M(11))+PSI( 310,12)*RHOK(N,12)*M(10)/(RHOK(N,11)*M(12))+A)+KG

CONTINUE
IF (MFK(N,11).LT.1.E-5) GO TO 27
A=APSI(11,1)*RHOK(N,1)*M(11)/(RHOK(N,11)*M(1))+PSI(11,2)*RHOK(N,2) 1*M(11)/(RHOK(N,11)*M(2))+PSI(11,3)*RHOK(N,3)*M(11)/(RHOK(N,11)*M(3) 2))+PSI(11,4)*RHOK(N,4)*M(11)/(RHOK(N,11)*M(4))+PSI(11,5)*RHOK(N,5) 3*M(11)/(RHOK(N,11)*M(5))+PSI(11,6)*RHOK(N,6)*M(11)/(RHOK(N,11)*M(6 4)))
KG=KGK(11)/(1+PSI(11,7)*RHOK(N,7)*M(11)/(RHOK(N,11)*M(7))+PSI(11,
27) \* RHO\text{K}(N, 8) \* M(11)/(RHO\text{K}(N, 11) \* M(8)) + PSI(11, 9) \* RHO\text{K}(N, 9) \* M(11)/(RHO\text{K}(N, 11) \* M(10)) + PSI(11, 10) \* RHO\text{K}(N, 10) \* M(11)/(RHO\text{K}(N, 11) \* M(10)) + PSI(11, 11) \* RHO\text{K}(N, 11) \* M(11)/(RHO\text{K}(N, 11) \* M(11)) + A) + KG

CONTINUE

IF (MFK(N, 12) < 1.E-5) GO TO 28

A = (PSI(12, 1) \* RHO\text{K}(N, 1) \* M(12)/(RHO\text{K}(N, 12) \* M(1)) + PSI(12, 2) \* RHO\text{K}(N, 2) \* M(12)/(RHO\text{K}(N, 12) \* M(2)) + PSI(12, 3) \* RHO\text{K}(N, 3) \* M(12)/(RHO\text{K}(N, 12) \* M(3)) + PSI(12, 4) \* RHO\text{K}(N, 4) \* M(12)/(RHO\text{K}(N, 12) \* M(4)) + PSI(12, 5) \* RHO\text{K}(N, 5) \* M(12)/(RHO\text{K}(N, 12) \* M(5)) + PSI(12, 6) \* RHO\text{K}(N, 6) \* M(12)/(RHO\text{K}(N, 12) \* M(6)) + PSI(12, 7) \* RHO\text{K}(N, 7) \* M(12)/(RHO\text{K}(N, 12) \* M(7)) + PSI(12, 8) \* RHO\text{K}(N, 8) \* M(12)/(RHO\text{K}(N, 12) \* M(8)) + PSI(12, 9) \* RHO\text{K}(N, 9) \* M(12)/(RHO\text{K}(N, 12) \* M(9)) + PSI(12, 10) \* RHO\text{K}(N, 10) \* M(12)/(RHO\text{K}(N, 12) \* M(10)) + PSI(12, 11) \* RHO\text{K}(N, 11) \* M(12)/(RHO\text{K}(N, 12) \* M(11)) + A) + KG

CONTINUE

P\text{R}(N) = MU(N)/KG*ROCPM(N)/RHO(N)

RETURN

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SUBROUTINE PDE1 (FS,CRNI)
SUBROUTINE FOR SOLVING SECOND ORDER LINEARIZED DIFFERENTIAL EQUA....
TIONS FOR TEMPERATURE OF THE CHAR AND UNCHARRED LAYERS.
DIMENSION AS(110), 8S(110), CS(110), ()S(1L)), BP(110), FS(11)), GP
1(110), ALPHB4(110), ALPHA2(110), ALP1B3(110), TSP(110), ALPHP2(110
2), KS(50), ALPHP1(110), ALPHA1(110), TP(50), KP(100), KPP(110), TF
3S(110), ALPHA3(110), ALPHA4(110), 4LPHP3(110), ALPHP4(110)
COMMON (DE1DE2t AS,BS,CS,DS,BP,GP
COMMON /PDE1/ ALPHI1,ALPHI2,ALPHI3,ALPHI4IALPHIPI I ALPHIP2,ALPAIP3,
1ALPHIP4,GAMMI1,GAMMI2,GAMMI4,GAMMIP1,GAMNUP2,GAMMIP3,GAMMIP4,SGMA,
2DX,ALPHAI,ALPHA2,ALPHP1,ALPHP2,ALPH83,ALPH84,DT,L,Q,KS,LP,QPT,KSP1
3,TSPDXP,IP,I,IJ,IN,I01,KP,LPP,LPPP,SPI I KPPI,MGDOT,D1P,MGDOTP,QNE
4T,QPNET,KPPIP,GAMP13,IM,EPSS,EPSPDXIOXPI,ALPHA4,ALPHP3tALPHP4,AL
5PHA3,HTSK,HTSKPOOPT1,IOPTI,T1BARITIBAR
COMMON /TS( IP1IIZ1,KPP,GAMIP1,GAMIP2 I GAMIP3,GAMIP4I G4MIPP1,34MIPP
12,GAMIPP3,GAMIPP4IKAPIPlyKAPIP2,KAPIP3,KAPIP4,KAPIPPI I KAPIPP2,IL,K
2APIPP3,KAPIPP4,0XPP,KPPPIP,KPPPIZ I IZ
DOUBLE PRECISION AS,BS,CS,DS,GSCNST,HSCNST,AISCNST,ZSCNST,YSCNST,X
1SCNST,AIS,BIS,CIS,DIS,BP,GP,WS,TFS
REAL KS,KPIL,LP,MCDOT,LPPILPPP,MGOOTP,KPPI,KSPI,KSP1,KPPIP,KAPIP1,
1KAPIP2,KAPIP3,K4PIP4,KAPIPP1,KAPIPP2,KAPIPP3,KAPIPP4,IL,KPPPIZ,KPP
2PIP,KPP
CALCULATE TRI-DIAGCNAL MATRIX COEFFICIENTS
DDX=DX1
IF (IOPTI.EQ.0) CC TO 1
IF ((FS(1)TIBAR).GT.1.E--6) GO TO 2
CCNTINUE
BS(1)=CRNI*((ALPHA1(1).-11./(6.*DDX))*L*SGMA*EPSS*FS(1)**3/KS(1)-3.
1/(2.*DDX**2)+4LPHA2(1))+ALPH84(1)0T
CS(1)=3.*CRNI/(4.*DDX**2)
GSCNST=CRNI*(3./(2.*DDX**2)-1./(6.*D)X**2))
HSCNST=....3.*CRNI/(4.*DDX**2)
AISCNST=CRNI/(6.*DDX**2)
DS(1)=-. ALPH83(1)+CRNI*(ALPHA1(1)-11./(6.*DDX))*Q*UKS(1)+(1.CRNI)
1*(ALPHP1(1)-11./(6.*DDX))*QPT*LPP/KSP1((1.-CRNI)*((ALPHP1(1)-11./
2(6.*DDX))*LPP*SGMA*EPSS*TSP(1)**WKSP1-3./(2.*DDX**2)+ALPHP2(1))-A

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3LPHB4(1)/DT*TSP(1)-(1.-CRNI)*(3./(4.*DDX**2)*TSP(2)+(3./(2.*DDX**2)))*TSP(3)-3./(4.*DDX**2)*TSP(4)+1./(6.*DDX**2)*TSP
GO TO 3
2 CONTINUE
BS(1)=1.
CS(1)=0.
GSCNST=0.
HSCNST=0.
AISCNST=0.
DS(1)=T13AR+1.E-4
3 CONTINUE
DO 5 N=2,IM
IF (N.NE.20) GO TO 4
DDX=DX
GO TO 5
4 AS(N)=CRNI*(1./DDX**2-4LPHAI(N)/(2.*DX))
BS(N)=CRNI*(ALPH42(N)-2./DDX**2+ALDH34(N)/(0T*CRNI))
CS(N)=CRNI*(1.0X**2+ALPhA1(N)/(2.*DDX))
DS(N)=-ALPH53(N)-(1-CRNI)*((1./DDX**2-ALPHB4(N)((DT*(1.-CRNI)))*TSP(N-1)1+(ALPHP2(N)-2./DDX**2-ALPHB4(N)/(DT*(1.-CRNI))))*TSP(N)+(1./DDX**22+2ALPHP1(N)/(2.*DDX)))*TSP(N+1))
5 CONTINUE
BS(1)=AS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*C
CS(1)=BS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*C
DS(1)=DS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*C
BS(20)=CRNI*(ALPHA1(20)*DX/(DX1*(DX1+DX))-2./(DX1*(DX1+DX)))
BS(20)=CRNI*(2./(DX*DX1)-ALPHA2(20)-ALPHA1(20)*((DX-DX1)/(DX1+DX))-
1ALPHB4(20)/DT
CS(20)=CRNI*(-2./(LX*(DX1+DX))-ALPHA1(20)*DX/(DX1*(DX1+DX))))
\[ DS(2J) = -ALPHB3(2J) - (1. - CRNI) \times (ALPHP1(2J) \times DX / (DX1 \times (DX1 + DX))) - 2. / (DX1) \]
\[ 1 \times (DX1 + DX)) \times TSP(1J) - (1. - CRNI) \times (2. / (DX \times DX1) - ALPHP2(20) - ALPHP1(20) \times 2(DX \times DX1) \times (DX1 + DX)) + ALPHB4(20) / DT) \times TSP(20) + (1. - CRNI) \times (2. / (DX \times (DX1 + DX)) \times ALPHP1(20) \times DX1 / (DX \times (DX1 + DX))) \times TSP(21) \]

\[ DDX = DXP1 \]

\[ \text{DO 7 N=IN,IC1} \]

\[ \text{IF (N.EQ.(I+20)) GO TO 6} \]

\[ \text{AS(N)} = CRNI \times (1./DOX**2 - ALPHAI(N)/((2.)*DA1)) \]
\[ \text{BS(N)} = CRNI \times (ALPHA2(N) - 2./DDX**2 + ALPHB4(N)/(DT*CRNI)) \]
\[ \text{CS(N)} = CRNI \times (1./DOX**2 + ALPHAI(N)/(2.)*DDX)) \]
\[ \text{DS(N)} = -ALPHB3(N) - (1. - CRNI) \times (1./DDX**2 - ALPHP1(N)/(2.*DX)) \times TSP(N-1) \]

\[ 1. + (ALPHP2(N) - 2./DDX**2 - ALPHB4(N)/(DT*(1. - CRNI))) \times TSP(N) + (1./DDX**2 + ALPHP1(N)/((2.*DDX)) \times TSP(N+1)) \]

\[ \text{GO TO 7} \]

\[ DDX = DXP \]

\[ \text{AS(N)} = CRNI \times (ALPHA1(N) \times DXP / (DX1 * (DX1 + DXP)) - 2. / (DX1 * (DX1 + DXP))) \]
\[ \text{BS(N)} = CRNI \times (2. / (DX1 * DXP) - ALPHP1(N)/(DX * DXP)) \]
\[ \text{CS(N)} = CRNI \times (ALPHA2(N) - 2./DDX**2 + ALPHB4(N)/(DT*CRNI)) \]
\[ \text{DS(N)} = -ALPHB3(N) - (1. - CRNI) \times (1./DDX**2 - ALPHP1(N)/(2.*DX)) \times TSP(N-1) \]

\[ 1. + (ALPHP2(N) - 2./DDX**2 - ALPHB4(N)/(DT*(1. - CRNI))) \times TSP(N) + (1./DDX**2 + ALPHP1(N)/((2.*DDX)) \times TSP(N+1)) \]

\[ \text{GO TO 7} \]

\[ 6 \]

\[ AS(N) = CRNI \times (ALPHA1(N) \times DXP / (DX1 * (DX1 + DXP)) - 2. / (DX1 * (DX1 + DXP))) \]
\[ BS(N) = CRNI \times (2. / (DX1 * DXP) - ALPHP1(N)/(DX * DXP)) \]
\[ CS(N) = CRNI \times (ALPHA2(N) - 2./DDX**2 + ALPHB4(N)/(DT*CRNI)) \]
\[ DS(N) = -ALPHB3(N) - (1. - CRNI) \times (1./DDX**2 - ALPHP1(N)/(2.*DX)) \times TSP(N-1) \]

\[ 1. + (ALPHP2(N) - 2./DDX**2 - ALPHB4(N)/(DT*(1. - CRNI))) \times TSP(N) + (1./DDX**2 + ALPHP1(N)/((2.*DDX)) \times TSP(N+1)) \]

\[ \text{GO TO 7} \]

\[ 7 \]

\[ \text{CONTINUE} \]

\[ \text{IF (IOPTI.EQ.0) GO TO 8} \]

\[ \text{IF ((FS(1)-TIBAR).GT.1.E-6) GO TO 9} \]

\[ 8 \]

\[ \text{CONTINUE} \]

\[ \text{AKSL=DX*KS(I) * ALPHI1/L} \]
\[ \text{AKPL=DX1*KP(I) * GAMMI4/LP} \]
\[ \text{AKAL=CRNI/(AKSL+AKPL)} \]
\[ \text{AKSLP=DX*KSPI*ALPHIP4/LPP} \]
\[ \text{AKPLP=DX1*KPPI*GAMMIP4/LPPP} \]
\[ \text{AKALP=(1. - CRNI)/(AKSLP+AKPLP)} \]
\[ \text{ZIS=-AKAL*KS(I)/(6.*DX*L)} \]

\[ \text{CONTINUE} \]

\[ \text{IF (IOPTI.EQ.0) GO TO 8} \]

\[ \text{IF ((FS(1)-TIBAR).GT.1.E-6) GO TO 9} \]

\[ 9 \]

\[ \text{CONTINUE} \]

\[ \text{AKSL=DX*KS(I) * ALPHI1/L} \]
\[ \text{AKPL=DX1*KP(I) * GAMMI4/LP} \]
\[ \text{AKAL=CRNI/(AKSL+AKPL)} \]
\[ \text{AKSLP=DX*KSPI*ALPHIP4/LPP} \]
\[ \text{AKPLP=DX1*KPPI*GAMMIP4/LPPP} \]
\[ \text{AKALP=(1. - CRNI)/(AKSLP+AKPLP)} \]
\[ \text{ZIS=-AKAL*KS(I)/(6.*DX*L)} \]
5*DS(I-1)*ZIS/(AS(I-1)*AS(I-2)*AS(I-3))-DS(I-3)*ZIS/AS(I-3)-DS(I-1)*XIS/AS(I-1)*ZIS/(AS(I-2)*AS(I-3))-DS(I-1)*XIS/AS(I-2)*AS(I-3)-DS(I-2)

GO TO 10

CONTINUE

AS(I)=0.
BS(I)=1.
CS(I)=0.
DS(I)=TIBAR+1.E-4

CONTINUE

DO 11 N=IP1,IZ1
AS(N)=CRNI*(1./OXPP**2-ALPHA1(N)/(2.*OXPP))
BS(N)=CRNI*(ALPH42(N)-2./DXPP**2+ALP1B4(N)/(DT*CRNI))
CS(N)=CRNI*(1./0XPP**2+ALPHAI(N)/(2.*OXPP))
DS(N)=-ALPH83(N)-(1.-CRNI)*((1./DXPP**2-ALPHPI(N)/(2.*DXPP))*TSP(N-1)-1)+(ALPH2(N)-2./CxPP**2-ALPHB4(N)/(DT*(1.-CRNI)))*TSP(N)+(1./DXP**2+ALPHP1(N)/(2.4 DOP))*TSP(N+1)))

AK=CRNI/(KP(IP)*GAMIP4*OXPP/LP+KPPI(IP)*KAPIP4*DXPP/IL-HTSK)
AKI =.(1.-CRNI)/(KPPIP*GAMIPP4*OXPILPPF )+KPPPIP*KAPIPP4*DXPP/IL-HTSK)
ZIS=-AK*KP(IP)/(6.*DXPP*LP)
YIS=AK*KP(IP)*(.75/DXPP+GAMIP1/3.)/LP
XIS=-AK*KP(IP)*((4./3.*DXPP)+1.5*GAMIP1)/LP
AIS=-AK*KP(IP)*(.75/DXPP-3.*GAMIP1)/LP
BIS=-1./DT+AK*(KP(IP)/LP*(1.5/DXPP-11.*GAMIP1/6.-GAMIP2*DXPP)+KPP(IP)/IL*(1.5/0XPP+11.*KAPIP1/6.-KAPIP2*DxpP))
CIS=-AK*KP(IP)*(.75/DXPP+3.*KAPIP1)/IL
EIS=-AK*KP(IP)**(4./3.*DXPP)-1.5*KAPIP1)/IL
FIS=AK*KP(IP)*(.75/DXPP-KAPIP1/3.)/IL
GIS=-AK*KP(IP)/(6.*DXPP*IL)
DIS=AK*(KP(IP)*GAMIP3*DXPP/LP+KPP(IP)*KAPIP3*DXPP/IL)-AK*KPPPIP/LPP
LPIP(-TSP(IP-4)/(6.*DXPP)+.75/DXPP+GAMIP1/3.)*TSP(IP-3)-(4./(3.*DXPP)
2+1.5*GAMIP1)*TSP(IP-2)+.75/DXPP+3.*GAMIP1)*TSP(IP-1)-(AKP*(KPP(IP)
3P/LPPP*(1.5/DXPP-11.*GAMIP2*DXPP)+KPPPIP/IL*(1.5/DXPP+11
4.*KAPIPPI/6.-KAPIP2*DXPP))+1./DT)*TSP(IP)+AKP*KPPPIP/IL*/(75/DXPP
\[ 5P^3 + 3 \cdot KAPIPP1 \cdot TSP(IP+1) + 4 \cdot (3 \cdot DXPP)^{-1.5} \cdot KAPIPP1 \cdot TSP(IP+2)^{-0.75} + 6DXPP \cdot KAPIPP1/3.3 \cdot TSP(IP+1) + TSP(IP+4)/(6 \cdot DXPP) + AKP \cdot (KPPIP \cdot GAMP III) \cdot 7 \cdot DXPP/LPPP + KPPIP \cdot KAPIPP3 \cdot DXPP/IL \]

\[ AS(IP) = -(BS(IP-1) \cdot XIS/AS(IP-1) - BS(IP-3) \cdot TSIP-3) - BS(IP-1) \cdot ZIS/(AS(IP-1) \cdot AS(IP+1) \cdot ZIS) - (BS(IP-2) \cdot XIS/(AS(IP-1) \cdot AS(IP+2) + AS(IP+1) \cdot BS(IP-2)) \]

\[ BS(IP) = -(BS(IP-1) \cdot ZIS/(AS(IP-1) \cdot AS(IP+1) \cdot AS(IP+2) + AS(IP+1) \cdot BS(IP-2)) \cdot TSIP-3) - BS(IP-1) \cdot ZIS/(AS(IP-1) \cdot AS(IP+1) \cdot AS(IP+2) + AS(IP+1) \cdot BS(IP-2)) \]

\[ CS(IP) = -(CS(IP+1) \cdot EIS/CS(IP+1) \cdot AS(IP+1) \cdot BS(IP+1) \cdot GIS/(CS(IP+1) \cdot CS(IP+2)) \]

\[ DS(IP) = -(DS(IP+1) \cdot EIS/CS(IP+1) \cdot AS(IP+1) \cdot BS(IP+1) \cdot GIS/(CS(IP+1) \cdot CS(IP+2)) \]

\[ DS(IP) = -(DS(IP+1) \cdot EIS/CS(IP+1) \cdot AS(IP+1) \cdot BS(IP+1) \cdot GIS/(CS(IP+1) \cdot CS(IP+2)) \]

\[ ZSCNST = CRNI \ast KPP(IZ)/16 \ast DXPP**2 \ast IP*(HTSKP*(ALPHA1(IZ)+11)/(6 \ast DXPP)) \]

\[ YSCNST = -(4.5 \ast ZSCNST) \]

\[ XSCNST = 8 \ast ZSCNST \]

\[ BS(I) = (6 \ast DXPP)**2 \ast ALPHA2(IZ) - 9) \ast ZSCNST - CRNI \ast SGMIMA \ast EPS \ast Fs(I) \ast 3 \ast \ast 1*(ALPHA1(IZ)+11)/(6 \ast DXPP)) \]

\[ DS(I) = -(CRNI*(ALPHA1(IZ)+11)/(6 \ast DXPP)) \]

\[ 4S/(AS(IP-1) \ast AS(IP-2) + BS(IP-2) \ast BS(IP-3) \ast CS(IP-3)) \ast ZIS/(AS(IP-1) \ast AS(IP+1) \ast AS(IP+2) \ast AS(IP+3) \ast ALPHAT(IZ) + 11)/(6 \ast DXPP)) \]

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C 212
21*(IZ)+11./(6.*DXPP))-((1.-CRNI)*(ALPHP1(IZ)+11./(6.*DXPP)))/(HTSPK
C 213
3*(ALPHP1(IZ)+11./(6.*DXPP))-ALPHP4(IZ)*KPPP/IL)*(QPN+ALP+P3(IZ
C 214
4)*KPPP/IL*(ALPHP1(IZ)+11./(6.*DXPP)))*KPPP/IL*(ALPHP1(IZ)+11
C 215
5.*(6.*DXPP)))*(TSP(IZ-4)/(6.*DXPP**2))-.75*TSP(IZ-3)/DXPP**2+.75*TSP
C 216
6*(IZ-2)/(3.*DXPP**2)+.75*TSP(IZ-1)/DXPP**2-(1.5/DXPP**2-ALPHP2(IZ))
C 217
7*TSP(IZ)))-SGMA*EPS*TS(IZ)**4)-TSP(IZ)/DT
C 218
AS(IZ)=AS(IZ-2)*BS(IZ-1)*(AS(IZ-1)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-1
C 219
1)*BS(IZ-2)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)+AS(IZ-1)*CS(IZ-2)*(AS
C 220
2*(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ)*AS(IZ-1)*AS(IZ-2)*AS(IZ-3)
C 221
BS(IZ)=AS(IZ-2)*CS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-2
C 222
1)*CS(IZ-1)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-BS(IZ-1)*AS(IZ-3)*BS(IZ
C 223
2)*BS(IZ)
C 224
DS(IZ)=AS(IZ-2)*DS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-2
C 225
1)*DS(IZ-1)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ-1)*AS(IZ-2)*AS(IZ
C 226
2)*(IZ-3)*DS(IZ)-DS(IZ-3)*ZSCNST)+AS(IZ-1)*DS(IZ-2)*(AS(IZ-3)*YSCNST-
C 227
3BS(IZ-3)*ZSCNST
C 228
CS(IZ)=0.
C 229
SOLVE TRI-DIAGONAL MATRIX FOR TS
C 230
BP(1)=CS(1)/BS(1)
C 231
GP(1)=DS(1)/BS(1)
C 232
DO 12 N=2,IZ
C 233
WS=BS(N)-AS(N)*GP(N-1)
C 234
BP(N)=CS(N)/WS
C 235
GP(N)=(DS(N)-AS(N)*GP(N-1))/WS
C 236
CONTINUE
C 237
TFS(IZ)=BP(IZ)
C 238
FS(IZ)=TFS(IZ)
C 239
KON=IZ1
C 240
DO 13 N=1,IZ1
C 241
TFS(KON)=GP(KON)-BP(KON)*TFS(KON+1)
C 242
FS(KON)=TFS(KON)
C 243
KON=KON-1
C 244
RETURN
C 245
END
SUBROUTINE PDP (CRNI, DT, L, DX, DX1, MGD, T, MGDOT, LPP, I, IM, RH0, P, MU, T, 
ITP, RU)
SUBROUTINE FOR SOLVING SECOND ORDER LINEARIZED DIFFERENTIAL EQUATIONS 
FOR PYROLYSIS GAS PRESSURE IN THE CHAR LAYER.
DIMENSION RHO(50), P(50), MU(50), AS(50), BS(50), CS(50), DS(50), 
1BP(50), GP(50), T(50), TP(50), ZP(50)
COMMON /PDP/ PAL1(50), PAL2(50), PAL3(50), PAL4(50), PAP1(50), PAP2(50)
1, PAP3(50), PAP4(50), PAB3(50), PAB4(50), PBP, PBP(50), PMP, PM(50), PMU, PPM, PRH 
20(50), ETA(50), ETAP(50), AVGMF(50), AVGMFP(50)
COMMON /DE1DE2/ AS, BS, CS, DS, RP, GP
REAL MUL, MGD, T, MGDOT, LPP, MGDOT
DOUBLE PRECISION AS, BS, CS, DS, PX, PY, PZ, PA, PB, PD, BP, GP, WP, ZP
CALCULATE TRI-DIAGONAL MATRIX COEFFICIENTS
N=1-2
DDX=DX1
DO 2 N=2, IM
IF (N. NE. 20) GO TO 1
AS(N)=CRNI*(1./DDX**2-PAL1(N)/(2.*DDX))
BS(N)=CRNI*(PAL2(N)-2./DDX**2+PAB4(N)/DT)
CS(N)=CRNI*(1./DDX**2+PAL1(N)/(2.*DDX))
DS(N)=PAB3(N)-(1.-CRNI)*((1./DDX**2-PAP1(N)/(2.*DDX))**2-P(N-1)**2- 
1(2./DDX**2-PAP2(N)+PAB4(N)/(DT*1.-CRNI))**2+(1./DDX**2+PAP 
21(N)/(2.*DDX))**2)*PP(N)**2+(1./DDX**2+PAP
CONTINUE
2 AS(20)=CRNI*(PAL1(20)*DX/(DX1*(DX1+DX))-2./DX)*PP(19)**2 
BS(20)=CRNI*(2./DX*DX1)-PAL2(20)-PAL1(20)*DX/(DX1+DX))**2-PAP4 
1(20)/DT
CS(20)=CRNI*(-2./DX**2-PAL1(20)*DX/(DX1+DX))
DS(20)=PAB3(20)-(1.-CRNI)*((PAP1(20)*DX/(DX1+DX))-2./DX)**2-PAP3 
1(DX))**2-PAP2(20)-PAP1(20)*DX/(DX1+DX))**2-PAP1(20)**2 
21/(DX1*DX))**2+(1.-CRNI)*(2./DX**2+PA 
3P1(20)*DX1/(DX1+DX))**2 
DS(2)=DS(2)-AS(2)*P(1)**2
AS(2)=0.
PX=CKNI/(6.*DX**2)
PY=-.75*CRNI/DX**2
PZ=4.*CRNI/(3.*DX**2)
PA=-PY
PB=PA*B4(I)/DT+CRNI*(PAL2(I)-3./(2.*DX**2))
PD=-PAB3(I)-(1.-CRNI)*(11./(6.*DX)+PAL1(I))*2.*MU(I)*L*MGDO*(RU*TP(I))/(AVGMF(I)*PPM(I))-(1.-CRNI)*(11./(0.*DX1+PAL1II))*(2.*MU(I)*L*MGDO*(RU*TII/lAVGMF(I)*PM(I)))-(1.-CRNIMPP(I-4)**2/(6.*DX**2)-.75*P13P(I-3)**2/(3.*DX**2)+2.75*PP(I-1)**2/DX**2+(PAP42(I)-1.5/DX**2-PA*B4(I)/DT*(1.-CRNI))*PP(I)**2)
AS(I)=PA-CS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3)-8S(I-1)/AS(I-1)*(PZ-PX*BS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3)))
BS(I)=PB-CS(I-1)/AS(I-1)*(PZ-PX*CS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3)))
DS(I)=PD-PX/AS(I-1)*DS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3))
CS(I)=0.
C SOLVE TRI-CIAGONAL MATRIX FOR P
BP(2)=CS(2)/BS(2)
GP(2)=DS(2)/BS(2)
DO 3 N=3,I
W=BS(N)-AS(N)*BP(N-1)
BP(N)=CS(N)/W
GP(N)=(DS(N)-AS(N)*GP(N-1))/W
3 CONTINUE
ZP(I)=DSQRT(GP(I))
P(I)=ZP(I)
KON=IM
DO 4 N=1,IN
ZP(KON)=DSQRT(GP(KON)-BP(KON)*ZP(KON+1)**2)
P(KON)=ZP(KON)
4 KON=KON-1
RETURN
END
SUBROUTINE PDF2 (BETAI,BETA3,BETP1,TP,F,CRNI,DX,DX1,DT,I)
SUBROUTINE FOR SOLVING FIRST ORDER LINEARIZED DIFFERENTIAL
EQUATIONS GOVERNING PYROLYSIS GAS TEMPERATURE AND FLOW RATE AND
CHAR LAYER POROSITY.
DIMENSION B(50), C(50), D(50), E(50), F(50), TP(50), BETAI(50), BE
TB2(50), BETB3(50), BETP1(50), TF(50)
COMMON /DIDE2/ B,C,D,E
DOUBLE PRECISION B,C,D,E,TF

CALCULATE TRI-DIAGONAL MATRIX COEFFICIENTS
IM=I-1
IN=I-2
IQ=I-3
DDX=DX1
B(N)=CRNI*(BETA1(N)-1.5/DDX)+BET83(N)/DT
C(N)=2.*CRNI/DDX
E(N)=-.5*CRNI/DDX
D(N)= -...BETB2(N)....((1.-CRNI)*(BETP1(N)1.5/DDX)-BETB3(IM)/DT)*TP(IM)....-(1.CRNI)/DX*TP(IM)

DO 2 N=1,IN
IF (N.NE.1) GO TC 1
DDX=DX
GO TO 2
CONTINUE
B(N)=CRNI*(BETA1(N)-1.5/DDX)+BET83(N)/DT
C(N)=2.*CRNI/DDX
E(N)=-.5*CRNI/DDX
D(N)= -...BETB2(N)....((1.-CRNI)*(BETP1(N)1.5/DDX)-BETB3(IM)/DT)*TP(N)-(1.CRNI)*TP(N+1)/DDX+TP(N+2)/(2.*DDX))

2 CONTINUE
B(IM)=CRNI*(BETA1(IM)-1./DX)+BETB3(IM)/DT
C(IM)=CRNI/DDX
E(IM)=0.
D(IM)= -...BETB2(IM)....((1.-CRNI)*(BETP1(IM)1.5/DDX)-BETB3(IM)/DT)*TP(IM)....-(1.CRNI)/DX*TP(IM)....
C SOLVE TRI-DIAGONAL MATRIX
TF(1)=F(1)
TF(IM)=(D(IM)-C(IM)*TF(I))/B(IM)
F(IM)=TF(IM)
KON=IN
DO 3 N=1,IN
TF(KON)=(D(KON)-C(KON)*TF(KON+1)-E(KON)*TF(KON+2))/B(KON)
F(KON)=TF(KON)
3 KON=KON-1
RETURN
END
SUBROUTINE CHCOM(TIME)  
SUBROUTINE FOR CALCULATING THE CHEMICAL REACTION RATES OF EACH SPECIES.

COMMON ACEF(12),ACER(12),BCEF(12),BCER(12),CRNI,KUPT(40,12),KUPTV(140),M(13),FKF(50,12),MNO,NNO,MU(50),MUKT(40,12),MUKTV(40),PR(50),R(250,12),RHO(50),RHOK(50,12),RHOKP(50,12),T(50),TEMP(40),NRCT,KT,RU(3),NSTEP,ROCPM(50),RS(50),RMR(50,12),R1S(50),DHK(50,12),DHJ(50,12),H
4RJSUM(50)

DIMENSION RMP(9),RMR(9),RJN(9)
REAL M
N=NSTEP
RMR(1)=RHCK(N,1)/M(1)
RMP(1)=1.
RMR(2)=RHOK(N,11)/M(11)
RMP(2)=RHOK(N,3)/M(3)*RHOK(N,2)/M(2)
RMR(3)=RHOK(N,3)/M(3)
RMP(3)=1.
RMR(4)=RHOK(4)/M(4)*RHOK(N,2)/M(2)
RMP(4)=1.
RMR(5)=RHOK(N,12)/M(12)
RMP(5)=1.
RMR(6)=RHOK(N,9)/M(9)
RMP(6)=1.
RMR(7)=RHCK(N,6)/M(6)
RMP(7)=1.
RMR(8)=RHOK(N,7)/M(7)
RMP(8)=1.
RMR(9)=RHOK(N,7)/M(7)
RMP(9)=1.
DO 1 J=1,9
AKF=ACEF(J)*EXP(-BCEF(J)/(RU*T(N))) IF(J.EQ.6)AKF=AKF/T(N)
AKK=ACER(J)*EXP(-BCER(J)/(RU*T(N))) RJSN(JJ)=AKF*RMP(JJ)-AKR*RMP(J)
1 CONTINUE
R(N,1)=-RJN(1)
\( R(N, 2) = 0.5 \times R(JN(1)) + R(JN(2)) + R(JN(3)) + R(JN(4)) + 3 \times R(JN(5)) + R(JN(7)) + 1.5 \times R(JN(8)) + 1 \times R(JN(9)) \)

\( R(N, 3) = R(JN(2)) - R(JN(3)) \)

\( R(N, 4) = R(JN(3)) - R(JN(4)) \)

\( R(N, 5) = 2 \times R(JN(6)) + R(JN(7)) \)

\( R(N, 6) = -R(JN(7)) \)

\( R(N, 7) = -R(JN(8)) - R(JN(9)) \)

\( R(N, 8) = 0.5 \times R(JN(8)) - R(JN(9)) \)

\( R(N, 9) = -R(JN(6)) \)

\( R(N, 10) = R(JN(9)) \)

\( R(N, 11) = 0.5 \times R(JN(1)) - R(JN(2)) \)

\( R(N, 12) = -R(JN(5)) \)

\( RS(N) = 2 \times R(JN(4)) + 6 \times R(JN(5)) \)

\( RHS(N) = -R(JN(6)) - R(JN(7)) - R(JN(9)) \)

\( RHR(N, 6) = R(JN(6)) \)

\( RHR(N, 7) = R(JN(7)) \)

\( RHR(N, 9) = R(JN(9)) \)

RETURN

END
APPENDIX D

PROGRAM TERMINOLOGY

A Dummy parameter used in computing viscosity of pyrolysis gas

AB2 Dummy array defined in solution of species continuity equation, single subscript

AC Specific reaction rate constant for first order oxidation of char layer

ACEF Specific reaction rate constant for forward chemical reaction, single subscript

ACER Specific reaction rate constant for reverse chemical reaction, single subscript

AEXP Specific reaction rate constant for pyrolysis gas of uncharred material

AINT Single subscripted parameter defined as $\int_{x(N)}^{1} \eta \rho \, dx$

AINT3 Single subscripted parameter defined as $\int_{x(N)}^{1} \left[ \frac{\partial}{\partial t} \eta \rho - \eta \sum_{i} R_{i} M_{i} \right] \, dx$

AIS Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer - insulation layer interface

AISCNST Coefficient in solid temperature finite difference equation evaluated at the front surface of the char layer

AK Parameter defined in solution of solid temperature equation

AKAL Parameter defined in solution of solid temperature equation

AKALP Parameter defined in solution of solid temperature equation

AKF Rate of homogeneous chemical reaction in forward direction, single subject
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AKP</td>
<td>Parameter defined in solution of solid temperature equation</td>
</tr>
<tr>
<td>AKPL</td>
<td>Parameter defined in solution of solid temperature equation</td>
</tr>
<tr>
<td>AKPLP</td>
<td>Parameter defined in solution of solid temperature equation</td>
</tr>
<tr>
<td>AKR</td>
<td>Rate of homogeneous chemical reaction in reverse direction, single subscript</td>
</tr>
<tr>
<td>AKSL</td>
<td>Parameter defined in solution of solid temperature equation</td>
</tr>
<tr>
<td>AKSLP</td>
<td>Parameter defined in solution of solid temperature equation</td>
</tr>
<tr>
<td>ALFC</td>
<td>Weighting factor for transpiration effectiveness of char mass loss</td>
</tr>
<tr>
<td>ALFP</td>
<td>Weighting factor for transpiration effectiveness of pyrolysis gases</td>
</tr>
<tr>
<td>ALPHA</td>
<td>Absorptivity of char surface</td>
</tr>
<tr>
<td>ALPHA 1, 2, 3, 4</td>
<td>Coefficients in linearized differential equations for solid temperature evaluated at end of time step, single subscript</td>
</tr>
<tr>
<td>ALPHB 3, 4</td>
<td>Coefficients in finite difference equation for solid temperature evaluated at mid point of time step, single subscript</td>
</tr>
<tr>
<td>ALPHI 1, 2, 3, 4</td>
<td>Values of ALPHA 1, etc. for the char layer at the pyrolysis zone evaluated at the start of the time step</td>
</tr>
<tr>
<td>ALPHI 1, 2, 3, 4</td>
<td>Values of ALPHA 1, etc. for the char layer at the pyrolysis zone evaluated at the end of the time step</td>
</tr>
<tr>
<td>ALPHP 1, 2, 3, 4</td>
<td>Values of ALPHA 1, etc. evaluated at the start of the time step, single subscript</td>
</tr>
</tbody>
</table>
AL1  Dummy array defined in solving species continuity equation, single subscript
AMDOT  Local mass flow rate of pyrolysis gas, single subscript
AMGDOT  Rate of pyrolysis of uncharred material given by rate equation
AMSDOT  Rate of char layer removed by oxidation
AMU  Dummy parameter defined in computing pyrolysis gas viscosity
AMJ  }
AP  Solution of pyrolysis gas pressure equation for previous iteration, single subscript
APR  Dummy parameter defined in computing pyrolysis gas Prandtl number
AP1  Dummy arrays defined in solution of species continuity equation, single subscript
ARH  }
AS  "AS" coefficient in matrix formed by second order differential equation, single subscript
AT  Pyrolysis gas temperature for previous iteration, single subscript
ATS  Solid temperature for previous iteration, single subscript
AVGMF  Average molecular weight of pyrolysis gas at end of time step, double subscript
AVGMFP  Average molecular weight of pyrolysis gas at start of time step, double subscript
B  "B" coefficient in matrix formed by first order equations, single subscript
BC  Activation temperature for first order oxidation of char layer
BCEF  Activation temperature for forward homogeneous chemical reaction involving gaseous species, single subscript
BCER  Activation temperature for reverse homogeneous chemical reaction involving gaseous species, single subscript
\( BETA_1 \) \( BETA_2 \) \( BETA_3 \) Coefficients in linearized differential equation of pyrolysis gas temperature evaluated at end of time step, single subscript

\( BETB_2 \) \( BETB_3 \) Coefficients in finite difference equation for pyrolysis gas temperature evaluated at mid point of time step, single subscript

\( BETP_1 \) \( BETP_2 \) \( BETP_3 \) Values of \( BETA_1 \), etc. evaluated at the start of the time step, single subscript

\( BEXP \) Activation temperature for pyrolysis of uncharred material

\( BIS \) Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer.

\( BMGDOT \) Rate of pyrolysis of uncharred material given by energy-balance

\( BMSDOT \) Rate of removal of char layer by sublimation

\( BP \) Parameter defined in algorithm for solving set of finite difference equations, single subscript

\( BRH \) Dummy array defined in solution of species continuity equation, single subscript

\( BS \) "BS" coefficient in matrix formed by second order differential equation, single subscript

\( C \) "C" coefficient in matrix formed by first order equations, single subscript

\( CE \) Mass fraction of oxygen at edge of boundary layer

\( CIS \) Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface

\( CPK \) Heat capacity of gaseous species, double subscript

\( CPKT \) Table of gaseous species heat capacity versus temperature, double subscript

\( CPKTV \) Dummy array defined for use in table-look-up routine to obtain \( CPK \), single subscript
CPP  Heat capacity of uncharred material, single subscript
CPPP  Heat capacity of insulation layer, single subscript
CPPPV  Constant heat capacity of insulation layer
CPPT  Table of uncharred material heat capacity versus temperature, single subscript
CPS  Heat capacity of char layer, single subscript
CPSA1  Dummy parameters defined in computing CPK
CPSA2  
CPSV  Constant heat capacity of char layer
CRNI  Crank-Nicolson factor - 1/2 for modified implicit solution
CS  "CS" coefficient in matrix formed by second order differential equation, single subscript
D  "D" coefficient in matrix formed by first order differential equations, single subscript
DDX  Distance between finite difference stations
DEB2  Coefficients in finite difference equation for conservation of species evaluated at mid point of time step, single subscript
DEB3  
DEP1  Values of DEP1, etc. evaluated at start of time step, double subscript
DEP2  
DEP3  
DETADX  Porosity gradient in char layer, single subscript
DHC  Heat of combustion of char layer
DHJ  Heat of reaction for heterogeneous chemical reaction, double subscript
DHK  Enthalpy of chemical species evaluated at solid temperature, double subscript
DHP  Heat of pyrolysis of uncharred material
DIFER  Convergence criteria
DIS  Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation interface
DKPDX  Gradient of uncharred material thermal conductivity, single subscript
DKSDX  Gradient of char layer thermal conductivity, single subscript
DL  Change in thickness of char layer
DLP  Change in thickness of uncharred layer
DMBRDX  Gradient of pyrolysis gas molecular weight, single subscript
DRHO  Difference in density of uncharred material and density of char layer at the pyrolysis zone
DRODX  Gradient of pyrolysis gas density at end of time step, single subscript
DS  "DS" coefficient in matrix formed by second order differential equation, single subscript
DT  Time increment
DTDX  Gradient of pyrolysis gas temperature at end of time step, single subscript
DVDX  Gradient of pyrolysis gas velocity, single subscript
DX  Distance between finite difference stations in char layer in region of course grid spacing
DXP  Distance between finite difference stations in uncharred layer in region of course grid spacing
DXPP  Distance between finite difference stations in insulation layer
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DXP1</td>
<td>Distance between finite difference stations in uncharred layer in region of the fine grid spacing</td>
</tr>
<tr>
<td>DXL</td>
<td>Distance between finite difference stations in char layer in region of fine grid spacing</td>
</tr>
<tr>
<td>E</td>
<td>&quot;E&quot; coefficient in matrix formed by first order equations, single subscript</td>
</tr>
<tr>
<td>EIS</td>
<td>Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer - insulation layer interface</td>
</tr>
<tr>
<td>EPSA1</td>
<td>Coefficients in linearized differential equation for char layer porosity evaluated at end of time step, single subscript</td>
</tr>
<tr>
<td>EPSA2</td>
<td></td>
</tr>
<tr>
<td>EPSA3</td>
<td></td>
</tr>
<tr>
<td>EPSB2</td>
<td>Coefficients in finite difference equation for char layer porosity evaluated at mid point of time step, single subscript</td>
</tr>
<tr>
<td>EPSB3</td>
<td></td>
</tr>
<tr>
<td>EPSP</td>
<td>Emissivity of radiating heat sink surface behind insulation</td>
</tr>
<tr>
<td>EPSP1</td>
<td>Values of EPSA1, etc. evaluated at the start of the time step, single subscript</td>
</tr>
<tr>
<td>EPSP2</td>
<td></td>
</tr>
<tr>
<td>EPSP3</td>
<td></td>
</tr>
<tr>
<td>EPSS</td>
<td>Emissivity of char layer surface</td>
</tr>
<tr>
<td>ETA</td>
<td>Porosity of char layer at end of time step, single subscript</td>
</tr>
<tr>
<td>ETAP</td>
<td>Porosity of char layer at start of time step, single subscript</td>
</tr>
<tr>
<td>F</td>
<td>Dummy array defined in solution of first order differential equations, single subscript</td>
</tr>
<tr>
<td>FIS</td>
<td>Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer insulation layer interface</td>
</tr>
<tr>
<td>FS</td>
<td>Dummy array defined in solution of solid temperature equations, single subscript</td>
</tr>
<tr>
<td>GAMIPPP1</td>
<td>Values of ALPHA1, etc. for the uncharred material at the uncharred layer-insulation layer interface evaluated at the start of the time step</td>
</tr>
</tbody>
</table>
Values of $\alpha_1$, etc., for the uncharred material at the uncharred layer-insulation layer interface evaluated at the end of the time step

Values of $\alpha_1$, etc. for the uncharred material at the pyrolysis zone evaluated at the end of the time step

Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface

Parameter defined in algorithm for solving set of finite difference equations, single subscript

Coefficient in solid temperature finite difference equation evaluated at the front surface of the char layer

Coefficient of convective heat transfer between char layer and pyrolysis gas, single subscript

Enthalpy of $N_2$ at char surface temperature evaluated at end of time step

Enthalpy of $O_2$ at char surface temperature evaluated at end of time step

Heat of sublimation of char layer material

Enthalpy of free stream

Enthalpy of gaseous species, double subscript

Table of gaseous species enthalpy versus temperature, double subscript

Dummy array defined for use in table look-up routine for single subscript

Parameters defined in computing coefficients in pyrolysis gas temperature equation, single subscript

Enthalpy of char layer evaluated at the char temperature, single subscript
HSA11  DUMMY PARAMETERS DEFINED IN COMPUTING HK
HSA12

HSCNST COEFFICIENT IN SOLID TEMPERATURE FINITE DIFFERENCE EQUATION EVALUATED AT THE FRONT SURFACE OF THE CHAR LAYER

HST ENTHALPY OF CHAR LAYER EVALUATED AT THE PYROLYSIS GAS TEMPERATURE, SINGLE SUBSCRIPT

HSTT TABLE OF CHAR LAYER ENTHALPY VERSUS TEMPERATURE, SINGLE SUBSCRIPT

HTSK VALUE OF $\rho C_p^l$ FOR HEAT SINK AT UNCHARRED LAYER-INSULATION LAYER INTERFACE

HTSKP VALUE OF $\rho C_p^l$ FOR HEAT SINK BEHIND INSULATION LAYER

HW ENTHALPY OF AIR AT CHAR SURFACE TEMPERATURE

I NUMBER OF FINITE DIFFERENCE STATIONS IN THE CHAR LAYER

IL THICKNESS OF INSULATION LAYER

IM IN IN2 IN 2 I0 I01 INDICES

IP TOTAL NUMBER OF FINITE DIFFERENCE STATIONS IN CHAR LAYER AND UNCHARRED MATERIAL

IPP1 INDICES

IZ TOTAL NUMBER OF FINITE DIFFERENCE STATIONS IN CHAR LAYER, UNCHARRED MATERIAL, AND INSULATION LAYER

IZ1 INDUMY INDICES

JK NUMBER OF FINITE DIFFERENCE STATIONS IN UNCHARRED MATERIAL

K DUMMY INDEX

KA PARAMETER DEFINED IN COMPUTING RATE OF CHAR LAYER REMOVAL BY FIRST ORDER OXIDATION
KAP'PP1) Value of ALPHAI, etc. for the insulation layer at the
uncharred layer-insulation layer interface evaluated at
the start of the time step

KAPIPP2) Value of ALPHAI, etc. for the insulation layer at the
uncharred layer-insulation layer interface evaluated at
the end of the time step

KG Conductivity of the pyrolysis gas

KGK Conductivity of gaseous species, single subscript

KI Dummy indices

KP Conductivity of uncharred material at end of time step,
single subscript

KPP Conductivity of insulation layer, single subscript

KPII Conductivity of uncharred material at pyrolysis zone
evaluated at start of time step

KPPIP Conductivity of uncharred material at uncharred layer -
insulation layer interface evaluated at start of time
step

KPPPIP Conductivity of insulation layer at uncharred layer -
insulation layer interface evaluated at start of time step

KPPPIZ Conductivity of insulation layer at back of insulation
evaluated at start of time step

KPPV Data input for insulation layer conductivity

KPT Table of uncharred material conductivity versus
temperature, single subscript

KS Conductivity of char layer at end of time step, single
subscript

KSPI Conductivity of char layer at pyrolysis zone evaluated
at start of time step

KSPI Conductivity of char layer at front surface evaluated at
start of time step
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>KST</td>
<td>Table of char layer conductivity versus temperature, single subscript</td>
</tr>
<tr>
<td>KT</td>
<td>Indices</td>
</tr>
<tr>
<td>KTT</td>
<td></td>
</tr>
<tr>
<td>KUPT</td>
<td>Table of gaseous species conductivity versus temperature, double subscript</td>
</tr>
<tr>
<td>KUPTV</td>
<td>Dummy array defined for use in table-look-up routine for KGK, single subscript</td>
</tr>
<tr>
<td>L</td>
<td>Char layer thickness at end of time step</td>
</tr>
<tr>
<td>LAM</td>
<td>Ratio of mass char layer removed to free stream oxygen consumed in first order oxidation of char</td>
</tr>
<tr>
<td>LP</td>
<td>Uncharred material thickness at end of time step</td>
</tr>
<tr>
<td>LPMIN</td>
<td>Minimum thickness of uncharred layer</td>
</tr>
<tr>
<td>LPP</td>
<td>Char layer thickness at start of time step</td>
</tr>
<tr>
<td>LPPP</td>
<td>Uncharred material thickness at start of time step</td>
</tr>
<tr>
<td>M</td>
<td>Molecular weight of chemical species, single subscript</td>
</tr>
<tr>
<td>MCPP</td>
<td>Order of interpolation in obtaining CPP</td>
</tr>
<tr>
<td>MFK</td>
<td>Mole fraction of gaseous species, double subscript</td>
</tr>
<tr>
<td>MFKI</td>
<td>Mole fraction of gaseous species at pyrolysis zone, single subscript</td>
</tr>
<tr>
<td>MGDOT</td>
<td>Rate of pyrolysis of uncharred material at end of time step</td>
</tr>
<tr>
<td>MGDOTP</td>
<td>Rate of pyrolysis of uncharred material at start of time step</td>
</tr>
<tr>
<td>MKP</td>
<td>Order of interpolation in obtaining KP</td>
</tr>
<tr>
<td>MKS</td>
<td>Order of interpolation in obtaining KS</td>
</tr>
<tr>
<td>MNO</td>
<td>Order of interpolation in obtaining HS, HST, HK, CPK, HBRKN2, HBRNKO2, MUK, and KGK</td>
</tr>
<tr>
<td>MPDOT</td>
<td>Effective mass injection rate at char surface</td>
</tr>
</tbody>
</table>
MQC  Order of interpolation in obtaining QC
MS   Molecular weight of carbon
MSDOT Rate of char layer removal by first order oxidation at end of time step
MSDOTP Rate of char layer removal by first order oxidation at start of time step
MSQPT Order of interpolation in obtaining SQPT
MU   Viscosity of pyrolysis gas mixture, single subscript
MUK  Viscosity of gaseous species, single subscript
MUKT Table of gaseous species viscosity versus temperature, double subscript
MUKTV Dummy array defined in computing pyrolysis gas viscosity, single subscript
N    Dummy index
NCPP Number of entries in CPPT table
NIT  Iteration count
NITA Trigger, set to 1 after first iteration following $\dot{\mathbf{m}}_g = 1.0 \times 10^{-3}$ kg/m$^2$-sec
NITC Trigger, set to 1 after first iteration
NITG Trigger, set to 1 if surface temperature changes more than .2% with respect to previous times
NITP Trigger, set to 1 when $\dot{\mathbf{m}}_g = 1.0 \times 10^{-3}$ kg/m$^2$-sec
NITS Trigger used in computing CPK and HK
NK1 Number of entries in KPT
NKS Number of entries in KST
NNO Number of entries in HSTT, HKT, CPKT, MUKT, and KUPT
NQC Number of entries in QCTAB
NRCT  Number of homogeneous chemical reactions treated

NRHOK  Trigger used in solving species continuity equation, single subscript

NSQPT  Number of entries in SQPT

NSTEP  Dummy index

P  Pyrolysis gas pressure at end of time step, single subscript

PA  "PA" coefficient in finite difference equation for pyrolysis gas pressure evaluated at the pyrolysis zone

PAB3  Coefficients in finite difference equation for pyrolysis gas pressure evaluated at mid-point of time step, single subscript

PAB4  

PAL1  Coefficients in linearized differential for pyrolysis gas pressure evaluated at end of time step, single subscript

PAL2  

PAL3  

PAL4  

PAMGDOT  Product of chemical species density and velocity at start of time step, double subscript

PAP1  Value of PAL1, etc. evaluated at the start of the time step, single subscript

PAP2  

PAP3  

PAP4  

PART  Parameter defined by |TS(1)-TSP(1)|

PB  "PB" coefficient in finite difference equation for pyrolysis gas pressure evaluated at the pyrolysis zone

PD  "PD" coefficient in finite difference equation for pyrolysis gas pressure evaluated at the pyrolysis zone

PHBRKN2  Enthalpy of N\textsubscript{2} at char surface temperature evaluated at start of time step

PHBRK02  Enthalpy of O\textsubscript{2} at char surface temperature evaluated at start of time step

PHI  Parameter defined in computing viscosity of pyrolysis gas, double subscript
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM</td>
<td>Permeability of char layer at end of time step, single subscript</td>
</tr>
<tr>
<td>PMU</td>
<td>Pyrolysis gas viscosity at pyrolysis zone, evaluated at start of time step</td>
</tr>
<tr>
<td>PMV</td>
<td>Data input for permeability of char layer</td>
</tr>
<tr>
<td>PP</td>
<td>Pyrolysis gas pressure at start of time step, single subscript</td>
</tr>
<tr>
<td>PPM</td>
<td>Permeability of char layer at pyrolysis zone, evaluated at start of time step</td>
</tr>
<tr>
<td>PR</td>
<td>Prandt number of pyrolysis gas</td>
</tr>
<tr>
<td>PRHO</td>
<td>Pyrolysis gas density at start of time step, single subscript</td>
</tr>
<tr>
<td>PRINTFQ</td>
<td>Time interval at which output is printed</td>
</tr>
<tr>
<td>PROM</td>
<td>Sum of mole density of all chemical species, single subscript</td>
</tr>
<tr>
<td>PROPC</td>
<td>Proportionality constant appearing in equation for HA</td>
</tr>
<tr>
<td>PSI</td>
<td>Parameter defined in computing conductivity of pyrolysis gas, double subscript</td>
</tr>
<tr>
<td>PT</td>
<td>Pyrolysis gas temperature at last table look up of data, single subscript</td>
</tr>
<tr>
<td>PTIME</td>
<td>Print time</td>
</tr>
<tr>
<td>PTS</td>
<td>Solid temperature at last table-look-up data, single subscript</td>
</tr>
<tr>
<td>PW</td>
<td>Dimensionless pressure at surface of char layer</td>
</tr>
<tr>
<td>PWP</td>
<td>Dimensional pressure at surface of char layer</td>
</tr>
<tr>
<td>PX, PY, PZ</td>
<td>&quot;PX&quot;, etc. coefficients in finite difference equation for pyrolysis gas pressure evaluated the pyrolysis zone</td>
</tr>
<tr>
<td>Q</td>
<td>Net heat transfer at char surface by conduction at end of time step</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>QC</td>
<td>Heat transfer to cold, non-ablating body</td>
</tr>
<tr>
<td>QCOND</td>
<td>Rate of energy transfer by conduction at char layer surface</td>
</tr>
<tr>
<td>QCT</td>
<td>Aerodynamic heat transfer to hot, ablating body</td>
</tr>
<tr>
<td>QCTAB</td>
<td>Table of QC versus time, single subscript</td>
</tr>
<tr>
<td>QFAC</td>
<td>Parameter define in computation of aerodynamic heat transfer</td>
</tr>
<tr>
<td>QNET</td>
<td>Heat transfer to back surface of insulation layer at end of time step</td>
</tr>
<tr>
<td>QPNET</td>
<td>Heat transfer to back surface of insulation layer at start of time step</td>
</tr>
<tr>
<td>QPT</td>
<td>Net heat transfer at char surface by conduction at start of time step</td>
</tr>
<tr>
<td>QRAT</td>
<td>Ratio of set heat transfer at surface by conduction to cold wall, non-ablating heat transfer</td>
</tr>
<tr>
<td>QRS</td>
<td>Radiant heat transfer at surface</td>
</tr>
<tr>
<td>RAD</td>
<td>Vehicle nose radius</td>
</tr>
<tr>
<td>RHO</td>
<td>Pyrolysis gas density at end of time step, single subscript</td>
</tr>
<tr>
<td>RHOK</td>
<td>Density of chemical species at end of time step, double subscript</td>
</tr>
<tr>
<td>RHOKP</td>
<td>Density of chemical species at start of time step, double subscript</td>
</tr>
<tr>
<td>RHOP</td>
<td>Density of uncharred layer at end of time step, single subscript</td>
</tr>
<tr>
<td>RHOPP</td>
<td>Density of insulation layer, single subscript</td>
</tr>
<tr>
<td>RHOPPV</td>
<td>Data input for insulation density</td>
</tr>
<tr>
<td>RHOSO</td>
<td>Density of char layer at front surface</td>
</tr>
<tr>
<td>RHOST</td>
<td>Theoretical density of char layer</td>
</tr>
<tr>
<td>RHR</td>
<td>Rate of function of chemical species by heterogeneous chemical reactions, double subscript</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>RHS</td>
<td>Rate of formation of solid by heterogeneous chemical reactions, single subscript</td>
</tr>
<tr>
<td>RJN</td>
<td>Rate of reaction of chemical reaction, single subscript</td>
</tr>
<tr>
<td>RM</td>
<td>Total mass rate of production, single subscript</td>
</tr>
<tr>
<td>RMP</td>
<td>Parameter defined by $\prod (\rho_i / M_i)^{v_i}$, single subscript</td>
</tr>
<tr>
<td>RMR</td>
<td>Parameter defined by $\prod (\rho_i / M_i)^{v_i}$, single subscript</td>
</tr>
<tr>
<td>ROCPM</td>
<td>Parameter defined by $\sum \rho_i C_{pi} / M_i$, single subscript</td>
</tr>
<tr>
<td>ROHM</td>
<td>Parameter defined by $\sum \rho_i H_i / M_i$, single subscript</td>
</tr>
<tr>
<td>ROM</td>
<td>Total mole density of pyrolysis gas, single subscript</td>
</tr>
<tr>
<td>RS</td>
<td>Mole rate of production of solid carbon at end of time step, single subscript</td>
</tr>
<tr>
<td>RT</td>
<td>Mole rate of production of chemical species, double subscript</td>
</tr>
<tr>
<td>RU</td>
<td>Universal gas constant</td>
</tr>
<tr>
<td>S</td>
<td>Trigger for surface removal mechanism</td>
</tr>
<tr>
<td>SGMA</td>
<td>Stephan-Boltzmann constant</td>
</tr>
<tr>
<td>SP</td>
<td>Trigger for selecting mode of calculation of pyrolysis rate of uncharred layer</td>
</tr>
<tr>
<td>SPECIES</td>
<td>Identification of gaseous species, single subscript</td>
</tr>
<tr>
<td>SQPT</td>
<td>Table of $(PW)^{1/2}$ versus time, single subscript</td>
</tr>
<tr>
<td>T</td>
<td>Pyrolysis gas temperature at end of time step, single subscript</td>
</tr>
<tr>
<td>TCPP</td>
<td>Temperature table for CPPT, single subscript</td>
</tr>
<tr>
<td>TEMP</td>
<td>Temperature table for HSTT, HKT, CPKT, MUKT, and KUPT, single subscript</td>
</tr>
<tr>
<td>TF</td>
<td>Pyrolysis gas temperature in double precision, single subscript</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>---------------------------------------------------------------------------</td>
</tr>
<tr>
<td>TFS</td>
<td>Solid temperature in double precision, single subscript</td>
</tr>
<tr>
<td>TIBAR</td>
<td>Maximum temperature at pyrolysis zone</td>
</tr>
<tr>
<td>TIME</td>
<td>Time from start of program</td>
</tr>
<tr>
<td>TIMET</td>
<td>Time table for QCTAB, single subscript</td>
</tr>
<tr>
<td>TKP</td>
<td>Temperature table for KPT, single subscript</td>
</tr>
<tr>
<td>TKS</td>
<td>Temperature table for KST, single subscript</td>
</tr>
<tr>
<td>TMPRES</td>
<td>Time table for SQPT, single subscript</td>
</tr>
<tr>
<td>TP</td>
<td>Pyrolysis gas temperature at start of time step, single subscript</td>
</tr>
<tr>
<td>TRAB</td>
<td>Trigger for selecting blocking approximation</td>
</tr>
<tr>
<td>TREF</td>
<td>Transpiration effectiveness</td>
</tr>
<tr>
<td>TS</td>
<td>Solid temperature at end of time step, single subscript</td>
</tr>
<tr>
<td>TSAVE</td>
<td>Parameter used in calculating DHK</td>
</tr>
<tr>
<td>TSP</td>
<td>Solid temperature at start of time step, single subscript</td>
</tr>
<tr>
<td>T1BAR</td>
<td>Sublimation temperature of char layer</td>
</tr>
<tr>
<td>V</td>
<td>Average velocity of gas in char layer, single subscript</td>
</tr>
<tr>
<td>VC</td>
<td>Velocity of moring coordinate, single subscript</td>
</tr>
<tr>
<td>W</td>
<td>Parameter defined in algorithm for solving finite difference equations for pyrolysis gas pressure</td>
</tr>
<tr>
<td>WS</td>
<td>Parameter defined in algorithm for solving finite difference equations for solid temperature</td>
</tr>
<tr>
<td>X</td>
<td>Dimensionless char layer coordinate</td>
</tr>
<tr>
<td>XIS</td>
<td>Coefficient in solid temperature finite difference equation at the pyrolysis zone and the uncharred layer insulation layer interface</td>
</tr>
<tr>
<td>XP</td>
<td>Dimensionless coordinate in uncharred layer</td>
</tr>
</tbody>
</table>
XSCNST  Coefficient in solid temperature finite difference equation evaluated at the back surface of the insulation layer

YETA  Time derivative of char layer porosity, single subscript

YIS  Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface

YP  Time derivative of pyrolysis gas pressure, single subscript

YRHO  Time derivative of pyrolysis gas density, single subscript

YRHOK  Time derivative of gaseous chemical species density, double subscript

YSCNST  Coefficient in solid temperature finite difference equation evaluated at the back surface of the insulation layer

YT  Time derivative of pyrolysis gas temperature, single subscript

YTS  Time derivative of solid temperature, single subscript

ZIS  Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer insulation layer interface

ZP  Pyrolysis gas pressure in double precision, single subscript

ZSCNST  Coefficient in solid temperature finite difference equation evaluated at the back surface of the insulation layer
The author was born [redacted] in [redacted]. After graduating from Lafayette High School in Mayo, Florida in 1955, he served three years on active duty with the U. S. Army before enrolling in the University of Florida. In 1962 he received the Bachelor of Mechanical Engineering Degree with Honors from the University of Florida and has been employed by the National Aeronautics and Space Administration at the Langley Research Center since that time. He has earned the Master of Aerospace Engineering Degree from the University of Virginia since being employed by NASA.

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