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

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by Ronald Keith Clark

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A NUMERICAL ANALYSIS OF THE TRANSIENT RESPONSE
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Ronald Keith Clark

(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 controlled 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.

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TABLE OF CONTENTS

PAGE

TITLE i

ACKNOWLEDGEMENTS. ii

TABLE OF CONTENTS iii

LIST OF FIGURES vi

LIST OF TABLES. viii

LIST OF SYMBOLS ix

CHAPTER

I. INTRODUCTION 1

II. GOVERNING EQUATIONS. 9

Char Layer Equations. 10

Char temperature differential equation. 10

Char porosity differential equation 17

Pyrolysis gas energy differential equation. . . . 18

Chemical species conservation equation. . . . 25

Total mass conservation equation 26

Pyrolysis gas pressure equation 33

Chemical reaction rate equations. 34

Uncharred Material and Insulation Equations 40

III. BOUNDARY CONDITIONS AND INITIAL CONDITIONS 41

Solid Phase Temperature Equations 43

Surface removal by oxidation 43

Front surface energy balance 50

Page

Pyrolysis zone energy balance 54

Rate of pyrolysis of uncharred material 55

Energy balance at uncharred material - insulation interface 55

Back surface energy balance 56

Initial conditions. 57

Char Porosity Equation 57

Pyrolysis Gas Temperature Equation 57

Pyrolysis Gas Pressure Equation. 58

Specified pressure at the front surface 58

Specified pressure gradient at the pyrolysis zone 58

Initial conditions. 60

Total Mass Conservation Equation 60

Chemical Species Conservation Equation 60

IV. TRANSFORMATION AND LINEARIZATION OF EQUATIONS AND BOUNDARY CONDITIONS. 62

Char Layer Equations 65

Char temperature equation 67

Char porosity equation. 68

Pyrolysis gas temperature equation. 69

Chemical species conservation equation. 72

Total mass conservation equation. 73

Pyrolysis gas pressure equation 74

Uncharred Layer Equation 75

Page

Insulation Layer Equation 78

Boundary Conditions 79

V. FINITE DIFFERENCE EQUATIONS. 82

Solid Phase Temperature Equations 84

Interior stations of the char layer 84

Interior stations of the uncharred layer. 89

Interior stations of the insulation layer 90

Boundary stations 91

Char Layer Porosity Equations 109

Pyrolysis Gas Temperature Equation. 112

Pyrolysis Gas Pressure Equation 115

Chemical Species Conservation Equation. 119

VI. SOLUTION OF EQUATIONS 123

VII. ANALYSIS VERIFICATION 134

VIII. RESULTS AND DISCUSSIONS. 156

IX. SUMMARY. 164

REFERENCES 165

APPENDICES 168

A. GENERAL FLOW CHART 168

B. PROGRAM USAGE INSTRUCTIONS 171

C. PROGRAM IN FORTRAN 600 STATEMENTS. 178

D. PROGRAM TERMINOLOGY. 229

VITA 247

LIST OF FIGURES

FIGURE		PAGE
1.	Schematic diagram of charring ablator	2
2.	Blocking effectiveness for a laminar boundary layer with air-to-air injection	52
3.	Location of system boundaries and coordinates	63
4.	Location of finite difference stations	83
5a.	Comparison of results for numerical and exact solutions to the Laplace equation for P^2 with P_w = 1013 N/m^2	137
5b.	Comparison of results for numerical and exact solutions to the Laplace equation for P^2 with P_w = 10130 N/m^2	138
6.	Flow of constant property incompressible fluid through an isothermal slab	139
7a.	Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with $\Delta x = 0.001$	143
7b.	Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with $\Delta x = 0.01$	144
8.	Comparison of numerical results with the exact solution for the heat sink problem	146
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	155
10.	The role of ablation analysis in the design of thermal protection system for aerospace applications	157
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	160
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.	162

PAGE

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. . . 163

LIST OF TABLES

TABLE		PAGE
1.	Chemical reactions involving pyrolysis gases and char layer	131
2.	Thermophysical properties of low-density phenolic-nylon ablation material.	132
3.	Inputs used in exact solution to heat sink case . . .	145
4.	Inputs used in exact solution to quasi-steady-state ablation case.	152
5.	Comparison of the exact solution and the numerical solution obtained with $K_h = 5x10^5\ m^{-1}$ for a quasi-steady-state condition	153
6.	Trajectory data used in making calculations for a typical ablation system.	159

LIST OF SYMBOLS

A	specific reaction rate constant for chemical reaction (various units) or radiant energy absorption of char layer (W/m^3)
A'	radiant energy absorption of pyrolysis gases (W/m^3) or specific reaction rate constant for pyrolysis of uncharred material (kg/m^2-sec)
A_i	chemical species i
$[A_i]$	mole density of chemical species i ($mole/m^3$)
A_s	specific surface area (area per unit volume) of char layer (1/m) or specific reaction rate constant for surface removal by oxidation (various units)
B	activation energy for chemical reaction (^oK)
B'	activation energy for pyrolysis of uncharred layer (^oK)
B_s	activation energy for surface removal by oxidation (^oK)
C	mass fraction of oxygen in boundary layer
$\bar{C}$	normalized mass fraction of oxygen in boundary layer
C_p	heat capacity of pyrolysis gases at constant pressure (J/mole-^oK)
$\hat{C}_p$	heat capacity of pyrolysis gases at constant pressure, per unit mass (J/kg-^oK)
$\hat{C}_{p_{HS}}$	heat capacity per unit mass of heat sink at interface of uncharred material and insulation layer (J/kg-^oK)
$\hat{C}_{p_{HSP}}$	heat capacity per unit mass of heat sink at back of insulation layer (J/kg-^oK)
C_{p_i}	heat capacity of chemical species i at constant pressure (J/mole-^oK)
C_{p_s}	heat capacity of solid at constant pressure (J/mole-^oK)

$\hat{C}_{p_s}$	heat capacity of solid at constant pressure, per unit mass (J/kg-^oK)
C_s	solid carbon
D	chemical diffusivity of boundary layer (m^2)
ε	radiant energy emission of char layer (W/m^3)
ε'	radiant energy emission of pyrolysis gases (W/m^3)
$\varepsilon_1, \varepsilon_2, \varepsilon_3$	coefficients in linearized differential equation for char layer porosity
G	free energy of pyrolysis gases (J/mole)
$\vec{g}$	resultant external force acting on pyrolysis gases (N/kg)
$\vec{g}_i$	external force acting on chemical species i (N/kg)
H	enthalpy of pyrolysis gases (J/mole)
$\bar{H}$	normalized enthalpy of boundary layer fluid
$\hat{H}$	enthalpy of pyrolysis gases, per unit mass (J/kg)
H_A	volumetric convective heat transfer coefficient (W/m^3-^oK)
H_c	heat of sublimation of char layer (J/kg)
$\hat{H}_e$	enthalpy of boundary layer fluid at edge of boundary layer, per unit mass (J/kg)
H_i	enthalpy of chemical species i (J/mole)
$\hat{H}_i$	enthalpy of chemical species i, per unit mass (J/kg)
H_s	enthalpy of char layer (J/mole)
$\hat{H}_s$	enthalpy of char layer, per unit mass (J/kg)
$\hat{H}_{s_o}$	heat of formation of char layer at 0 ^oK, per unit mass (J/kg)
$H(T)_{O_2}$	enthalpy of O_2 at temperature T (J/mole)

$\hat{H}(T)_s$	enthalpy of solid at temperature T, per unit mass (J/kg)
$H(T_s)_{CO}$	enthalpy of CO at temperature T_s (J/mole)
$H(T_s)_{C_s}$	enthalpy of solid carbon at temperature T_s (J/mole)
I	number of finite difference stations in char layer
J	number of finite difference stations in uncharred layer
J_i	molar flux of chemical species i relative to mass average velocity (moles/m^2-sec)
j_i	mass flux of chemical species i relative to mass average velocity (kg/m^2-sec)
K	permeability of char layer (m^2) or number of finite difference stations in insulation layer
K_h	constant in equation for H_A(Eq. 2-1) (1/m)
k	thermal conductivity of boundary layer fluid (W/m-^oK) or specific reaction rate (various units)
k_f	forward reaction rate of chemical reaction (various units)
k_r	reverse reaction rate of chemical reaction (various units)
k_s	thermal conductivity of solid (W/m-^oK)
ℓ	thickness of char layer (m)
ℓ'	thickness of uncharred layer (m)
ℓ''	thickness of insulation layer (m)
ℓ_{HS}	thickness of heat sink between uncharred layer and insulation layer (m)
ℓ_{HSP}	thickness of heat sink at back of insulation layer (m)
ℓ_o	initial thickness of char layer (m)
ℓ'_o	initial thickness of uncharred layer (m)
$\bar{M}$	average molecular weight of pyrolysis gases (kg/mole)

$\dot{m}$	mass flow rate of pyrolysis gases (kg/m^2-sec)
M_i	molecular weight of chemical species i (kg/mole)
M_{O_2}	molecular weight of O_2 (kg/mole)
M_s	molecular weight of char layer (kg/mole)
$\dot{m}_g$	rate of pyrolysis of uncharred material (kg/m^2-sec)
$\dot{m}_i$	mass flow rate of chemical species i (kg/m^2-sec)
$\dot{m}_{O_2}$	mass rate of diffusion of O_2 through the boundary layer to the char layer surface (kg/m^2-sec)
$\dot{m}_s$	mass rate of char removal (kg/m^2-sec)
$\dot{m}_T$	effective rate of mass injection into the boundary layer (kg/m^2-sec)
n	order of chemical reaction
$\vec{n}$	unit vector normal to the surface
$\vec{n}_i$	mass flux of chemical species i relative to a fixed coordinate system (kg/m^2-sec)
N_{Le}	dimensionless parameter ($k/\rho C_p D$), Lewis Number
N_{Pr}	dimensionless parameter ($\mu C_p/k$), Prandtl Number
N_{Sc}	dimensionless parameter ($\mu/\rho D$), Schmidt Number
P	Laplace transform of T' defined by $\int_0^\infty e^{-st}\, T'(X',t)dt$ or pressure (N/m^2)
P_1	pyrolysis gas pressure at finite difference station 1 (N/m^2)
P_e	pressure at edge of boundary layer (N/m^2)
P_{O_2}	partial pressure of O_2 (N/m^2)
$P_{w,o}$	initial pressure at char layer surface (N/m^2)
$P_{w,s}$	stagnation wall pressure (N/m^2)
$\vec{q}$	rate of energy transfer in pyrolysis gases by conduction (W/m^2)

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)
$\vec{q}_s$	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 $r^{\underline{th}}$ chemical reaction ($1/m^3$-sec)
Rad	radius of curvature of surface (m)
$r_h^{(r)}$	net rate of progress of $r^{\underline{th}}$ 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)

r_{T_i}	net mass rate of production of chemical species i (kg/m^3-sec)
R_u	universal gas constant (J/mole-^oK)
S	surface area (m^2) or entropy of pyrolysis gases (J/mole-^oK)
s	exponent on T in chemical reaction rate equation (Eq. 2-67)
$\hat{S}$	entropy of pyrolysis gases per unit mass, (J/kg-K)
$\hat{S}_i$	entropy of chemical species i per unit mass, (J/kg-K)
$S(T_{s_1} - \bar{T}_1)$	step function defined for use in Eq. 3-41
T	pyrolysis gas temperature (^oK)
t	time (seconds)
T'	dimensionless temperature defined by Eq. 7-7
$\bar{T}_I$	maximum temperature of pyrolysis zone used when limiting temperature at that station (^oK)
T_o	initial temperature of pyrolysis gases (^oK) or reservoir temperature (^oK)
T_s	solid temperature (^oK)
$\bar{T}_1$	maximum char surface temperature used when limiting temperature at that station (^oK)
u	component of velocity vector (m/sec)
$\hat{U}$	internal energy per unit mass of pyrolysis gases (J/kg)
V	volume (m^3)
$\hat{V}$	volume of pyrolysis gases per unit mass (m^3/kg)
v	component of velocity vector (m/sec) or velocity of pyrolysis gases in char layer (m/sec)
V_c	velocity of finite difference station in moving coordinate system (m/sec)

v_o	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)

<u>Greek letters</u>:

α	absorptivity of front surface
α_c	weighting factor for char material injected into boundary layer
α_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
β	trigger for selecting blocking approximation; $\beta = 0$ for 2nd order approximation, $\beta = 1$ for linear approximation

$\beta_1, \beta_2, \beta_3$	coefficients in linearized differential equation for pyrolysis gas temperature
$\gamma_1, \gamma_2, \gamma_3, \gamma_4$	coefficients in linearized differential equation for pyrolysis gas pressure
$\bar{\bar{\delta}}$	unit tensor
$\Delta_{1_i}, \Delta_{2_i}, \Delta_{3_i}$	coefficients in linearized chemical species conservation equation
ΔH	heat of reaction for heterogeneous chemical reaction
ΔH_c	heat of combustion of char (J/mole)
ΔH_p	heat of pyrolysis of uncharred material (J/kg)
Δt	increment in time (sec)
$\Delta T_{surface}$	change in temperature of char layer surface (^oK)
Δx	dimensionless distance between finite difference stations
$\Delta \rho$	difference in density of uncharred material and char layer at the pyrolysis zone (kg/m^3)
ε_s	emissivity of char surface
ε_s''	emissivity of back surface
η	char layer porosity
η_I	char layer porosity at pyrolysis zone
η_o	initial char layer porosity
$\bar{\eta}$	blocking coefficient used with linear ablation theory
θ_j	fraction of surface sites occupied by molecules of chemical species j
θ_o	fraction of surface sites which are void
λ	ratio of char layer mass removed to mass of oxygen diffusing to the surface
μ	viscosity of pyrolysis gases or boundary layer fluid ($N - sec/m^2$)

$\hat{\mu}_i$	chemical potential of chemical species i (J/kg)
ν_i'	coefficient of chemical species i appearing as a reactant in a stoichiometric representation of a chemical reaction (moles)
ν_i''	coefficient of chemical species i appearing as a product in a stoichiometric representation of a chemical reaction (moles)
ρ	density of pyrolysis gases or boundary layer fluid (kg/m^3)
$\bar{\rho}$	normalized density of boundary layer fluid
ρ_{HS}	density of heat sink at interface of uncharred layer and insulation layer (kg/m^3)
ρ_{HSP}	density of heat sink at back of insulation layer (kg/m^3)
ρ_i	density of chemical species i (kg/m^3)
ρ_s	density of solid (kg/m^3)
ρ_{s_o}	density of char layer at the front surface (kg/m^3)
ρ_∞	flow field density external to the boundary layer (kg/m^3)
σ	Stefan-Boltzmann constant (W/m^2-sec-$^oK^4$)
$\bar{\bar{\tau}}$	viscous stress tensor (N/m^2)
τ_{xx}	xx-element of the viscous stress tensor in moving coordinate system (N/m^2)
τ_{yy}	yy-element of the viscous stress tensor in fixed coordinate system (N/m^2)

<u>Overlines</u>

$-$	normalized or averaged
$\hat{}$	per unit mass
$\rightarrow$	vector
$\bar{\bar{}}$	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
1	char layer surface

CHAPTER I

INTRODUCTION

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,

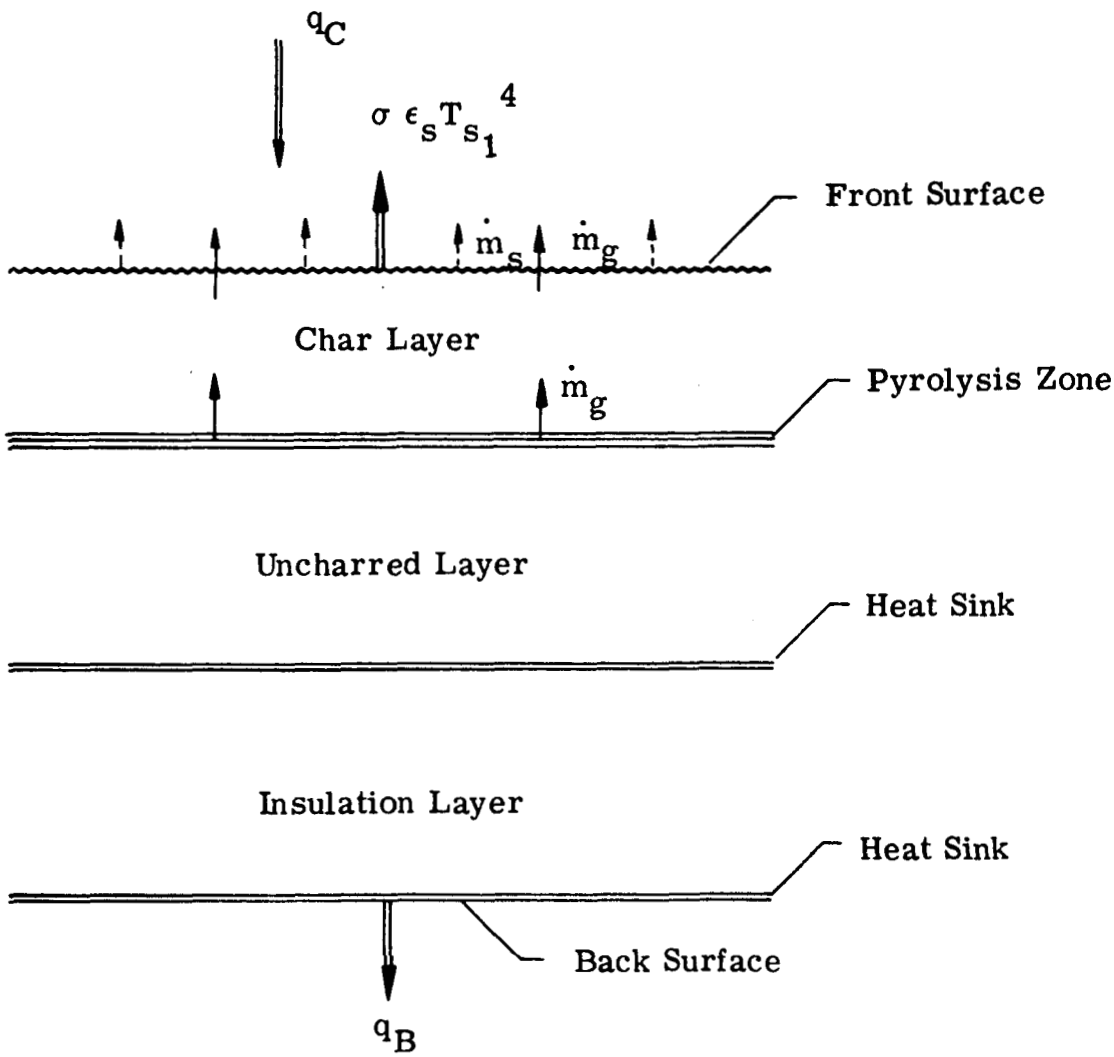

Figure 1.- Schematic diagram of charring ablator.

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 ablator. However, their analysis also invokes the assumption of thermal equilibrium between the char layer and pyrolysis gases. Ref. 16 presents 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 occuring 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.

CHAPTER II

GOVERNING EQUATIONS

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 η 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

$$\int_V \frac{\partial}{\partial t} [(1 - \eta) \rho_s \hat{H}_s] \, dV$$

Conduction heat transfer term

$$- \int_S \vec{q}_s \cdot \vec{n} \, dS$$

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

$$H_A = \frac{K_h v}{N_{Pr}} \sum_i \frac{\rho_i C_{pi}}{M_i} \tag{2-1}$$

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

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

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

$$\int_V \eta \, r_{hs} \, \hat{H}_s \, dV$$

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

$$- \int_V \eta \sum_r r_h^{(r)} \, \Delta H^{(r)} \, dV$$

Radiation of energy to the solid

$$\int_V (1 - \eta)(A - \varepsilon) \, dV$$

Energy produced within the solid by any internal source

$$\int_V (1 - \eta) \, q_s''' \, dV$$

Combining these terms in equation form gives

$$\int_V \frac{\partial}{\partial t} [(1 - \eta)\ \rho_s\ \hat{H}_s]\ dV = - \int_S \vec{q}_s \cdot \vec{n}\ dS - \int_V H_A\ (T_s - T)\ dV$$

$$+ \int_V \eta\ r_s\ \hat{H}(T_s)\ \ dV + \int_V \eta\ r_{hs}\ \hat{H}_s\ dV - \int_V \eta \sum_r r_h^{(r)}\ \Delta H^{(r)}\ dV$$

$$+ \int_V (1 - \eta)(A - \varepsilon)\ dV + \int_V (1 - \eta)\ q_s'''\ dV \qquad (2\text{-}2)$$

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 $r^{\underline{th}}$ heterogeneous chemical reaction which is the oxidation of solid carbon to form carbon monoxide. The stoichiometric equation representing this reaction is

$$O_2 + 2C_s \rightarrow 2CO \qquad (2\text{-}3)$$

and the heat supplied to the reaction is just the difference in enthalpy of the products and the reactants, or in equation form

$$\Delta H^{(r)} = 2\ H(T_s)_{CO} - H(T)_{O_2} - H(T_s)_{C_s} \tag{2-4}$$

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

$$\int_V \{ \frac{\partial}{\partial t} [(1 - \eta)\ \rho_s\ \hat{H}_s] + \vec{\nabla} \cdot \vec{q}_s + H_A\ (T_s - T) - \eta\ r_s\ \hat{H}(T)_s - \eta\ r_{hs}\ \hat{H}_s$$

$$+ \eta \sum_r r_h^{(r)}\ \Delta H^{(r)} - (1 - \eta)(A - \varepsilon) - (1 - \eta)\ q'''\}\ dV = 0. \tag{2-5}$$

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

$$\frac{\partial}{\partial t} [(1 - \eta)\ \rho_s\ \hat{H}_s] + \vec{\nabla} \cdot \vec{q}_s + H_A\ (T_s - T) - \eta\ r_s\ \hat{H}(T_s) - \eta\ r_{hs}\ \hat{H}_s$$

$$+ \eta \sum_r r_h^{(r)} \Delta H^{(r)} - (1 - \eta)(A - \varepsilon) - (1 - \eta)\ q''' = 0. \tag{2-6}$$

The non-stationary term is expanded to obtain

$$\frac{\partial}{\partial t} [(1 - \eta)\ \rho_s\ \hat{H}_s] = (1 - \eta)\ \rho_s\ \frac{\partial \hat{H}_s}{\partial t} + (1 - \eta)\ \hat{H}_s\ \frac{\partial \rho_s}{\partial t} - \rho_s\ \hat{H}_s\ \frac{\partial \eta}{\partial t}. \tag{2-7}$$

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

$$\frac{\partial}{\partial t} [(1 - \eta)\ \rho_s \hat{H}_s] = (1 - \eta)\ \rho_s\ \frac{\partial \hat{H}_s}{\partial t} - \rho_s\ \hat{H}_s\ \frac{\partial \eta}{\partial t}. \tag{2-8}$$

The char layer energy equation now takes the form

$$(1 - \eta)\rho_s \frac{\partial \hat{H}_s}{\partial t} = - \vec{\nabla} \cdot \vec{q}_s - H_A(T_s - T) + \eta\, r_s\, \hat{H}(T)_s + \eta\, r_{hs} \hat{H}_s$$

$$- \eta \sum_r r_r^{(r)}\, \Delta H^{(4)} + (1 - \eta)(A - \varepsilon) + (1 - \eta) q_s''' + \rho_s\, \hat{H}_s \frac{\partial \eta}{\partial t} . \qquad (2\text{-}9)$$

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

$$\hat{H}_s = \int_0^{T_s} \hat{C}_{p_s}\, dT_s + \hat{H}_{s_o} . \qquad (2\text{-}10)$$

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

$$\frac{\partial \hat{H}_s}{\partial t} = \frac{\partial}{\partial t} \int_0^{T_s} \hat{C}_{p_s}\, dT_s + \frac{\partial}{\partial t} \hat{H}_{s_o} . \qquad (2\text{-}11)$$

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

$$\frac{\partial \hat{H}_s}{\partial t} = \int_0^{T_s} \frac{\partial}{\partial t} \hat{C}_{p_s}\, dT_s + \hat{C}_{p_s} \frac{\partial T_s}{\partial t} + \frac{\partial}{\partial t} \hat{H}_{s_o} , \qquad (2\text{-}12)$$

but $\hat{C}_{ps}$ is not a function of time and $\hat{H}_{s_o}$ is constant so

$$\frac{\partial \hat{H}_s}{\partial t} = \hat{C}_{p_s} \frac{\partial T_s}{\partial t} . \tag{2-13}$$

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

$$\vec{q}_s = - k_s \vec{\nabla} T_s \quad , \tag{2-14}$$

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

$$(1 - \eta) \rho_s \hat{C}_{p_s} \frac{\partial T_s}{\partial t} = \vec{\nabla} \cdot (k_s \vec{\nabla} T_s) - H_A (T_s - T) + \eta r_s \hat{H}(T)_s$$

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

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

The specific quantities $\hat{C}_{p_s}$, $\hat{H}_s(T)$, $\Delta\hat{H}_j$ and $\hat{H}_s$ and the chemical production terms r_s and r_{h_s} may be expressed in terms of the respective mole quantities and Eq. 2-15 becomes

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

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

$$+ (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \frac{\partial \eta}{\partial t} . \tag{2-16}$$

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

$$\text{Mass Rate of Deposition} = \eta\, M_s R_s \,. \tag{2-17}$$

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

$$\left(\frac{\partial \eta}{\partial t}\right)_{hom} = -\,\eta\,\frac{M_s R_s}{\rho_s} \,. \tag{2-18}$$

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

$$\left(\frac{\partial \eta}{\partial t}\right)_h = - \eta \frac{M_s}{\rho_s} R_{hs} \quad . \tag{2-19}$$

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

$$\frac{\partial \eta}{\partial t} = - \frac{\eta M_s}{\rho_s} (R_{hs} + R_s) \quad . \tag{2-20}$$

<u>Pyrolysis gas energy differential equation</u>.- 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

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

Convection by mass average velocity

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

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

$$- \int_S \vec{q} \cdot \vec{n} \, dS$$

Radiation term

$$\int_V \eta(A' - \varepsilon') \, dV$$

Work by external forces

$$\int_V \eta \sum_i \vec{n}_i \cdot \vec{g}_i \, dV$$

where $\vec{n}_i$ 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

$$\vec{n}_i = \rho_i \vec{v} + \vec{j}_i \ . \tag{2-21}$$

Work by pressure forces

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

Work by viscous forces

$$\int_S [\bar{\bar{\tau}} \cdot \vec{v}_o] \cdot \vec{n} \, dS$$

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

$$- \int_V \eta \; r_{hs} \; \hat{H}_s \; dV$$

Energy gain resulting from heterogeneous chemical reactions

$$\int_V \eta \sum_r r_h^{(r)} \; \Delta H^{(r)} \; dV \; .$$

Combining these terms in equation form gives

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

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

$$+ \int_V \eta(A' - \varepsilon') dV + \int_V \eta \sum_i \vec{n}_i \cdot \vec{g}_i \; dV$$

$$- \int_S P \; \vec{v}_o \cdot \vec{n} \; dS + \int_S [\bar{\bar{\tau}} \cdot \vec{v}_o] \cdot \vec{n} \; dS$$

$$+ \int_V H_A \; (T_s - T) \; dV - \int_V \eta \; r_s \; \hat{H}(T)_s \; dV$$

$$- \int_V \eta \; r_{hs} \; \hat{H}_s dV + \int_V \eta \sum_r r_h^{(r)} \; \Delta H^{(r)} \; dV \; . \qquad (2\text{-}22)$$

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

$$\int_V \{ \frac{\partial}{\partial t} [\eta \rho(\hat{U} + \frac{1}{2} v^2)] + \vec{\nabla} \cdot [(\hat{U} + \frac{1}{2} v^2) \rho \vec{v}_o]$$

$$+ \vec{\nabla} \cdot \vec{q} - \eta (A' - \varepsilon') - \eta \sum_i \vec{n}_i \cdot \vec{g}_i + \vec{\nabla} \cdot P \vec{v}_o$$

$$- \vec{\nabla} \cdot [\bar{\bar{\tau}} \cdot \vec{v}_o] - H_A(T_s - T) + \eta r_s \hat{H}(T)_s + \eta r_{hs} \hat{H}_s$$

$$- \eta \sum_r r_r^{(r)} \Delta H^{(r)} \} dV = 0 \quad . \tag{2-23}$$

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

$$\frac{\partial}{\partial t} [\eta \rho(\hat{U} + \frac{1}{2} v^2)] + \vec{\nabla} \cdot [(\hat{U} + \frac{1}{2} v^2) \rho \vec{v}_o] + \vec{\nabla} \cdot \vec{q}$$

$$- \eta(A' - \varepsilon) - \eta \sum_i \vec{n}_i \cdot \vec{g}_i + \vec{\nabla} \cdot P \vec{v}_o$$

$$- \vec{\nabla} \cdot [\bar{\bar{\tau}} \cdot \vec{v}_o] - H_A(T_s - T) + \eta r_s \hat{H}(T)_s + \eta r_{hs} \hat{H}_s$$

$$- \eta \sum_r r_h^{(r)} \Delta H^{(r)} = 0 \quad . \tag{2-24}$$

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

$$\int_V \frac{\partial}{\partial t} (\eta \rho \vec{v}) \, dV = - \int_s (\rho \vec{v}) \vec{v}_o \cdot \vec{n} \, dS - \int_S \eta P \bar{\bar{\delta}} \cdot \vec{n} \, dS$$

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

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

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

$$- \vec{\nabla} \cdot \eta \bar{\bar{\tau}} - \eta \rho \vec{g} \} \, dV = 0 \quad . \qquad (2\text{-}26)$$

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

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

$$- \vec{\nabla} \cdot \eta \bar{\bar{\tau}} - \eta \rho \vec{g} = 0 \quad . \tag{2-27}$$

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

$$\frac{1}{2}\frac{\partial}{\partial t}(\eta \rho v^2) + \frac{1}{2}\eta v^2 \frac{\partial \rho}{\partial t} + \frac{1}{2}\rho v^2 \frac{\partial \eta}{\partial t} + \frac{1}{2}\vec{\nabla} \cdot \rho v^2 \vec{v}_o$$

$$+ \frac{1}{2} v^2 \vec{v}_o \cdot \vec{\nabla} \rho + \frac{1}{2}\rho v^2 \vec{\nabla} \cdot \vec{v}_o + \vec{\nabla} \cdot P \vec{v}_o$$

$$- \eta P \vec{\nabla} \cdot \vec{v} - \vec{\nabla} \cdot [\bar{\bar{\tau}} \cdot \vec{v}_o] + \eta \bar{\bar{\tau}} : \vec{\nabla} \cdot \vec{v}$$

$$- \eta \rho v g = 0 \quad . \tag{2-28}$$

Equation 2-28 is subtracted from Eq. 2-24 to obtain the thermal energy equation of the pyrolysis gases as

$$\eta\,\rho\,\frac{D\hat{U}}{Dt} + \rho(\hat{U} - \frac{1}{2}v^2)\,\frac{D\eta}{Dt} + \eta(\hat{U} - \frac{1}{2}v^2)(\frac{D\rho}{Dt} + \rho\,\vec{\nabla}\cdot\vec{v})$$

$$+ \eta\,P\,\vec{\nabla}\cdot\vec{v} - \eta\,\bar{\bar{\tau}} : \nabla v - \eta \sum_i \vec{j}_i \cdot \vec{g}_i + \vec{\nabla}\cdot\vec{q}$$

$$- \eta\,(A' - \varepsilon') - H_A(T_s - T) + \eta\,r_s\,\hat{H}(T)_s + \eta\,r_{hs}\,\hat{H}_s$$

$$- \eta \sum_r r_h^{(r)}\,\Delta H_j^{(r)} = 0\ . \qquad (2\text{-}29)$$

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

$$\hat{U} = \hat{H} - P/\rho \qquad (2\text{-}30)$$

yields

$$\frac{D\hat{U}}{Dt} = \frac{D\hat{H}}{Dt} - \frac{1}{\rho}\frac{DP}{Dt} + \frac{P}{\rho^2}\frac{D\rho}{Dt}\ , \qquad (2\text{-}31)$$

<u>Chemical species continuity equation</u>.- 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

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

$$+ \int_V \eta \, r_{T_i} \, dV - \int_S \eta \vec{j}_i \cdot \vec{n} \, dS \, . \qquad (2\text{-}32)$$

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

$$\int_V \left[\frac{\partial}{\partial t} (\eta \rho_i) + \vec{\nabla} \cdot (\rho_i v_o) - \eta \, r_{T_i} + \vec{\nabla} \cdot \eta \vec{j}_i \right] dV = 0 \qquad (2\text{-}33)$$

which yields the chemical species conservation equation

$$\frac{\partial}{\partial t} (\eta \rho_i) + \vec{\nabla} \cdot (\rho_i \vec{v}_o) + \vec{\nabla} \cdot \eta \vec{j}_i - \eta \, r_{T_i} = 0 \, . \qquad (2\text{-}34)$$

<u>Total mass conservation equation</u>.- The total mass conservation equation is obtained by summing the chemical species conservation equation over all species. Thus

$$\frac{\partial}{\partial t} (\eta \rho) + \vec{\nabla} \cdot (\rho \vec{v}_o) - \eta \sum_i r_{T_i} = 0 \, . \qquad (2\text{-}35)$$

Equations 2-29, 2-31 and 2-35 are combined to give the pyrolysis gas energy equation in terms of enthalpy as

$$\eta \rho \frac{D\hat{H}}{Dt} = \eta \frac{DP}{Dt} + P \frac{D\eta}{Dt} - \eta (\hat{H} - \frac{1}{2} v^2) \Sigma r_{T_i}$$

$$+ \eta \bar{\bar{\tau}} : \vec{\nabla} \vec{v} + \eta \sum_i \vec{j}_i \cdot \vec{g}_i - \vec{\nabla} \cdot \vec{q} + \eta (A' - \varepsilon')$$

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

$$+ \eta \sum_r r_h^{(r)} \Delta H^{(r)} . \qquad (2\text{-}36)$$

It is more convenient to work with the pyrolysis gas energy equation written in terms of $\hat{C}_p$ 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

$$d\hat{H} = T\, d\hat{S} + \hat{V}\, d\, P + \sum_i \hat{\mu}_i\, d(\rho_i/\rho) . \qquad (2\text{-}37)$$

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

$$\frac{D\hat{H}}{Dt} = T\frac{D\hat{S}}{Dt} + \hat{V}\frac{DP}{Dt} + \sum_i \hat{\mu}_i \frac{D}{Dt}(\rho_i/\rho) \ . \tag{2-38}$$

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

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

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

$$d\hat{S} = \frac{\hat{C}_p}{T}\,dT - \frac{\hat{V}}{T}\,dP - \frac{1}{T}\sum_i \hat{\mu}_i\ d(\rho_i/\rho) \ . \tag{2-41}$$

Equating the coefficients for dT in Eqs. 2-40 and 2-41 gives

$$\left(\frac{\partial \hat{S}}{\partial T}\right)_{P,\rho_i/\rho} = \frac{\hat{C}_p}{T} . \tag{2-42}$$

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

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

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

$$d\hat{S} = \frac{\hat{C}_p}{T} dT - \left(\frac{\partial \hat{V}}{\partial T}\right)_{P,\rho_i/\rho} dT + \sum_i \left(\frac{\partial \hat{S}}{\partial \rho_i/\rho}\right)_{P,T} d(\rho_i/\rho) . \tag{2-44}$$

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

$$\frac{D\hat{S}}{Dt} = \frac{\hat{C}_p}{T}\frac{DT}{Dt} - \left(\frac{\partial \hat{V}}{\partial T}\right)_{P,\rho_i/\rho}\frac{DP}{Dt} + \sum_i \left(\frac{\partial \hat{S}}{\partial \rho_i/\rho}\right)_{P,T}\frac{D}{Dt}(\rho_i/\rho) . \tag{2-45}$$

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

$$\frac{D\hat{H}}{Dt} = \hat{C}_p\frac{DT}{Dt} + \hat{V}\frac{DP}{Dt} - T\left(\frac{\partial \hat{V}}{\partial T}\right)_{P,\rho_i/\rho}\frac{DP}{Dt}$$

$$+ \sum_i \left[\hat{\mu}_i + T\left(\frac{\partial \hat{S}}{\partial \rho_i/\rho}\right)_{P,T}\right]\frac{D}{Dt}(\rho_i/\rho) . \tag{2-46}$$

The summation term in this equation can be reduced by considering the relation between partial properties. The entropy of a system is written as

$$\hat{S} = \sum_i (\rho_i/\rho)\,\hat{S}_i \ . \tag{2-47}$$

From Eq. 2-47 we have that

$$d\hat{S} = \sum_i \frac{\rho_i}{\rho}\, d\hat{S}_i + \sum_i \hat{S}_i \quad d\left(\frac{\rho_i}{\rho}\right) . \tag{2-48}$$

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

$$d\hat{S} = \sum_i \hat{S}_i \quad d(\rho_i/\rho) . \tag{2-49}$$

Thus

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

The partial specific Gibbs function is defined as

$$\hat{\mu}_i = \left(\frac{\partial G}{\partial M_i}\right)_{P,T} . \tag{2-51}$$

But

$$G = H - TS \tag{2-52}$$

or

$$G = \sum_i M_i \, (\hat{H}_i - T\hat{S}_i) \; . \tag{2-53}$$

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

$$\hat{\mu}_i = \hat{H}_i - T \, \hat{S}_i \; . \tag{2-54}$$

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

$$\frac{D\hat{H}}{Dt} = \hat{C}_p \frac{DT}{Dt} + \hat{V} \frac{DP}{Dt} - T \left(\frac{\partial \hat{V}}{\partial T} \right)_{P,\rho_i/\rho} \frac{DP}{Dt}$$

$$+ \sum_i \hat{H}_i \frac{D}{Dt} (\rho_i/\rho) \; . \tag{2-55}$$

Equation 2-55 is combined with Eq. 2-36 to give the pyrolysis gas energy equation in terms of $\hat{C}_p$ as

$$\eta \rho \hat{C}_p \frac{DT}{Dt} = - \eta \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_{P,\rho_i/\rho} \frac{DP}{Dt} - \eta \rho \sum_i \hat{H}_i \frac{D}{Dt} (\rho_i/\rho)$$

$$+ P \frac{D\eta}{Dt} - \eta (\hat{H} - \frac{1}{2} v^2) \sum_i r_{T_i} + \eta \bar{\bar{\tau}} : \vec{\nabla} \vec{v} + \eta \sum_i \vec{j}_i \cdot \vec{g}_i$$

$$- \vec{\nabla} \cdot \vec{q} + \eta (A' - \varepsilon') + H_A (T_s - T) - \eta r_s \hat{H}(T)_s - \eta r_{hs} \hat{H}_s$$

$$+ \eta \sum_r r_h^{(r)} \Delta H^{(r)} . \qquad (2\text{-}56)$$

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

$$\frac{D}{Dt} (\rho_i/\rho) = \frac{1}{\rho} r_{T_i} - \frac{1}{\eta \rho} \vec{\nabla} \cdot \vec{j}_i - \frac{\rho_i}{\rho^2} \sum_i r_{T_i} . \qquad (2\text{-}57)$$

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

$$\eta \sum_i \frac{\rho_i C_{p_i}}{M_i} \frac{DT}{Dt} = - \eta \left(\frac{\partial \ln \rho}{\partial \ln T} \right)_{P,x_i} \frac{DP}{Dt} - \eta \sum_i H_i R_{T_i}$$

$$+ \sum_i H_i \vec{\nabla} \cdot \vec{J}_i + P \frac{D\eta}{Dt} + \frac{1}{2} \eta v^2 \sum_i R_{T_i} M_i$$

$$+ \eta \bar{\bar{\tau}} : \vec{\nabla} \vec{v} + \eta \sum_i \frac{\vec{J}_i}{M_i} \cdot \vec{g}_i - \vec{\nabla} \cdot \vec{q} + \eta (A' - \varepsilon')$$

$$+ H_A (T_s - T) - \eta R_s H(T)_s - \eta R_{hs} H_s$$

$$+ \eta \sum_r r_h^{(r)} \Delta H^{(r)} . \qquad (2\text{-}58)$$

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

$$\vec{v}_o = - \frac{K}{\mu} \vec{\nabla} P \qquad (2\text{-}59)$$

or

$$\vec{v} = - \frac{K}{\mu\eta} \vec{\nabla} P . \qquad (2\text{-}60)$$

Equation 2-59 may be combined with the total mass conservation equation to give

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

The equation of state for the pyrolysis gases,

$$P = \rho\ R_u T/\bar{M} \qquad (2\text{-}62)$$

and the identity

$$P\ \vec{\nabla}\ P = \frac{1}{2} \vec{\nabla}\ P^2 \qquad (2\text{-}63)$$

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

$$\vec{\nabla} \cdot \vec{\nabla}\ P^2 + \frac{\mu T}{K\bar{M}} \vec{\nabla} \left(\frac{K\bar{M}}{\mu T} \right) \cdot \vec{\nabla}\ P^2$$

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

<u>Chemical reaction rate equations</u>.- 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

$$\sum_i \nu_i' A_i \rightarrow \sum_i \nu_i'' A_i \tag{2-65}$$

is

$$\text{reaction rate} = k \prod_i [A_i]^{\nu_i'}, \tag{2-66}$$

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

$$k = A\, T^S \exp\,(-B/T) \tag{2-67}$$

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

Simultaneous forward and reverse chemical reactions are represented by

$$\sum_i \nu_i^{(r)'} A_i \underset{k_r^{(r)}}{\overset{k_f^{(r)}}{\rightleftarrows}} \sum_i \nu_i^{(r)''} A_i \tag{2-68}$$

where

$$r = 1,2, \text{---} \ m \text{ independent reactions.}$$

The rate of forward reaction for the chemical reaction represented by the $r^{\underline{th}}$ equation is

$$\text{rate of forward reaction} = k_f^{(r)} \prod_i [A_i]^{\nu_i^{(r)'}} \tag{2-69}$$

and the rate of reverse reaction is

$$\text{rate of reverse reaction} = k_r^{(r)} \prod_i [A_i]^{\nu_i^{(r)''}} \quad . \tag{2-70}$$

Thus the net rate of progress of the $r^{\underline{th}}$ reaction in the forward direction is given by

$$r^{(r)} = k_f^{(r)} \prod_i [A_i]^{\nu_i^{(r)'}} - k_r^{(r)} \prod_i [A_i]^{\nu_i^{(r)''}} \quad . \tag{2-71}$$

Now this reaction yields a predetermined number of moles of chemical species 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

$$R_i = \sum_r [\nu_i^{(r)''} - \nu_i^{(r)'}]\{k_f^{(r)} \prod_i [A_i]^{\nu_i^{(r)'}} - k_r^{(r)} \prod_i [A_i]^{\nu_i^{(r)''}}\} . \tag{2-72}$$

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

$$\sum_j \nu'_j A_j \rightarrow \sum_j \nu''_j A_j \tag{2-73}$$

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

$$\text{reaction rate} = k \prod_j [\theta_j]^{\nu'_j} \theta_o^n \tag{2-74}$$

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

$$k = A \exp(-B/T) \tag{2-75}$$

and

$$n = \sum_j (\nu_j'' - \nu_j') \,. \tag{2-76}$$

Simultaneous forward and reverse heterogeneous chemical reactions are represented by

$$\sum_j \nu_j^{(r)'} A_j \underset{k_r^{(r)}}{\overset{k_f^{(r)}}{\rightleftarrows}} \sum_j \nu_j^{(r)''} A_j \tag{2-77}$$

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

$$\text{rate of forward reaction} = k_f^{(r)} \prod_j [\theta_j]^{\nu_j^{(r)'}} \theta_o^{n^{(r)}} \tag{2-78}$$

and the rate of the reverse reaction is

$$\text{rate of reverse reaction} = k_r^{(r)} \prod_j [\theta_j]^{\nu_j^{(r)''}} \theta_o^{n^{(r)}} \,. \tag{2-79}$$

Thus the net rate of the $r^{\underline{th}}$ reaction is given by

$$r_h^{(r)} = \left\{ k_f^{(r)} \prod_j [\theta_j]^{\nu_j^{(r)'}} - k_r^{(r)} \prod_j [\theta_j]^{\nu_j^{(r)''}} \right\} \theta_o^{n^{(r)}} A_s \tag{2-80}$$

and the molar rate of production of chemical species j resulting from the set of reactions (Eq. 2-77) is

$$R_{h_j} = \sum_r [\nu_j^{(r)''} - \nu_j^{(r)'}] \left\{ k_f^{(r)} \prod_j [\theta_j]^{\nu_j^{(r)'}} - k_r^{(r)} \prod_j [\theta_j]^{\nu_j^{(r)''}} \right\} A_s \, \theta_o^{n^{(r)}} \tag{2-81}$$

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

$$\vec{\nabla} \cdot k_s' \vec{\nabla} T_s' = \rho_s' \hat{C}_{p_s}' \frac{\partial T_s'}{\partial t} \tag{2-82}$$

and

$$\vec{\nabla} \cdot k_s'' \vec{\nabla} T_s'' = \rho_s'' \hat{C}_{p_s}'' \frac{\partial T_s''}{\partial t} , \tag{2-83}$$

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

$$(1 - \eta) \frac{\rho_s C_{ps}}{M_s} \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial y} \left(k_s \frac{\partial T_s}{\partial y} \right) - H_A (T_s - T)$$

$$+ \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \varepsilon)$$

$$+ (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \frac{\partial \eta}{\partial t} \tag{3-1}$$

Char porosity

$$\frac{\partial \eta}{\partial t} = - \eta \frac{M_s}{\rho_s} (R_{hs} + R_s) \tag{3-2}$$

Pyrolysis gas temperature

$$\eta \sum_i \frac{\rho_i C_{pi}}{M_i} \left(\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial y} \right) = -\eta \left(\frac{\partial \ln \rho}{\partial \ln T} \right)_{P, x_i} \left(\frac{\partial P}{\partial t} \right.$$

$$\left. + v \frac{\partial P}{\partial y} \right) - \eta \sum_i H_i R_{T_i} + \sum_i H_i \frac{\partial}{\partial y} J_i + P \frac{\partial \eta}{\partial t} + P v \frac{\partial \eta}{\partial y}$$

$$+ \frac{1}{2} \eta v^2 \sum_i R_{T_i} M_i + \eta \bar{\bar{\tau}}_{yy} \frac{\partial v}{\partial y} + \eta \sum_i \frac{J_i g_i}{M_i} - \frac{\partial}{\partial y} q_y$$

$$+ \eta (A' - \varepsilon') + H_A (T_s - T) - \eta R_s H(T)_s - \eta R_{hs} H_s$$

$$+ \eta \sum_r r_h^{(r)} \Delta H^{(r)} \tag{3-3}$$

Chemical species continuity equation

$$\frac{\partial}{\partial t} (\eta \rho_i) + \frac{\partial}{\partial y} (\rho_i v_o) + \frac{\partial}{\partial y} \eta j_i - \eta r_{T_i} = 0 \tag{3-4}$$

Total mass conservation equation

$$\frac{\partial}{\partial t} (\eta \rho) + \frac{\partial}{\partial y} (\rho v_o) - \eta \sum_i r_{T_i} = 0 \tag{3-5}$$

Pressure of pyrolysis gas

$$\frac{\partial^2 P^2}{\partial y^2} + \frac{\mu T}{K\bar{M}} \frac{\partial}{\partial y} \left(\frac{K\bar{M}}{\mu T} \right) \frac{\partial P^2}{\partial y} - \frac{2\mu R_u T}{K\bar{M}} \left[\frac{\partial}{\partial t} (\eta \rho) \right.$$

$$\left. - \eta \sum_i R_{T_i} M_i \right] = 0 \tag{3-6}$$

Uncharred Layer and Substrate Insulation Equations.-

Uncharred layer temperature

$$\frac{\partial}{\partial y} \left(k_s' \frac{\partial T_s'}{\partial y} \right) = \rho_s' \hat{C}_{p_s}' \frac{\partial T_s'}{\partial t} \tag{3-7}$$

Substrate insulation temperature

$$\frac{\partial}{\partial y}\left(k_s'' \frac{\partial T_s''}{\partial y}\right) = \rho_s'' \hat{C}_{p_s}'' \frac{\partial T_s''}{\partial t} . \tag{3-8}$$

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, writting the mass loss rate as

$$\dot{m}_s = k\ (P_{O_2})_w^n \tag{3-9}$$

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

$$k = A_s\ \exp(-B_s/T_{s_1}). \tag{3-10}$$

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

$$(P_{O_2})_w = (x_{O_2})_w\ P_e \tag{3-11}$$

$$P_w = P_e \tag{3-12}$$

$$(x_{O_2})_w = C_w\ \bar{M}_w/M_{O_2}. \tag{3-13}$$

Therefore,

$$(P_{O_2})_w = \frac{C_w \bar{M}_w}{M_{O_2}} P_e \ . \tag{3-14}$$

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

$$\dot{m}_s = A_s \exp(-B_s/T_{s_1}) \left(\frac{C_w \bar{M}_w}{M_{O_2}} P_e \right)^n . \tag{3-15}$$

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

$$P_{w,s} = \frac{11}{12} \rho_e v_e^2 \ . \tag{3-16}$$

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

$$q_c \ \alpha \ \sqrt{\rho_e/\mathrm{Rad}} \ v_e^3 \tag{3-17}$$

and

$$\hat{H}_e \ \alpha \ v_e^2 \ . \tag{3-18}$$

Thus the wall pressure is approximated by

$$P_{w,s} = 5.693 \times 10^6 \text{ Rad } (q_c/\hat{H}_e)^2 \ . \tag{3-19}$$

In the current problem,

$$P_w = P_{w,s} \tag{3-20}$$

thus

$$P_w = 5.693 \times 10^6 \text{ Rad } (q_c/\hat{H}_e)^2 \ . \tag{3-21}$$

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

$$\dot{m}_s = \lambda \ \dot{m}_{O_2} \tag{3-22}$$

where λ 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

$$\bar{\rho} \ u \frac{\partial C}{\partial z} + \bar{\rho} \ v \frac{\partial C}{\partial y} = \frac{\partial}{\partial y} \left(\frac{\mu}{N_{Sc}} \frac{\partial C}{\partial y} \right) \tag{3-23}$$

and the boundary layer energy equation is

$$\bar{\rho}\, u \frac{\partial \hat{H}}{\partial z} + \bar{\rho}\, v \frac{\partial \hat{H}}{\partial y} = \frac{\partial}{\partial y}\left[\frac{\mu}{N_{Pr}} \frac{\partial \hat{H}}{\partial y} + \frac{\mu}{2}\left(1 - \frac{1}{N_{Pr}}\right) \frac{\partial u^2}{\partial y}\right]. \tag{3-24}$$

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

$$\left.\begin{aligned} C &= C_w \\ \hat{H} &= \hat{H}_w \end{aligned}\right\} \text{ at } y = 0 \tag{3-25}$$

and

$$\left.\begin{aligned} C &= C_e \\ \hat{H} &= \hat{H}_e \end{aligned}\right\} \text{ at } y = \infty\,. \tag{3-26}$$

Nondimensionalizing Eqs. 3-23 and 3-24 with

$$\left.\begin{aligned} \bar{C} &= \frac{C - C_w}{C_e - C_w} \\ \bar{H} &= \frac{\hat{H} - \hat{H}_w}{\hat{H}_e - \hat{H}_w} \end{aligned}\right\} \tag{3-27}$$

gives

$$\left.\begin{aligned} \bar{\rho}\, u \frac{\partial \bar{C}}{\partial z} + \bar{\rho}\, v \frac{\partial \bar{C}}{\partial y} &= \frac{\partial}{\partial y} \frac{\mu}{N_{sc}} \frac{\partial \bar{C}}{\partial y} \\ \bar{\rho}\, u \frac{\partial \bar{H}}{\partial z} + \bar{\rho}\, v \frac{\partial \bar{H}}{\partial y} &= \frac{\partial}{\partial y} \frac{\mu}{N_{Pr}} \frac{\partial \bar{H}}{\partial y} \\ \bar{C} = \bar{H} &= 0 \text{ at } y = 0 \\ \bar{C} = \bar{H} &= 1 \text{ at } y = \infty . \end{aligned}\right\} \tag{3-28}$$

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

$$\bar{H} = F_1\ (z, y, N_{Pr}) \tag{3-29}$$

then the solution of the oxygen conservation equation is

$$\bar{C} = F_1\ (z, y, N_{Sc})\ . \tag{3-30}$$

The rate of oxygen transfer to the surface by diffusion may be expressed as

$$\dot{m}(O_2) = (C_e - C_w) \left(\frac{\mu}{N_{Sc}} \frac{\partial \bar{C}}{\partial y} \right)_w \tag{3-31}$$

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

$$q = (H_e - H_w) \left(\frac{\mu}{N_{Pr}} \frac{\partial \bar{H}}{\partial y} \right)_w . \tag{3-32}$$

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

$$q_{c,net} = 0.76\, N_{Pr}^{-0.6} \, (\rho_w \, \mu_w)^{0.1} \, (\rho_s \, \mu_s)^{0.4} \, (\hat{H}_e - \hat{H}_w) \sqrt{\frac{du_e}{dz}} . \tag{3-33}$$

Therefore, the rate of oxygen diffusion to the surface is

$$\dot{m}_{O_2} = 0.76\, N_{Sc}^{-0.6} \, (\rho_w \, \mu_w)^{0.1} \, (\rho_s \, \mu_s)^{0.4} \, (C_e - C_w) \sqrt{\frac{du_e}{dz}} . \tag{3-34}$$

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

$$\dot{m}_{O_2} = \frac{N_{Sc}^{-0.6} \, (C_e - C_w)}{N_{Pr}^{-0.6} \, (\hat{H}_e - \hat{H}_w)} \, q_{c,net} \tag{3-35}$$

or

$$\dot{m}_{O_2} = \frac{C_e - C_w}{H_e - H_w} N_{Le}^{0.6} \bar{M}_w q_{c,net} . \tag{3-36}$$

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

$$\dot{m}_s = \frac{C_e - C_w}{H_e - H_w} \lambda N_{Le}^{0.6} \bar{M}_w q_{c,net} . \tag{3-37}$$

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,

$$\dot{m}_s = \frac{k P_e C_e \bar{M}_w}{M_{O_2} + \dfrac{k P_e (H_e - H_w)}{\lambda N_{Le}^{0.6} q_{c,net}}} \tag{3-38}$$

where

$$k = A_s \exp (- B_s/T_{s_1}) . \tag{3-39}$$

<u>Front surface energy balance</u>.- 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

$$q_{c,net} = q_c \ (1 - H_w/H_e) \ [1 - \bar{\eta} \ \dot{m}_T \ \hat{H}_e/q_c] \tag{3-40}$$

where

$$\dot{m}_T = \alpha_c \ \dot{m}_s + \alpha_p \ \dot{m}_1 \tag{3-41}$$

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

$$q_{c,net} = q_c \ (1 - H_w/H_e) \ \{1.- [.724 \ \dot{m}_T \ \hat{H}_e/q_c - .13 \ (\dot{m}_T \ \hat{H}_e/q_c)^2]\} \ . \tag{3-42}$$

Figure 2 shows the linear approximation to be good for values of $\dot{m}_T\hat{H}_e/q_c \leq 1$. The second-order approximation is good for $\dot{m}_T\hat{H}_e/q_c < 2.25$. In Ref. 16 Swann, Pittman and Smith specify a minimum value of

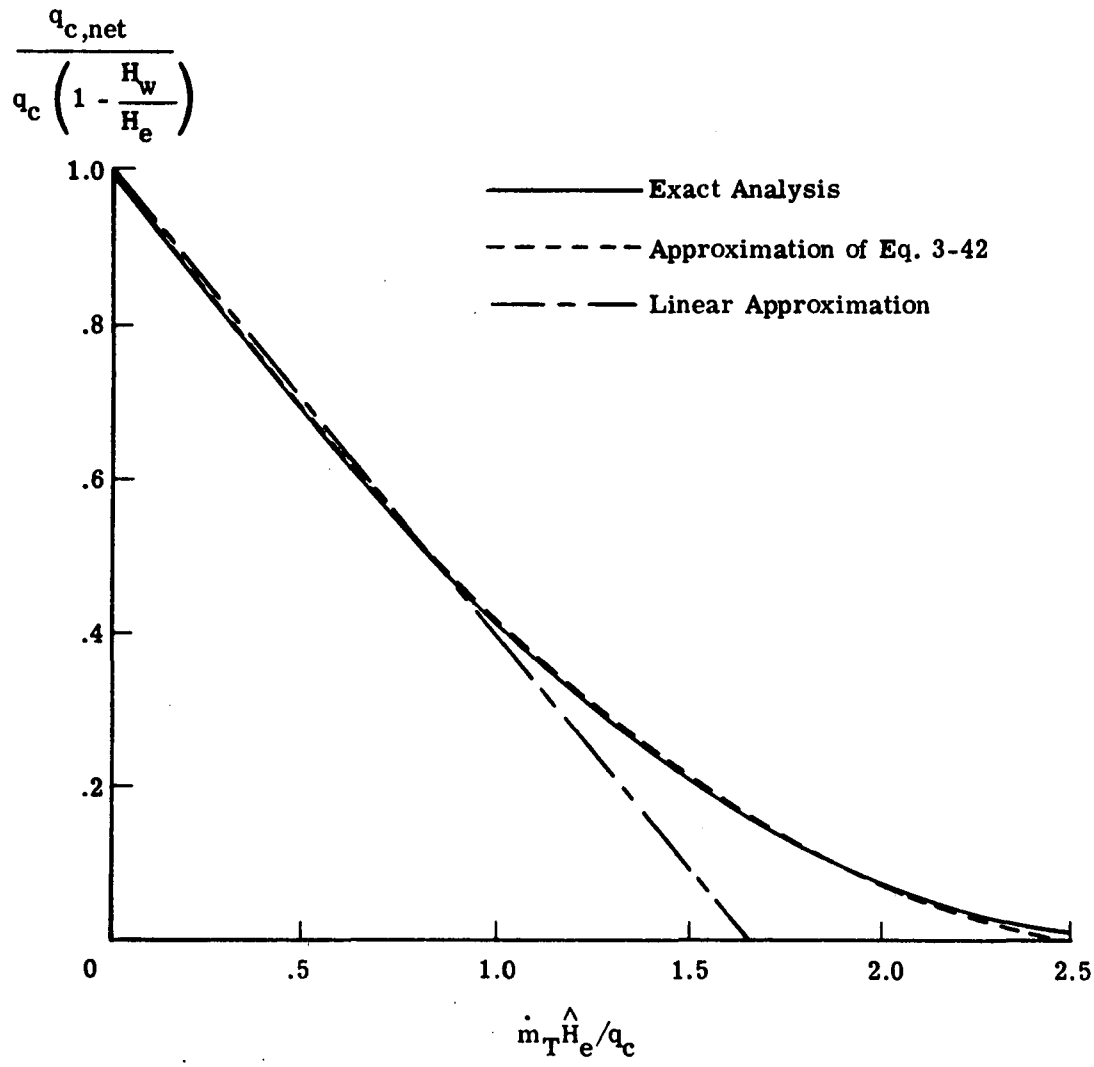

Figure 2.- Blocking effectiveness for a laminar boundary layer with air-to-air injection.

$\dfrac{q_{c,net}}{q_c(1 - H_w/H_e)}$ of 0.04 at $\dot{m}_T\hat{H}_e/q_c = 2.25$, where the second order curve departs the exact curve.

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

$$q_c \quad (1 - H_w/H_e) \quad \{1 - (1 - \beta)\ [0.724\ \dot{m}_T \hat{H}_e/q_c$$

Cold Wall Convective Heating Rate — Hot-wall correction — Aerodynamic

Net Convective

$$-0.13\ (\dot{m}_T\ \hat{H}_e/q_c)^2] - \beta\ \bar{\eta}\ \dot{m}_T\ H_e/q_c\} + \alpha\ q_R$$

Blocking — Radiative Heating Rate

Heating

$$+ [1 - S(T_{s_1} - \bar{T}_1)]\ \dot{m}_s\ \Delta H_c = \sigma\ \varepsilon_s\ T_{s_1}^4$$

Combustion Heating Rate — Reradiation

$$- k_s \frac{\partial T_s}{\partial y} \qquad + S(T_{s_1} - \bar{T}_1)\ \dot{m}_s\ H_c \tag{3-43}$$

Conduction to Interior — Heat of Sublimation of Char

where

$$\beta = 1 \text{ when } \dot{m}_T \hat{H}_e/q_c \leq 1.0$$

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

$S(T_{s_1} - \bar{T}_1)$ is a step function defined by

$$S(T_{s_1} - \bar{T}_1) = 1 \text{ when } T_{s_1} = \bar{T}_1$$

$$S(T_{s_1} - \bar{T}_1) = 0 \text{ when } T_{s_1} < \bar{T}_1 .$$

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

$$- \left(k_s \frac{\partial T_s}{\partial y}\right)_I = \dot{m}_g \, \Delta H_p - \left(k'_s \frac{\partial T'_s}{\partial y}\right)_I . \tag{3-44}$$

Also, the temperature of the char layer equals the temperature of the uncharred layer at their interface.

$$T_{s_I} = T'_{s_I} . \tag{3-45}$$

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

$$\dot{m}_g = A' \exp\left(-B'/T_{s_I}\right) . \tag{3-46}$$

It is sometimes desirable to limit the temperature at the pyrolysis zone to some value $\bar{T}_I$. When such a restriction is used Eqs. 3-44 and 3-46 are employed as described until the pyrolysis zone temperature reaches $\bar{T}_I$, 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 $T_{s_I} = \bar{T}_I$.

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

$$- \left(k'_s \frac{\partial T'_s}{\partial y}\right)_{I+J} = - \left(k''_s \frac{\partial T''_s}{\partial y}\right)_{I+J} + \rho_{Hs} \hat{C}_{p_{Hs}} \ell_{Hs} \left(\frac{\partial T'_s}{\partial t}\right)_{I+J} \tag{3-47}$$

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

$$T'_{s\ I+J} = T''_{s\ I+J} \ . \tag{3-48}$$

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

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

$$+ \rho_{HSP} \hat{C}_{p_{HSP}} \ell_{HSP} \left(\frac{\partial T''_s}{\partial t}\right)_{I+J+K} \ . \tag{3-49}$$

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

$$q_B = \sigma \, \varepsilon_s'' \, T_s''^{\,4} \, I + J + K \, . \tag{3-50}$$

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

$$T_s \, (y,t) = T_{s_o}(y) \text{ at } t = 0 \tag{3-51}$$

where the superscript on T_s is neglected.

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

$$\eta \, (y,t) = \eta_o(y) \text{ at } t = 0. \tag{3-52}$$

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

$$T\ (y,t) = T_o(y) \text{ at } t = 0. \tag{3-53}$$

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,

$$P_1 = P_w\ . \tag{3-54}$$

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

$$v_o = -\frac{K}{\mu}\frac{\partial P}{\partial y} \tag{3-55}$$

Equation 3-55 is multiplied by ρ and the equation of state is used to give

$$\rho\, v_o = -\frac{K\bar{M}}{\mu R_u T} P \frac{\partial P}{\partial y} . \tag{3-56}$$

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

$$(\rho\, v_o)_I = -\dot{m}_g \tag{3-57}$$

to obtain

$$\left(\frac{\partial P}{\partial y}\right)_I = R_u \left(\frac{\mu T}{K\bar{M}P}\right)_I \dot{m}_g . \tag{3-58}$$

But

$$\frac{\partial P}{\partial y} = \frac{1}{2P}\frac{\partial P^2}{\partial y} \tag{3-59}$$

therefore

$$\left(\frac{\partial P^2}{\partial y}\right)_I = 2\, R_u \left(\frac{\mu T}{K\bar{M}}\right)_I \dot{m}_g . \tag{3-60}$$

Initial conditions.- The initial condition for the pyrolysis gas pressure is

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

Total Mass Conservation Equation

The mass conservation equation is solved for the product ρv_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

$$(\rho\ v_o)_I = -\ \dot{m}_g\ . \tag{3-62}$$

The initial condition for the mass flow rate is

$$(\rho\ v_o)_{y,t} = -\dot{m}_o(y) \text{ at } t = 0. \tag{3-63}$$

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

$$(\rho_i \ v)_I = -\left(\frac{x_i}{\eta \bar{M}}\right)_I M_i \dot{m}_g \ . \tag{3-64}$$

The initial condition for the species continuity equation is

$$(\rho_i \ v)_{y,t} = (\rho_i v)_{y,o} \text{ at } t = 0. \tag{3-65}$$

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_o 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

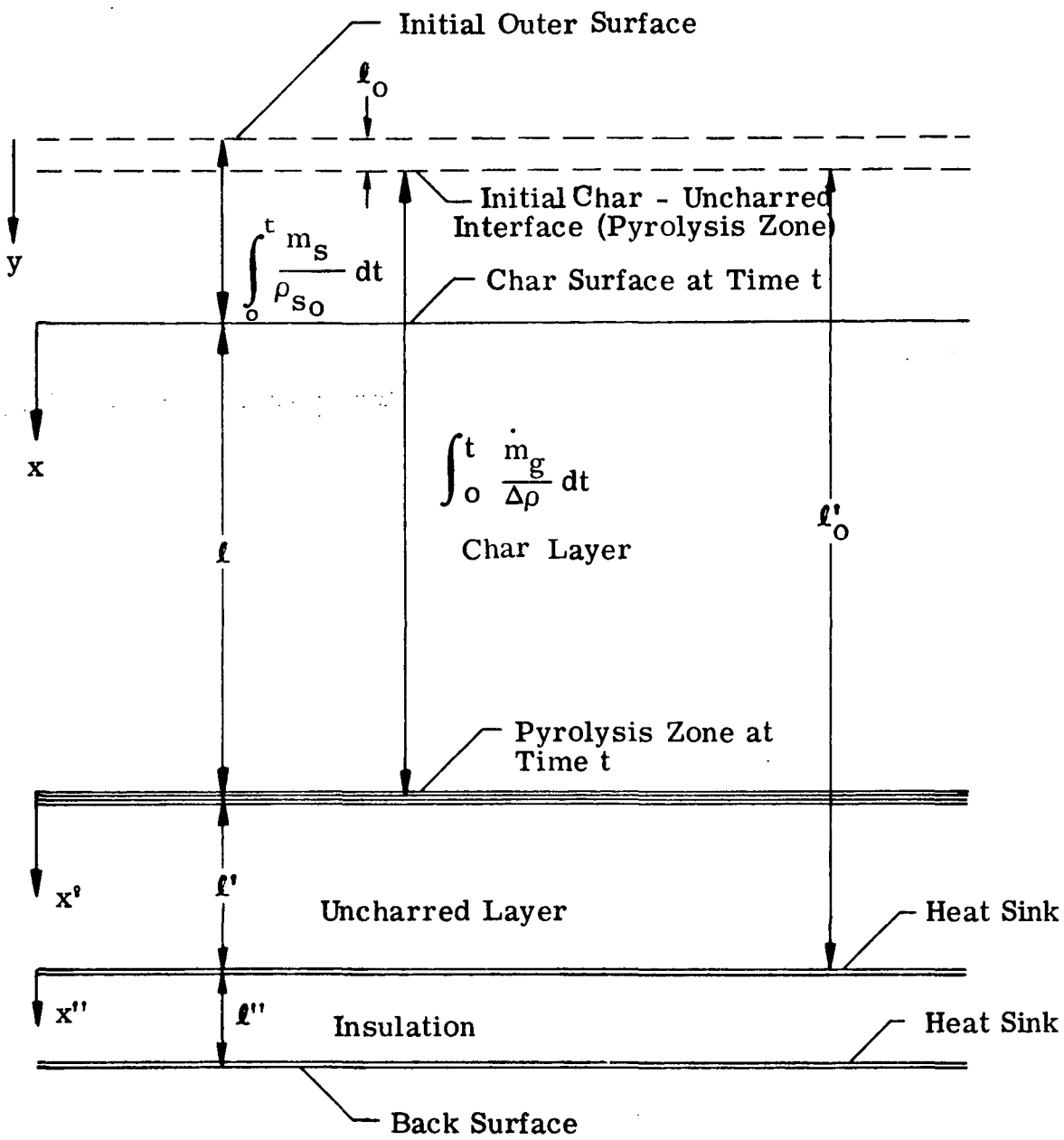

Figure 3.- Location of system boundaries and coordinates.

$$x_d = y - \int_0^t \frac{\dot{m}_s}{\rho_{s_o}} \, dt \tag{4-1}$$

where the integral representsthe total surface recession at some time t. Equation 4-1 is nondimensionalized by the char layer thickness ℓ to give the transformed dimensionless coordinate for the char layer as

$$x = \frac{y - \int_0^t \dot{m}_s/\rho_{s_o} \, dt}{\ell} \, . \tag{4-2}$$

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

$$x'_d = y - \ell_o - \int_0^t \dot{m}_g/\Delta\rho \, dt \tag{4-3}$$

where ℓ_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 ℓ' to give the transformed dimensionless coordinate for the uncharred layer as

$$x' = \frac{y - \ell_o - \int_0^t \dot{m}_g/\Delta\rho \, dt}{\ell'} \quad . \tag{4-4}$$

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

$$x'' = \frac{y - (\ell_o + \ell'_o)}{\ell''} \quad . \tag{4-5}$$

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:

$$\left(\frac{\partial}{\partial t}\right)_{\text{Old}} = \left(\frac{\partial}{\partial t}\right)_{\text{New}} + \left[\frac{\partial x}{\partial y}\frac{\partial y}{\partial t} + \frac{\partial x}{\partial \ell}\frac{\partial \ell}{\partial t} + \frac{\partial x}{\partial t}\right]\frac{\partial}{\partial x} \tag{4-6}$$

but

$$\left.\begin{aligned}
\frac{\partial x}{\partial y} &= \frac{1}{\ell} \\
\frac{\partial x}{\partial \ell} &= -\, x/\ell \\
\frac{\partial x}{\partial t} &= -\,\frac{1}{\ell}\,\dot{m}_s/\rho_{s_o} \\
\ell &= \ell_o + \int_0^t [\dot{m}_g/\Delta\rho - \dot{m}_s/\rho_{s_o}]\, dt \\
\frac{\partial \ell}{\partial t} &= \dot{m}_g/\Delta\rho - \dot{m}_s/\rho_{s_o} \;.
\end{aligned}\right\} \tag{4-7}$$

Therefore

$$\left(\frac{\partial}{\partial t}\right)_{\text{Old}} = \left(\frac{\partial}{\partial t}\right)_{\text{New}} - V_c\,\frac{\partial}{\partial x} \tag{4-8}$$

where

$$V_c = \frac{1}{\ell}\,[\dot{m}_s/\rho_{s_o} + x(\dot{m}_g/\Delta\rho - \dot{m}_s/\rho_{s_o})] \;. \tag{4-9}$$

Also

$$\frac{\partial}{\partial y} = \frac{\partial x}{\partial y}\,\frac{\partial}{\partial x} \tag{4-10}$$

or

$$\frac{\partial}{\partial y} = \frac{1}{\ell} \frac{\partial}{\partial x} \tag{4-11}$$

and

$$\frac{\partial^2}{\partial y^2} = \frac{1}{\ell^2} \frac{\partial^2}{\partial x^2} \quad . \tag{4-12}$$

Char temperature equation.- Using these derivative expressions the char temperature equation becomes

$$(1 - \eta) \frac{\rho_s C_{p_s}}{M_s} \left[\frac{\partial T_s}{\partial t} - V_c \frac{\partial T_s}{\partial x}\right] = \frac{k_s}{\ell^2} \frac{\partial^2 T_s}{\partial x^2} + \frac{1}{\ell^2} \frac{\partial k_s}{\partial x} \frac{\partial T_s}{\partial x}$$

$$- H_A(T_s - T) + \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \varepsilon)$$

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

This equation can be written as

$$\frac{\partial^2 T_s}{\partial x^2} + \alpha_1 \frac{\partial T_s}{\partial x} + \alpha_2 T_s + \alpha_3 + \alpha_4 \frac{\partial T_s}{\partial t} = 0 \tag{4-14}$$

where

$$\alpha_1 = \frac{1}{k_s}\left[\frac{\partial k_s}{\partial x} + \rho_s \ell^2 (1 - \eta) \frac{C_{p_s}}{M_s} V_c\right] \tag{4-15}$$

$$\alpha_2 = - H_A \ell^2/k_s \tag{4-16}$$

$$\alpha_3 = \frac{\ell^2}{k_s}\left[H_A T + \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \varepsilon)\right.$$

$$\left. + (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s}\left(\frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial x}\right) - \eta \sum_j R_{hj} \Delta H_j\right] \tag{4-17}$$

$$\alpha_4 = - (1 - \eta) \ell^2 \rho_s C_{p_s}/M_s k_s \tag{4-18}$$

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 α'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

$$\frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial x} + \eta \frac{M_s}{\rho_s} (R_{hs} + R_s) = 0 \tag{4-19}$$

or, writing it in the linear form,

$$\frac{\partial \eta}{\partial x} + \varepsilon_1 \eta + \varepsilon_2 + \varepsilon_3 \frac{\partial \eta}{\partial t} = 0 \tag{4-20}$$

where

$$\varepsilon_1 = -\frac{M_s}{\rho_s}(R_{hs} + R_s)/V_c \tag{4-21}$$

$$\varepsilon_2 = 0 \tag{4-22}$$

$$\varepsilon_3 = 1/V_c \tag{4-23}$$

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

$$\eta \sum_i \frac{\rho_i C_{pi}}{M_i}\left[\frac{\partial T}{\partial t} + (v/\ell - V_c)\frac{\partial T}{\partial x}\right] = -\eta\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_{P,x_i}\left[\frac{\partial P}{\partial t}\right.$$

$$\left. + (v/\ell - V_c)\frac{\partial P}{\partial x}\right] - \eta \sum_i H_i R_{T_i} + \sum_i H_i \frac{1}{\ell}\frac{\partial}{\partial x} J_i$$

$$+ P\left[\frac{\partial \eta}{\partial t} + (v/\ell - V_c)\frac{\partial \eta}{\partial x}\right] + \frac{1}{2}\eta v^2 \sum_i R_{T_i} M_i$$

$$+ \eta/\ell^3 \tilde{\tilde{\tau}}_{xx}\frac{\partial v}{\partial x} + \eta \sum_i \frac{J_i g_i}{M_i} - \frac{1}{\ell}\frac{\partial}{\partial x} q_x$$

$$+ \eta (A' - \varepsilon') + H_A (T_s - T) - \eta R_s H(T)_s - \eta R_{hs} H_s$$

$$+ \eta \sum_r r_h^{(r)} \Delta H^{(r)} . \tag{4-24}$$

Since

$$\rho = P\bar{M}/R_u T \tag{4-25}$$

$$\left(\frac{\partial \ \ell n \ \rho}{\partial \ \ell n \ T}\right)_{P,x_i} = -1 \ . \tag{4-26}$$

Also

$$\frac{\partial P}{\partial t} = \sum_i \rho_i/M_i \ R_u \frac{\partial T}{\partial t} + R_u T \frac{\partial}{\partial t} \sum_i \rho_i/M_i \tag{4-27}$$

and

$$\frac{\partial P}{\partial x} = \sum_i \rho_i/M_i \ R_u \frac{\partial T}{\partial x} + R_u \ T \frac{\partial}{\partial x} \sum_i \rho_i/M_i \ . \tag{4-28}$$

Therefore Eq. 4-24 can be written as

$$\eta \ (v/\ell - V_c) \left[\sum_i \frac{\rho_i \ C_{p_i}}{M_i} - R_u \sum_i \rho_i/M_i\right] \frac{\partial T}{\partial x} + \Bigg\{ H_A$$

$$- \eta \ R_u \left[\frac{\rho}{\eta \bar{M}} \left(\frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial x}\right) + \frac{\partial}{\partial t}\left(\sum_i \rho_i/M_i\right)\right.$$

$$\left. + (v/\ell - V_c) \frac{\partial}{\partial x}\left(\sum_i \rho_i/M_i\right)\right]\Bigg\} T + \eta \sum_i H_i \ R_{T_i}$$

$$- \frac{1}{\ell} \sum_i H_i \frac{\partial}{\partial x} J_i - \eta \frac{v^2}{2} \sum_i R_{T_i} \ M_i - \frac{\tau_{xx}}{\ell^3} \frac{\partial v}{\partial x}$$

$$- \eta \sum_i \frac{J_i \ g_i}{M_i} + \frac{1}{\ell^2} \frac{\partial}{\partial x} q_x - \eta \ (A' - \varepsilon') - H_A T_s$$

$$+ \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + \eta \left(\sum_i \frac{\rho_i C_{p_i}}{M_i} \right.$$

$$\left. - R_u \sum_i \rho_i / M_i \right) \frac{\partial T}{\partial t} = 0 \tag{4-29}$$

or, in the linear form,

$$\frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 \tag{4-30}$$

where

$$\beta_1 = \{H_A - \eta R_u \left[\frac{\rho}{\eta \bar{M}} \left(\frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial x} \right) + \frac{\partial}{\partial t} \left(\sum_i \rho_i / M_i \right) \right.$$

$$\left. \left. + (v/\ell - V_c) \frac{\partial}{\partial x} \left(\sum_i \rho_i / M_i \right) \right] \right\} / D1 \tag{4-31}$$

$$D1 = \eta (v/\ell - V_c) \left[\sum_i \frac{\rho_i C_{p_i}}{M_i} - R_u \sum_i \rho_i / M_i \right] \tag{4-32}$$

$$\beta_2 = \left[\eta \sum_i H_i R_{T_i} - \frac{1}{\ell} \sum_i H_i \frac{\partial}{\partial x} J_i - \eta \frac{v^2}{2} \sum_i R_{T_i} M_i \right.$$

$$- \frac{\tau_{xx}}{\ell^3} \frac{\partial v}{\partial x} - \eta \sum_i \frac{J_i g_i}{M_i} + \frac{1}{\ell^2} \frac{\partial}{\partial x} q_x$$

$$- \eta (A' - \varepsilon') - H_A T_s + \eta R_s H(T)_s + \eta R_{hs} H_s$$

$$\left. - \eta \sum_r r_h^{(r)} \Delta H^{(r)} \right] / D1 \tag{4-33}$$

$$\beta_3 = \eta \left(\sum_i \frac{\rho_i \, C_{p_i}}{M_i} - R_u \sum_i \rho_i / M_i \right) / D1 \tag{4-34}$$

<u>Chemical species continuity equation</u>.- The transformed chemical species continuity equation is

$$\frac{\partial}{\partial t} (\eta \, \rho_i) - V_c \frac{\partial}{\partial x} (\eta \, \rho_i) + \frac{1}{\ell} \frac{\partial}{\partial x} (\rho_i \, v_o) + \frac{1}{\ell} \frac{\partial}{\partial x} \eta j_i - \eta \, R_{T_i} \, M_i = 0 \tag{4-35}$$

This equation is combined with the identities

$$\dot{m}_i = - \rho_i \, v \tag{4-36}$$

and

$$v_o = \eta \, v \tag{4-37}$$

to obtain

$$\eta \left(\frac{V_c}{v} - \frac{1}{\ell} \right) \frac{\partial}{\partial x} \dot{m}_i + \left[\left(\frac{V_c}{v} - \frac{1}{\ell} \right) \frac{\partial \eta}{\partial x} - \frac{\eta}{v^2} \frac{\partial v}{\partial x} - \frac{1}{v} \frac{\partial \eta}{\partial t} \right] \dot{m}_i + \frac{1}{\ell} \frac{\partial}{\partial x} \eta j_i - \eta \, R_{T_i} \, M_i + \eta \frac{\partial \rho_i}{\partial t} = 0 \tag{4-38}$$

or, in linear form,

$$\frac{\partial \dot{m}_i}{\partial x} + \Delta_{1_i} \, \dot{m}_i + \Delta_{2_i} + \Delta_{3_i} \frac{\partial \dot{m}_i}{\partial t} = 0 \tag{4-39}$$

where

$$\Delta_{1_i} = \frac{1}{\eta}\frac{\partial\eta}{\partial x} + \left[\frac{\eta\ R_{T_i}\ M_i}{\rho_i} - \eta\ \frac{V_c}{v}\frac{\partial v}{\partial x} - \frac{\partial\eta}{\partial t}\right] \quad /D2 \tag{4-40}$$

$$D2 = \eta(V_c - \frac{v}{\ell}) \tag{4-41}$$

$$\Delta_{2_i} = v\left(\frac{1}{\ell}\frac{\partial}{\partial x}\eta j_i + \eta\ \frac{\partial\rho_i}{\partial t}\right) \quad /D2 \tag{4-42}$$

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

Total mass conservation equation.- The transformed total mass conservation equation is

$$\frac{\partial}{\partial t}(\eta\ \rho) - V_c\frac{\partial}{\partial x}(\eta\ \rho) + \frac{1}{\ell}\frac{\partial}{\partial x}(\rho\ v_o) - \eta\sum_i R_{T_i}\ M_i = 0\ . \tag{4-44}$$

This equation is combined with the identity

$$\dot{m} = -\ \rho\ v_o \tag{4-45}$$

to obtain

$$\frac{\partial}{\partial x}\dot{m} = \ell\left[\frac{\partial}{\partial t}(\eta\ \rho) - \eta\sum_i R_{T_i}\ M_i - V_c\left(\eta\frac{\partial\rho}{\partial x} + \rho\frac{\partial\eta}{\partial x}\right)\right] \tag{4-46}$$

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

$$\frac{\partial^2 P^2}{\partial x^2} + \frac{\mu T}{K\bar{M}} \frac{\partial}{\partial x} \left(\frac{K\bar{M}}{\mu T}\right) \frac{\partial}{\partial x} P^2 - 2 \frac{\mu R_u T}{K\bar{M}} \left[\frac{\partial}{\partial t} (\eta \rho) - V_c \frac{\partial}{\partial x} (\eta \rho) - \eta \sum_i R_{T_i} M_i\right] = 0 . \tag{4-47}$$

This equation is combined with the equation of state to give

$$\begin{aligned} &\frac{\partial^2 P^2}{\partial x^2} + \frac{\mu}{K}\left[\frac{T}{\bar{M}} \frac{\partial}{\partial x} \left(\frac{K\bar{M}}{\mu T}\right) + \frac{\eta V_c}{P}\right] \frac{\partial P^2}{\partial x} \\ &- \frac{2\mu}{\bar{M}KP}\left[\eta \left(\frac{\partial \bar{M}}{\partial t} - \frac{\bar{M}}{T} \frac{\partial T}{\partial t}\right) + \bar{M} \left(\frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial t}\right) + \eta \left(\frac{\bar{M}}{T} \frac{\partial T}{\partial x} - V_c \frac{\partial \bar{M}}{\partial x}\right)\right] P^2 \\ &+ \frac{2\mu\eta}{K\rho} \sum_i R_{T_i} M_i - \frac{\mu\eta}{KP} \frac{\partial P^2}{\partial t} = 0 \end{aligned} \tag{4-48}$$

or, in the linear form,

$$\frac{\partial^2 P^2}{\partial x^2} + \gamma_1 \frac{\partial P^2}{\partial x} + \gamma_2 P^2 + \gamma_3 + \gamma_4 \frac{\partial P^2}{\partial t} = 0 \tag{4-49}$$

where

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

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

$$\left. + \bar{M}\left(\frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial x}\right) + \eta\left(\frac{\bar{M}}{T}\frac{\partial T}{\partial x} - V_c \frac{\partial \bar{M}}{\partial x}\right)\right] \tag{4-51}$$

$$\gamma_3 = \frac{2\mu\eta}{K\rho} \sum_i R_{T_i} M_i \tag{4-52}$$

$$\gamma_4 = -\frac{\mu\eta}{KP} \tag{4-53}$$

Uncharred Layer Equation

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

$$\left(\frac{\partial}{\partial t}\right)_{\text{Old}} = \left(\frac{\partial}{\partial t}\right)_{\text{New}} + \left[\frac{\partial x'}{\partial y}\frac{\partial y}{\partial t} + \frac{\partial x'}{\partial \ell'}\frac{\partial \ell'}{\partial t} + \frac{\partial x'}{\partial t}\right]\frac{\partial}{\partial x} \tag{4-54}$$

but

$$\left.\begin{aligned}
\frac{\partial x'}{\partial y} &= \frac{1}{\ell'} \\
\frac{\partial x'}{\partial \ell'} &= -\frac{x'}{\ell'} \\
\frac{\partial x'}{\partial t} &= -\frac{1}{\ell'}\,\dot{m}_g/\Delta\rho \\
\ell' &= \ell'_o - \int_0^t \dot{m}_g/\Delta\rho \; dt \\
\frac{\partial \ell'}{\partial t} &= -\,\dot{m}_g/\Delta\rho \;.
\end{aligned}\right\} \tag{4-55}$$

Therefore

$$\left(\frac{\partial}{\partial t}\right)_{\text{Old}} = \left(\frac{\partial}{\partial t}\right)_{\text{New}} + \frac{\dot{m}_g}{\Delta\rho}\left(\frac{x' - 1}{\ell'}\right)\frac{\partial}{\partial x'} \;. \tag{4-56}$$

Also

$$\frac{\partial}{\partial y} = \frac{\partial x'}{\partial y}\,\frac{\partial}{\partial x'} \tag{4-57}$$

or

$$\frac{\partial}{\partial y} = \frac{1}{\ell'}\,\frac{\partial}{\partial x'} \tag{4-58}$$

and

$$\frac{\partial^2}{\partial y^2} = \frac{1}{\ell'^2} \frac{\partial^2}{\partial x'^2} \quad . \tag{4-59}$$

These equations are employed to obtain the transformed energy equation for the uncharred layer as

$$\frac{k'_s}{\ell'^2} \frac{\partial^2 T_s}{\partial x'^2} + \left[\frac{1}{\ell'^2} \frac{\partial k'_s}{\partial x'} + \frac{\rho'_s \hat{C}'_{p_s} \dot{m}_g (1 - x')}{\ell' \Delta\rho} \right] \frac{\partial T_s}{\partial x'}$$

$$- \rho'_s \hat{C}'_{p_s} \frac{\partial T_s}{\partial t} = 0 \tag{4-60}$$

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

$$\frac{\partial^2 T_s}{\partial x'^2} + \alpha'_1 \frac{\partial T_s}{\partial x'} + \alpha'_2 T_s + \alpha'_3 + \alpha'_4 \frac{\partial T_s}{\partial t} = 0 \tag{4-61}$$

where

$$\alpha'_1 = \frac{1}{k'_s} \left[\frac{\partial k'_s}{\partial x'} + \frac{\ell' \rho'_s \hat{C}'_{p_s} \dot{m}_g}{\Delta\rho} (1 - x') \right] \tag{4-62}$$

$$\alpha'_2 = 0 \tag{4-63}$$

$$\alpha'_3 = 0 \tag{4-64}$$

$$\alpha_4' = -\rho_s' \hat{C}_{p_s}' \ell'^2/k_s' \ . \tag{4-65}$$

Insulation Layer Equation

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

$$\left(\frac{\partial}{\partial t}\right)_{\text{Old}} = \left(\frac{\partial}{\partial t}\right)_{\text{New}}$$

$$\frac{\partial}{\partial y} = \frac{\partial x''}{\partial y}\frac{\partial}{\partial x''} \tag{4-66}$$

$$= \frac{1}{\ell''}\frac{\partial}{\partial x''}$$

$$\frac{\partial^2}{\partial y^2} = \frac{1}{\ell''^2}\frac{\partial^2}{\partial x''^2} \ .$$

The insulation layer temperature equation becomes

$$\frac{k_s''}{\ell''^2}\frac{\partial^2 T_s}{\partial x''^2} + \frac{1}{\ell''^2}\frac{\partial k_s''}{\partial x''}\frac{\partial T_s}{\partial x''} - \rho_s''\hat{C}_{p_s}''\frac{\partial T_s}{\partial t} = 0 \tag{4-67}$$

or

$$\frac{\partial^2 T_s}{\partial x''^2} + \alpha_1''\frac{\partial T_s}{\partial x''} + \alpha_2'' T_s + \alpha_3'' + \alpha_4''\frac{\partial T_s}{\partial t} = 0 \tag{4-68}$$

where

$$\alpha_1'' = \frac{1}{k_s''} \frac{\partial k_s''}{\partial x''} \tag{4-69}$$

$$\alpha_2'' = 0 \tag{4-70}$$

$$\alpha_3'' = 0 \tag{4-71}$$

$$\alpha_4'' = - \frac{\rho_s'' \hat{C}_{p_s}'' \ell''^2}{k_s''} \quad . \tag{4-72}$$

Boundary Conditions

The transformed boundary conditions are as follows:

Rate of surface removal by oxidation

$$\dot{m}_s = \frac{k P_e C_e \bar{M}_w}{M_{O_2} + \dfrac{k P_e (H_e - H_w)}{\lambda N_{Le}^{0.6} q_{c,net}}} \tag{4-73}$$

Energy balance at the front surface

$$q_c (1 - H_w/H_e) \left\{ 1 - (1 - \beta) \left[0.724 \frac{\hat{H}_e \dot{m}_T}{q_c} - 0.13 \left(\frac{\hat{H}_e \dot{m}_T}{q_c} \right)^2 \right] - \beta \bar{\eta} \dot{m}_T \frac{\hat{\hat{H}}_e}{q_c} \right\} + \alpha q_R + \left[1 - S(T_{s_I} - \bar{T}_1) \right] \dot{m}_s \Delta H_c$$

$$= \sigma \varepsilon_s T_{s_1}^4 - \frac{k_s}{\ell} \frac{\partial T_s}{\partial x} + s(T_{s_1} - \bar{T}_1) \dot{m}_s H_c \tag{4-74}$$

Energy balance at the pyrolysis zone

$$- \left(\frac{k_s}{\ell} \frac{\partial T_s}{\partial x}\right)_{x = 1} = \dot{m}_g \, \Delta H_p - \left(\frac{k_s'}{\ell'} \frac{\partial T_s}{\partial x'}\right)_{x' = 0} \tag{4-75}$$

Rate of pyrolysis of uncharred material

$$\dot{m}_g = A' \exp\left(-B'/T_{s \; x = 1}\right) \tag{4-76}$$

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

$$- \left(\frac{k_s'}{\ell'} \frac{\partial T_s}{\partial x'}\right)_{x' = 1} = - \left(\frac{k_s''}{\ell''} \frac{\partial T_s}{\partial x''}\right)_{x'' = 0}$$

$$+ \rho_{HS} \, \hat{C}_{P_{HS}} \, \ell_{HS} \left(\frac{\partial T_s}{\partial t}\right)_{x' = 1} \tag{4-77}$$

Energy balance at the back surface of the insulation layer

$$- \left(\frac{k_s''}{\ell''} \frac{\partial T_s}{\partial x''}\right)_{x'' = 1} = \sigma \, \varepsilon_s'' \, T_s^{\,4}{}_{x'' = 1} - q_B$$

$$+ \rho_{HSP} \, \hat{C}_{P_{HSP}} \, \ell_{HSP} \left(\frac{\partial T_s}{\partial t}\right)_{x'' = 1} \tag{4-78}$$

Specified char porosity at the pyrolysis zone

$$\eta_{x = 1} = \eta_o \tag{4-79}$$

Specified temperature of pyrolysis gas at the pyrolysis interface

$$T_{x = 1} = T_{s_{x = 1}} \tag{4-80}$$

Specified pressure at the front surface

$$P_{x = 0} = P_w \tag{4-81}$$

Specified pressure gradient at the pyrolysis interface

$$\left(\frac{\partial}{\partial x} P^2\right)_{x = 1} = 2\ell \, R_u \left(\frac{\mu T}{K\bar{M}}\right)_{x = 1} \dot{m}_g \tag{4-82}$$

Specified mass flow rate at the pyrolysis interface

$$(\dot{m})_{x = 1} = \dot{m}_g \tag{4-83}$$

Specified chemical species mass flow rate at the pyrolysis interface

$$(\rho_i \, v)_{x = 1} = -\left(\frac{x_i}{\eta \bar{M}}\right)_{x = 1} M_i \dot{m}_g \, . \tag{4-84}$$

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

$$\left.\begin{aligned} \Delta x &= 1/I - 1 \\ \Delta x' &= 1/J \\ \Delta x'' &= 1/K \end{aligned}\right\} \qquad (5\text{-}1)$$

The station coordinates are

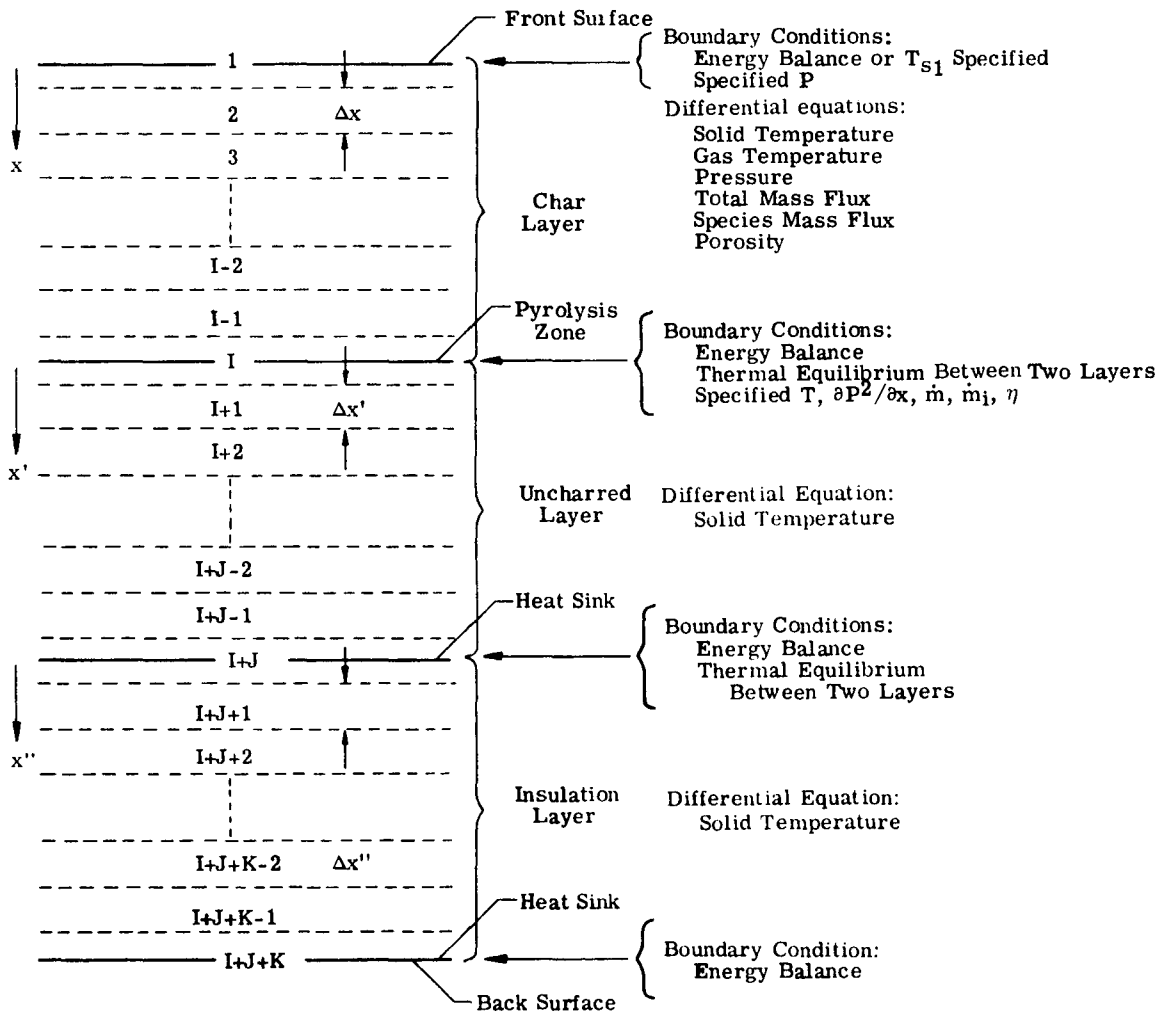

Figure 4.- Location of finite difference stations.

$$x = (N - 1)\Delta x \tag{5-2}$$

for the char layer,

$$x' = (N - I)\Delta x' \tag{5-3}$$

for the uncharred layer, and

$$x'' = (N - I - J)\ \Delta x'' \tag{5-4}$$

for the insulation layer.

Solid Phase Temperature Equations

The differential equation for the char temperature is

$$\frac{\partial^2 T_s}{\partial x^2} + \alpha_1 \frac{\partial T_s}{\partial x} + \alpha_2\ T_s + \alpha_3 + \alpha_4 \frac{\partial T_s}{\partial t} = 0\ . \tag{5-5}$$

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

$$T_s(N + 1) = T_s(N) + \left(\frac{\partial T_s}{\partial x}\right)_N \Delta x + \left(\frac{\partial^2 T_s}{\partial x^2}\right)_N \frac{\Delta x^2}{2!}$$

$$+ \left(\frac{\partial^3 T_s}{\partial x^3}\right)_N \frac{\Delta x^3}{3!} + --- \tag{5-6}$$

$$T_s(N - 1) = T_s(N) - \left(\frac{\partial T_s}{\partial x}\right)_N \Delta x + \left(\frac{\partial^2 T_s}{\partial x^2}\right)_N \frac{\Delta x^2}{2!}$$

$$- \left(\frac{\partial^3 T_s}{\partial x^3}\right)_N \frac{\Delta x^3}{3!} + --- \tag{5-7}$$

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

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

Therefore the equation

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

is accurate to terms of the order Δx^2. Similarly, adding Eqs. 5-6 and 5-7 gives

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

which is accurate to terms of the order Δx^2.

Equations 5-9 and 5-10 are used in Eq. 5-5 to obtain

$$\frac{1}{\Delta x^2}\,[T_s(N+1) - 2\,T_s(N) + T_s(N-1)] + \frac{\alpha_1(N)}{2\Delta x}\,[T_s(N+1)$$

$$- T_s(N-1)] + \alpha_2(N)\,T_s(N) + \alpha_3(N)$$

$$+ \alpha_4(N)\left(\frac{\partial T_s}{\partial t}\right)_N = 0\,. \tag{5-11}$$

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

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

$$+ \frac{\Delta t^2}{4}\left[\frac{\partial^2}{\partial t^2}\left(\alpha_4 \frac{\partial T_s}{\partial t}\right)\right]^{P+\Delta t/2} + \text{---} \tag{5-12}$$

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

$$+ \frac{\Delta t^2}{4}\left[\frac{\partial^2}{\partial t^2}\left(\alpha_4 \frac{\partial T_s}{\partial t}\right)\right]^{P+\Delta t/2} + \text{---}\ ; \tag{5-13}$$

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

$$\left(\alpha_4 \frac{\partial T_s}{\partial t}\right)^{P+\Delta t/2} = \frac{1}{2}\left[\alpha_4^P \frac{\partial T_s}{\partial t}^P + \alpha_4^{P+\Delta t} \frac{\partial T_s}{\partial t}^{P+\Delta t}\right] \tag{5-14}$$

which is accurate to terms of the order Δt^2. Now

$$\alpha_4^{P + \Delta t/2} = \frac{1}{2}\left(\alpha_4^{P} + \alpha_4^{P + \Delta t}\right) \tag{5-15}$$

$$\left.\frac{\partial T_s}{\partial t}\right|^{P + \Delta t/2} = \frac{T_s^{P + \Delta t} - T_s^{P}}{\Delta t} \tag{5-16}$$

and $\alpha_4^P \left.\frac{\partial T_s}{\partial t}\right|^P$ and $\alpha_4^{P + \Delta t} \left.\frac{\partial T_s}{\partial t}\right|^{P + \Delta t}$ are obtained from the explicit and implicit formulations of Eq. 5-11, that is

$$\left(\alpha_4 \frac{\partial T_s}{\partial t}\right)_N^P = -\frac{1}{\Delta x^2}\left[T_s(N+1)^P - 2\,T_s(N)^P + T_s(N-1)^P\right]$$

$$-\left.\frac{\alpha_1(N)}{2\Delta x}\right|^P \left[T_s(N+1)^P - T_s(N-1)^P\right] - \alpha_2(N)^P\, T_s(N)^P$$

$$-\,\alpha_3(N)^P \tag{5-17}$$

$$\left(\alpha_4 \frac{\partial T_s}{\partial t}\right)_N^{P + \Delta t} = -\frac{1}{\Delta x^2}\left[T_s(N+1)^{P + \Delta t} - 2\,T_s(N)^{P + \Delta t} + T_s(N-1)^{P + \Delta t}\right.$$

$$-\frac{\alpha_1(N)^{P + \Delta t}}{2\Delta x}\left[T_s(N+1)^{P + \Delta t} - T_s(N-1)^{P + \Delta t}\right] - \alpha_2(N)^{P+\Delta t} T_s(N)^{P+\Delta t}$$

$$-\,\alpha_3(N)^{P + \Delta t}\,. \tag{5-18}$$

Therefore, the modified implicit finite difference equation for T_s at interior stations is

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

$$- 2\, T_s(N)^P + T_s(N-1)^P] + \frac{\alpha_1(N)^P}{2\Delta x} [T_s(N+1)^P - T_s(N-1)^P]$$

$$+ \alpha_2(N)^P\, T_s(N)^P + \alpha_3(N)^P + \frac{1}{\Delta x^2} [T_s(N+1)^{P+\Delta t} - 2\, T_s(N)^{P+\Delta t}$$

$$+ T_s(N-1)^{P+\Delta t}] + \frac{\alpha_1(N)^{P+\Delta t}}{2\Delta x} [T_s(N+1)^{P+\Delta t} - T_s(N-1)^{P+\Delta t}]$$

$$+ \alpha_2(N)^{P+\Delta t}\, T_s(N)^{P+\Delta t} + \alpha_3(N)^{P+\Delta t} = 0 \qquad (5\text{-}19)$$

or

$$A_s(N)\, T_s(N-1)^{P+\Delta t} + B_s(N)\, T_s(N)^{P+\Delta t} + C_s(N)\, T_s(N+1)^{P+\Delta t}$$

$$= D_s(N) \qquad (5\text{-}20)$$

where

$$A_s(N) = 1/\Delta x^2 - \alpha_1(N)^{P+\Delta t}/2\Delta x \qquad (5\text{-}21)$$

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

$$C_s(N) = 1/\Delta x^2 + \alpha_1(N)^{P+\Delta t}/2\Delta x \qquad (5\text{-}23)$$

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

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

$$- \left[\frac{1}{\Delta x^2} + \frac{\alpha_1(N)^P}{2\Delta x}\right] T_s(N+1)^P . \qquad (5\text{-}24)$$

<u>Interior stations of the uncharred layer</u>.- 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

$$A_s'(N)\ T_s(N-1)^{P+\Delta t} + B_s'(N)\ T_s(N)^{P+\Delta t} + C_s'\ T_s(N+1)^{P+\Delta t}$$

$$= D_s'(N) \qquad (5\text{-}25)$$

where

$$A_s'(N) = 1/\Delta x'^2 - \frac{\alpha_1(N)^{P+\Delta t}}{2\Delta x'} \qquad (5\text{-}26)$$

$$B_s'(N) = \alpha_2'(N)^{P+\Delta t} - \frac{2}{\Delta x'^2} + \frac{1}{\Delta t}[\alpha_4'(N)^P + \alpha_4'(N)^{P+\Delta t}] \qquad (5\text{-}27)$$

$$C_s'(N) = 1/\Delta x'^2 + \frac{\alpha_1(N)^{P+\Delta t}}{2\Delta x'} \qquad (5\text{-}28)$$

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

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

$$- \left[\frac{1}{\Delta x'^2} + \frac{\alpha_1'(N)^P}{2\Delta x'}\right] T_s(N+1)^P \qquad (5\text{-}29)$$

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

$$A_s''(N)\; T_s(N-1)^{P+\Delta t} + B_s''(N)\; T_s(N)^{P+\Delta t} + C_s''(N)\; T_s(N+1)^{P+\Delta t}$$

$$= D_s''(N) \qquad (5\text{-}30)$$

where

$$A_s''(N) = 1/\Delta x''^2 - \frac{\alpha_1''(N)^{P+\Delta t}}{2\Delta x''} \qquad (5\text{-}31)$$

$$B_s''(N) = \alpha_2''(N)^{P+\Delta t} - 2/\Delta x''^2 + \frac{1}{\Delta t}\,[\alpha_4''(N)^P + \alpha_4''(N)^{P+\Delta t}] \qquad (5\text{-}32)$$

$$C_s''(N) = 1/\Delta x''^2 + \frac{\alpha_1''(N)^{P+\Delta t}}{2\Delta x''} \qquad (5\text{-}33)$$

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

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

$$- \left[\frac{1}{\Delta x''^2} + \frac{\alpha_1''(N)^P}{2\Delta x''}\right] T_s(N + 1)^P . \tag{5-34}$$

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

$$- \frac{1}{\ell} \left(k_s \frac{\partial T_s}{\partial x}\right)_{N = 1} = q_{c,net} - \sigma \varepsilon_s T_{s_1}^4 . \tag{5-35}$$

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

$$\frac{\partial^2 T_s}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial T_s}{\partial x}\right) . \tag{5-36}$$

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

$$\left(\frac{\partial T_s}{\partial x}\right)_{N=2} = \left(\frac{\partial T_s}{\partial x}\right)_{N=1} + \Delta x \left[\frac{\partial}{\partial x}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} + \frac{\Delta x^2}{2}\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1}$$

$$+ \frac{\Delta x^3}{6}\left[\frac{\partial^3}{\partial x^3}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} + \frac{\Delta x^4}{24}\left[\frac{\partial^4}{\partial x^4}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} + --- \qquad (5\text{-}37)$$

$$\left(\frac{\partial T_s}{\partial x}\right)_{N=3} = \left(\frac{\partial T_s}{\partial x}\right)_{N=1} + 2\Delta x\left[\frac{\partial}{\partial x}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} + 2\Delta x^2\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1}$$

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

$$\left(\frac{\partial T_s}{\partial x}\right)_{N=4} = \left(\frac{\partial T_s}{\partial x}\right)_{N=1} + 3\Delta x\left[\frac{\partial}{\partial x}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} + \frac{9\Delta x^2}{2}\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1}$$

$$+ \frac{9}{2}\Delta x^3\left[\frac{\partial^3}{\partial x^3}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} + \frac{27}{8}\Delta x^4\left[\frac{\partial^4}{\partial x^4}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} + --- \qquad (5\text{-}39)$$

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

$$\left[\frac{\partial}{\partial x}\left(\frac{\partial T_s}{\partial x}\right)\right]_{N=1} = \frac{1}{6\Delta x}\left[-11\left(\frac{\partial T_s}{\partial x}\right)_{N=1} + 18\left(\frac{\partial T_s}{\partial x}\right)_{N=2}\right.$$

$$\left. - 9\left(\frac{\partial T_s}{\partial x}\right)_{N=3} + 2\left(\frac{\partial T_s}{\partial x}\right)_{N=4}\right] \qquad (5\text{-}40)$$

which is accurate to terms of the order Δx^3. Therefore,

$$\left(\frac{\partial^2 T_s}{\partial x^2}\right)_{N=1} = \frac{1}{6\Delta x}\left[-11\left(\frac{\partial T_s}{\partial x}\right)_{N=1} + 18\left(\frac{\partial T_s}{\partial x}\right)_{N=2} - 9\left(\frac{\partial T_s}{\partial x}\right)_{N=3} + 2\left(\frac{\partial T_s}{\partial x}\right)_{N=4}\right]. \tag{5-41}$$

Combining Eq. 5-41 with Eq. 5-5 written for station $N = 1$ gives

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

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

$$\left\{\left[\alpha_1(1) - \frac{11}{6\Delta x}\right]\frac{\ell}{k_s(1)}\sigma\,\varepsilon_s\,T_s(1)^3 - \frac{3}{2\Delta x^2} + \alpha_2(1)\right\}T_s(1) + \frac{3}{4\Delta x^2}T_s(2) + \left(\frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2}\right)T_s(3) - \frac{3}{4\Delta x^2}T_s(4) + \frac{1}{6\Delta x^2}T_s(5) + \alpha_3(1) - \frac{q_{c,net}\,\ell}{k_s(1)}\left[\alpha_1(1) - \frac{11}{6\Delta x}\right] + \alpha_4(1)\left(\frac{\partial T_s}{\partial t}\right)_{N=1} = 0 \tag{5-43}$$

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

$$\{[\alpha_1(1)^{P+\Delta t} - \frac{11}{6\Delta x}]\frac{\ell^{P+\Delta t}}{k_s(1)^{P+\Delta t}}\sigma\,\varepsilon_s[T_s(1)^{P+\Delta t}]^3 - \frac{3}{2\Delta x^2}$$

$$+ \alpha_2(1)^{P+\Delta t} + \frac{1}{\Delta t}[\alpha_4(1)^P + \alpha_4(1)^{P+\Delta t}]\}T_s(1)^{P+\Delta t}$$

$$+ 3/4\Delta x^2\, T_s(2)^{P+\Delta t} + \left(\frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2}\right) T_s(3)^{P+\Delta t} - \frac{3}{4\Delta x^2}\, T_s(4)^{P+\Delta t}$$

$$+ \frac{1}{6\Delta x^2}\, T_s(5)^{P+\Delta t} = -\alpha_3(1)^P - \alpha_3(1)^{P+\Delta t} + [\alpha_1(1)^{P+\Delta t}$$

$$- \frac{11}{6\Delta x}]\, q_{c,net}^{P+\Delta t}\quad \frac{\ell^{P+\Delta t}}{k_s(1)^{P+\Delta t}} + [\alpha_1(1)^P - \frac{11}{6\Delta x}]q_{c,net}^P\,\frac{\ell^P}{k_s(1)^P}$$

$$- \{[\alpha_1(1)^P - \frac{11}{6\Delta x}]\frac{\ell^P}{k_s(1)^P}\sigma\,\varepsilon_s[T_s(1)^P]^3 - \frac{3}{2\Delta x^2}$$

$$+ \alpha_2(1)^P - \frac{1}{\Delta t}[\alpha_4(1)^P + \alpha_4(1)^{P+\Delta t}]\}\, T_s(1)^P$$

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

$$- \frac{1}{6\Delta x^2}\, T_s(5)^P \qquad (5\text{-}44)$$

or

$$B1_s\ T_s(1)^{P+\Delta t} + C1_s\ T_s(2)^{P+\Delta t} + G1_s\ T_s(3)^{P+\Delta t}$$

$$+ H1_s\ T_s(4)^{P+\Delta t} + I1_s\ T_s(5)^{P+\Delta t} = D1_s \tag{5-45}$$

where

$$B1_s = [\alpha_1(1)^{P+\Delta t} - \frac{11}{6\Delta x}]\ \frac{\ell^{P+\Delta t}}{k_s(1)^{P+\Delta t}}\ \sigma\ \varepsilon_s[T_s(1)^{P+\Delta t}]^3$$

$$- \frac{3}{2\Delta x^2} + \alpha_2(1)^{P+\Delta t} + \frac{1}{\Delta t}\ [\alpha_4(1)^P + \alpha_4(1)^{P+\Delta t}] \tag{5-46}$$

$$C1_s = 3/8\Delta x^2 \tag{5-47}$$

$$G1_s = \frac{3}{4\Delta x^2} - \frac{1}{12\Delta x^2} \tag{5-48}$$

$$H1_s = -\frac{3}{8\Delta x^2} \tag{5-49}$$

$$I1_s = \frac{1}{12\Delta x^2} \tag{5-50}$$

$$D1_s = -\alpha_3(1)^P - \alpha_3(1)^{P+\Delta t} + [\alpha_1(1)^{P+\Delta t} - \frac{11}{6\Delta x}]\ q^{P+\Delta t}_{c,net}\ \frac{\ell^{P+\Delta t}}{k_s(1)^{P+\Delta t}}$$

$$+ [\alpha_1(1)^P - \frac{11}{6\Delta x}]\ q^P_{c,net}\ \frac{\ell^P}{k_s(1)^P} - \{[\alpha_1(1)^P$$

$$- \frac{11}{6\Delta x}]\ \frac{\ell^P}{k_s(1)^P}\ \sigma\ \varepsilon_s[T_s(1)^P]^3 - \frac{3}{2\Delta x^2} + \alpha_2(1)^P$$

$$- \frac{1}{\Delta t} [\alpha_4(1)^P + \alpha_4(1)^{P + \Delta t}]\} T_s(1)^P - \frac{3}{4\Delta x^2} T_s(2)^P$$

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

$$- \frac{1}{6\Delta x^2} T_s(5)^P . \tag{5-51}$$

<u>At the pyrolysis zone (N = I).</u>- The boundary condition at the pyrolysis zone is

$$- \frac{1}{\ell} \left(k_s \frac{\partial T_s}{\partial x}\right)_{N = I} = \dot{m}_g \Delta H_p - \frac{1}{\ell'} \left(k_s' \frac{\partial T_s}{\partial x'}\right)_{N = I} . \tag{5-52}$$

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

$$\left(\frac{\partial^2 T_s}{\partial x^2}\right)_{N = I} = \frac{1}{6\Delta x} [11 \left(\frac{\partial T_s}{\partial x}\right)_{N = I} - 18 \left(\frac{\partial T_s}{\partial x}\right)_{N = I - 1}$$

$$+ 9 \left(\frac{\partial T_s}{\partial x}\right)_{N = I - 2} - 2 \left(\frac{\partial T_s}{\partial x}\right)_{N = I - 3}] . \tag{5-53}$$

Using this equation in the governing equation for char layer temperature and solving for the char layer temperature gradient at the pyrolysis zone gives

$$\left(\frac{\partial T_s}{\partial x}\right)_{N=1} = \frac{6}{11}\left[3\left(\frac{\partial T_s}{\partial x}\right)_{N=I-1} - \frac{3}{2}\left(\frac{\partial T_s}{\partial x}\right)_{N=I-2}\right.$$

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

$$- \alpha_2(I)\ \Delta x\ T_s(I) - \alpha_3(I)\ \Delta x$$

$$\left. - \alpha_4(I)\ \Delta x\ \frac{\partial T_s}{\partial t}_{N=I}\right] \quad . \tag{5-54}$$

The analogous expression for the uncharred layer temperature gradient is

$$\left(\frac{\partial T_s}{\partial x'}\right)_{N=I} = \frac{6}{11}\left[3\left(\frac{\partial T_s}{\partial x}\right)_{N=I+1} - \frac{3}{2}\left(\frac{\partial T_s}{\partial x}\right)_{N=I+2} + \frac{1}{3}\left(\frac{\partial T_s}{\partial x}\right)_{N=I+3}\right.$$

$$+ \alpha_1'(I)\ \Delta x'\left(\frac{\partial T_s}{\partial x}\right)_{N=I} + \alpha_2'(I)\ \Delta x'\ T_s(I)$$

$$\left. + \alpha_3'(I)\ \Delta x' + \alpha_4'(I)\ \Delta x'\left(\frac{\partial T_s}{\partial t}\right)_{N=I}\right] , \tag{5-55}$$

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

$$\left(\frac{\partial T_s}{\partial t}\right)_{N=I} = \frac{1}{\dfrac{\Delta x\ k_s(I)\alpha_4(I)}{\ell} + \dfrac{\Delta x'\ k_s'(I)\alpha_4'(I)}{\ell'}}\left\{\frac{k_s(I)}{\ell}\left[3\left(\frac{\partial T_s}{\partial x}\right)_{N=I-1}\right.\right.$$

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

$$- \alpha_3(I)\Delta x\Big] + \frac{11}{6}\dot{m}_g \Delta H_p - \frac{k_s'(I)}{\ell'}\left[3\left(\frac{\partial T_s}{\partial x}\right)_{N = I + 1} - \frac{3}{2}\left(\frac{\partial T_s}{\partial x}\right)_{N = I + 2}\right.$$

$$+ \frac{1}{3}\left(\frac{\partial T_s}{\partial x}\right)_{N = I + 3} + \alpha_1'(I)\Delta x'\left(\frac{\partial T_s}{\partial x'}\right)_I + \alpha_2'(I)\Delta x' T_s(I)$$

$$\left.+ \alpha_3'(I)\Delta x'\right]\Bigg\} \tag{5-56}$$

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

$$\left(\frac{\partial T_s}{\partial t}\right)_{N = I} = \frac{1}{\dfrac{k_s(I)\alpha_4(I)\Delta x}{\ell} + \dfrac{k_s'(I)\alpha_4'(I)\Delta x'}{\ell'}}\Bigg\{\frac{k_s(I)}{\ell}\Bigg[-\frac{1}{6\Delta x}T_s(I - 4)$$

$$+ \left(\frac{3}{4\Delta x} + \frac{\alpha_1(I)}{3}\right)T_s(I - 3) - \left(\frac{4}{3\Delta x} + \frac{3\alpha_1(I)}{2}\right)T_s(I - 2)$$

$$- \left(\frac{3}{4\Delta x} - 3\alpha_1(I)\right)T_s(I - 1)\Bigg] + \Bigg[\frac{k_s(1)}{\ell}\left(\frac{3}{2\Delta x} - \frac{11}{6}\alpha_1(I)\right.$$

$$\left.- \alpha_2(I)\Delta x\right) + \frac{k_s'(I)}{\ell'}\left(\frac{3}{2\Delta x} + \frac{11}{6}\alpha_1'(I) - \alpha_2'(I)\Delta x'\right)\Bigg]T_s(I)$$

$$+ \frac{11}{6}\dot{m}_g \Delta H_p - \frac{k_s(I)\alpha_3(I)\Delta x}{\ell} - \frac{k_s'(I)\alpha_3'(I)\Delta x'}{\ell}$$

$$- \frac{k_s'(I)}{\ell'}\Bigg[\left(\frac{3}{4\Delta x'} + 3\alpha_1'(I)\right)T_s(I + 1) + \left(\frac{4}{3\Delta x'} - \frac{3\alpha_1(I)}{2}\right)T_s(I + 2)$$

$$-\left(\frac{3}{4\Delta x'} - \frac{\alpha_1(I)}{3}\right)T_s(I + 3) + \frac{1}{6\Delta x'}T_s(I + 4)\Bigg]\Bigg\} \quad . \tag{5-57}$$

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

$$
\begin{aligned}
ZI_s\ T_s(I-4)^{P+\Delta t} &+ YI_s\ T_s(I-3)^{P+\Delta t} + XI_s\ T_s(I-2)^{P+\Delta t} \\
&+ AI_s\ T_s(I-1)^{P+\Delta t} + BI_s\ T_s(I)^{P+\Delta t} \\
&+ CI_s\ T_s(I+1)^{P+\Delta t} + EI_s\ T_s(I+2)^{P+\Delta t} \\
&+ FI_s\ T_s(I+3)^{P+\Delta t} + GI_s\ T_s(I+4)^{P+\Delta t} \\
&= DI_s
\end{aligned}
\tag{5-58}
$$

where

$$
ZI_s = \frac{-k_s(I)^{P+\Delta t}/(12\ \Delta x\ \ell^{P+\Delta t})}{\dfrac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \dfrac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{}}
\tag{5-59}
$$

$$
YI_s = \frac{k_s(I)^{P+\Delta t}\left[\dfrac{3}{4\Delta x} + \dfrac{\alpha_1(x)^{P+\Delta t}}{3}\right]/\ell^{P+\Delta t}}{2\left[\dfrac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \dfrac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]}
\tag{5-60}
$$

$$XI_s = \frac{-k_s(I)^{P+\Delta t}\left[\frac{4}{3\Delta x} + \frac{3\alpha_1(x)^{P+\Delta t}}{2}\right]/\ell^{P+\Delta t}}{2\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]} \tag{5-61}$$

$$AI_s = \frac{-k_s(I)^{P+\Delta t}\left[\frac{3}{4\Delta x} - 3\alpha_1(I)^{P+\Delta t}\right]/\ell^{P+\Delta t}}{2\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]} \tag{5-62}$$

$$BI_s = -\frac{1}{\Delta t} + \frac{1}{2\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell^{P+\Delta t}}\right]}$$

$$\left\{\frac{k_s(I)^{P+\Delta t}}{\ell^{P+\Delta t}}\left[\frac{3}{2\Delta x} - \frac{11}{6}\alpha_1(I)^{P+\Delta t} - \alpha_2(I)^{P+\Delta t}\Delta x\right]\right.$$

$$\left. + \frac{k_s'(I)^{P+\Delta t}}{\ell'^{P+\Delta t}}\left[\frac{3}{2\Delta x'} + \frac{11}{6}\alpha_1'(I)^{P+\Delta t} - \alpha_2'(I)^{P+\Delta t}\right]\right\} \tag{5-63}$$

$$CI_s = \frac{-k_s'(I)^{P+\Delta t}\left[\frac{3}{4\Delta x'} + 3\alpha_1'(I)^{P+\Delta t}\right]/\ell'^{P+\Delta t}}{2\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]} \tag{5-64}$$

$$EI_s = \frac{-k_s'(I)^{P+\Delta t}\left[\frac{4}{3\Delta x'} + 3\alpha_1'(I)^{P+\Delta t}\right]/\ell'^{P+\Delta t}}{2\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]} \tag{5-65}$$

$$FI_s = \frac{k_s'(I)^{P+\Delta t}\left[\frac{3}{4\Delta x'} - \frac{1}{3}\alpha_1'(I)^{P+\Delta t}\right]/\ell'^{P+\Delta t}}{2\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]} \tag{5-66}$$

$$GI_s = \frac{-k_s'(I)^{P+\Delta t}/(12\,\Delta x'\ell'^{P+\Delta t})}{\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]} \tag{5-67}$$

$$DI_s = \frac{1}{2\left[\frac{k_s(I)^{P+\Delta t}\alpha_4(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}} + \frac{k_s'(I)^{P+\Delta t}\alpha_4'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}}\right]}$$

$$\left[\frac{k_s(I)^{P+\Delta t}\alpha_3(I)^{P+\Delta t}\Delta x}{\ell^{P+\Delta t}}\right.$$

$$\left. + \frac{k_s'(I)^{P+\Delta t}\alpha_3'(I)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} - \frac{11}{6}\dot{m}_g^{P+\Delta t}\,\Delta H_p\right]$$

$$+ \frac{1}{2\left[\frac{k_s(I)^P\alpha_4(I)^P\Delta x}{\ell^P} + \frac{k_s'(I)^P\alpha_4'(I)^P\Delta x'}{\ell'^P}\right]}\left[\frac{k_s(I)^P\alpha_3(I)^P\Delta x}{\ell^P}\right.$$

$$\left. + \frac{k_s'(I)^P\alpha_3'(I)^P\Delta x'}{\ell'^P} - \frac{11}{6}\dot{m}_g^P\,\Delta H_p\right]$$

$$- \frac{k_s(I)^P/\ell^P}{2\left[\frac{k_s(I)^P\alpha_4(I)^P\Delta x}{\ell^P} + \frac{k_s'(I)^P\alpha_4'(I)^P\Delta x'}{\ell'^P}\right]}\left\{-\frac{1}{6\Delta x}T_s(I-4)^P\right.$$

$$+\left[\frac{3}{4\Delta x}+\frac{\alpha_1(I)^P}{3}\right]T_s(I-3)^P-\left[\frac{4}{3\Delta x}+\frac{3}{2}\,\alpha_1(I)^P\right]T_s(I-2)^P$$

$$-\left[\frac{3}{4\Delta x}-3\alpha_1(I)^P\right]T_s(I-1)^P\Bigg\}$$

$$-\Bigg[\frac{1}{2\left[\frac{k_s(I)^P\alpha_4(I)^P\Delta x}{\ell^P}+\frac{k_s'(I)^P\alpha_4'(I)^P\Delta x'}{\ell'^P}\right]}\Bigg\{\frac{k_s(I)^P}{\ell^P}\Bigg[\frac{3}{2\Delta x}$$

$$-\frac{11}{6}\,\alpha_1(I)^P-\alpha_2(I)^P\Delta x\Bigg]+\frac{k_s'(I)^P}{\ell'^P}\Bigg[\frac{3}{2\Delta x'}+\frac{11}{6}\,\alpha_1'(I)^P$$

$$-\alpha_2'(I)^P\Delta x'\Bigg]\Bigg\}+\frac{1}{\Delta t}\Bigg]T_s(I)^P$$

$$+\frac{k_s'(I)^P/\ell'^P}{2\left[\frac{k_s(I)^P\alpha_4(I)^P\Delta x}{\ell^P}+\frac{k_s'(I)^P\alpha_4'(I)^P\Delta x'}{\ell'^P}\right]}\Bigg\{\Bigg[\frac{3}{4\Delta x'}$$

$$+3\alpha_1'(I)^P\Bigg]T_s(I+1)^P+\left[\frac{4}{3\Delta x'}-\frac{3}{2}\,\alpha_1'(I)^P\right]T_s(I+2)^P$$

$$-\left[\frac{3}{4\Delta x'}-\frac{1}{3}\,\alpha_1'(I)^P\right]T_s(I+3)^P+\frac{1}{6\Delta x'}\,T_s(I+4)^P\Bigg\} \qquad (5\text{-}68)$$

<u>At the uncharred material - insulation interface (N = I + J)</u>.- The boundary condition at the interface of the uncharred material and the insulation is

$$- \frac{1}{\ell'} \left(k_s' \frac{\partial T_s}{\partial x'} \right)_{N = I + J} = - \frac{1}{\ell''} \left(k_s'' \frac{\partial T_s}{\partial x''} \right)_{N = I + J}$$

$$+ \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \left(\frac{\partial T_s}{\partial t} \right)_{N = I + J} . \tag{5-69}$$

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

$$ZP_s \; T_s(I + J - 4)^{P + \Delta t} + YP_s \; T_s(I + J - 3)^{P + \Delta t}$$

$$+ XP_s \; T_s(I + J - 2)^{P + \Delta t} + AP_s \; T_s(I + J - 1)^{P + \Delta t}$$

$$+ BP_s \; T_s(I + J)^{P + \Delta t} + CP_s \; T_s(I + J + 1)^{P + \Delta t}$$

$$+ EP_s \; T_s(I + J + 2)^{P + \Delta t} + FP_s \; T_s(I + J + 3)^{P + \Delta t}$$

$$+ GP_s \; T_s(I + J + 4)^{P + \Delta t} = DP_s \tag{5-70}$$

where

$$ZP_s = \frac{k_s'(I+J)^{P+\Delta t}/(12 \; \Delta' \ell'^{P+\Delta t})}{\left[\frac{k_s'(I+J)^{P+\Delta t} \alpha_4'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_4''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]} \tag{5-71}$$

$$YP_s = \frac{k_s'(I+J)^{P+\Delta t}/\ell'^{P+\Delta t}\left[\frac{3}{4\Delta x'} + \alpha_1'(I+J)^{P+\Delta t}/3\right]}{2\left[\frac{k_s'(I+J)^{P+\Delta t}\alpha_4'(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t}\alpha_4''(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]} \tag{5-72}$$

$$XP_s = \frac{-k_s'(I+J)^{P+\Delta t}/\ell'^{P+\Delta t}\left[\frac{4}{3\Delta x'} + \frac{3}{2}\alpha_1'(I+J)^{P+\Delta t}\right]}{2\left[\frac{k_s'(I+J)^{P+\Delta t}\alpha_4'(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t}\alpha_4''(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]} \tag{5-73}$$

$$AP_s = \frac{-k_s'(I+J)^{P+\Delta t}/\ell'^{P+\Delta t}\left[\frac{3}{4\Delta x'} - 3\alpha_1'(I+J)^{P+\Delta t}\right]}{2\left[\frac{k_s'(I+J)^{P+\Delta t}\alpha_4'(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s'(I+J)^{P+\Delta t}\alpha_4''(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]} \tag{5-74}$$

$$BP_s = \frac{1}{2\left[\frac{k_s'(I+J)^{P+\Delta t}\alpha_4'(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t}\alpha_4''(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

$$\left\{\frac{k_s'(I+J)^{P+\Delta t}}{\ell'^{P+\Delta t}}\left[\frac{3}{2\Delta x'} - \frac{11}{6}\alpha_1'(I+J)^{P+\Delta t} - \alpha_2'(I+J)^{P+\Delta t}\Delta x'\right] + \frac{k_s''(I+J)^{P+\Delta t}}{\ell''^{P+\Delta t}}\left[\frac{3}{2\Delta x''} + \frac{11}{6}\alpha_1''(I+J)^{P+\Delta t} - \alpha_2''(I+J)^{P+\Delta t}\Delta x''\right]\right\} - \frac{1}{\Delta t} \tag{5-75}$$

$$CP_s = \frac{-k''_s(I+J)^{P+\Delta t}/\ell''^{P+\Delta t}\left[\frac{3}{4\Delta x''} + 3\alpha''_1(I+J)^{P+\Delta t}\right]}{2\left[\frac{k'_s(I+J)^{P+\Delta t}\alpha'_4(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k''_s(I+J)^{P+\Delta t}\alpha''_4(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

(5-76)

$$EP_s = \frac{-k''_s(I+J)^{P+\Delta t}/\ell''^{P+\Delta t}\left[\frac{4}{3\Delta x''} - \frac{3}{2}\alpha''_1(I+J)^{P+\Delta t}\right]}{2\left[\frac{k'_s(I+J)^{P+\Delta t}\alpha'_4(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k''_s(I+J)^{P+\Delta t}\alpha''_4(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

(5-77)

$$FP_s = \frac{k''_s(I+J)^{P+\Delta t}/\ell''^{P+\Delta t}\left[\frac{3}{4\Delta x''} - \frac{1}{3}\alpha''_1(I+J)^{P+\Delta t}\right]}{2\left[\frac{k'_s(I+J)^{P+\Delta t}\alpha'_4(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k''_s(I+J)^{P+\Delta t}\alpha''_4(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

(5-78)

$$GP_s = \frac{-k''_s(I+J)^{P+\Delta t}/(12\ \Delta x''\ell''^{P+\Delta t})}{\left[\frac{k'_s(I+J)^{P+\Delta t}\alpha'_4(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k''_s(I+J)^{P+\Delta t}\alpha''_4(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HE}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

(5-79)

$$DP_s = \frac{\left[k'_s(I+J)^{P+\Delta t}\alpha'_3(I+J)^{P+\Delta t}\ \Delta x'/\ell'^{P+\Delta t} + k''_s(I+J)^{P+\Delta t}\alpha''_3(I+J)^{P+\Delta t}\ \Delta x''/\ell''^{P+\Delta t}\right]}{2\left[\frac{k'_s(I+J)^{P+\Delta t}\alpha'_4(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k''_s(I+J)^{P+\Delta t}\alpha''_4(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

$$- \frac{k'_s\ (I+J)^{P}/\ell'^{P}}{2\left[\frac{k'_s(I+J)^{P+\Delta t}\alpha'_4(I+J)^{P+\Delta t}\Delta x'}{\ell'^{P+\Delta t}} + \frac{k''_s(I+J)^{P+\Delta t}\alpha''_4(I+J)^{P+\Delta t}\Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

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

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

$$-\left[\frac{1}{2\left[\frac{k_s'(I+J)^P\alpha_4'(I+J)^P\Delta x'}{\ell'^P} + \frac{k_s''(I+J)^P\alpha_4''(I+J)^P\Delta x''}{\ell''^P} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]} \right.$$

$$\left\{ \frac{k_s'(I+J)^P}{\ell'^P}\left[\frac{3}{2\Delta x'} - \frac{11}{6}\alpha_1'(I+J)^P - \alpha_2'(I+J)^P\Delta x'\right] + \frac{k_s''(I+J)^P}{\ell''^P}\left[\frac{3}{2\Delta x''}\right.\right.$$

$$\left.\left. + \frac{11}{6}\alpha_1''(I+J)^P - \alpha_2''(I+J)^P\Delta x''\right]\right\} + \left.\frac{1}{\Delta t}\right] T_s(I+J)^P$$

$$+ \frac{k_s''(I+J)^P/\ell''^P}{2\left[\frac{k_s'(I+J)^P\alpha_4'(I+J)^P\Delta x'}{\ell'^P} + \frac{k_s''(I+J)^P\alpha_4''(I+J)^P\Delta x''}{\ell''^P} - \rho_{HS}\hat{C}_{P_{HS}}\ell_{HS}\right]}$$

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

$$\left. -\left[\frac{3}{4\Delta x''} - \frac{1}{3}\alpha_1''(I+J)^P\right] T_s(I+J+3)^P + \frac{1}{6\Delta x''} T_s(I+J+4)^P \right\} . \qquad (5\text{-}80)$$

<u>At the back surface (N = I + J + K)</u>.- The back surface boundary condition is

$$-\frac{1}{\ell''}\left(k_s''\ \frac{\partial T_s}{\partial x''}\right)_{N = I+J+K} = \sigma\,\varepsilon_s''\,T_s(I+J+K)^4$$

$$- q_B + \rho_{HSP}\hat{C}_{P_{HSP}}\ell_{HSP}\left(\frac{\partial T_s}{\partial t}\right)_{N = I+J+K} . \qquad (5\text{-}81)$$

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

$$ZZ_s\ T_s(I + J + K - 4)^{P + \Delta t} + YZ_s\ T_s(I + J + K - 3)^{P + \Delta t}$$

$$+ XZ_s\ T_s(I + J + K - 2)^{P + \Delta t} + AZ_s\ T_s(I + J + K - 1)^{P + \Delta t}$$

$$+ BZ_s\ T_s(I + J + K)^{P + \Delta t} = DZ_s \tag{5-82}$$

where

$$ZZ_s = \frac{k_s''(I+J+K)^{P+\Delta t}/(12\ \Delta x''^2 \ell'')}{\left[\rho_{HSP}\hat{C}_{P_{HSP}}\ell_{HSP}\ [\alpha_1''(I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}\ ] - \alpha_4''\ \frac{\alpha_4''(I+J+K)^{P+\Delta t}k_s''(I+J+K)^{P+\Delta t}}{\ell''}\right]} \tag{5-83}$$

$$YZ_s = -4.5\ ZZ_s \tag{5-84}$$

$$XZ_s = 8\ ZZ_s \tag{5-85}$$

$$AZ_s = -\ YZ_s \tag{5-86}$$

$$BZ_s = [6\alpha_2''(I+J+K)^{P+\Delta t}\Delta x''^2 - 9]\ ZZ_s - \frac{1}{\Delta t}$$

$$- \frac{\sigma\ \varepsilon''_s\ [T_s(I+J+K)^{P+\Delta t}]^3\ [\alpha''_1(I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}]}{2\left\{\rho_{HSP}\hat{C}_{P_{HSP}}\ \ell_{HSP}\left[\alpha''_1(I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}\right] - \frac{\alpha''_4(I+J+K)^{P+\Delta t}k''_s(I+J+K)^{P+\Delta t}}{\ell''}\right\}} \tag{5-87}$$

$$DZ_s = - \frac{\alpha''_1(I+J+K)^{P+\Delta t} + 11/6\Delta x''}{2\left\{\rho_{HSP}\hat{C}_{P_{HSP}}\ \ell_{HSP}[\alpha''_1(I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}] - \frac{\alpha''_4(I+J+K)^{P+\Delta t}k''_s(I+J+K)^{P+\Delta t}}{\ell''}\right\}}$$

$$\left\{q_B^{P+\Delta t} + \frac{\alpha''_3(I+J+K)^{P+\Delta t}\ k''_s(I+J+K)^{P+\Delta t}/\ell''}{\alpha''_1(I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}}\right\}$$

$$- \frac{\alpha''_1(I+J+K)^{P} + 11/6\Delta x''}{2\left\{\rho_{HSP}\hat{C}_{P_{HSP}}\ \ell_{HSP}[\alpha''_1(I+J+K)^{P} + \frac{11}{6\Delta x''}] - \frac{\alpha''_4(I+J+K)^{P}k''_s(I+J+K)^{P}}{\ell''}\right\}}$$

$$\left[q_B^P + \frac{\alpha''_3(I+J+K)^P k''_s(I+J+K)^P/\ell''}{\alpha''_1(I+J+K)^P + 11/6\Delta x''} + \frac{k''_s(I+J+K)^P/\ell''}{\alpha''_1(I+J+K)^P + 11/6\Delta x''}\right.$$

$$\left\{\frac{1}{6\Delta x''^2}\ T_s(I+J+K)^P - \frac{3}{4\Delta x''^2}\ T_s(I+J+K-3)^P + \frac{4}{3\Delta x''^2}\ T_s(I+J+K-2)^P\right.$$

$$\left. + \frac{3}{4\Delta x''^2}\ T_s(I+J+K-1)^P - \left[\frac{3}{2\Delta x''^2} - \alpha''_2(I+J+K)^P\right] T_s(I+J+K)^P\right\}$$

$$\left. - \sigma\ \varepsilon''_s\ [T_s(I+J+K)^P]^4\right] - \frac{1}{\Delta t}\ T_s(I+J+K)^P.. \tag{5-88}$$

Char Layer Porosity Equation

The differential equation for the char layer porosity is

$$\frac{\partial \eta}{\partial x} + \varepsilon_1 \eta + \varepsilon_2 + \varepsilon_3 \frac{\partial \eta}{\partial t} = 0 \ . \tag{5-89}$$

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

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

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

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

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

which is accurate to terms of the order Δx^2.

Combining Eqs. 5-89 and 5-92 gives

$$[\varepsilon_1(N) - \frac{3}{2\Delta x}]\eta(N) + \frac{2}{\Delta x}\eta(N+1) - \frac{1}{2\Delta x}\eta(N+2)$$

$$+ \varepsilon_2(N) + \varepsilon_3(N)\left(\frac{\partial\eta}{\partial t}\right)_N = 0 \qquad (5\text{-}93)$$

which yields the following modified implicit finite difference equation.

$$B(N)\ \eta(N)^{P+\Delta t} + C(N)\ \eta(N+1)^{P+\Delta t} + E(N)\ \eta(N+2)^{P+\Delta t}$$

$$= D(N) \qquad (5\text{-}94)$$

where

$$B(N) = \frac{1}{2\Delta t}\ [\varepsilon_3(N)^P + \varepsilon_3(N)^{P+\Delta t}]$$

$$+ \frac{1}{2}\ [\varepsilon_1(N)^{P+\Delta t} - \frac{3}{2\Delta x}] \qquad (5\text{-}95)$$

$$C(N) = \frac{1}{\Delta x} \qquad (5\text{-}96)$$

$$E(N) = -\frac{1}{4\Delta x} \qquad (5\text{-}97)$$

$$D(N) = -\frac{1}{2}\,[\varepsilon_2(N)^P + \varepsilon_2(N)^{P+\Delta t}]$$

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

$$-\frac{1}{\Delta x}\,\eta(N+1)^P + \frac{1}{4\Delta x}\,\eta(N+2)^P\,. \qquad (5\text{-}98)$$

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:

$$\left(\frac{\partial\eta}{\partial x}\right)_{N = I - 1} = \frac{\eta(I) - \eta(I - 1)}{\Delta x} \qquad (5\text{-}99)$$

which is accurate to terms of the order Δx. The resulting modified implicit finite difference equation for station $I - 1$ is

$$B(I - 1)\eta(I - 1)^{P+\Delta t} + C(I - 1)\eta(I)^{P+\Delta t} = D(I - 1) \qquad (5\text{-}100)$$

where

$$B(I - 1) = \frac{1}{\Delta t} [\varepsilon_3(I - 1)^P + \varepsilon_3(I - 1)^{P+\Delta t}] + \varepsilon_1(I - 1)^{P+\Delta t} - \frac{1}{\Delta x} \tag{5-101}$$

$$C(I - 1) = \frac{1}{\Delta x} \tag{5-102}$$

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

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

$$- \frac{1}{\Delta x} \eta(I)^P \ . \tag{5-103}$$

The single boundary condition for char layer porosity equation is

$$\eta(I) = \eta_I \quad . \tag{5-104}$$

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

$$\frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 \ . \tag{5-105}$$

The single boundary condition for this equation is

$$T(I) = T_s(I) \ . \tag{5-106}$$

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 $1 \leq N \leq I - 2$

$$B(N)\ T(N)^{P + \Delta t} + C(N)\ T(N + 1)^{P + \Delta t} + E(N)\ T(N + 2)^{P + \Delta t}$$

$$= D(N) \tag{5-107}$$

where

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

$$C(N) = \frac{1}{\Delta x} \tag{5-109}$$

$$E(N) = -\frac{1}{4\Delta x} \tag{5-110}$$

$$D(N) = -\frac{1}{2}\ [\beta_2(N)^P + \beta_2(N)^{P + \Delta t}] - \frac{1}{2}\ \{\beta_1(N)^P - \frac{3}{2\Delta x}$$

$$- \frac{1}{\Delta t}\ [\beta_3(N)^P + \beta_3(N)^{P + \Delta t}]\}T(N)^P - \frac{1}{\Delta x}\ T(N + 1)^P + \frac{1}{4\Delta x}\ T(N + 2)^P$$

(5-111)

and, for $N = I - 1$,

$$B(I - 1)\ T(I - 1)^{P + \Delta t} + C(I - 1)\ T(I)^{P + \Delta t} = D(I - 1) \qquad (5\text{-}112)$$

where

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

$$+ \beta_1(I - 1)^{P + \Delta t} - \frac{1}{\Delta x} \qquad (5\text{-}113)$$

$$C(I - 1) = \frac{1}{\Delta x} \qquad (5\text{-}114)$$

$$D(I - 1) = - [\beta_2(I - 1)^P + \beta_2(I - 1)^{P + \Delta t}] - \{\beta_1(I - 1)^P$$

$$- \frac{1}{\Delta x} - \frac{1}{\Delta t}\ [\beta_3(I - 1)^P + \beta_3(I - 1)^{P + \Delta t}]\}\ T(I - 1)^P$$

$$- \frac{1}{\Delta x}\ T(I)^P\ . \qquad (5\text{-}115)$$

The equation applied at $N = I$ is

$$T(I) = T_s(I)\ . \qquad (5\text{-}116)$$

Pyrolysis Gas Pressure Equation

The differential equation for the pyrolysis gas pressure is

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

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

$$A_P(N)\ P^2(N - 1)^{P + \Delta t} + B_P(N)\ P^2(N)^{P + \Delta t}$$

$$+ C_P(N)\ P^2(N + 1)^{P + \Delta t} = D_P(N) \tag{5-118}$$

where

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

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

$$C_P(N) = \frac{1}{\Delta x^2} + \frac{\gamma_1(N)^{P + \Delta t}}{2\Delta x} \tag{5-121}$$

$$D_P(N) = -\gamma_3(N)^P - \gamma_3(N)^P + \Delta t \left[\frac{1}{\Delta x^2} - \frac{\gamma_1(N)^P}{2\Delta x}\right] P^2(N-1)^P$$

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

$$- \left[\frac{1}{\Delta x^2} + \frac{\gamma_1(N)^P}{2\Delta x}\right] P^2(N+1)^P \quad . \tag{5-122}$$

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

$$P(1) = P_w \tag{5-123}$$

or

$$P^2(1) = P_w^2 \tag{5-124}$$

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 -

$$\left(\frac{\partial P^2}{\partial x}\right)_{N=I} = 2\, R_u\, \ell \left(\frac{\mu T}{K\bar{M}}\right)_{N=I} \dot{m}_g \quad . \tag{5-125}$$

The second order derivative of Eq. 5-117 is written as the first derivative of the gradient of P^2,

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

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 $N = I - 1$, $N = 1 - 2$, and $N = I - 3$. Thus

$$\left(\frac{\partial^2 P^2}{\partial x^2}\right)_{N = I} = \frac{1}{6\Delta x}\left[11\left(\frac{\partial P^2}{\partial x}\right)_{N = I} - 18\left(\frac{\partial P^2}{\partial x}\right)_{N = I - 1}\right.$$

$$\left. + 9\left(\frac{\partial P^2}{\partial x}\right)_{N = I - 2} - 2\left(\frac{\partial P^2}{\partial x}\right)_{N = I - 3}\right] \quad . \tag{5-127}$$

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

$$\left[\frac{11}{6\Delta x} + \gamma_1(I)\right]\left(\frac{\partial P^2}{\partial x}\right)_{N = I} - \frac{3}{\Delta x}\left(\frac{\partial P^2}{\partial x}\right)_{N = I - 1} + \frac{3}{2\Delta x}\left(\frac{\partial P^2}{\partial x}\right)_{N = I - 2}$$

$$- \frac{1}{3\Delta x}\left(\frac{\partial P^2}{\partial x}\right)_{N = I - 3} + \gamma_2(I)\, P^2(I) + \gamma_3(I)$$

$$+ \gamma_4(I)\left(\frac{\partial P^2}{\partial t}\right)_{N = I} = 0 \quad . \tag{5-128}$$

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

$$\frac{1}{6\Delta x^2} P^2(I-4) - \frac{3}{4\Delta x^2} P^2(I-3) + \frac{4}{3\Delta x^2} P^2(I-2)$$

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

$$+ \left[\frac{11}{6\Delta x} + \gamma_1(I)\right] 2 \ell R_u \left(\frac{\mu T}{K\bar{M}}\right)_{N=I} \dot{m}_g$$

$$+ \gamma_4(I) \left(\frac{\partial P^2}{\partial t}\right)_{N=I} = 0 \quad . \tag{5-129}$$

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,

$$PX\ P^2(I-4)^{P+\Delta t} + PY\ P^2(I-3)^{P+\Delta t} + PZ\ P^2(I-2)^{P+\Delta t}$$

$$+ AP\ P^2(I-1)^{P+\Delta t} + BP\ P^2(I)^{P+\Delta t}$$

$$= DP \tag{5-130}$$

where

$$PX = \frac{1}{12\Delta x^2} \tag{5-131}$$

$$PY = -\frac{3}{8\Delta x^2} \tag{5-132}$$

$$PZ = \frac{3}{3\Delta x^2} \tag{5-133}$$

$$AP = - PY \tag{5-134}$$

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

$$- \frac{3}{2\Delta x^2}] \tag{5-135}$$

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

$$\left. + \gamma_1(I)^P \right] R_u \ell^P \dot{m}_g^P \left(\frac{\mu T}{K\bar{M}} \right)^P_{N = I}$$

$$- \left[\frac{11}{6\Delta x} + \gamma_1(I)^{P+\Delta t} \right] R_u \ell^{P+\Delta t} \dot{m}_g^{P+\Delta t} \left(\frac{\mu T}{K\bar{M}} \right)^{P+\Delta t}_{N = I}$$

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

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

$$+ \gamma_4(I)^{P + \Delta t}]\} P^2(I)^P \quad . \tag{5-136}$$

Chemical Species Conservation Equation

The differential equation for conservation of chemical species is

$$\frac{\partial}{\partial x} \dot{m}_i + \Delta_{1_i} \dot{m}_i + \Delta_{2_i} + \Delta_{3_i} \frac{\partial \dot{m}_i}{\partial t} = 0 \cdot \tag{5-137}$$

The single boundary condition for this equation is

$$(\dot{m}_i)_{N = I} = - M_i \left(\frac{x_i}{\eta \bar{M}}\right)_{N = I} \dot{m}_g \quad . \tag{5-138}$$

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

$$B_i(N)\ \dot{m}_i(N)^{P + \Delta t} + C_i(N)\ \dot{m}_i(N + 1)^{P + \Delta t}$$

$$+ E_i(N)\ \dot{m}_i(N + 2)^{P + \Delta t} = D_i(N) \tag{5-139}$$

for $1 \leq N \leq I - 2$

where

$$B_i(N) = \frac{1}{2\Delta t}\ [\Delta_{1_i}(N)^P + \Delta_{1_i}(N)^{P + \Delta t}]$$

$$+ \frac{1}{2}\ [\Delta_{1_i}(N)^{P + \Delta t} - \frac{3}{2\Delta x}\ ] \tag{5-140}$$

$$C_i(N) = \frac{1}{\Delta x} \tag{5-141}$$

$$E_i(N) = - \frac{1}{4\Delta x} \tag{5-142}$$

$$D_i(N) = -\frac{1}{2}\,[\Delta_{2_i}(N)^P + \Delta_{2_i}(N)^{P+\Delta t}]$$

$$-\frac{1}{2}\,\{\Delta_{1_i}(N)^P - \frac{3}{2\Delta x} - \frac{1}{\Delta t}\,[\Delta_{3_i}(N)^P$$

$$+ \Delta_{3_i}(N)^{P+\Delta t}]\}\,\dot{m}_i(N)^P - \frac{1}{\Delta x}\,\dot{m}_i(N+1)^P$$

$$+ \frac{1}{4\Delta x}\,\dot{m}_i(N+2)^P \tag{5-143}$$

and, for $N = I - 1$,

$$B_i(I-1)\dot{m}_i(I-1)^{P+\Delta t} + C_i(I-1)\dot{m}_i(I)^{P+\Delta t} = D_i(I-1) \tag{5-144}$$

where

$$B_i(I-1) = \frac{1}{\Delta t}\,[\Delta_{3_i}(I-1)^P + \Delta_{3_i}(I-1)^{P+\Delta t}]$$

$$+ \Delta_{1_i}(I-1)^{P+\Delta t} - \frac{1}{\Delta x} \tag{5-145}$$

$$C_i(I-1) = \frac{1}{\Delta x} \tag{5-146}$$

$$D_i(I-1) = -\Delta_{2_i}(I-1)^P - \Delta_{2_i}(I-1)^{P+\Delta t} - \{\Delta_{1_i}(I-1)^P$$

$$-\frac{1}{\Delta x} - \frac{1}{\Delta t}\,[\Delta_{3_i}(I-1)^P + \Delta_{3_i}(I-1)^P]\}\dot{m}_i(I-1)^P - \frac{1}{\Delta x}\,\dot{m}_i(I)^P \tag{5-147}$$

and, for $N = I$,

$$\dot{m}_i(I) = - M_i \left(\frac{x_i}{\eta \bar{M}}\right)_{N = I} \dot{m}_g \cdot \tag{5-148}$$

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):

$$B1_s \; T_s(1)^{P + \Delta t} + C1_s \; T_s(2)^{P + \Delta t} + G1_s \; T_s(3)^{P + \Delta t}$$

$$+ H1_s \; T_s(4)^{P + \Delta t} + I1_s \; T_s(5)^{P + \Delta t} = D1_s \qquad (6\text{-}1)$$

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

$$A_s(N) \; T_s(N - 1)^{P + \Delta t} + B_s(N) \; T_s(N)^{P + \Delta t} + C_s(N) \; T_s(N + 1)^{P + \Delta t} = D_s(N). \qquad (6\text{-}2)$$

At the pyrolysis zone (N = I):

$$ZI_s\ T_s(I-4)^{P+\Delta t} + YI_s\ T_s(I-3)^{P+\Delta t} + XI_s\ T_s(I-2)^{P+\Delta t}$$

$$+ A_s(I)\ T_s(I-1)^{P+\Delta t} + B_s(I)\ T_s(I)^{P+\Delta t} + C_s(I)\ T_s(I+1)^{P+\Delta t}$$

$$+ EI_s\ T_s(I+2)^{P+\Delta t} + FI_s\ T_s(I+3)^{P+\Delta t} + GI_s\ T_s(I+4)^{P+\Delta t}$$

$$= D_s(I) \qquad (6\text{-}3)$$

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

$$A_s(N)\ T_s(N-1)^{P+\Delta t} + B_s(N)\ T_s(N)^{P+\Delta t} + C_s(N)\ T_s(N+1)^{P+\Delta t} = D_s(N) \qquad (6\text{-}4)$$

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

$$ZP_s\ T_s(I+J-4)^{P+\Delta t} + YP_s\ T_s(I+J-3)^{P+\Delta t} + XP_s\ T_s(I+J-2)^{P+\Delta t}$$

$$+ AP_s\ T_s(I+J-1)^{P+\Delta t} + BP_s\ T_s(I+J)^{P+\Delta t}$$

$$+ CP_s\ T_s(I+J+1)^{P+\Delta t} + EP_s\ T_s(I+J+2)^{P+\Delta t}$$

$$+ FP_s\ T_s(I+J+3)^{P+\Delta t} + GP_s\ T_s(I+J+4)^{P+\Delta t}$$

$$= D_s(I+J) \qquad (6\text{-}5)$$

Within the insulation layer $(I + J < N < I + J + K)$:

$$A_s(N)\ T_s(N - 1)^{P + \Delta t} + B_s(N)\ T_s(N)^{P + \Delta t} + C_s(N)\ T_s(N + 1)^{P + \Delta t} = D_s(N) \tag{6-6}$$

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

$$ZZ_s\ T_s(I + J + K - 4)^{P + \Delta t} + YZ_s\ T_s(I + J + K - 3)^{P + \Delta t}$$

$$+ XZ_s\ T_s\ (I + J + K - 2)^{P + \Delta t} + Az_s\ T_s\ (I + J + K - 1)^{P + \Delta t}$$

$$+ Bz_s\ T_s\ (I + J + K)^{P + \Delta t} = Dz_s\ . \tag{6-7}$$

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

$$\left.\begin{array}{ll}
B_s(1)\ T_s(1)^{P+\Delta t} + C_s(1)\ T_s(2)^{P+\Delta t} = D_s(1) & N = 1 \\
A_s(N)\ T_s(N-1)^{P+\Delta t} + B_s(N)\ T_s(N)^{P+\Delta t} & \\
\quad + C_s(N)\ T_s(N+1)^{P+\Delta t} = D_s(N) & 1 < N < I + J + K \\
A_s(I + J + K)\ T_s(I + J + K - 1)^{P+\Delta t} + B_s(I + J + K) & \\
\quad T_s(I + K + K)^{P+\Delta t} = D_s(I + J + K) & N = I + J + K
\end{array}\right\} \quad (6\text{-}8)$$

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

$$\left.\begin{array}{ll}
W(1) = B_s(1) & \\
W(N) = B_s(N) - A_s(N)\ B(N-1) & 2 \leq N \leq I + J + K \\
B(N) = C_s(N)/W(N) & 1 \leq N \leq I + J + K - 1
\end{array}\right\} \quad (6\text{-}9)$$

and

$$\left.\begin{aligned} G(1) &= D_s(1)/W(1) \\ G(N) &= [D_s(N) - A_s(N)\ G(N-1)]/W(N) \quad 2 \le N \le I + J + K. \end{aligned}\right\} \quad (6\text{-}10)$$

The solution is

$$\left.\begin{aligned} T_s(I + J + K)^{P + \Delta t} &= G(I + J + K) \\ T_s(N)^{P + \Delta t} &= G(N) - B(N)\ T_s(N + 1)^{P + \Delta t} \quad 1 \le N \le I + J + K - 1. \end{aligned}\right\} \quad (6\text{-}11)$$

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

$$\left.\begin{aligned} B(N)\ T(N)^{P + \Delta t} + C(N)\ T(N + 1)^{P + \Delta t} + E(N)\ T(N + 2)^{P + \Delta t} &= D(N) \qquad 1 \le N \le I - 2 \\ B(I - 1)\ T(I - 1)^{P + \Delta t} + C(I - 1)\ T(I)^{P + \Delta t} &= D(I - 1) \\ T(I)^{P + \Delta t} &= T_s(I)^{P + \Delta t} \ . \end{aligned}\right\} \quad (6\text{-}12)$$

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

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

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

$$\int_a^b \frac{\partial}{\partial x}(\dot{m})\ dx = \ell \int_a^b \left[\frac{\partial}{\partial t}(\eta\rho) - \eta \sum_i R_{T_i} M_i - V_c \frac{\partial}{\partial x}(\eta\rho)\right] dx\ . \quad (6\text{-}14)$$

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

$$\dot{m}_b = \dot{m}_a + \ell \int_a^b \left[\frac{\partial}{\partial t}(\eta\rho) - \eta \sum_i R_{T_i} M_i - V_c \frac{\partial}{\partial x}(\eta\rho)\right] dx\ . \quad (6\text{-}15)$$

If the lower limit of integration is station N and the upper limit is the pyrolysis zone (N = I), Eq. 6-14 becomes

$$\dot{m}(N) = \dot{m}(I) - \ell \int_{x(N)}^{I} \left[\frac{\partial}{\partial t} (\eta\rho) - \eta \sum_i R_{T_i} M_i \right] dx$$

$$+ \int_{x(N)}^{I} V_c \frac{\partial}{\partial x} (\eta\rho)\, dx \,. \tag{6-16}$$

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

$$\dot{m}(N) = \dot{m}(I) - \ell \int_{x(N)}^{I} \left[\frac{\partial}{\partial t} (\eta\rho) - \eta \sum_i R_{T_i} M_i \right] dx$$

$$+ V_c(I)\, \eta(I)\, \rho(I) - V_c(N)\, \eta(N)\, \rho(N)$$

$$- (\dot{m}_g/\Delta\rho - \dot{m}_s/\rho_{s_o}) \int_{x(N)}^{I} \eta\, \rho\, dx. \tag{6-17}$$

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: $aA + bB + \ldots \underset{k_r}{\overset{k_F}{\rightleftarrows}} nN + oO + \ldots$)

$k = A \exp(-B/T)$

	Reaction	Type	Rate law	Frequency factor, A	Activation energy, B °K
1.	$CH_4 \rightarrow \frac{1}{2} C_2H_6 + \frac{1}{2} H_2$	Homogeneous	$k_F A$	7.6×10^{14}	4.775×10^4
2.	$C_2H_6 \rightarrow C_2H_4 + H_2$	Homogeneous	$k_F A$	3.14×10^{15}	3.019×10^4
3.	$C_2H_4 \rightarrow C_2H_2 + H_2$	Homogeneous	$k_F A$	2.57×10^8	1.157×10^5
4.	$C_2H_2 \rightarrow 2C + H_2$	Homogeneous	$k_F A^2$	2.14×10^{10}	2.009×10^4
5.	$C_6H_6 \rightarrow 6C + 3H_2$	Homogeneous	$k_F A$	1.4×10^{11}	2.622×10^4
6.	$C + CO_2 \rightarrow 2CO$	Heterogeneous	$k_F B$	1.2×10^{12}	4.282×10^4
7.	$C + H_2O \rightarrow CO + H_2$	Heterogeneous	$k_F B$	9.26×10^3	3.524×10^4
8.	$NH_3 \rightarrow \frac{1}{2} N_2 + 1.5H_2$	Homogeneous	$k_F A$	2.86×10^6	3.055×10^4
9.	$NH_3 + C \rightarrow HCN + H_2$	Heterogeneous	$k_F A$	8.78×10^6	3.885×10^4

Table 2.- Thermophysical Properties of Low-Density Phenolic-Nylon Ablation Material (Dow and Bush, Ref. 38).

Char

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

Uncharred Material

Pyrolysis kinetics -	
Specific reaction rate constant, kg/m^2-sec-atm	7.74×10^6
Activation energy, ^oK	1.289×10^4
Effective heat of pyrolysis, J/kg	1.28×10^6
Specific heat, J/kg-^oK, at temperature of -	
311^oK	1.51×10^3
367^oK	1.80×10^3
423^oK	2.07×10^3
478^oK	2.24×10^3
533^oK	2.28×10^3
589^oK	2.28×10^3
Thermal conductivity, W/m-^oK, at temperature of -	
300^oK	0.080
390^oK	0.084
500^oK	0.088
610^oK	0.092
710^oK	0.094

Table 2.- Concluded

Initial composition of pyrolysis gases - mole fraction of chemical species at pyrolysis zone -

CH_4	0.0
H_2	0.294
C_2H_4	0.0
C_2H_2	0.0
CO	0.59
H_2O	0.0
NH_3	0.0
N_2	0.009
CO_2	0.0
HCN	0.0
C_2H_6	0.0
C_6H_6	0.107

CHAPTER VII

ANALYSIS VERIFICATION

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 "α_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

$$\frac{\partial^2 P^2}{\partial x^2} + \gamma_1 \frac{\partial P^2}{\partial x} + \gamma_2 P^2 + \gamma_3 + \gamma_4 \frac{\partial P^2}{\partial t} = 0 . \tag{7-1}$$

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

$$\left.\begin{aligned} P^2_{x=0} &= P^2_w \\ \left(\frac{\partial P^2}{\partial x}\right)_{x=1} &= 2\,\ell R_u \left(\frac{\mu T}{K\bar{M}}\right)_{x=1} \dot{m}_g \\ P^2(x,0) &= P^2_{w,0} . \end{aligned}\right\} \tag{7-2}$$

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

$$P = \left[\frac{2\mu \ \ell R_u T \ \dot{m}_g}{K\bar{M}} \ x + P_w^2 \right]^{1/2} . \tag{7-3}$$

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.

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

$$\frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 \tag{7-4}$$

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

$$\left. \begin{aligned} T(1,t) &= T_{s_{x=1}} \quad \text{for } t > 0 \\ T(x,0) &= T_{s_o} \end{aligned} \right\} \tag{7-5}$$

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

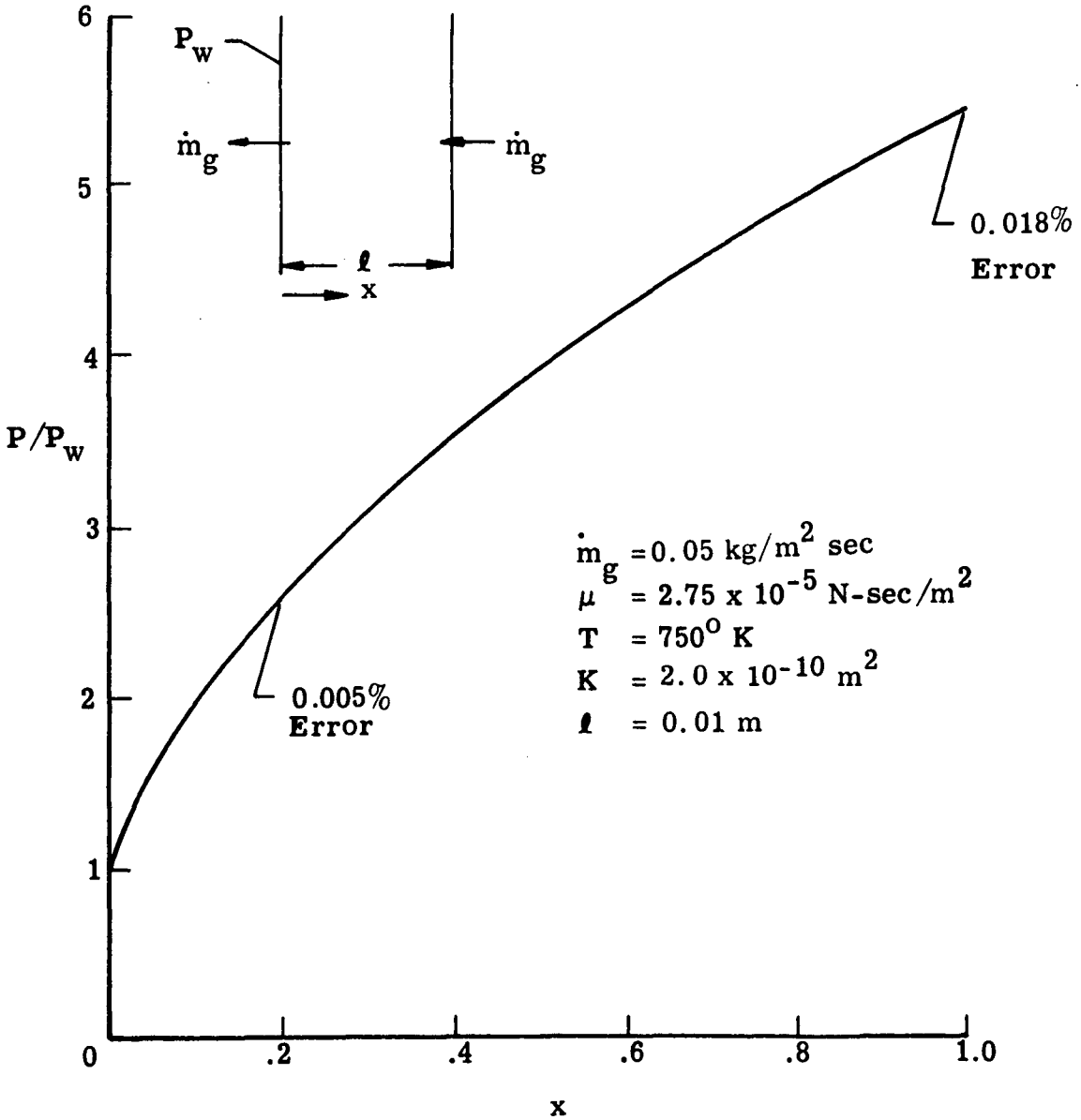

Figure 5a.- Comparison of results for numerical and exact solutions to the Laplace equation for P^2 with P_w = 0.01 ATM.

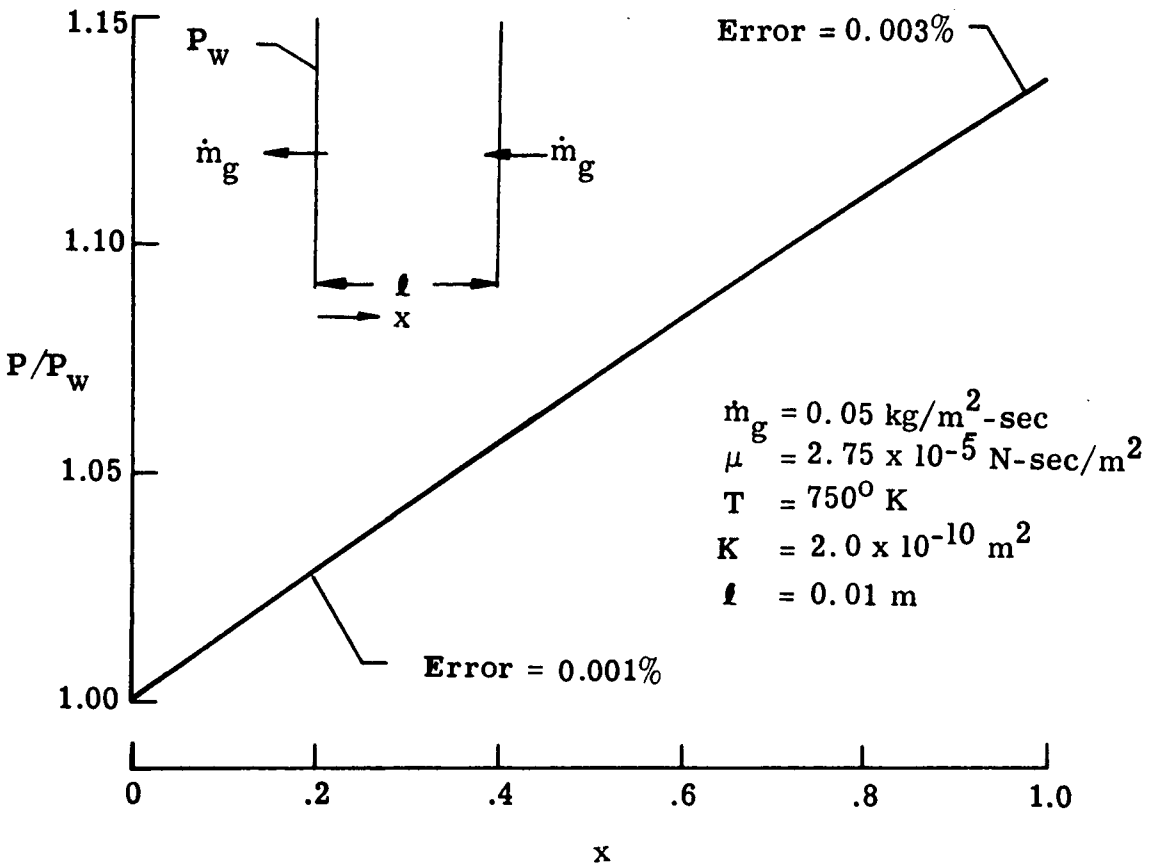

Figure 5b.- Comparison of results for numerical and exact solutions to the Laplace equation for P^2 with $P_w = 0.1$ ATM.

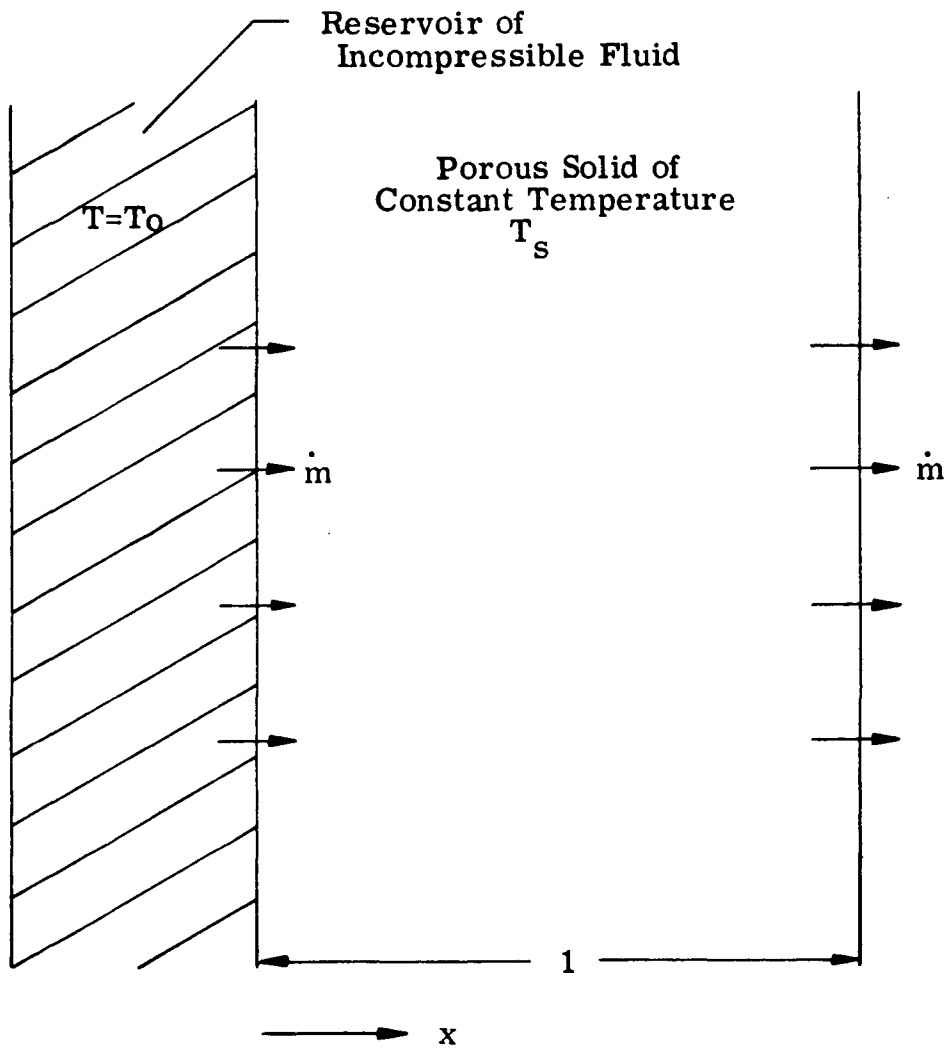

Figure 6.- Flow of constant property incompressible fluid through an isothermal slab.

$$\frac{\partial T'}{\partial x'} + AT' + \frac{\partial T'}{\partial t} = 0 \tag{7-6}$$

where

$$\left.\begin{aligned} T' &= \frac{T - T_s}{T_0 - T_s} \\ x' &= x\ell/v \\ A &= \frac{H_A}{\eta\rho C_p} \end{aligned}\right\} \tag{7-7}$$

and the boundary and initial conditions for T' are

$$\left.\begin{aligned} T'(0,t) &= 1.0 \quad \text{for} \quad t > 0 \\ T'(x',0) &= 0. \end{aligned}\right\} \tag{7-8}$$

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

$$P = \int_0^\infty e^{-St}\, T'(x',t)\, dt \tag{7-9}$$

is introduced. Equations 7-6 and 7-8 become

$$\left.\begin{aligned} &\frac{\partial P}{\partial x'} + (A + S)\ P = 0 \\ &P(0,t) = 1./S \\ &P(x',0) = 0. \end{aligned}\right\} \tag{7-10}$$

The solution to Eq. 7-10 is

$$P = \exp\ (-\ Ax')\ \frac{1}{S}\ \exp\ (-\ Sx')\ . \tag{7-11}$$

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

$$T'(x',t) = \exp(-\ Ax')\ S(t - x') \tag{7-12}$$

where

$$S(t - x') = \begin{cases} 0 \text{ when } 0 < t < x' \\ 1 \text{ when } t > x' \ . \end{cases} \tag{7-13}$$

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

This idealized case was solved with $A = 1.0$ and $\ell/v = 1.0$ 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)

$$T_s = T_{s_0} + q(\ell + \ell')/k_s \left\{ \frac{k_s\, t}{\rho_s \hat{C}_{p_s} (\ell + \ell')^2} + \frac{1}{2}(1 - x)^2 - \frac{1}{6} - \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos\left[n\pi(1 - x)\right] \exp\left[n^2 \pi^2 \frac{k_s\, t}{\rho_s \hat{C}_{p_s} (\ell + \ell')^2} \right] \right\}. \qquad (7\text{-}14)$$

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.

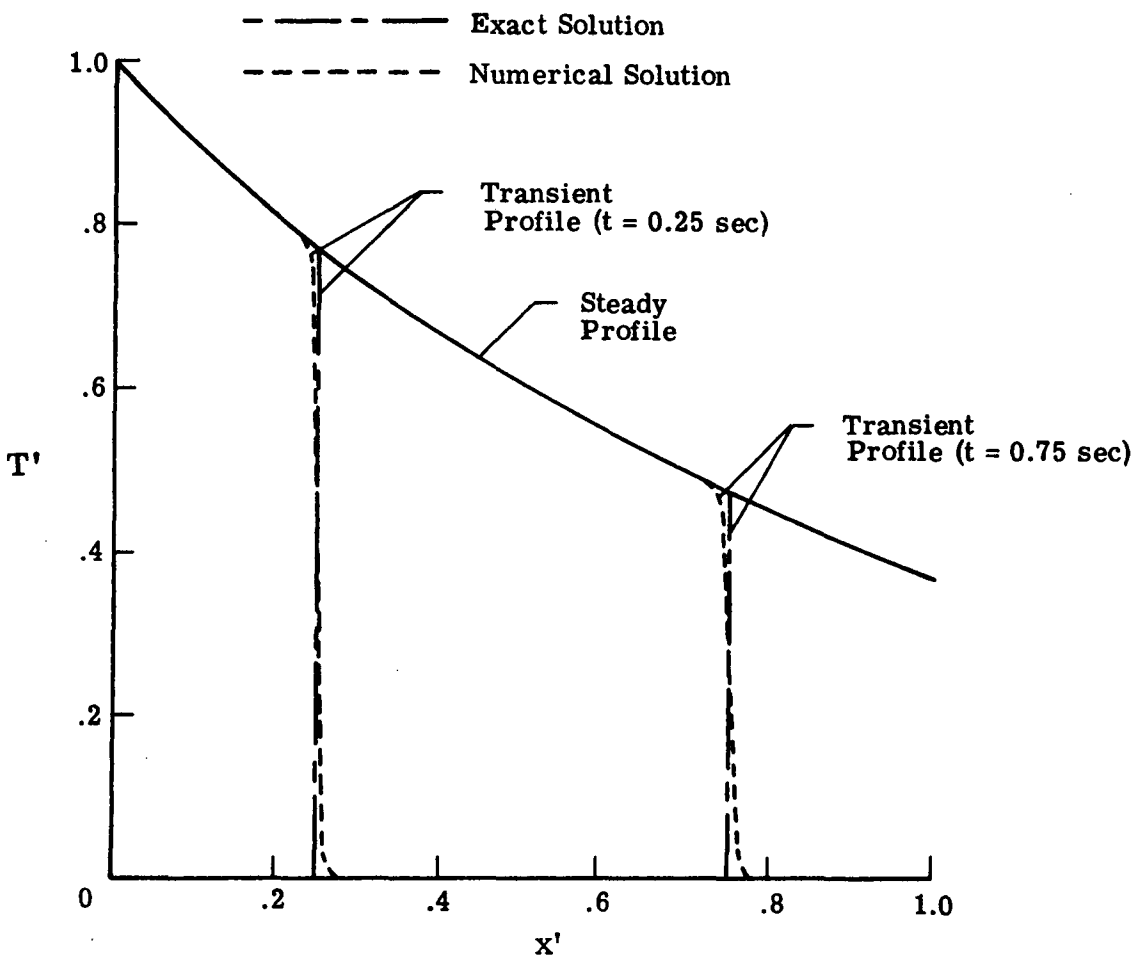

Figure 7a.- Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with $\Delta x = .001$.

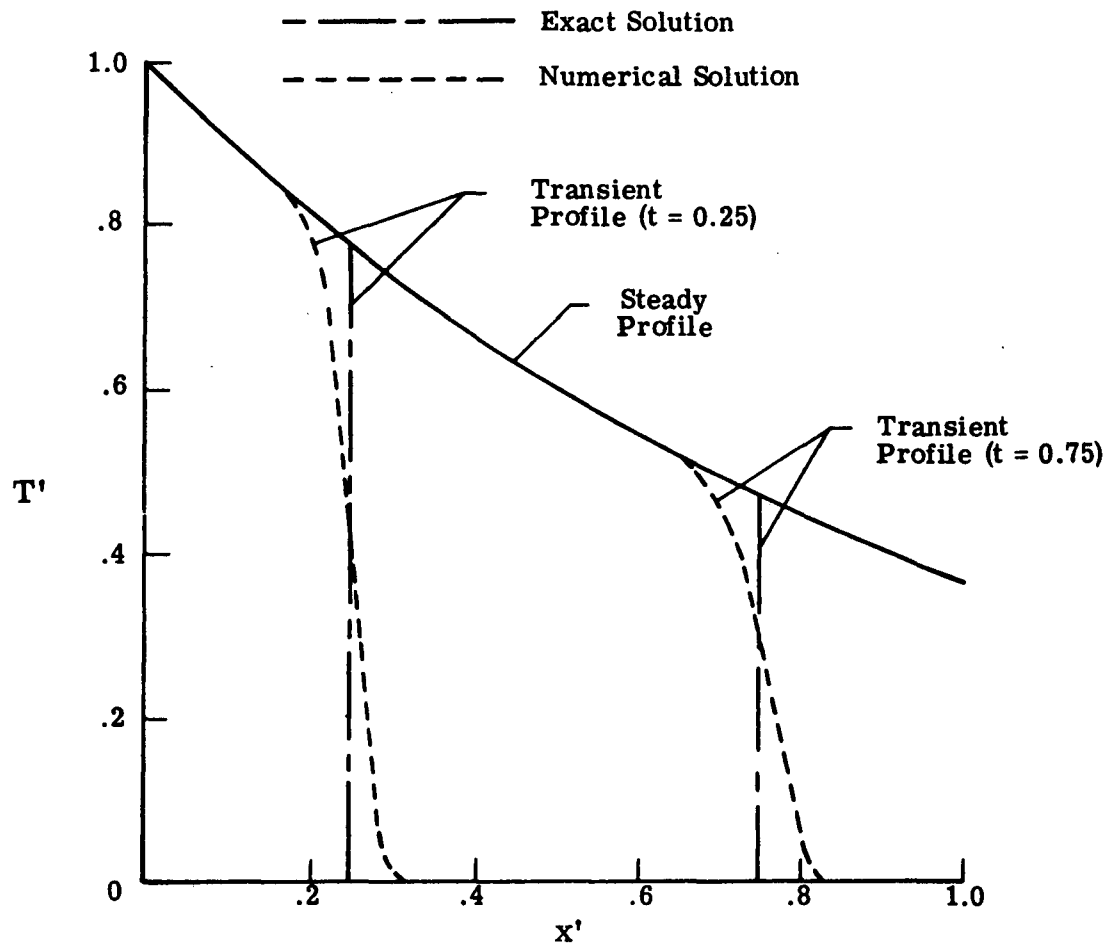

Figure 7b.- Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with $\Delta X = .01$.

Table 3.- Inputs Used in Exact Solution to Heat Sink Case.

Quantity	Value
q	$1. \times 10^6$ W/m^2
ℓ	0.01 m
ℓ'	0.01 m
k_s	0.624 W/m^2-$^\circ$K
ρ_s	2140 kg/m^3
$\hat{C}_{P_s}$	715.16 J/kg-$^\circ$K
T_{s_o}	300° K

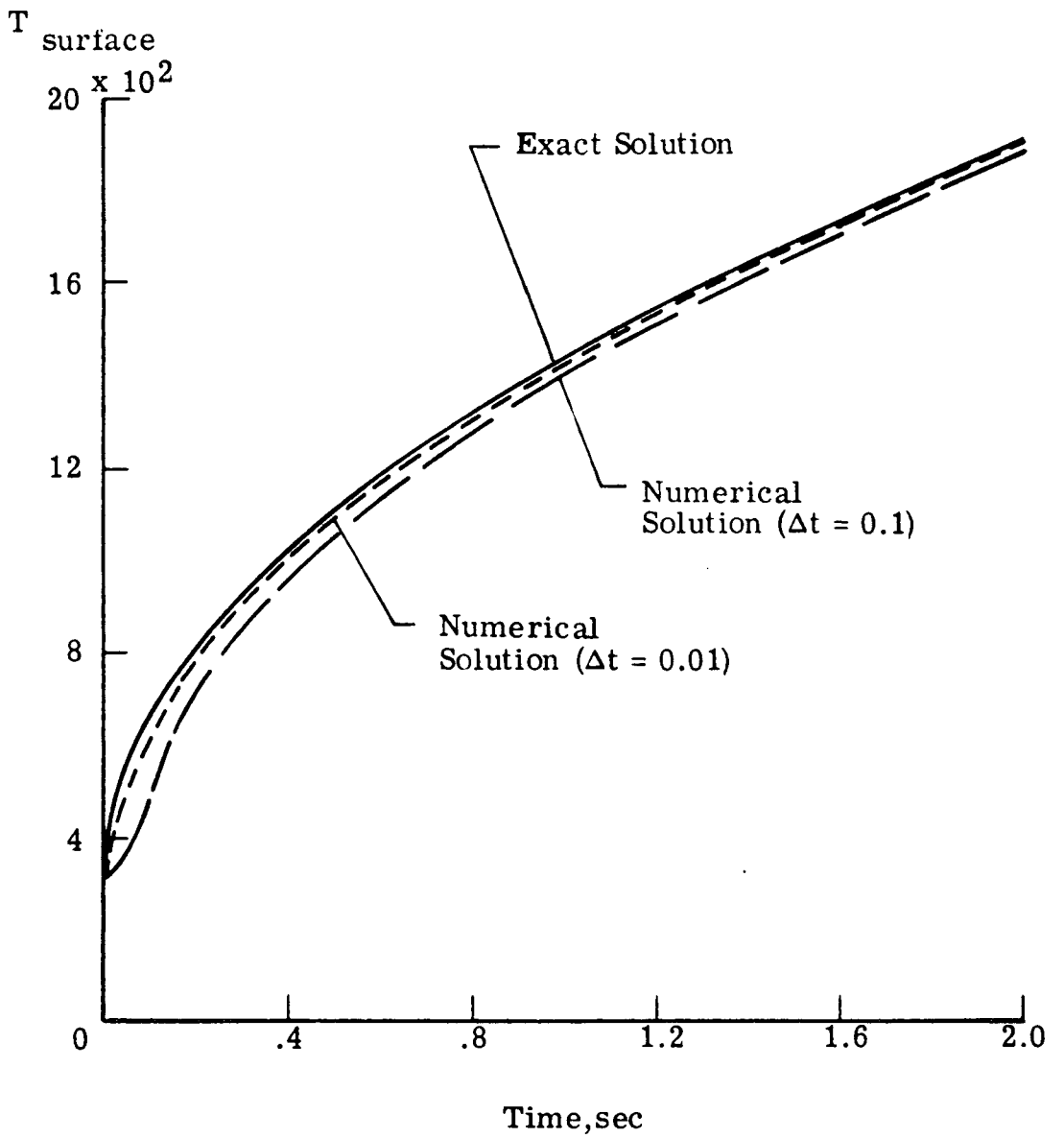

Figure 8.- Comparison of numerical results with the exact solution for the heat sink problem.

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)

$$(1 - \eta) \frac{\rho_s C_{P_s}}{M_s} \left[\frac{\partial T_s}{\partial t} - V_c \frac{\partial T_s}{\partial x} \right] = \frac{k_s}{\ell^2} \frac{\partial^2 T_s}{\partial x^2}$$

$$+ \frac{1}{\ell^2} \frac{\partial k_s}{\partial x} \frac{\partial T_s}{\partial x} - H_A(T_s - T) + \eta R_s H(T)_s$$

$$+ \eta R_{h_s} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \varepsilon)$$

$$+ (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \left(\frac{\partial \eta}{\partial x} - V_c \frac{\partial \eta}{\partial x} \right) . \qquad (7\text{-}15)$$

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

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

$$- \eta R_u \left[\frac{\rho}{\eta \bar{M}} \left(\frac{\partial \eta}{\partial t} - V_c \frac{\partial \eta}{\partial x} \right) + \frac{\partial}{\partial t} \left(\sum_i \rho_i / M_i \right) + (v/\ell \right.$$

$$- V_c) \frac{\partial}{\partial x} \left(\sum_i \rho_i/M_i\right)\Bigg] \; T + \eta \sum_i H_i R_{T_i} - \frac{1}{\ell} \sum_i H_i \frac{\partial}{\partial x} J_i$$

$$- \frac{v^2}{2} \sum_i R_{T_i} M_i - \frac{\tau_{xx}}{\ell^3} \frac{\partial v}{\partial x} - \eta \sum_i \frac{J_i g_i}{M_i} + \frac{1}{\ell^2} \frac{\partial}{\partial x} q_x$$

$$- \eta(A' - \varepsilon') + \eta R_s \; H(T)_s + \eta R_{h_s} \; H_s$$

$$- \eta \sum_r r_h^{(r)} \; \Delta H^{(r)} + \eta \left(\sum_i \frac{\rho_i C_{P_i}}{M_i} - R_u \sum_i \rho_i/M_i\right) \frac{\partial T}{\partial t} = 0 , \quad (7\text{-}16)$$

With quasi-steady-state ablation, ℓ, $\dot{m}_g$, and $\dot{m}_s$ are constant and

$$\left.\begin{aligned} \dot{m}_g/\Delta_\rho &= \dot{m}_s/\rho_{s_o} \\ \frac{\partial T_s}{\partial t} &= 0 \\ \frac{\partial T}{\partial t} &= 0 \; . \end{aligned}\right\} \quad (7\text{-}17)$$

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

$$\frac{\partial^2 T_s}{\partial x^2} + \frac{\ell}{k_s} \hat{C}_{P_s} \; \dot{m}_s \frac{\partial T_s}{\partial x} - \frac{\ell^2}{k_s} H_A(T_s - T) = 0 \quad (7\text{-}18)$$

$$\eta(v/\ell - \dot{m}_s/\rho_{s_o}\ell)\left[\rho\hat{C}_P - R_u \sum_i \rho_i/M_i\right]\frac{\partial T}{\partial x} - H_A(T_s - T) = 0 . \tag{7-19}$$

Equations 7-18 and 7-19 are combined to eliminate the term, $H_A(T_s - T$, thus

$$\frac{\partial^2 T_s}{\partial x^2} + \frac{\ell}{k_s}\left[\hat{C}_{P_s}\ \dot{m}_s \frac{\partial T_s}{\partial x} - \eta\ (v - \dot{m}_s/\rho_{s_o})(\rho\hat{C}_P - R_u \sum_i(\rho_i/M_i)\ \frac{\partial T}{\partial x}\right] = 0 . \tag{7-20}$$

Invoking the assumption of local thermal equilibrium between the pyrolysis gases and char layer $\left(T = T_s \text{ and } \frac{\partial T}{\partial x} = \frac{\partial T_s}{\partial x}\right)$ gives

$$\frac{\partial^2 T_s}{\partial x^2} + D\frac{\partial T_s}{\partial x} = 0 \tag{7-21}$$

where

$$D = \frac{\ell}{k_s}\left[\dot{m}_s\ \hat{C}_{P_s} + \left(\dot{m}_g + \eta\frac{\rho\dot{m}_s}{\rho_{s_o}}\right)\left(\hat{C}_P - \frac{R_u}{\bar{M}}\right)\right] . \tag{7-22}$$

The solution of Eq. 7-21 is

$$T_s = C_1 + C_2 \exp(-Dx). \tag{7-23}$$

The integration constants are determined from the boundary conditions:

$$\left.\begin{aligned} T_s(0) &= \bar{T}_1 \\ T_s(1) &= \bar{T}_I \end{aligned}\right\} \tag{7-24}$$

and the final solution is

$$T_s = \frac{\bar{T}_I - \bar{T}_1 \exp(-D) + (\bar{T}_1 - \bar{T}_I) \exp(-Dx)}{1 - \exp(-D)} \quad . \tag{7-25}$$

The mass loss rates $\dot{m}_s$ and $\dot{m}_g$ and the char layer thickness ℓ are obtained from this equation with the following equations

$$\left.\begin{aligned} \dot{m}_g/\Delta\rho &= \dot{m}_s/\rho_{s_o} \\ \left(\frac{\partial T_s}{\partial x}\right)_{x=0} &= \frac{\ell}{k_s}\left(\dot{m}_s H_C - q_{aero}\right) \\ \left(\frac{\partial T_s}{\partial x}\right)_{x=1} &= -\dot{m}_g \Delta H_P \frac{\ell}{k_s} \end{aligned}\right\} \tag{7-26}$$

where energy transfer into the uncharred layer is neglected. Thus

$$\left.\begin{aligned} \dot{m}_s &= \frac{\frac{\rho_{s_o}}{\Delta\rho} q_{aero}}{H_C + \Delta H_P + D'(\bar{T}_1 - \bar{T}_I)} \\ \dot{m}_g &= \frac{q_{aero}}{H_C + \Delta H_P + D'(\bar{T}_1 - \bar{T}_I)} \\ \ell &= \frac{k_s}{q_{aero} D'}\left[H_C + \Delta H_P + D'(\bar{T}_1 - \bar{T}_I)\right] \ln\left[\frac{\Delta H_P + D'(\bar{T}_1 - \bar{T}_I)}{\Delta H_P}\right] \end{aligned}\right\} \tag{7-27}$$

where

$$D' = \hat{C}_{P_s} + \left(\hat{C}_P - \frac{R_u}{\bar{M}}\right)\left(\frac{\Delta\rho + \eta\rho}{\rho_{s_o}}\right) \tag{7-28}$$

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,

$$H_A = \frac{K_h v}{N_{Pr}} \sum_i \frac{\rho_i C_{P_i}}{M_i} . \tag{7-29}$$

Calculations were made using a value for K_h of 5×10^5 1/m yet a temperature difference of 1.5° 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.

Quantity	Value
q_{aero}	0.8×10^5 W/m^2
k_s	0.624 W/m^2-^{o}K
ρ_{s_o}	320. kg/m^3
$\Delta\rho$	320. kg/m^3
$\hat{C}_{P_s}$	2090. J/kg-^{o}K
$\hat{C}_P$	2090. J/kg-^{o}K
$\bar{T}_1$	2222. ^{o}K
$\bar{T}_I$	556. ^{o}K
ΔH_P	2.324×10^6 J/kg
H_C	2.324×10^6 J/kg
$\bar{M}$	0.029 kg/g-mole ^{o}K

Table 5.- Comparison of the Exact Solution and the Numerical Solution Obtained with $K_h = 5. \times 10^5$ 1/m for a Quasi-Steady State Condition.

Parameter	Numerical Solution	Exact Solution	% Error
$\dot{m}_s$, kg/m^{2}sec	7.304×10^{-2}	7.185×10^{-2}	1.66
$\dot{m}_g$, kg/m^{2}sec	7.301×10^{-2}	7.185×10^{-2}	1.61
ℓ,m	2.924×10^{-3}	2.973×10^{-3}	-1.65

$$H_A(T_s - T) = \frac{1}{\ell}\left(\dot{m}_g - \eta\rho\dot{m}_s/\rho_{s_o}\right)\left[\hat{C}_p - \frac{R_u}{\bar{M}}\frac{\partial T_s}{\partial x}\right] . \quad (7\text{-}30)$$

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.

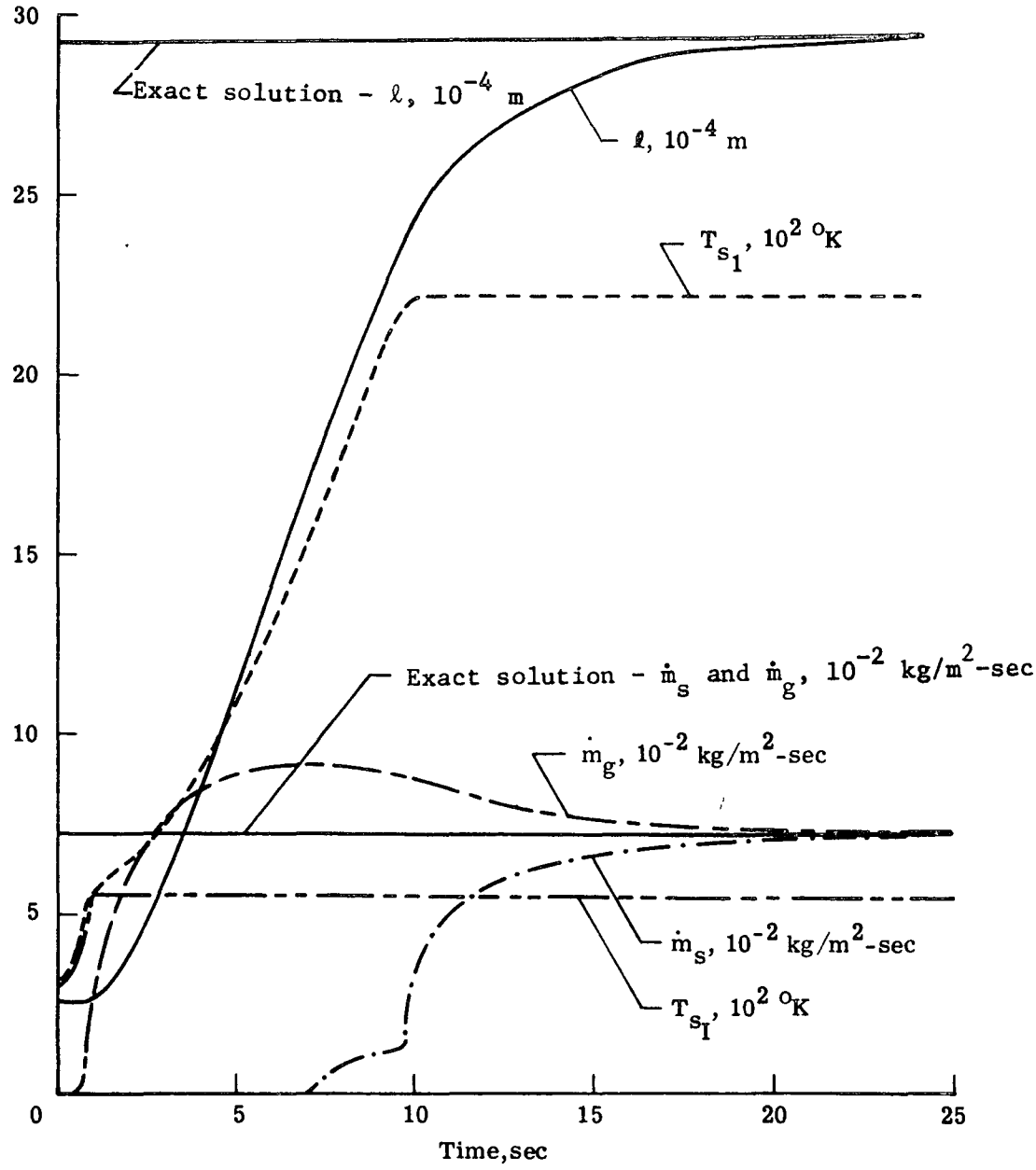

Figure 9.- Numerical results for $\dot{m}_s$, $\dot{m}_g$, ℓ, surface temperature, and pyrolysis temperature for a case run to quasi-steady-state condition.

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

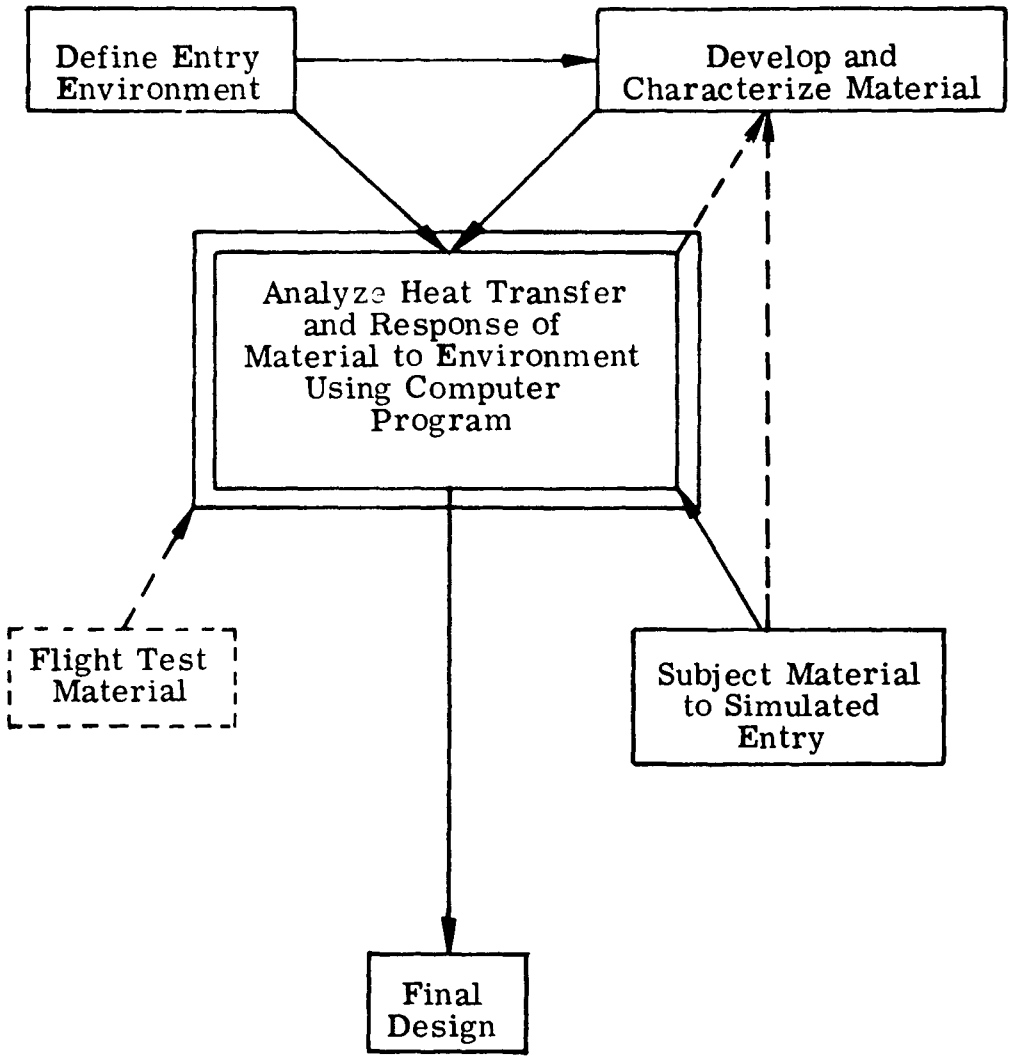

Figure 10.- The role of ablation analysis in the design of thermal protection systems for aerospace applications.

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.

Parameter	Value
q_c, W/m^2, at time, sec	
0	2.162×10^3
10	8.0×10^5
1000	8.0×10^5
P_w, N/m^2, at time, sec	
0	1.0×10^{-6}
9	1.0×10^{-4}
29	9.0×10^{-4}
39	1.0×10^{-1}
1000	1.0×10^{-1}
H_e, J/kg	3.1×10^5
C_e	0.23

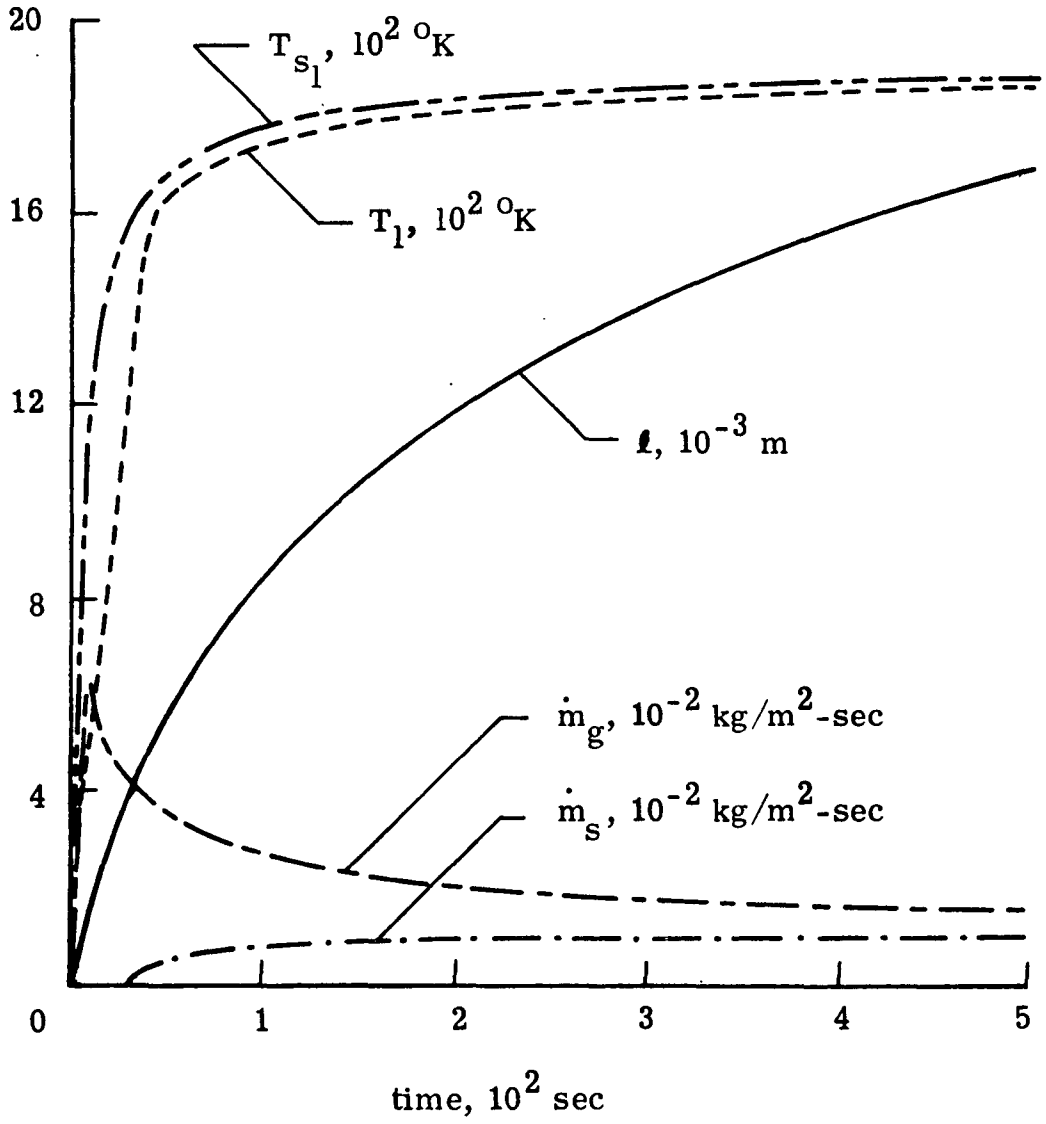

Figure 11.- Typical time histories of $\dot{m}_s$, $\dot{m}_g$, ℓ, surface temperature, and pyrolysis gas temperature at the surface for an ablation system subjected to a square heat pulse.

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.

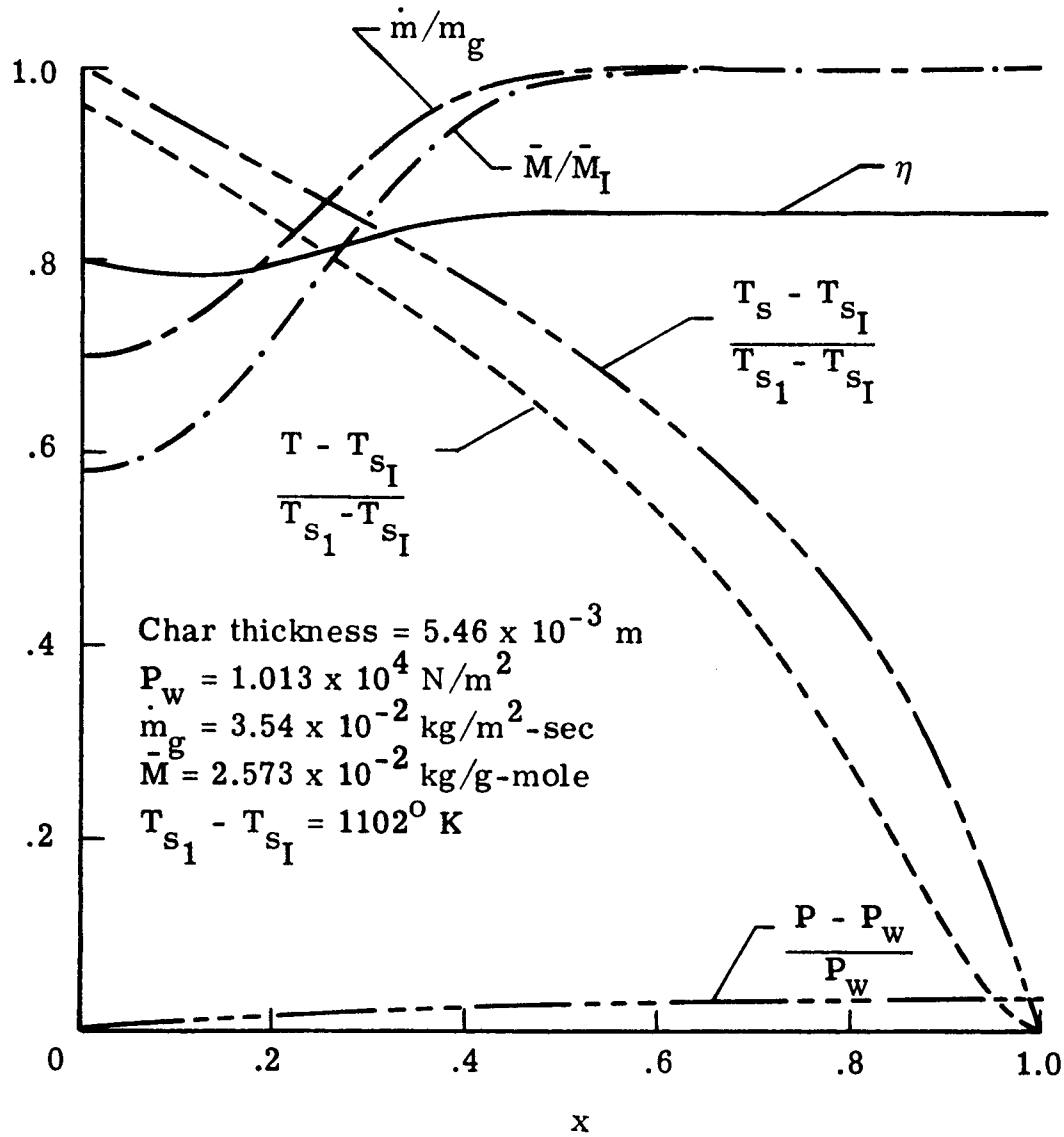

Figure 12.- Profiles of pyrolysis gas temperature, char layer temperature, pyrolysis gas molecular weight, char porosity, local mass flow rate, and pyrolysis gas pressure at a time of 50 sec for the case represented in Fig. 11.

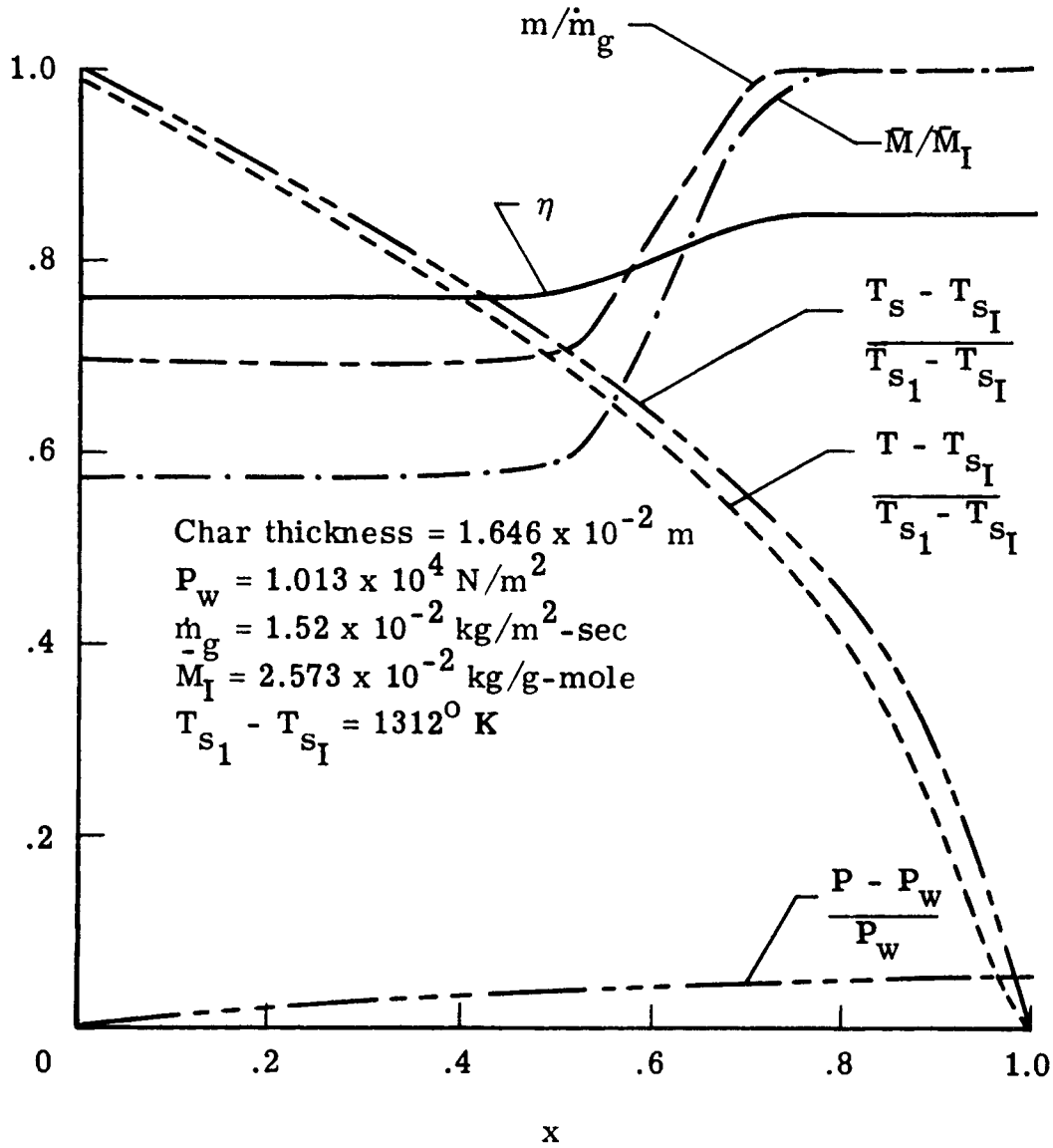

Figure 13.- Profiles of pyrolysis gas temperature, char layer temperature, pyrolysis gas molecular weight, char porosity, local mass flow rate, and pyrolysis gas pressure at a time of 500 sec for the case represented in Fig. 11.

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.

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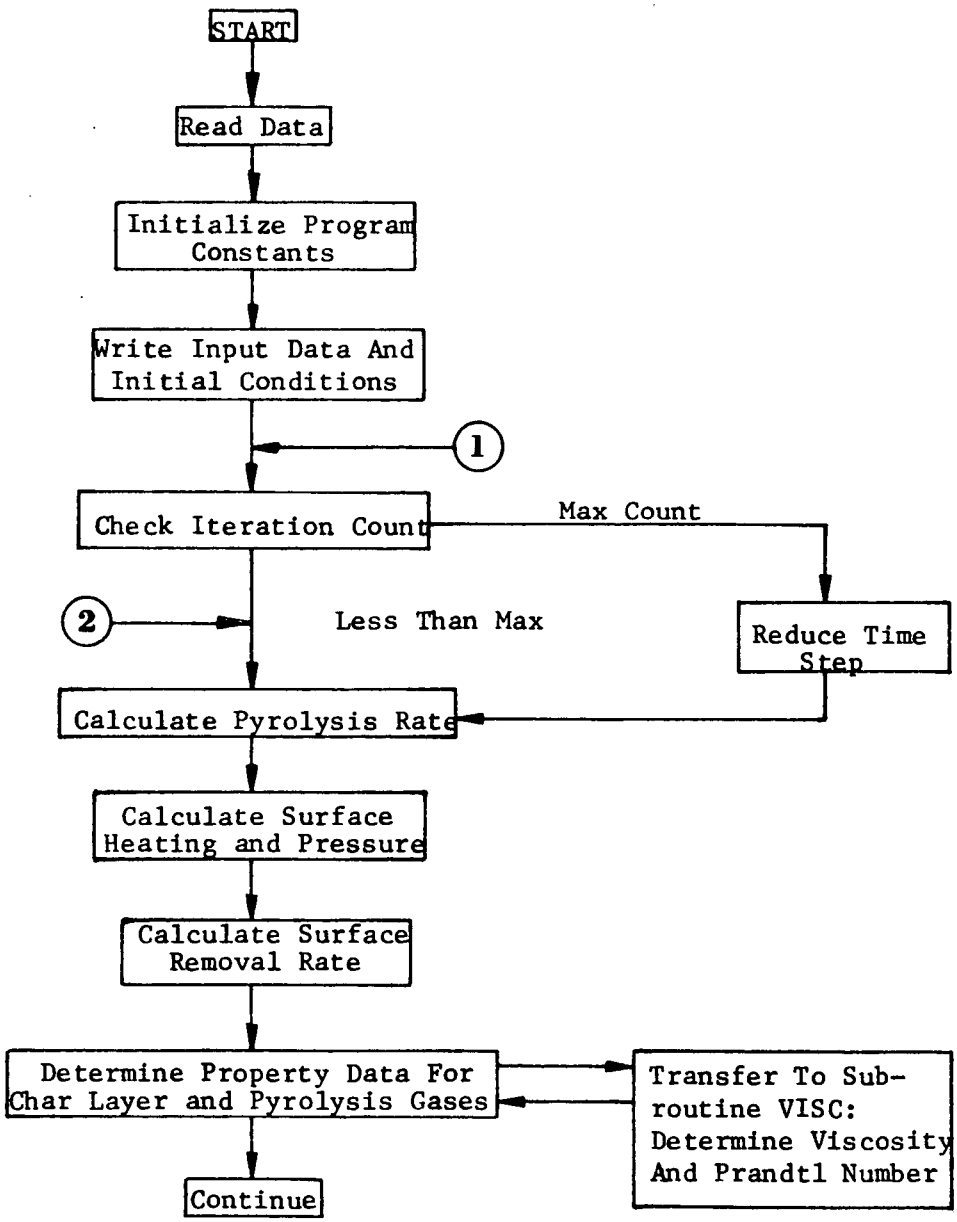
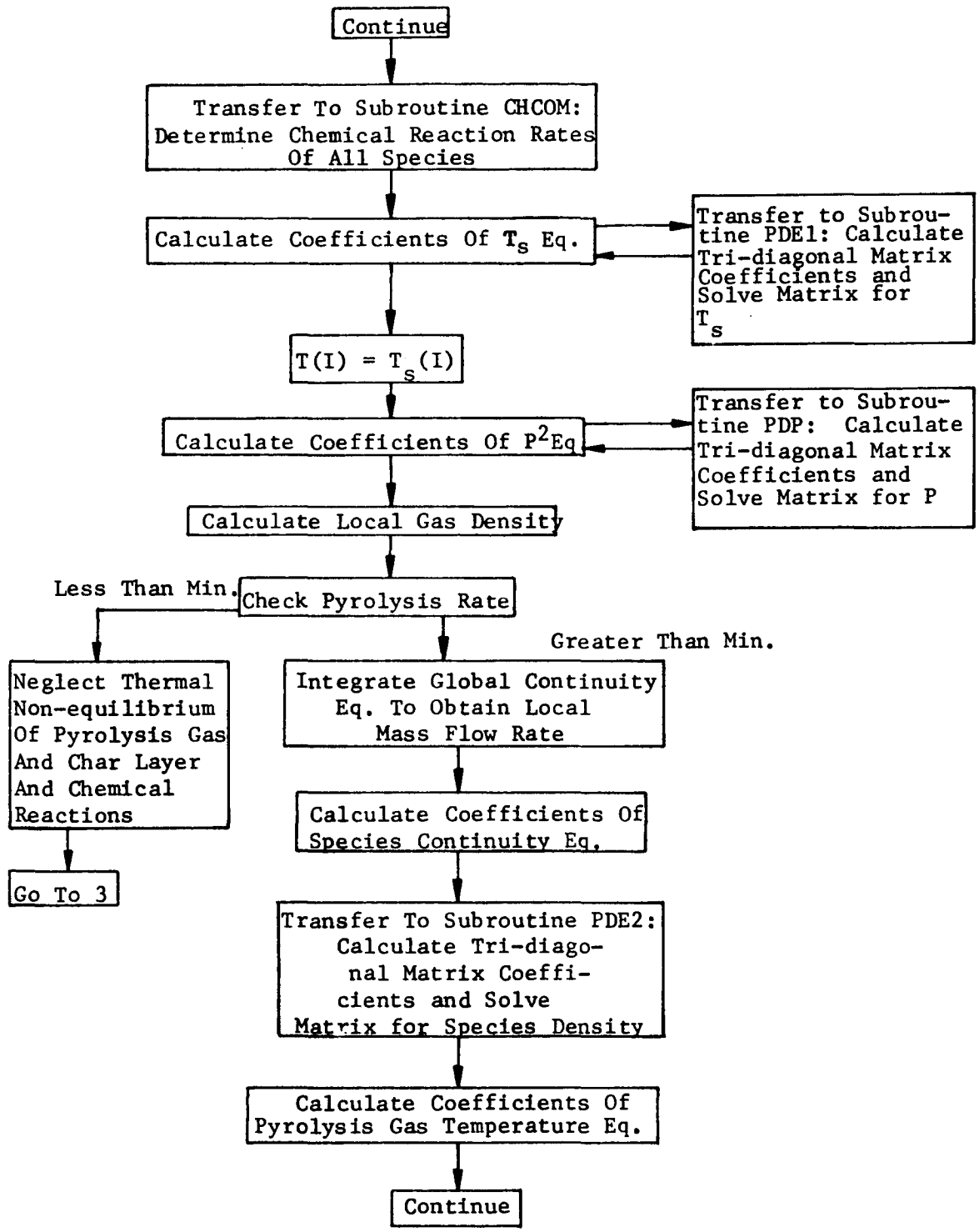
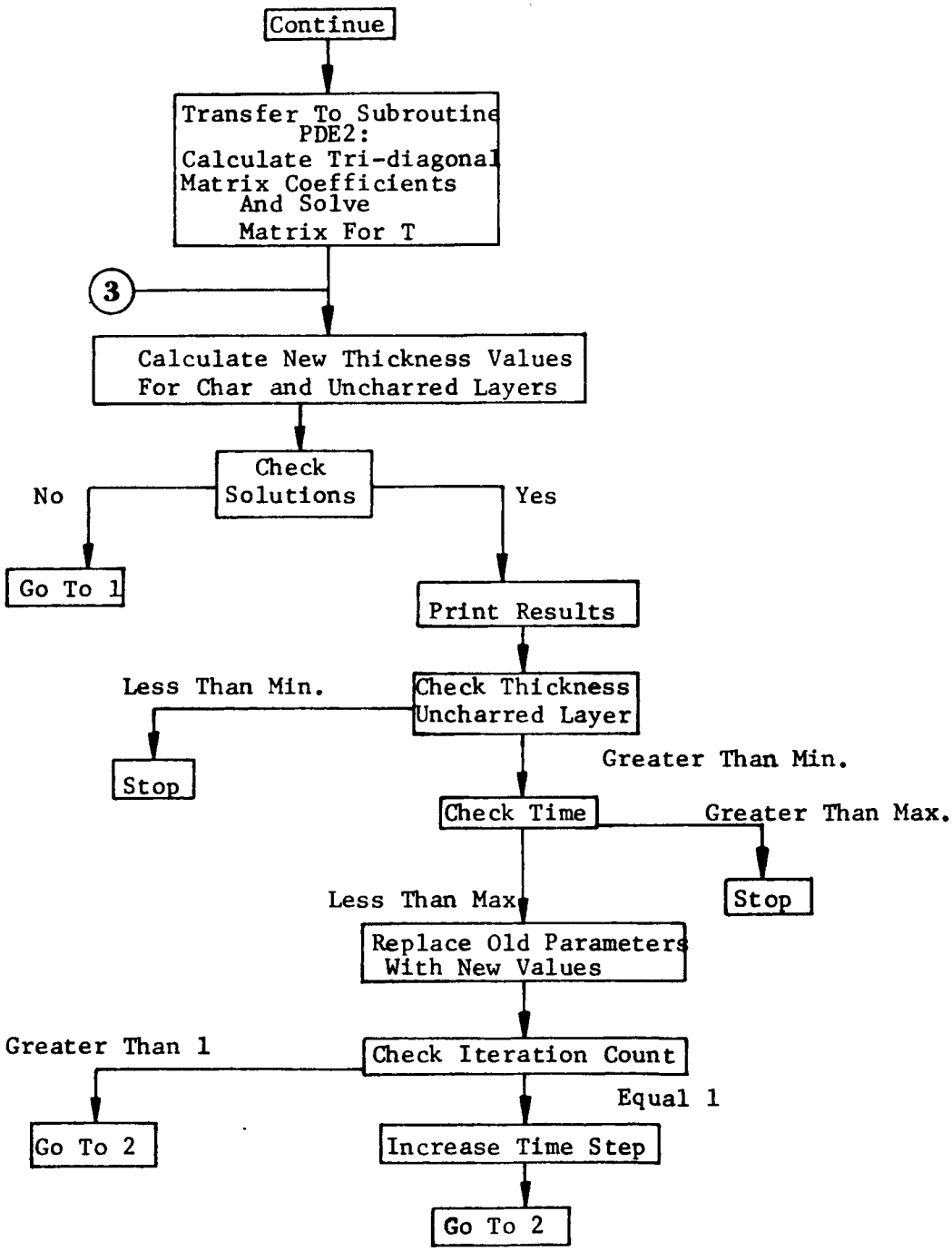
APPENDIX A

GENERAL FLOW CHART




Continue
Transfer To Subroutine CHCOM: Determine Chemical Reaction Rates Of All Species
Calculate Coefficients Of T_s Eq.
Transfer to Subroutine PDE1: Calculate Tri-diagonal Matrix Coefficients and Solve Matrix for T_s
$T(I) = T_s(I)$
Calculate Coefficients Of P^2Eq
Transfer to Subroutine PDP: Calculate Tri-diagonal Matrix Coefficients and Solve Matrix for P
Calculate Local Gas Density
Less Than Min.
Check Pyrolysis Rate
Greater Than Min.
Neglect Thermal Non-equilibrium Of Pyrolysis Gas And Char Layer And Chemical Reactions
Go To 3
Integrate Global Continuity Eq. To Obtain Local Mass Flow Rate
Calculate Coefficients Of Species Continuity Eq.
Transfer To Subroutine PDE2: Calculate Tri-diagonal Matrix Coefficients and Solve Matrix for Species Density
Calculate Coefficients Of Pyrolysis Gas Temperature Eq.
Continue


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
Yes
Go To 1
Print Results
Less Than Min.
Check Thickness Uncharred Layer
Stop
Greater Than Min.
Check Time
Greater Than Max.
Stop
Less Than Max
Replace Old Parameters With New Values
Greater Than 1
Check Iteration Count
Equal 1
Go To 2
Increase Time Step
Go To 2

APPENDIX B

PROGRAM USAGE INSTRUCTIONS

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.

FORTRAN VARIABLE	DESCRIPTION
AC	Specific reaction rate constant for first order oxidation of char layer (LIST).
ACEF(12)	Specific reaction rate constant for forward chemical reaction (PERM).
ACER(12)	Specific reaction rate constant for reverse chemical reaction (PERM).
AEXP	Specific reaction rate constant for pyrolysis of uncharred material (LIST).
ALFC	Weight factor for transpiration effectiveness of mass removal by oxidation or sublimation (LIST).
ALFP	Weight factor for transpiration effectiveness of pyrolysis gases (LIST).
ALPHA	Absorptivity of char surface (LIST).
BC	Activation temperature for first order oxidation of char layer (LIST).
BCEF(12)	Activation temperature for forward chemical reaction (PERM).
BCER(12)	Activation temperature for reverse chemical reaction (PERM).
BEXP	Activation temperature for pyrolysis of uncharred material (LIST).
CE	Mass fraction of oxygen at edge of boundary layer (LIST).

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 $\rho\hat{C}_p\ell$ for heat sink at uncharred layer insulation layer interface (LIST).
HTSKP	Value of $\rho\hat{C}_p\ell$ 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).

C.3

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).

PMV	Constant permeability of char layer (LIST).
PRNTFRQ	Time interval for printing output (PIKUP).
PROPC	Proportionality constant in expression for H_A(LIST).
PTIME	Time at start of calculation (PIKUP).
QCTAB(40)	Table of cold wall heating rate versus time (LIST).
QRS	Radiant heat transfer at surface (LIST).
RAD	Vehicle nose radius for hypersonic velocities (LIST).
RHOPPV	Constant density of insulation layer (LIST).
RHOST	Theoretical density of char layer (LIST).
RU	Universal gas constant (PERM).
SGMA	Stephan-Boltzman constant (PERM).
SQPT(40)	Table of square root of wall pressure versus time (LIST).
T	Initial pyrolysis gas temperature (PIKUP).
T1BAR	Sublimation temperature of char layer (LIST).
TCPP(40)	Temperature table for CPPT (LIST).
TEMP (40)	Temperature table for HSTT, HKT, CPKT, MUKT and KUPT (PERM).
TIBAR	Maximum temperature of pyrolysis zone (LIST).
TIME	Time at start of calculation (PIKUP).
TIMET(40)	Time table for QCTAB(LIST).
TKP(40)	Temperature table for KPT (LIST).
TKS(40)	Temperature table for KST (LIST).
TMPRESS(40)	Time table for SQPT (LIST).
TRAB	Trigger for selecting blocking approximation (LIST).
TREF	Transpiration effectiveness (LIST).
TS	Initial char layer temperature (PIKUP).

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-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=OUTPUT)
C
C
C     A NUMERICAL SOLUTION OF THE DIFFERENTIAL EQUATIONS GOVERNING THE
C     TRANSIENT RESPONSE OF A ONE-DIMENSIONAL ABLATION SYSTEM INCLUDING
C     EFFECTS OF THERMAL NON-EQUILIBRIUM, MASS TRANSFER, AND CHEMICAL
C     REACTIONS.
C     REFERENCE--  CLARK, RONALD K.-  A NUMERICAL ANALYSIS OF THE TRAN-
C        SIENT RESPONSE OF AN ABLATION SYSTEM INCLUDING EFFECTS OF THER-
C        MAL NON-EQUILIBRIUM, MASS TRANSFER, AND CHEMICAL KINETICS.
C        DOCTOR OF PHILOSOPHY DISSERTATION, VIRGINIA POLYTECHNIC IN-
C        STITUTE AND STATE UNIVERSITY, BLACKSBURG, VA. 1972.
C
C     PRIMARY INPUTS
C        DHC        HEAT OF COMBUSTION OF CHAR LAYER
C        DHP        HEAT OF PYROLYSIS
C        DRHO       DENSITY CHANGE ACROSS PYROLYSIS INTERFACE
C        DT         TIME INCREMENT
C        EPSP       BACK SURFACE EMISSIVITY
C        EPSS       CHAR SURFACE EMISSIVITY
C        HC         HEAT OF SUBLIMATION OF CHAR LAYER
C        HE         ENTHALPY OF FREE STREAM
C        HTSK       VALUE OF THERMAL CAPACITY OF HEAT SINK AT BACK OF
C                   UNCHARRED MATERIAL
C        HTSKP      VALUE OF THERMAL CAPACITY OF HEAT SINK AT BACK OF
C                   INSULATION LAYER
C        IOPTI      TRIGGER FOR SELECTING METHOD OF COMPUTING PYROLYSIS
C                   RATE.  (IOPTI=0  NO RESTRICTION ON TEMPERATURE OF PY-
C                   ROLYSIS ZONE- PYROLYSIS RATE COMPUTED USING ARR-
C                   HENIUS TYPE RATE EQUATION, IOPTI=1  TEMPERATURE OF
C                   PYROLYSIS ZONE LIMITED TO TIBAR- PYROLYSIS RATE COM-
C                   PUTED USING ENERGY BALANCE WHEN TS(I)=TIBAR)
C        IOPT1      TRIGGER FOR SELECTING MODE OF BEHAVIOR OF SURFACE
C                   TEMPERATURE DURING SUBLIMATION.  (IOPT1=0  NO RE-
C                   STRICTION ON SURFACE TEMPERATURE, IOPT1=1  SURFACE
C                   TEMPERATURE LIMITED TO T1BAR)
```

```
C        IOPTP     TRIGGER FOR SELECTING METHOD OF COMPUTING WALL PRES-   A  37
C                  SURE.  (IOPTP=1 USE TABLE LOOKUP, IOPTP=0 COMPUTE      A  38
C                  WALL PRESSURE FROM HYPERSONIC FLOW THEORY)             A  39
C        KT        NUMBER OF GASEOUS SPECIES CONSIDERED                   A  40
C        LOP       INITIAL THICKNESS OF UNCHARRED LAYER                   A  41
C        NRCT      NUMBER OF CHEMICAL REACTIONS CONSIDERED                A  42
C        QCTAB     TABLE OF COLD WALL CONVECTIVE HEATING RATE VS TIME     A  43
C        QRS       RADIANT HEATING RATE                                   A  44
C        RAD       RADIUS OF BODY                                         A  45
C        RHOST     THEORETICAL DENSITY OF CHAR MATERIAL                   A  46
C        SQPT      TABLE OF WALL PRESSURE VS TIME                         A  47
C        TIBAR     MAXIMUM TEMPERATURE OF PYROLYSIS ZONE USED WITH        A  48
C        T1BAR     SUBLIMATION TEMPERATURE OF CHAR LAYER                  A  49
C                                                                         A  50
C        CHEMICAL SPECIES IDENTIFICATION-                                 A  51
C                  1.  CH4        2.  H2         3.  C2H4                 A  52
C                  4.  C2H2       5.  CO         6.  H2O                  A  53
C                  7.  NH3        8.  N2         9.  CO2                  A  54
C                 10.  HCN       11.  C2H6      12.  C6H6                 A  55
C                 13.  C (SOLID)                                          A  56
C                                                                         A  57
C     FOR DOUBLE SUBSCRIPTED QUANTITIES-  FIRST SUBSCRIPT REFERS TO       A  58
C        REACTION, STATION, OR TEMPERATURE AND SECOND SUBSCRIPT REFERS    A  59
C        TO CHEMICAL SPECIES.                                             A  60
C                                                                         A  61
C                                                                         A  62
      DIMENSION ALPHA1(110), ALPHA2(110), ALPHA3(110), ALPHA4(110), ARH(  A  63
     150), ALPHB3(110), ALPHB4(110), ALPHP1(110), ALPHP2(110), ALPHP3(11  A  64
     20), ALPHP4(110), BETA1(50), BETA2(50), BETA3(50), YP(50), BRH(50),  A  65
     3 BETB3(50), BETP1(50), BETP2(50), BETP3(50), CPK(50,12), BET32(50)  A  66
     4, CPKT(40,12), CPKTV(40), CPP(100), CPPT(40), CPS(50), AL1(50), DE  A  67
     5B2(50,12), DEB3(50), DEL1(50,12), DEL2(50,12), DEL3(50), DEP1(50,1  A  68
     62), DEP2(50,12), DEP3(50), DETADX(50), AB2(50), ROHM(50), DKPDX(10  A  69
     70), DKSDX(50), DVDX(50), AB3(50), TP(50), HA(50), PAMGDOT(50,12),   A  70
     8EPSB3(50), HK(50,13), HKT(40,13), HKTV(40), HRSUM(50), HS(50), HST  A  71
```

```
9(50), AP1(50), HSTT(40), KG(50), KP(100), KPT(40), KS(50), P(50),
$TIMET(40), QCTAB(40), TMPRES(40), SQPT(40), TCPP(40), TKP(40), EPS
$P1(50), RHOP(100), RM(50), ROM(50), TS(110), EPSA1(50), EPSA2(50),
$ TSP(110), V(50), MFKI(12), EPSA3(50), EPSP2(50), EPSP3(50), EPSB2
$(50), PROM(50), AMDOT(50), AP(50), KPP(110), CPPP(110), RHOPP(110)
$, DRODX(50), YETA(50), NRHOK(12), AT(50), ATS(110), YTS(110), YT(5
$0), YRHO(50), YRHOK(50,12), TKS(40), KST(40), PTS(110), PT(50), VC
$(50), DMBRDX(50), DTDX(50), AINT1(50), AINT3(50), SPECIES(13)
 COMMON ACEF(12),ACER(12),BCEF(12),BCER(12),CRNI,KUPT(40,12),KJPTV(
140),M(13),MFK(50,12),MNO,NNO,MU(50),MUKT(40,12),MUKTV(40),PR(50),R
2(50,12),RHO(50),RHOK(50,12),RHOKP(50,12),T(50),TEMP(40),NRCT,KT,RU
3,NSTEP,ROCPM(50),RS(50),RHR(50,12),RHS(50),DHK(50,12),DHJ(50,12),H
4RJSUM(50)
 COMMON /PDE1/ ALPHI1,ALPHI2,ALPHI3,ALPHI4,ALPHIP1,ALPHIP2,ALPHIP3,
1ALPHIP4,GAMMI1,GAMMI2,GAMMI4,GAMMIP1,GAMMIP2,GAMMIP3,GAMMIP4,SGMA,
2DX,ALPHA1,ALPHA2,ALPHP1,ALPHP2,ALPHB3,ALPHB4,DT,L,Q,KS,LP,QPT,KSP1
3,TSP,DXP,IP,I,IO,IN,IO1,KP,LPP,LPPP,KSPI,KPPI,MGDOT,DHP,MGDOTP,QNE
4T,QPNET,KPPIP,GAMMI3,IM,EPSS,EPSP,DX1,DXP1,ALPHA4,ALPHP3,ALPHP4,AL
5PHA3,HTSK,HTSKP,IOPT1,IOPTI,TIBAR,TI3AR
 COMMON /PDP/ PAL1(50),PAL2(50),PAL3(50),PAL4(50),PAP1(50),PAP2(50)
1,PAP3(50),PAP4(50),PAB3(50),PAB4(50),PWP,PP(50),PM(50),PMU,PPM,PRH
2O(50),ETA(50),ETAP(50),AVGMF(50),AVGMFP(50)
 COMMON /TS/ IP1,IZ1,KPP,GAMIP1,GAMIP2,GAMIP3,GAMIP4,GAMIPP1,GAMIPP
12,GAMIPP3,GAMIPP4,KAPIP1,KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPIPP2,IL,K
2APIPP3,KAPIPP4,DXPP,KPPPIP,KPPPIZ,IZ
 EQUIVALENCE (EPSA2,EPSB2,EPSP2), (AB3,DEB3)
 REAL KS,MU,MUK,KPPV,KP,M,L,LP,MS,MSDOT,MGDOT,MPDOT,KST,KPT,KUPT,MU
1KTV,MUKT,KUPTV,KG,LAM,KA,LPP,MFKI,LPPP,MFK,MGDOTP,KPPI,KSPI,KSP1,K
2PPIP,IL,KPP,KPPPIZ,KPPPIP,KAPIP1,KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPI
3PP2,KAPIPP3,KAPIPP4,LPMIN,MSDOTP
 NAMELIST /PERM/ SGMA,I,JK,CRNI,KT,RU,M,ACEF,BCEF,NRCT,ACER,BCER,DX
11,DX,DXP,DXPP,IZ,DIFER,DXP1,LPMIN,TEMP,MNO,NNO,HSTT,CPKT,HKT,KUPT,
2MUKT,SPECIES
 NAMELIST /PIKUP/ TS,P,T,ETA,MGDOT,MSDOT,MFK,L,LP,TIME,PTIME,DT,KSP
```

```
     11,KSPI,KPPI,PRNTFRQ                                               A 106
      NAMELIST /LIST/ PROPC,ALFC,ALFP,ALPHA,DHC,ITR,QRS,EPSS,EPSP,HC,RHO  A 107
     1ST,RAD,T1BAR,DHP,LAM,CE,AC,BC,HE,TREF,TRAB,MFKI,AEXP,BEXP,IL,CPPPV  A 108
     2,KPPV,RHOPPV,HTSK,HTSKP,CPSV,PMV,KPT,TKP,MKS,NKS,KST,CPPT,TCPP,MCP  A 109
     3P,NCPP,MKP,TIMET,QCTAB,MQC,NQC,TMPRES,SQPT,MSQPT,NSQPT,TKS,NKP,IOP  A 110
     4T1,IOPTI,TIBAR,IOPTP,DRHO                                         A 111
C     READ INPUT DATA                                                   A 112
      READ (5,PERM)                                                     A 113
      READ (5,PIKUP)                                                    A 114
      READ (5,LIST)                                                     A 115
C     INITIALIZE PROGRAM CONSTANTS                                      A 116
      KTT=KT+1                                                          A 117
      KM=KT-2                                                           A 118
      IM=I-1                                                            A 119
      IN=I+1                                                            A 120
      IN2=I+2                                                           A 121
      IP=I+JK                                                           A 122
      IO1=IP-1                                                          A 123
      IO=IP-2                                                           A 124
      NITC=0                                                            A 125
      NITA=0                                                            A 126
      MS=M(13)                                                          A 127
      AINT1(I)=0.                                                       A 128
      AINT3(I)=0.                                                       A 129
      IP1=IP+1                                                          A 130
      IZ1=IZ-1                                                          A 131
      NIT=0                                                             A 132
      NITG=0                                                            A 133
      ICHCOM=0                                                          A 134
      NTIME=0                                                           A 135
C     CONVERT INPUT DATA TO PROPER UNITS (SYSTEM INTERNATIONAL)         A 136
C        DATA FOR HEAT CAPACITY OF CHAR LAYER- SOLID CARBON- ARE INPUT  A 137
C        IN UNITS OF JOULES/KILOGRAM (.012 KILOGRAM/G-MOLE)             A 138
C        DATA FOR HEAT CAPACITY AND ENTHALPY ARE INPUT WITH ENERGY IN   A 139
C        UNITS OF THERMOCHEMICAL CALORIE (4.184 J/CAL)                  A 140
C        DATA FOR VISCOSITY OF GASEOUS SPECIES ARE INPUT IN UNITS OF    A 141
```

```
C        POISES (0.0000001 NEWTON-SECOND/METER SQ PER POISE)
      CPSV=.012*CPSV
      DO 1 K=1,NRCT
      BCEF(K)=4.184*BCEF(K)
      ACER(K)=0.
1     BCER(K)=4.184*BCER(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,PIKUP)
      WRITE (2,LIST)
C     INITIALIZE ALL PARAMETERS
      KS(1)=KSP1
      KS(I)=KSPI
      KP(I)=KSPI
      MGDOTP=MGDOT
      MSDOTP=MSDOT
      LPP=L
      LPPP=LP
      QPNET=SGMA*EPSP*TS(IZ)**4
      DO 6 N=1,I
      DETADX(N)=0.
      DRODX(N)=0.
      AMDOT(N)=MGDOT
      PP(N)=P(N)
```

```
      RHO(N)=0.                                                         A 177
      RHS(N)=0.                                                         A 178
      RS(N)=0.                                                          A 179
      ROM(N)=0.                                                         A 180
      DO 4 KI=1,KT                                                      A 181
      RHOK(N,KI)=P(N)*M(KI)*MFK(N,KI)/(RU*T(N))                         A 182
      ROM(N)=ROM(N)+RHOK(N,KI)/M(KI)                                    A 183
      RHOKP(N,KI)=RHOK(N,KI)                                            A 184
      DHJ(N,KI)=0.                                                      A 185
      R(N,KI)=0.                                                        A 186
      RHR(N,KI)=0.                                                      A 187
4     RHO(N)=RHO(N)+RHOK(N,KI)                                          A 188
      PROM(N)=ROM(N)                                                    A 189
      V(N)=-MGDOTP/(RHO(N)*ETA(N))                                      A 190
      ROCPM(N)=P(N)*200./(RU*T(N))                                      A 191
      DO 5 K=1,KT                                                       A 192
5     PAMGDOT(N,K)=-RHOK(N,K)*V(N)                                      A 193
      DVDX(N)=0.                                                        A 194
6     PRHO(N)=RHO(N)                                                    A 195
      DO 7 N=1,IP                                                       A 196
      TSP(N)=TS(N)                                                      A 197
      PTS(N)=300.                                                       A 198
      IF (N.GT.I) GO TO 7                                               A 199
      PT(N)=300.                                                        A 200
      AP(N)=0.                                                          A 201
      TP(N)=T(N)                                                        A 202
      ETAP(N)=.85                                                       A 203
7     CONTINUE                                                          A 204
      DO 8 N=IP,IZ                                                      A 205
      PTS(N)=300.                                                       A 206
      TSP(N)=TS(N)                                                      A 207
8     CONTINUE                                                          A 208
      QCT=SGMA*EPSS*TS(1)**4+KS(1)*(11.*TS(1)-18.*TS(2)+9.*TS(3)-2.*TS(4  A 209
     1))/(6.*DX1*L)                                                     A 210
      QPT=SGMA*EPSS*TS(1)**4+KS(1)*(11.*TS(1)-18.*TS(2)+9.*TS(3)-2.*TS(4  A 211
```

```
     1))/(6.*DX1*L)                                                    A 212
      GO TO 12                                                         A 213
C     BEGIN ITERATION                                                  A 214
9     CONTINUE                                                         A 215
      IF (NITG.EQ.0) GO TO 12                                          A 216
C     ESTIMATE SOLUTION AT NEXT TIME STEP                              A 217
      DO 11 N=1,IZ                                                     A 218
      TS(N)=TS(N)+YTS(N)*DT                                            A 219
      IF (N.GT.I) GO TO 11                                             A 220
      RHO(N)=RHO(N)+YRHO(N)*DT                                         A 221
      T(N)=T(N)+YT(N)*DT                                               A 222
      P(N)=P(N)+YP(N)*DT                                               A 223
      ETA(N)=ETA(N)+YETA(N)*DT                                         A 224
      DO 10 K=1,KT                                                     A 225
10    RHOK(N,K)=RHOK(N,K)+YRHOK(N,K)*DT                                A 226
11    CONTINUE                                                         A 227
12    NIT=NIT+1                                                        A 228
      RHOSO=RHOST*(1.-ETA(1))                                          A 229
C     DETERMINE HEATING AT BACK SURFACE                                A 230
      QNET=SGMA*EPSP*TS(IZ)**4                                         A 231
C     CHECK ITERATION COUNT- REDUCE TIME STEP IF MAX ITER EXCEEDED     A 232
      IF (NIT.LT.ITR) GO TO 15                                         A 233
      TIME=TIME-DT                                                     A 234
      MGDOT=MGDOTP                                                     A 235
      DO 14 N=1,IZ                                                     A 236
      IF (N.GT.I) GO TO 14                                             A 237
      DO 13 K=1,KT                                                     A 238
13    RHOK(N,K)=RHOKP(N,K)                                             A 239
      T(N)=TP(N)                                                       A 240
      RHO(N)=PRHO(N)                                                   A 241
      P(N)=PP(N)                                                       A 242
      ETA(N)=ETAP(N)                                                   A 243
14    TS(N)=TSP(N)                                                     A 244
      HBRKN2=PHBRKN2                                                   A 245
      HBRKO2=PHBRKO2                                                   A 246
```

```
      L=LPP                                                             A 247
      LP=LPPP                                                           A 248
      DT=.75*DT                                                         A 249
      GO TO 109                                                         A 250
15    CONTINUE                                                          A 251
C                                                                       A 252
C     COMPUTE MASS RATE OF PYROLYSIS GAS GENERATED AT INTERFACE         A 253
C                                                                       A 254
C     CALCULATE PYROLYSIS RATE                                          A 255
C     CHECK IOPTI- IOPTI=1 AND TS(I)=TIBAR USE EQ 3-42 FOR MGDOT        A 256
C                  IOPTI=0 USE EQ 3-44 FOR MGDOT                        A 257
      IF (NIT.GT.1) GO TO 20                                            A 258
      SP=1.                                                             A 259
      IF (TS(I).LE.(TIBAR-6.)) GO TO 16                                 A 260
      SP=(TIBAR-TS(I))/6.                                               A 261
      IF (SP.LT.0.) SP=0.                                               A 262
16    CONTINUE                                                          A 263
      IF ((MGDOT.GT.1.E-5).AND.(NITA.EQ.1)) GO TO 17                    A 264
      NITP=0                                                            A 265
      IF (MGDOT.GT.1.E-3) NITP=1                                        A 266
      IF ((NITP.EQ.1).AND.(NITA.EQ.0)) DT=.0625                         A 267
17    TIME=TIME+DT                                                      A 268
      GO TO 19                                                          A 269
18    MGDOT=AEXP*EXP(-BEXP/TS(I))                                       A 270
19    CONTINUE                                                          A 271
      IF (MGDOT.GT.0.) GO TO 21                                         A 272
      MGDOT=0.                                                          A 273
      IF (IOPTI.EQ.0) GO TO 21                                          A 274
      TS(I)=TS(I)-1.E-4                                                 A 275
20    CONTINUE                                                          A 276
      IF (IOPTI.EQ.0) GO TO 18                                          A 277
      AMGDOT=AEXP*EXP(-BEXP/TS(I))                                      A 278
      BMGDOT=(-KS(I)*(11.*TS(I)-18.*TS(IM)+9.*TS(I-2)-2.*TS(I-3))/(6.*DX A 279
     1*L)-KP(I)*(11.*TS(I)-18.*TS(I+1)+9.*TS(I+2)-2.*TS(I+3))/(6.*DXP1*L A 280
     2P))/DHP                                                           A 281
```

```
      MGDOT=SP*AMGDOT+(1.-SP)*BMGDOT                                    A 282
21    CONTINUE                                                          A 283
      MGDOT=.875*MGDOTP+.125*MGDOT                                      A 284
      IF (NIT.EQ.1) GO TO 22                                            A 285
      GO TO 26                                                          A 286
22    CONTINUE                                                          A 287
      IF (NITC.EQ.0) GO TO 23                                           A 288
      AMDOT(1)=AMDOT(1)*MGDOT/MGDOTP                                    A 289
23    CONTINUE                                                          A 290
C     DETERMINE SURFACE HEATING AND PRESSURE                            A 291
      CALL FTLUP (TIME,QC,MQC,NQC,TIMET,QCTAB)                          A 292
      IF (IOPTP.EQ.1) GO TO 24                                          A 293
      PWP=5.69306E6*RAD*(QC/HE)**2                                      A 294
      GO TO 25                                                          A 295
24    CONTINUE                                                          A 296
      CALL FTLUP (TIME,PW,MSQPT,NSQPT,TMPRES,SQPT)                      A 297
      PW=PW**2                                                          A 298
      PWP=1.013E5*PW                                                    A 299
25    CONTINUE                                                          A 300
      P(1)=PWP                                                          A 301
26    CONTINUE                                                          A 302
      AMDOT(1)=MGDOT                                                    A 303
      DO 27 N=1,NNO                                                     A 304
27    HKTV(N)=HKT(N,8)                                                  A 305
      CALL FTLUP (TS(1),HBRKN2,MNO,NNO,TEMP,HKTV)                       A 306
      DO 28 N=1,NNO                                                     A 307
28    HKTV(N)=HKT(N,13)                                                 A 308
      CALL FTLUP (TS(1),HBRKO2,MNO,NNO,TEMP,HKTV)                       A 309
      HW=.790795*HBRKN2+.209205*HBRKO2                                  A 310
C     CALCULATE SURFACE REMOVAL RATE                                    A 311
C     CHECK IOPT1-  IOPT1=1 AND TS(1)=T1BAR USE EQ 3-41 FOR MSDOT       A 312
C                   IOPT1=0 USE EQ 3-36 FOR MSDOT                       A 313
      IF (NIT.GT.1) GO TO 29                                            A 314
      S=1.                                                              A 315
      IF (TS(1).LE.(T1BAR-22.)) GO TO 29                                A 316
```

```
      S=(T1BAR-TS(1))/22.                                               A 317
      IF (S.LT.0.) S=0.                                                 A 318
29    CONTINUE                                                          A 319
      QCOND=KS(1)*(11.*TS(1)-18.*TS(2)+9.*TS(3)-2.*TS(4))/(6.*DX1*L)    A 320
      KA=AC*EXP(-BC/TS(1))                                              A 321
      AMSDOT=KA*PW*CE*.901/(1.+KA*PW*(HE-HW)/(.032*LAM*QCT))            A 322
      BMSDOT=(QCT+ALPHA*QRS-SGMA*EPSS*TS(1)**4-QCOND)/HC                A 323
      MSDOT=S*AMSDOT+(1.-S)*BMSDOT                                      A 324
      IF (MSDOT.GT.0.) GO TO 30                                         A 325
      MSDOT=0.                                                          A 326
      IF (IOPT.EQ.0) GO TO 30                                           A 327
      TS(1)=TS(1)-1.E-4                                                 A 328
30    CONTINUE                                                          A 329
      MSDOT=.875*MSDOTP+.125*MSDOT                                      A 330
      MPDOT=ALFC*MSDOT+ALFP*AMDOT(1)                                    A 331
C     CALCULATE NET AERODYNAMIC HEATING RATE TO SURFACE- EQ. 3-40       A 332
      QFAC=HE*MPDOT/(QC*.029)                                           A 333
      IF (QFAC.GT.2.25) GO TO 31                                        A 334
      QCT=QC*(1.-HW/HE)*(1.-TREF*TRAB*MPDOT*HE/(QC*.029)-(1.-TRAB)*(.724 A 335
     1*HE/(QC*.029)*MPDOT-.13*(HE*MPDOT/(QC*.029))**2))                 A 336
      GO TO 32                                                          A 337
31    QCT=QC*(1.-HW/HE)*.04                                             A 338
32    CONTINUE                                                          A 339
      Q=QCT+ALPHA*QRS+S*MSDOT*DHC-(1.-S)*MSDOT*HC                       A 340
      DDX=DX1                                                           A 341
C     DETERMINE PROPERTY DATA FOR CHAR LAYER AND PYROLYSIS GASES        A 342
      IF (T(20).GT.1000.) ICHCOM=1                                      A 343
      X=-DDX                                                            A 344
      IF (NIT.GT.1) GO TO 37                                            A 345
      DO 34 N=5,I,5                                                     A 346
      J=N                                                               A 347
      IF (N.EQ.5) J=1                                                   A 348
      NSTEP=J                                                           A 349
      IF (T(J).LT.299.) GO TO 33                                        A 350
C     CALL SUBROUTINE VISC TO COMPUTE VISCOSITY AND PRANDTL NUMBER OF   A 351
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C          PYROLYSIS GASES                                          A 352
      CALL VISC                                                     A 353
33    CONTINUE                                                      A 354
34    CONTINUE                                                      A 355
      DO 35 N=2,9                                                   A 356
      ANJ=(N-1)/9.                                                  A 357
      MU(N)=MU(1)+ANJ*(MU(10)-MU(1))                                A 358
35    PR(N)=PR(1)+ANJ*(PR(10)-PR(1))                                A 359
      DO 36 N=15,I,5                                                A 360
      KON=4                                                         A 361
      APR=(PR(N)-PR(N-5))/5.                                        A 362
      AMU=(MU(N)-MU(N-5))/5.                                        A 363
      DO 36 J=1,4                                                   A 364
      PR(N-KON)=PR(N-5)+J*APR                                       A 365
      MU(N-KON)=MU(N-5)+J*AMU                                       A 366
36    KON=KON-1                                                     A 367
      PMU=MU(I)                                                     A 368
37    CONTINUE                                                      A 369
      DO 53 N=1,I                                                   A 370
      CALL FTLJP (T(N),HK(N,13),MNO,NNO,TEMP,HKTV)                  A 371
      AVGMF(N)=0.                                                   A 372
      DO 38 K=1,KT                                                  A 373
      AVGMF(N)=AVGMF(N)+MFK(N,K)*M(K)                               A 374
38    CONTINUE                                                      A 375
      IF (N.EQ.21) DDX=DX                                           A 376
      X=X+DDX                                                       A 377
      VC(N)=(MSDOT/RHOSO+X*(MGDOT/DRHO-MSDOT/RHOSO))/L              A 378
      IF (NITC.EQ.0) GO TO 39                                       A 379
      IF (ABS(TS(N)-PTS(N)).LT.5.) GO TO 40                         A 380
      PTS(N)=TS(N)                                                  A 381
39    CONTINUE                                                      A 382
      CALL FTLJP (TS(N),HS(N),MNO,NNO,TEMP,HSTT)                    A 383
      IF (NITC.GT.0) GO TO 40                                       A 384
      AVGMFP(N)=AVGMF(N)                                            A 385
      PM(N)=PMV                                                     A 386
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```
      CPS(N)=CPSV                                                       A 387
40    CONTINUE                                                          A 388
      CALL FTLUP (TS(N),KS(N),MKS,NKS,TKS,KST)                          A 389
C     NEGLECT HEAT CONDUCTION IN FLUID                                  A 390
      NSTEP=N                                                           A 391
      IF (ICHCOM.EQ.0) GO TO 41                                         A 392
C     CALL SUBROUTINE CHCOM TO DETERMINE CHEMICAL REACTION RATES OF     A 393
C        EACH SPECIES                                                   A 394
      CALL CHCOM (TIME)                                                 A 395
41    CONTINUE                                                          A 396
      IF (NITC.EQ.0) GO TO 42                                           A 397
      IF (ABS(T(N)-PT(N)).LT.5.) GO TO 50                               A 398
      PT(N)=T(N)                                                        A 399
      IF (T(N).LT.300.) GO TO 43                                        A 400
42    CONTINUE                                                          A 401
43    CONTINUE                                                          A 402
      CALL FTLUP (T(N),HST(N),MNO,NNO,TEMP,HSTT)                        A 403
      DO 45 K=1,KM                                                      A 404
      DO 44 J=1,NNO                                                     A 405
      CPKTV(J)=CPKT(J,K)                                                A 406
      HKTV(J)=HKT(J,K)                                                  A 407
44    CONTINUE                                                          A 408
      CALL FTLUP (T(N),HK(N,K),MNO,NNO,TEMP,HKTV)                       A 409
      CALL FTLUP (T(N),CPK(N,K),MNO,NNO,TEMP,CPKTV)                     A 410
      CALL FTLUP (TS(N),DHK(N,K),MNO,NNO,TEMP,HKTV)                     A 411
45    CONTINUE                                                          A 412
      NITS=0                                                            A 413
46    CONTINUE                                                          A 414
      IF (T(N).GT.1500.) GO TO 47                                       A 415
      CPK(N,11)=(2.882035E00+2.*5.16099E-03*T(N)+3.*3.971480E-06*T(N)**2  A 416
     1-4.*3.708198E-09*T(N)**3+5.*8.949908E-13*T(N)**4)*RU              A 417
      CPK(N,12)=(3.511186E-01+2.*1.876996E-02*T(N)-3.*2.649069E-06*T(N)*  A 418
     1*2-4.*1.877262E-09*T(N)**3+5.*6.077093E-13*T(N)**4)*RU            A 419
      HK(N,11)=(2.882035E00*T(N)+5.160995E-03*T(N)**2+3.971480E-06*T(N)*  A 420
     1*3-3.708198E-09*T(N)**4+8.949908E-13*T(N)**5)*RU-1.157984E04      A 421
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      HK(N,12)=(3.511186E-01*T(N)+1.876996E-02*T(N)**2-2.649069E-05*T(N)   A 422
     1**3-1.877262E-09*T(N)**4+6.077093E-13*T(N)**5)*RU+1.143849E04        A 423
      GO TO 48                                                             A 424
47    CPK(N,11)=(1.430804E00+2.*9.444913E-03*T(N)-3.*2.348033E-06*T(N)**   A 425
     12-4.*2.968006E-10*T(N)**3-5.*1.489961E-14*T(N)**4)*RJ                A 426
      CPK(N,12)=(4.619871E00+2.*1.440481E-02*T(N)-3.*3.748451E-06*T(N)**   A 427
     12+4.*4.894085E-10*T(N)**3-5.*2.515503E-14*T(N)**4)*RU                A 428
      HK(N,11)=(1.430804E00*T(N)+9.444913E-03*T(N)**2-2.348033E-06*T(N)*   A 429
     1*3-2.968006E-10*T(N)**4-1.489961E-14*T(N)**5)*RU-1.157984E04         A 430
      HK(N,12)=(4.619871E00*T(N)+1.440481E-02*T(N)**2-3.748451E-06*T(N)*   A 431
     1*3+4.894085E-10*T(N)**4-2.515503E-14*T(N)**5)*RU+1.143849E04         A 432
48    CONTINUE                                                             A 433
      IF (NITS.EQ.1) GO TO 49                                              A 434
      TSAVE=T(N)                                                           A 435
      CPSA11=CPK(N,11)                                                     A 436
      CPSA12=CPK(N,12)                                                     A 437
      HSA11=HK(N,11)                                                       A 438
      HSA12=HK(N,12)                                                       A 439
      T(N)=TS(N)                                                           A 440
      NITS=NITS+1                                                          A 441
      GO TO 46                                                             A 442
49    T(N)=TSAVE                                                           A 443
      DHK(N,11)=HK(N,11)                                                   A 444
      DHK(N,12)=HK(N,12)                                                   A 445
      HK(N,11)=HSA11                                                       A 446
      HK(N,12)=HSA12                                                       A 447
      CPK(N,11)=CPSA11                                                     A 448
      CPK(N,12)=CPSA12                                                     A 449
      DHJ(N,6)=2.*DHK(N,5)-HK(N,9)-HS(N)                                   A 450
      DHJ(N,7)=DHK(N,5)+DHK(N,2)-HK(N,6)-HS(N)                             A 451
      DHJ(N,9)=DHK(N,10)+DHK(N,2)-HK(N,7)-HS(N)                            A 452
50    CONTINUE                                                             A 453
      HRJSUM(N)=0.                                                         A 454
      HRSUM(N)=0.                                                          A 455
      RM(N)=0.                                                             A 456
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      ROCPM(N)=0.                                                       A 457
      ROHM(N)=0.                                                        A 458
      DO 51 K=1,KT                                                      A 459
51    RM(N)=RM(N)+R(N,K)*M(K)                                           A 460
      DO 52 K=1,KT                                                      A 461
      HRJSUM(N)=HRJSUM(N)+RHR(N,K)*DHJ(N,K)                             A 462
      HRSUM(N)=HRSUM(N)+R(N,K)*HK(N,K)                                  A 463
      ROHM(N)=ROHM(N)+RHOK(N,K)*HK(N,K)/M(K)                            A 464
52    ROCPM(N)=ROCPM(N)+RHOK(N,K)*CPK(N,K)/M(K)                         A 465
53    CONTINUE                                                          A 466
      DMBRDX(1)=(-11.*AVGMF(1)+18.*AVGMF(2)-9.*AVGMF(3)+2.*AVGMF(4))/(6.  A 467
     1*DX1)                                                             A 468
      DTDX(1)=(-11.*T(1)+18.*T(2)-9.*T(3)+2.*T(3))/(6.*DX1)             A 469
      DDX=DX1                                                           A 470
      DO 55 N=2,IM                                                      A 471
      IF (N.EQ.20) GO TO 54                                             A 472
      DMBRDX(N)=(AVGMF(N+1)-AVGMF(N-1))/(2.*DDX)                        A 473
      DTDX(N)=(T(N+1)-T(N-1))/(2.*DDX)                                  A 474
      GO TO 55                                                          A 475
54    DMBRDX(N)=(DX1**2*AVGMF(N+1)-(DX1**2-DX**2)*AVGMF(N)-DX**2*AVGMF(N  A 476
     1-1))/(DX1*DX*(DX1+DX))                                            A 477
      DTDX(N)=(DX1**2*T(N+1)-(DX1**2-DX**2)*T(N)-DX**2*T(N-1))/(DX1*DX*(  A 478
     1DX1+DX))                                                          A 479
      DDX=DX                                                            A 480
55    CONTINUE                                                          A 481
      DMBRDX(I)=(11.*AVGMF(I)-18.*AVGMF(IM)+9.*AVGMF(I-2)-2.*AVGMF(I-3))  A 482
     1/(6.*DX)                                                          A 483
      DTDX(I)=(11.*T(I)-18.*T(IM)+9.*T(I-2)-2.*T(I-3))/(6.*DX)          A 484
      PPM=PM(I)                                                         A 485
C     DETERMINE PROPERTIES OF UNCHARRED LAYER AND INSULATION LAYER      A 486
      DO 57 N=1,IP                                                      A 487
      IF (NITC.EQ.0) GO TO 56                                           A 488
      IF (ABS(TS(N)-PTS(N)).LT.5.) GO TO 57                             A 489
      PTS(N)=TS(N)                                                      A 490
56    CONTINUE                                                          A 491
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      CALL FTLUP (TS(N),KP(N),MKP,NKP,TKP,KPT)                          A 492
      CALL FTLUP (TS(N),CPP(N),MCPP,NCPP,TCPP,CPPT)                     A 493
      RHOP(N)=576.                                                      A 494
57    CONTINUE                                                          A 495
      IF (NITC.GT.0) GO TO 60                                           A 496
      DO 58 N=1,I                                                       A 497
      HA(N)=PROPC*ROCPM(N)*V(N)/PR(N)                                   A 498
58    CONTINUE                                                          A 499
      DO 59 N=IP,IZ                                                     A 500
      KPP(N)=KPPV                                                       A 501
      CPPP(N)=CPPPV                                                     A 502
      RHOPP(N)=RHOPPV                                                   A 503
59    CONTINUE                                                          A 504
      KPPPIP=KPP(IP)                                                    A 505
      KPPPIZ=KPP(IZ)                                                    A 506
      KSP1=KS(1)                                                        A 507
      KSPI=KS(I)                                                        A 508
      KPPI=KP(I)                                                        A 509
      KPPIP=KP(IP)                                                      A 510
60    CONTINUE                                                          A 511
      DKSDX(1)=(-11.*KS(1)+18.*KS(2)-9.*KS(3)+2.*KS(4))/(6.*DX1)        A 512
      DKSDX(I)=(11.*KS(I)-18.*KS(IM)+9.*KS(I-2)-2.*KS(I-3))/(6.*DX)     A 513
      DDX=DX1                                                           A 514
      DO 62 N=2,IM                                                      A 515
      IF (N.EQ.20) GO TO 61                                             A 516
      DKSDX(N)=(KS(N+1)-KS(N-1))/(2.*DDX)                               A 517
      GO TO 62                                                          A 518
61    DDX=DX                                                            A 519
      DKSDX(20)=(DX1**2*KS(21)+(DX**2-DX1**2)*KS(20)-DX**2*KS(19))/(DX1* A 520
     1DX*(DX1+DX))                                                      A 521
62    CONTINUE                                                          A 522
      DKPDX(I)=(-11.*KP(I)+18.*KP(IN)-9.*KP(IN2)+2.*KP(I+4))/(6.*DXP1)  A 523
      DKPDX(IP)=(11.*KP(IP)-18.*KP(IO1)+9.*KP(IO)-2.*KP(IP-3))/(6.*DXP) A 524
      DDX=DXP1                                                          A 525
      DO 64 N=IN,IO1                                                    A 526
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      IF (N.EQ.(I+20)) GO TO 63                                         A 527
      DKPDX(N)=(KP(N+1)-KP(N-1))/(2.*DXP)                               A 528
      GO TO 64                                                          A 529
63    DKPDX(I+20)=(DXP1**2*KP(I+21)+(DXP**2-DXP1**2)*KP(I+20)-DXP**2*KP(  A 530
     1I+19))/(DXP1*DXP*(DXP1+DXP))                                      A 531
      DDX=DXP                                                           A 532
64    CONTINUE                                                          A 533
C                                                                       A 534
C     SOLUTION OF PARTIAL DIFFERENTIAL EQUATION FOR CHAR LAYER          A 535
C                                                                       A 536
C     CALCULATE COEFFICIENTS IN DIFFERENTIAL EQ FOR SOLID TEMPERATURE   A 537
      DO 66 N=1,I                                                       A 538
      ATS(N)=TS(N)                                                      A 539
      ALPHA1(N)=(DKSDX(N)+L**2*(1.-ETA(N))*CPS(N)*RHOST/MS*VC(N))/KS(N) A 540
      ALPHA2(N)=0.                                                      A 541
      ALPHA3(N)=L**2/KS(N)*(HA(N)*(TP(N)-TSP(N))+ETA(N)*(HST(N)*RS(N)+RH  A 542
     1S(N)*HS(N)-HRJSUM(N))+RHOST*HS(N)/MS*((ETA(N)-ETAP(N))/DT-VC(N)*DE  A 543
     2TADX(N)))                                                         A 544
      ALPHA4(N)=-(1.-ETA(N))*L**2*RHOST*CPS(N)/(MS*KS(N))               A 545
      IF (NITC.NE.0) GO TO 65                                           A 546
      ALPHP1(N)=ALPHA1(N)                                               A 547
      ALPHP2(N)=ALPHA2(N)                                               A 548
      ALPHP3(N)=ALPHA3(N)                                               A 549
      ALPHP4(N)=ALPHA4(N)                                               A 550
65    CONTINUE                                                          A 551
      ALPHB3(N)=CRNI*ALPHA3(N)+(1.-CRNI)*ALPHP3(N)                      A 552
      ALPHB4(N)=CRNI*ALPHA4(N)+(1.-CRNI)*ALPHP4(N)                      A 553
66    CONTINUE                                                          A 554
      IF (NITC.NE.0) GO TO 67                                           A 555
      ALPHIP1=ALPHA1(I)                                                 A 556
      ALPHIP2=ALPHA2(I)                                                 A 557
      ALPHIP3=ALPHA3(I)                                                 A 558
      ALPHIP4=ALPHA4(I)                                                 A 559
67    CONTINUE                                                          A 560
      ALPHI1=ALPHA1(I)                                                  A 561
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      ALPHI2=ALPHA2(I)                                                  A 562
      ALPHI3=ALPHA3(I)                                                  A 563
      ALPHI4=ALPHA4(I)                                                  A 564
      DDX=DXP1                                                          A 565
      XP=0.                                                             A 566
      DO 68 N=I,IP                                                      A 567
      IF (N.EQ.(I+20)) DDX=DXP                                          A 568
      ATS(N)=TS(N)                                                      A 569
      ALPHA1(N)=(DKPDX(N)+LP*RHOP(N)*CPP(N)*MGDOT*(1.-XP)/DRHO)/KP(N)   A 570
      XP=XP+DDX                                                         A 571
      ALPHA2(N)=0.                                                      A 572
      ALPHA3(N)=0.                                                      A 573
      ALPHA4(N)=-RHOP(N)*CPP(N)*LP**2/KP(N)                             A 574
      ALPHB3(N)=0.                                                      A 575
      IF (NITC.NE.0) GO TO 68                                           A 576
      ALPHP1(N)=ALPHA1(N)                                               A 577
      ALPHP2(N)=ALPHA2(N)                                               A 578
      ALPHP3(N)=ALPHA3(N)                                               A 579
      ALPHP4(N)=ALPHA4(N)                                               A 580
68    ALPHB4(N)=CRNI*ALPHA4(N)+(1.-CRNI)*ALPHP4(N)                      A 581
      IF (NITC.NE.0) GO TO 69                                           A 582
      GAMMIP1=ALPHA1(I)                                                 A 583
      GAMMIP2=ALPHA2(I)                                                 A 584
      GAMMIP3=ALPHA3(I)                                                 A 585
      GAMMIP4=ALPHA4(I)                                                 A 586
      GAMIPP1=ALPHA1(IP)                                                A 587
      GAMIPP2=ALPHA2(IP)                                                A 588
      GAMIPP3=ALPHA3(IP)                                                A 589
      GAMIPP4=ALPHA4(IP)                                                A 590
69    CONTINUE                                                          A 591
      GAMMI1=ALPHA1(I)                                                  A 592
      GAMMI2=ALPHA2(I)                                                  A 593
      GAMMI3=ALPHA3(I)                                                  A 594
      GAMMI4=ALPHA4(I)                                                  A 595
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      GAMIP1=ALPHA1(IP)                                                 A 596
      GAMIP2=ALPHA2(IP)                                                 A 597
      GAMIP3=ALPHA3(IP)                                                 A 598
      GAMIP4=ALPHA4(IP)                                                 A 599
      DO 71 N=IP,IZ                                                     A 600
      ATS(N)=TS(N)                                                      A 601
      ALPHA1(N)=0.                                                      A 602
      ALPHA2(N)=0.                                                      A 603
      ALPHA3(N)=0.                                                      A 604
      ALPHA4(N)=-RHOPP(N)*CPPP(N)*IL**2/KPP(N)                          A 605
      IF (NITC.NE.0) GO TO 70                                           A 606
      ALPHP1(N)=ALPHA1(N)                                               A 607
      ALPHP2(N)=ALPHA2(N)                                               A 608
      ALPHP3(N)=ALPHA3(N)                                               A 609
      ALPHP4(N)=ALPHA4(N)                                               A 610
      ALPHB3(N)=0.                                                      A 611
70    CONTINUE                                                          A 612
71    ALPHB4(N)=CRNI*ALPHA4(N)+(1.-CRNI)*ALPHP4(N)                      A 613
      IF (NITC.NE.0) GO TO 72                                           A 614
      KAPIPP1=ALPHA1(IP)                                                A 615
      KAPIPP2=ALPHA2(IP)                                                A 616
      KAPIPP3=ALPHA3(IP)                                                A 617
      KAPIPP4=ALPHA4(IP)                                                A 618
72    CONTINUE                                                          A 619
      KAPIP1=ALPHA1(IP)                                                 A 620
      KAPIP2=ALPHA2(IP)                                                 A 621
      KAPIP3=ALPHA3(IP)                                                 A 622
      KAPIP4=ALPHA4(IP)                                                 A 623
C     CALL SUBROUTINE PDE1 TO SOLVE FOR TS                              A 624
      CALL PDE1 (TS,CRNI)                                               A 625
C     CALCULATE COEFFICIENTS IN DIFFERENTIAL EQ FOR P                   A 626
      DDX=DX1                                                           A 627
      DO 74 N=1,I                                                       A 628
      AP(N)=P(N)                                                        A 629
      IF (N.EQ.1) GO TO 74                                              A 630
      PAL2(N)=2.*MU(N)*ETA(N)*L**2/(PM(N)*RHO(N)*RU*T(N))*(AVGMF(N)*(T(N  A 631
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```
     1)-TP(N))/(DT*T(N))-AVGMF(N)*VC(N)*DTDX(N)/T(N)+VC(N)*DMBRDX(N)-(AV
     2GMF(N)-AVGMFP(N))/DT)
      PAL3(N)=2.*MU(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)*RU*T(N))
      IF (N.EQ.I) GO TO 74
      IF (N.EQ.20) GO TO 73
      PAL1(N)=MU(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)*RU*T(N))*VC(N
     3)
      GO TO 74
73    CONTINUE
      DDX=DX
      PAL1(20)=MU(20)*ETA(20)*T(20)/(PM(20)*AVGMF(20))*(DX1**2*PM(21)*AV
     1GMF(21)/(MU(21)*ETA(21)*T(21))-(DX1**2-DX**2)*PM(20)*AVGMF(20)/(MU
     2(20)*ETA(20)*T(20))-DX**2*PM(19)*AVGMF(19)/(MU(19)*ETA(19)*T(19)))
     3/(DX1*DX*(DX1+DX))+MU(20)*ETA(20)*AVGMF(20)*L**2/(PM(20)*RHO(20)*T
     4(20)*RU)*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(IM)*AVGMF(IM)/(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)/(
     3MU(I-3)*ETA(I-3)*T(I-3)))/(6.*DX)+MU(I)*ETA(I)*AVGMF(I)*L**2*VC(I)
     4/(PM(I)*RHO(I)*RU*T(I))
      DO 76 N=2,I
      IF (NITC.GT.0) GO TO 75
      PAP1(N)=0.
      PAP2(N)=0.
      PAP3(N)=0.
      PAP4(N)=0.
75    PAB3(N)=CRNI*PAL3(N)+(1.-CRNI)*PAP3(N)
76    PAB4(N)=CRNI*PAL4(N)+(1.-CRNI)*PAP4(N)
C     CALL SUBROUTINE PDP TO SOLVE FOR P
      CALL PDP (CRNI,DT,L,DX,DX1,MGDOT,MGDOTP,LPP,I,IM,RHO,P,MU,T,TP,RU)
C     CALCULATE LOCAL PYROLYSIS GAS DENSITY
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```
      DO 77 N=1,I                                                       A 667
      RHO(N)=P(N)*AVGMF(N)/(RU*T(N))                                    A 668
77    CONTINUE                                                          A 669
      DRODX(1)=(-11.*RHO(1)+18.*RHO(2)-9.*RHO(3)+2.*RHO(4))/(6.*DX1)    A 670
      DDX=DX1                                                           A 671
      DO 79 N=2,IM                                                      A 672
      IF (N.EQ.20) GO TO 78                                             A 673
      DRODX(N)=(RHO(N+1)-RHO(N-1))/(2.*DDX)                             A 674
      GO TO 79                                                          A 675
78    DDX=DX                                                            A 676
      DRODX(N)=(DX1**2*RHO(N+1)+(DX**2-DX1**2)*RHO(N)-DX**2*RHO(N-1))/(D A 677
     1X1*DX*(DX1+DX))                                                   A 678
79    CONTINUE                                                          A 679
      DRODX(I)=(11.*RHO(I)-18.*RHO(IM)+9.*RHO(I-2)-2.*RHO(I-3))/(6.*DX) A 680
C     CHECK PYROLYSIS RATE-  IF LESS THAN MIN NEGLECT THERMAL NON-      A 681
C        EQUILIBRIUM OF PYROLYSIS GASES AND CHAR LAYER AND CHEMICAL     A 682
C        REACTIONS                                                      A 683
      IF (NITP.GT.0) GO TO 81                                           A 684
      DO 80 N=1,I                                                       A 685
      ETA(N)=ETA(I)                                                     A 686
      AT(N)=T(N)                                                        A 687
      T(N)=TS(N)                                                        A 688
      AMDOT(N)=MGDOT                                                    A 689
      V(N)=-MGDOT/(RHO(N)*ETA(N))                                       A 690
      DO 80 K=1,KT                                                      A 691
      RHOK(N,K)=MFK(N,K)*RHO(N)*M(K)/AVGMF(N)                           A 692
80    CONTINUE                                                          A 693
      GO TO 101                                                         A 694
81    CONTINUE                                                          A 695
C     CALCULATE LOCAL MASS FLOW RATE OF PYROLYSIS GASES                 A 696
      AINT1(IM)=DX/2.*(ETA(I)*RHO(I)+ETA(IM)*RHO(IM))                   A 697
      AINT3(IM)=DX/2.*(ETA(I)*((RHO(I)-PRHO(I))/DT-RM(I))+RHO(I)*(ETA(I) A 698
     1-ETAP(I))/DT+ETA(IM)*((RHO(IM)-PRHO(IM))/DT-RM(IM))+RHO(IM)*(ETA(I A 699
     2M)-ETAP(IM))/DT)                                                  A 700
      KON=I-2                                                           A 701
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      DDX=DX                                                            A 702
      DO 83 N=3,I                                                       A 703
      IF (KON.EQ.19) GO TO 82                                           A 704
      AINT1(KON)=AINT1(KON+2)+DDX/3.*(ETA(KON+2)*RHO(KON+2)+4.*ETA(KON+1  A 705
     1)*RHO(KON+1)+ETA(KON)*RHO(KON))                                   A 706
      AINT3(KON)=AINT3(KON+2)+DDX/3.*(ETA(KON+2)*((RHO(KON+2)-PRHO(KON+2  A 707
     1))/DT-RM(KON+2))+RHO(KON+2)*(ETA(KON+2)-ETAP(KON+2))/DT+4.*(ETA(KO  A 708
     2N+1)*((RHO(KON+1)-PRHO(KON+1))/DT-RM(KON+1))+RHO(KON+1)*(ETA(KON+1  A 709
     3)-ETAP(KON+1))/DT)+ETA(KON)*((RHO(KON)-PRHO(KON))/DT-RM(KON))+RHO(  A 710
     4KON)*(ETA(KON)-ETAP(KON))/DT)                                     A 711
      GO TO 83                                                          A 712
82    DDX=DX1                                                           A 713
      AINT1(KON)=AINT1(KON+1)+DDX/2.*(ETA(KON+1)*RHO(KON+1)+ETA(KON)*RHO  A 714
     1(KON))                                                            A 715
      AINT3(KON)=AINT3(KON+1)+DDX/2.*(ETA(KON+1)*((RHO(KON+1)-PRHO(KON+1  A 716
     1))/DT-RM(KON))+RHO(KON+1)*(ETA(KON+1)-ETAP(KON+1))/DT+ETA(KON)*((R  A 717
     2HO(KON)-PRHO(KON))/DT-RM(KON))+RHO(KON)*(ETA(KON)-ETAP(KON))/DT)  A 718
83    KON=KON-1                                                         A 719
      DO 84 N=1,IM                                                      A 720
      AMDOT(N)=MGDOT+L*(VC(I)*ETA(I)*RHO(I)-VC(N)*ETA(N)*RHO(N))-L*AINT3  A 721
     1(N)-(MGDOT/DRHO-MSDOT/RHOSO)*AINT1(N)                             A 722
84    KON=KON-1                                                         A 723
      DO 85 N=1,I                                                       A 724
      V(N)=-AMDOT(N)/(RHO(N)*ETA(N))                                    A 725
85    CONTINUE                                                          A 726
      DO 86 N=1,I                                                       A 727
86    DVDX(N)=L*((VC(N)-V(N)/L)*(DRODX(N)/RHO(N)+DETADX(N)/ETA(N))-((RHO  A 728
     1(N)-PRHO(N))/(DT*RHO(N))+(ETA(N)-ETAP(N))/(DT*ETA(N))+RM(N)/RHO(N)  A 729
     2))                                                                A 730
      DO 91 K=1,KT                                                      A 731
      NRHOK(K)=0.                                                       A 732
      DO 87 N=1,I                                                       A 733
      IF ((MFK(N,K).GT.1.E-5).OR.(R(N,K).GT.1.E-5)) NRHOK(K)=1          A 734
87    CONTINUE                                                          A 735
      IF (NRHOK(K).EQ.0) GO TO 91                                       A 736
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      ARH(I)=M(K)*MFKI(K)*MGDOT/(AVGMF(I)*ETA(I))                       A 737
C     CALCULATE COEFFICIENTS IN SPECIES CONTINUITY EQ                   A 738
      DO 89 N=1,I                                                       A 739
      BRH(N)=PAMGDOT(N,K)                                               A 740
      DEN=ETA(N)*(VC(N)-V(N)/L)                                         A 741
      DEL1(N,K)=DETADX(N)/ETA(N)-(ETA(N)*VC(N)/V(N)*DVDX(N)+(ETA(N)-ETAP A 742
     1(N))/DT)/DEN                                                      A 743
      DEL2(N,K)=V(N)*ETA(N)*((RHOK(N,K)-RHOKP(N,K))/DT-R(N,K)*M(K))/DEN A 744
      DEL3(N)=0.                                                        A 745
      IF (NITA.GT.0) GO TO 88                                           A 746
      DEP1(N,K)=DEL1(N,K)                                               A 747
      DEP2(N,K)=DEL2(N,K)                                               A 748
      DEP3(N)=DEL3(N)                                                   A 749
88    DEB2(N,K)=CRNI*DEL2(N,K)+(1.-CRNI)*DEP2(N,K)                      A 750
      DEB3(N)=CRNI*DEL3(N)+(1.-CRNI)*DEP3(N)                            A 751
      AL1(N)=DEL1(N,K)                                                  A 752
      AP1(N)=DEP1(N,K)                                                  A 753
      AB2(N)=DEB2(N,K)                                                  A 754
89    CONTINUE                                                          A 755
C                                                                       A 756
C     COMPUTE GAS DENSITY THROUGH CHAR LAYER                            A 757
C                                                                       A 758
C     CALL SUBROUTINE PDE2 TO SOLVE FOR THE LOCAL MASS FLOW OF          A 759
C        SPECIES                                                        A 760
      CALL PDE2 (AL1,AB2,AB3,AP1,BRH,ARH,CRNI,DX,DX1,DT,I)              A 761
      DO 90 N=1,I                                                       A 762
      IF (ARH(N).LT.1.E-100) ARH(N)=1.E-100                             A 763
      RHOK(N,K)=.875*RHOKP(N,K)-.125*ARH(N)/V(N)                        A 764
90    CONTINUE                                                          A 765
91    CONTINUE                                                          A 766
      DO 92 N=1,I                                                       A 767
      ROM(N)=0.                                                         A 768
      DO 92 K=1,KT                                                      A 769
92    ROM(N)=ROM(N)+RHOK(N,K)/M(K)                                      A 770
      DO 93 N=1,IM                                                      A 771
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      DO 93 K=1,KT                                                      A 772
93    MFK(N,K)=RHOK(N,K)/(ROM(N)*M(K))                                  A 773
C     CALCULATE COEFFICIENTS IN PYROLYSIS GAS TEMPERATURE DIFFERENTIAL  A 774
C        EQUATION                                                       A 775
      DO 95 N=1,I                                                       A 776
      AT(N)=T(N)                                                        A 777
      DEN=ETA(N)*(V(N)/L-VC(N))*(ROCPM(N)-RHO(N)*RU/AVGMF(N))           A 778
      BETA1(N)=(HA(N)*TP(N)/T(N)-ETA(N)*RU*((ROM(N)-PROM(N))/DT+(V(N)/L-  A 779
     1VC(N))*(DRODX(N)/AVGMF(N)-RHO(N)*DMBRDX(N)/AVGMF(N)**2))-RHO(N)*RU  A 780
     2*((ETA(N)-ETAP(N))/DT-VC(N)*DETADX(N))/AVGMF(N))/DEN              A 781
      BETA2(N)=(ETA(N)*(HRSUM(N)-V(N)**2/2.*RM(N)+RS(N)*HST(N)+RHS(N)*HS  A 782
     1(N)-HRJSUM(N))-HA(N)*TSP(N))/DEN                                  A 783
      BETA3(N)=ETA(N)*(ROCPM(N)-RHO(N)*RU/AVGMF(N))/DEN                 A 784
      IF (NITA.GT.0) GO TO 94                                           A 785
      BETP1(N)=BETA1(N)                                                 A 786
      BETP2(N)=BETA2(N)                                                 A 787
      BETP3(N)=BETA3(N)                                                 A 788
94    CONTINUE                                                          A 789
      BETB2(N)=CRNI*BETA2(N)+(1.-CRNI)*BETP2(N)                         A 790
      BETB3(N)=CRNI*BETA3(N)+(1.-CRNI)*BETP3(N)                         A 791
95    CONTINUE                                                          A 792
      T(I)=TS(I)                                                        A 793
C     CALL SUBROUTINE PDE2 TO SOLVE FOR T                               A 794
      CALL PDE2 (BETA1,BETB2,BETB3,BETP1,TP,T,CRNI,DX,DX1,DT,I)         A 795
      DO 96 N=1,I                                                       A 796
C     CALCULATE COEFFICIENTS IN POROSITY DIFFERENTIAL EQUATION          A 798
96    T(N)=.875*TP(N)+.125*T(N)                                         A 797
      DO 98 N=1,I                                                       A 799
      EPSA1(N)=-MS*(RHS(N)+RS(N))/(RHOST*VC(N))                         A 800
      EPSA2(N)=0.                                                       A 801
      EPSA3(N)=-1./VC(N)                                                A 802
      IF (NITA.NE.0) GO TO 97                                           A 803
      EPSP1(N)=EPSA1(N)                                                 A 804
      EPSP3(N)=EPSA3(N)                                                 A 805
97    CONTINUE                                                          A 806
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      EPSB3(N)=CRNI*EPSA3(N)+(1.-CRNI)*EPSP3(N)                         A 807
98    CONTINUE                                                          A 808
C     CALL SUBROUTINE PDE2 TO SOLVE FOR ETA                             A 809
      CALL PDE2 (EPSA1,EPSB2,EPSB3,EPSP1,ETAP,ETA,CRNI,DX,DX1,DT,I)     A 810
      DETADX(1)=(-11.*ETA(1)+18.*ETA(2)-9.*ETA(3)+2.*ETA(4))/(6.*DX1)   A 811
      DDX=DX1                                                           A 812
      DO 100 N=2,IM                                                     A 813
      IF (N.EQ.20) GO TO 99                                             A 814
      DETADX(N)=(ETA(N+1)-ETA(N-1))/(2.*DDX)                            A 815
      GO TO 100                                                         A 816
99    DDX=DX                                                            A 817
      DETADX(20)=(DX1**2*ETA(21)-(DX1**2-DX**2)*ETA(20)-DX**2*ETA(19))/(  A 818
     1DX1*DX*(DX1+DX))                                                  A 819
100   CONTINUE                                                          A 820
      DETADX(I)=(11.*ETA(I)-18.*ETA(IM)+9.*ETA(I-2)-2.*ETA(I-3))/(6.*DX)  A 821
      NITA=1                                                            A 822
101   CONTINUE                                                          A 823
      NITC=1                                                            A 824
C     CALCULATE NEW THICKNESS VALUES FOR CHARRED AND UNCHARRED LAYERS   A 825
      DLP=(MGDOTP/DRHO+4.*(CRNI*MGDOT+(1.-CRNI)*MGDOTP)/DRHO+MGDOT/DRHO)  A 826
     1*DT/6.                                                            A 827
      DL=DLP-(MSDOTP/(1.-ETAP(1))+4.*(CRNI*MSDOT/(1.-ETA(1))+(1.-CRNI)*M  A 828
     1SDOTP/(1.-ETAP(1)))+MSDOT/(1.-ETA(1)))*DT/(6.*RHOST)              A 829
      LP=LPPP-DLP                                                       A 830
      IF (LP.LT.LPMIN) GO TO 110                                        A 831
      L=LPP+DL                                                          A 832
C     CHECK SOLUTIONS-  IF NO CHECK ITERATE AGAIN                       A 833
      DO 102 N=1,IZ                                                     A 834
      IF (ABS((TS(N)-ATS(N))/TS(N)).GT.DIFER) GO TO 12                  A 835
      IF (N.GT.I) GO TO 102                                             A 836
      IF (ABS((P(N)-AP(N))/P(N)).GT.DIFER) GO TO 12                     A 837
      IF (ABS((T(N)-AT(N))/T(N)).GT.DIFER) GO TO 12                     A 838
102   CONTINUE                                                          A 839
      PART=2.*DIFER*TS(1)                                               A 840
      NITG=0                                                            A 841
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      IF (ABS(TS(1)-TSP(1)).GT.PART) NITG=1                             A 842
      IF (ABS(TIME-PTIME-PRNTFRQ).LE.DT/2.) GO TO 103                   A 843
      IF ((TIME-PTIME-PRNTFRQ).GT.0.) GO TO 103                         A 844
      GO TO 105                                                         A 845
103   CONTINUE                                                          A 846
      QRAT=Q/QC                                                         A 847
C     PRINT RESULTS                                                     A 848
      WRITE (2,112) TIME,DT,NIT,TS(1),T(1),QRAT,MSDOT,MGDOT,AMDOT(1),L,L  A 849
     1P                                                                 A 850
      WRITE (2,118)                                                     A 851
      WRITE (2,120) (TS(N),N=1,IZ)                                      A 852
      WRITE (2,113)                                                     A 853
      WRITE (2,120) (ETA(N),N=1,I)                                      A 854
      WRITE (2,117)                                                     A 855
      WRITE (2,120) (T(N),N=1,I)                                        A 856
      WRITE (2,119)                                                     A 857
      WRITE (2,120) (P(N),N=1,I)                                        A 858
      WRITE (2,114)                                                     A 859
      DO 104 K=1,KT                                                     A 860
      WRITE (2,111) SPECIES(K)                                          A 861
      WRITE (2,120) (MFK(N,K),N=1,I)                                    A 862
104   CONTINUE                                                          A 863
      WRITE (2,115)                                                     A 864
      WRITE (2,120) (AVGMF(N),N=1,I)                                    A 865
      WRITE (2,116)                                                     A 866
      WRITE (2,120) (AMDOT(N),N=1,I)                                    A 867
      PTIME=PTIME+10.                                                   A 868
105   CONTINUE                                                          A 869
C     IF SOLUTIONS CHECK RETAIN CURRENT VALUES OF PARAMETERS            A 870
      DO 108 N=1,IZ                                                     A 871
      YTS(N)=(TS(N)-TSP(N))/DT                                          A 872
      IF (N.GT.I) GO TO 107                                             A 873
      YETA(N)=(ETA(N)-ETAP(N))/DT                                       A 874
      YRHO(N)=(RHO(N)-PRHO(N))/DT                                       A 875
      YP(N)=(P(N)-PP(N))/DT                                             A 876
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      PAP1(N)=PAL1(N)                                                   A 877
      PAP2(N)=PAL2(N)                                                   A 878
      PAP3(N)=PAL3(N)                                                   A 879
      PAP4(N)=PAL4(N)                                                   A 880
      PROM(N)=ROM(N)                                                    A 881
      PRHO(N)=RHO(N)                                                    A 882
      AVGMFP(N)=AVGMF(N)                                                A 883
      PP(N)=P(N)                                                        A 884
      EPSP1(N)=EPSA1(N)                                                 A 885
      EPSP3(N)=EPSA3(N)                                                 A 886
      BETP1(N)=BETA1(N)                                                 A 887
      BETP2(N)=BETA2(N)                                                 A 888
      BETP3(N)=BETA3(N)                                                 A 889
      YT(N)=(T(N)-TP(N))/DT                                             A 890
      DEP3(N)=DEL3(N)                                                   A 891
      DO 106 K=1,KT                                                     A 892
      DEP1(N,K)=DEL1(N,K)                                               A 893
      DEP2(N,K)=DEL2(N,K)                                               A 894
      YRHOK(N,K)=(RHOK(N,K)-RHOKP(N,K))/DT                              A 895
      PAMGDOT(N,K)=-RHOK(N,K)*V(N)                                      A 896
106   RHOKP(N,K)=RHOK(N,K)                                              A 897
      HA(N)=ABS(PROPC*ROCPM(N)*V(N)/PR(N))                              A 898
      TP(N)=T(N)                                                        A 899
      ETAP(N)=ETA(N)                                                    A 900
107   CONTINUE                                                          A 901
      ALPHP1(N)=ALPHA1(N)                                               A 902
      ALPHP2(N)=ALPHA2(N)                                               A 903
      ALPHP3(N)=ALPHA3(N)                                               A 904
      ALPHP4(N)=ALPHA4(N)                                               A 905
108   TSP(N)=TS(N)                                                      A 906
      MSDOTP=MSDOT                                                      A 907
      ALPHIP1=ALPHI1                                                    A 908
      ALPHIP2=ALPHI2                                                    A 909
      ALPHIP3=ALPHI3                                                    A 910
      ALPHIP4=ALPHI4                                                    A 911
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      GAMMIP1=GAMMI1                                                    A 912
      GAMMIP2=GAMMI2                                                    A 913
      GAMMIP3=GAMMI3                                                    A 914
      GAMMIP4=GAMMI4                                                    A 915
      GAMIPP1=GAMIP1                                                    A 916
      GAMIPP2=GAMIP2                                                    A 917
      GAMIPP3=GAMIP3                                                    A 918
      GAMIPP4=GAMIP4                                                    A 919
      KAPIPP1=KAPIP1                                                    A 920
      KAPIPP2=KAPIP2                                                    A 921
      KAPIPP3=KAPIP3                                                    A 922
      KAPIPP4=KAPIP4                                                    A 923
      QPNET=QNET                                                        A 924
      PHBRKN2=HBRKN2                                                    A 925
      PHBRKO2=HBRKO2                                                    A 926
      QPT=Q                                                             A 927
      KSP1=KS(1)                                                        A 928
      KSPI=KS(I)                                                        A 929
      KPPI=KP(I)                                                        A 930
      KPPIP=KP(IP)                                                      A 931
      LPP=L                                                             A 932
      LPPP=LP                                                           A 933
      MGDOTP=MGDOT                                                      A 934
C     CHECK ITERATION COUNT-  INCREASE TIME STEP IF ITERATION= 1        A 935
      IF (NIT.GT.1) GO TO 109                                           A 936
      IF (NTIME.LT.5) GO TO 109                                         A 937
      DT=1.5*DT                                                         A 938
      IF (DT.GT.10) DT=10.                                              A 939
      NTIME=0                                                           A 940
109   NIT=0                                                             A 941
      NTIME=NTIME+1                                                     A 942
      GO TO 9                                                           A 943
110   CONTINUE                                                          A 944
      WRITE (2,121) LP                                                  A 945
      STOP                                                              A 946
```

```
C                                                                       A 947
C                                                                       A 948
C                                                                       A 949
111   FORMAT (50X,A10)                                                  A 950
112   FORMAT (/12X,7HTIME = ,F9.4,18X,5HDT = ,F7.4,24X,23HNUMBER OF ITER  A 951
     1ATIONS = ,I2/12X,8HTS(1) = ,F9.2,17X,7HT(1) = ,F9.2,20X,7HQRAT = ,  A 952
     2F7.4/12X,8HMSDOT = ,E15.8,11X,8HMGDOT = ,E15.8,13X,11HAMDOT(1) = ,  A 953
     3E15.8/12X,16HCHAR THICKNESS =,E16.8,2X,18HUNCHAR THICKNESS =,E16.8  A 954
     4)                                                                 A 955
113   FORMAT (2X,19HCHAR LAYER POROSITY)                                A 956
114   FORMAT (2X,29HMOLE FRACTION GASEOUS SPECIES)                      A 957
115   FORMAT (2X,40HAVERAGE MOLECULAR WEIGHT PYROLYSIS GASES)           A 958
116   FORMAT (2X,39HLOCAL MASS FLOW RATE OF PYROLYSIS GASES)            A 959
117   FORMAT (//2X,17HFLUID TEMPERATURE)                                A 960
118   FORMAT (//2X,17HSOLID TEMPERATURE)                                A 961
119   FORMAT (2X,8HPRESSURE)                                            A 962
120   FORMAT (2X,5E25.15)                                               A 963
121   FORMAT (20X,36HMINIMUM THICKNESS VIRGIN MATERIAL = ,E20.10)       A 964
      END                                                               A 965-
```

```
      SUBROUTINE VISC                                                   B   1
C     CALCULATION OF FLUID VISCOSITY AND PRANDTL NUMBER AT LOCAL TEMP-  B   2
C        ERATURE (REF.  BROKAW- NASA TR R-81)                           B   3
      DIMENSION MUK(12), KGK(12)                                        B   4
      COMMON /DE1DE2/ PSI(12,12),PHI(12,12),DUMMY(1032)                 B   5
      COMMON ACEF(12),ACER(12),BCEF(12),BCER(12),CRNI,KUPT(40,12),KUPTV(  B   6
     140),M(13),MFK(50,12),MNO,NNO,MU(50),MUKT(40,12),MUKTV(40),PR(50),R  B   7
     2(50,12),RHO(50),RHOK(50,12),RHOKP(50,12),T(50),TEMP(40),NRCT,KT,RU  B   8
     3,NSTEP,ROCPM(50),RS(50)                                           B   9
      REAL MU,MUK,M,KUPT,MUKTV,MUKT,KUPTV,KG,KGK                        B  10
      N=NSTEP                                                           B  11
      DO 2 K=1,KT                                                       B  12
      IF (MFK(N,K).LT.1.E-5) GO TO 2                                    B  13
      DO 1 J=1,NNO                                                      B  14
      MUKTV(J)=MUKT(J,K)                                                B  15
      KUPTV(J)=KUPT(J,K)                                                B  16
1     CONTINUE                                                          B  17
      CALL FTLUP (T(N),MUK(K),MNO,NNO,TEMP,MUKTV)                       B  18
      CALL FTLJP (T(N),KGK(K),MNO,NNO,TEMP,KUPTV)                       B  19
      IF (T(N).GE.300.) GO TO 2                                         B  20
      MUK(K)=MUKTV(1)                                                   B  21
      KGK(K)=KUPTV(1)                                                   B  22
2     CONTINUE                                                          B  23
      DO 4 K=1,KT                                                       B  24
      DO 4 J=1,KT                                                       B  25
      IF (K.EQ.J) GO TO 4                                               B  26
      IF (MFK(N,K).LT.1.E-5) GO TO 3                                    B  27
      PHI(K,J)=(1.+SQRT(MUK(K)/MUK(J))*SQRT(SQRT(M(J)/M(K))))**2/(2.*SQR  B  28
     1T(2.)*SQRT(1.+M(K)/M(J)))                                         B  29
      PSI(K,J)=PHI(K,J)*(1.+2.41*(M(K)-M(J))*(M(K)-.142*M(J))/(M(K)+M(J)  B  30
     1)**2)                                                             B  31
      GO TO 4                                                           B  32
3     CONTINUE                                                          B  33
      PHI(K,J)=0.                                                       B  34
      PSI(K,J)=0.                                                       B  35
4     CONTINUE                                                          B  36
```

```
      MU(N)=0.                                                          B   37
      IF (MFK(N,1).LT.1.E-5) GO TO 5                                    B   38
      A=1.+PHI(1,2)*RHOK(N,2)*M(1)/(RHOK(N,1)*M(2))+PHI(1,3)*RHOK(N,3)*M  B   39
     1(1)/(RHOK(N,1)*M(3))+PHI(1,4)*RHOK(N,4)*M(1)/(RHOK(N,1)*M(4))+PHI(  B   40
     21,5)*RHOK(N,5)*M(1)/(RHOK(N,1)*M(5))+PHI(1,6)*RHOK(N,6)*M(1)/(RHOK  B   41
     3(N,1)*M(6))                                                       B   42
      MU(N)=MUK(1)/(PHI(1,7)*RHOK(N,7)*M(1)/(RHOK(N,1)*M(7))+PHI(1,8)*RH  B   43
     1OK(N,8)*M(1)/(RHOK(N,1)*M(8))+PHI(1,9)*RHOK(N,9)*M(1)/(RHOK(N,1)*M  B   44
     2(9))+PHI(1,10)*RHOK(N,10)*M(1)/(RHOK(N,1)*M(10))+PHI(1,11)*RHOK(N,  B   45
     311)*M(1)/(RHOK(N,1)*M(11))+PHI(1,12)*RHOK(N,12)*M(1)/(RHOK(N,1)*M(  B   46
     412))+A)                                                           B   47
5     CONTINUE                                                          B   48
      IF (MFK(N,2).LT.1.E-5) GO TO 6                                    B   49
      A=1.+PHI(2,1)*RHOK(N,1)*M(2)/(RHOK(N,2)*M(1))+PHI(2,3)*RHOK(N,3)*M  B   50
     1(2)/(RHOK(N,2)*M(3))+PHI(2,4)*RHOK(N,4)*M(2)/(RHOK(N,2)*M(4))+PHI(  B   51
     22,5)*RHOK(N,5)*M(2)/(RHOK(N,2)*M(5))+PHI(2,6)*RHOK(N,6)*M(2)/(RHOK  B   52
     3(N,2)*M(6))                                                       B   53
      MU(N)=MUK(2)/(PHI(2,7)*RHOK(N,7)*M(2)/(RHOK(N,2)*M(7))+PHI(2,8)*RH  B   54
     1OK(N,8)*M(2)/(RHOK(N,2)*M(8))+PHI(2,9)*RHOK(N,9)*M(2)/(RHOK(N,2)*M  B   55
     2(9))+PHI(2,10)*RHOK(N,10)*M(2)/(RHOK(N,2)*M(10))+PHI(2,11)*RHOK(N,  B   56
     311)*M(2)/(RHOK(N,2)*M(11))+PHI(2,12)*RHOK(N,12)*M(2)/(RHOK(N,2)*M(  B   57
     412))+A)+MU(N)                                                     B   58
6     CONTINUE                                                          B   59
      IF (MFK(N,3).LT.1.E-5) GO TO 7                                    B   60
      A=1.+PHI(3,1)*RHOK(N,1)*M(3)/(RHOK(N,3)*M(1))+PHI(3,2)*RHOK(N,2)*M  B   61
     1(3)/(RHOK(N,3)*M(2))+PHI(3,4)*RHOK(N,4)*M(3)/(RHOK(N,3)*M(4))+PHI(  B   62
     23,5)*RHOK(N,5)*M(3)/(RHOK(N,3)*M(5))+PHI(3,6)*RHOK(N,6)*M(3)/(RHOK  B   63
     3(N,3)*M(6))                                                       B   64
      MU(N)=MUK(3)/(PHI(3,7)*RHOK(N,7)*M(3)/(RHOK(N,3)*M(7))+PHI(3,8)*RH  B   65
     1OK(N,8)*M(3)/(RHOK(N,3)*M(8))+PHI(3,9)*RHOK(N,9)*M(3)/(RHOK(N,3)*M  B   66
     2(9))+PHI(3,10)*RHOK(N,10)*M(3)/(RHOK(N,3)*M(10))+PHI(3,11)*RHOK(N,  B   67
     311)*M(3)/(RHOK(N,3)*M(11))+PHI(3,12)*RHOK(N,12)*M(3)/(RHOK(N,3)*M(  B   68
     412))+A)+MU(N)                                                     B   69
7     CONTINUE                                                          B   70
      IF (MFK(N,4).LT.1.E-5) GO TO 8                                    B   71
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```
      A=1.+PHI(4,1)*RHOK(N,1)*M(4)/(RHOK(N,4)*M(1))+PHI(4,2)*RHOK(N,2)*M   B   72
     1(4)/(RHOK(N,4)*M(2))+PHI(4,3)*RHOK(N,3)*M(4)/(RHOK(N,4)*M(3))+PHI(   B   73
     24,5)*RHOK(N,5)*M(4)/(RHOK(N,4)*M(5))+PHI(4,6)*RHOK(N,6)*M(4)/(RHOK   B   74
     3(N,4)*M(6))                                                          B   75
      MU(N)=MUK(4)/(PHI(4,7)*RHOK(N,7)*M(4)/(RHOK(N,4)*M(7))+PHI(4,8)*RH   B   76
     1OK(N,8)*M(4)/(RHOK(N,4)*M(8))+PHI(4,9)*RHOK(N,9)*M(4)/(RHOK(N,4)*M   B   77
     2(9))+PHI(4,10)*RHOK(N,10)*M(4)/(RHOK(N,4)*M(10))+PHI(4,11)*RHOK(N,   B   78
     311)*M(4)/(RHOK(N,4)*M(11))+PHI(4,12)*RHOK(N,12)*M(4)/(RHOK(N,4)*M(   B   79
     412))+A)+MU(N)                                                        B   80
8     CONTINUE                                                             B   81
      IF (MFK(N,5).LT.1.E-5) GO TO 9                                       B   82
      A=1.+PHI(5,1)*RHOK(N,1)*M(5)/(RHOK(N,5)*M(1))+PHI(5,2)*RHOK(N,2)*M   B   83
     1(5)/(RHOK(N,5)*M(2))+PHI(5,3)*RHOK(N,3)*M(5)/(RHOK(N,5)*M(3))+PHI(   B   84
     25,4)*RHOK(N,4)*M(5)/(RHOK(N,5)*M(4))+PHI(5,6)*RHOK(N,6)*M(5)/(RHOK   B   85
     3(N,5)*M(6))                                                          B   86
      MU(N)=MUK(5)/(PHI(5,7)*RHOK(N,7)*M(5)/(RHOK(N,5)*M(7))+PHI(5,8)*RH   B   87
     1OK(N,8)*M(5)/(RHOK(N,5)*M(8))+PHI(5,9)*RHOK(N,9)*M(5)/(RHOK(N,5)*M   B   88
     2(9))+PHI(5,10)*RHOK(N,10)*M(5)/(RHOK(N,5)*M(10))+PHI(5,11)*RHOK(N,   B   89
     311)*M(5)/(RHOK(N,5)*M(11))+PHI(5,12)*RHOK(N,12)*M(5)/(RHOK(N,5)*M(   B   90
     412))+A)+MU(N)                                                        B   91
9     CONTINUE                                                             B   92
      IF (MFK(N,6).LT.1.E-5) GO TO 10                                      B   93
      A=1.+PHI(6,1)*RHOK(N,1)*M(6)/(RHOK(N,6)*M(1))+PHI(6,2)*RHOK(N,2)*M   B   94
     1(6)/(RHOK(N,6)*M(2))+PHI(6,3)*RHOK(N,3)*M(6)/(RHOK(N,6)*M(3))+PHI(   B   95
     26,4)*RHOK(N,4)*M(6)/(RHOK(N,6)*M(4))+PHI(6,5)*RHOK(N,5)*M(6)/(RHOK   B   96
     3(N,6)*M(5))                                                          B   97
      MU(N)=MUK(6)/(PHI(6,7)*RHOK(N,7)*M(6)/(RHOK(N,6)*M(7))+PHI(6,8)*RH   B   98
     1OK(N,8)*M(6)/(RHOK(N,6)*M(8))+PHI(6,9)*RHOK(N,9)*M(6)/(RHOK(N,6)*M   B   99
     2(9))+PHI(6,10)*RHOK(N,10)*M(6)/(RHOK(N,6)*M(10))+PHI(6,11)*RHOK(N,   B  100
     311)*M(6)/(RHOK(N,6)*M(11))+PHI(6,12)*RHOK(N,12)*M(6)/(RHOK(N,6)*M(   B  101
     412))+A)+MU(N)                                                        B  102
10    CONTINUE                                                             B  103
      IF (MFK(N,7).LT.1.E-5) GO TO 11                                      B  104
      A=1.+PHI(7,1)*RHOK(N,1)*M(7)/(RHOK(N,7)*M(1))+PHI(7,2)*RHOK(N,2)*M   B  105
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     1(7)/(RHOK(N,7)*M(2))+PHI(7,3)*RHOK(N,3)*M(7)/(RHOK(N,7)*M(3))+PHI(   B 106
     27,4)*RHOK(N,4)*M(7)/(RHOK(N,7)*M(4))+PHI(7,5)*RHOK(N,5)*M(7)/(RHOK   B 107
     3(N,7)*M(5))+PHI(7,6)*RHOK(N,6)*M(7)/(RHOK(N,7)*M(6))                 B 108
      MU(N)=MUK(7)/(PHI(7,8)*RHOK(N,8)*M(7)/(RHOK(N,7)*M(8))+PHI(7,9)*RH   B 109
     1OK(N,9)*M(7)/(RHOK(N,7)*M(9))+PHI(7,10)*RHOK(N,10)*M(7)/(RHOK(N,7)   B 110
     2*M(10))+PHI(7,11)*RHOK(N,11)*M(7)/(RHOK(N,7)*M(11))+PHI(7,12)*RHOK   B 111
     3(N,12)*M(7)/(RHOK(N,7)*M(12))+A)+MU(N)                               B 112
11    CONTINUE                                                             B 113
      IF (MFK(N,8).LT.1.E-5) GO TO 12                                      B 114
      A=1.+PHI(8,1)*RHOK(N,1)*M(8)/(RHOK(N,8)*M(1))+PHI(8,2)*RHOK(N,2)*M   B 115
     1(8)/(RHOK(N,8)*M(2))+PHI(8,3)*RHOK(N,3)*M(8)/(RHOK(N,8)*M(3))+PHI(   B 116
     28,4)*RHOK(N,4)*M(8)/(RHOK(N,8)*M(4))+PHI(8,5)*RHOK(N,5)*M(8)/(RHOK   B 117
     3(N,8)*M(5))+PHI(8,6)*RHOK(N,5)*M(8)/(RHOK(N,8)*M(6))                 B 118
      MU(N)=MUK(8)/(PHI(8,7)*RHOK(N,7)*M(8)/(RHOK(N,8)*M(7))+PHI(8,9)*RH   B 119
     1OK(N,9)*M(8)/(RHOK(N,8)*M(9))+PHI(8,10)*RHOK(N,10)*M(8)/(RHOK(N,8)   B 120
     2*M(10))+PHI(8,11)*RHOK(N,11)*M(8)/(RHOK(N,8)*M(11))+PHI(8,12)*RHOK   B 121
     3(N,12)*M(8)/(RHOK(N,8)*M(12))+A)+MU(N)                               B 122
12    CONTINUE                                                             B 123
      IF (MFK(N,9).LT.1.E-5) GO TO 13                                      B 124
      A=1.+PHI(9,1)*RHOK(N,1)*M(9)/(RHOK(N,9)*M(1))+PHI(9,2)*RHOK(N,2)*M   B 125
     1(9)/(RHOK(N,9)*M(2))+PHI(9,3)*RHOK(N,3)*M(9)/(RHOK(N,9)*M(3))+PHI(   B 126
     29,4)*RHOK(N,4)*M(9)/(RHOK(N,9)*M(4))+PHI(9,5)*RHOK(N,5)*M(9)/(RHOK   B 127
     3(N,9)*M(5))+PHI(9,6)*RHOK(N,6)*M(9)/(RHOK(N,9)*M(6))                 B 128
      MU(N)=MUK(9)/(PHI(9,7)*RHOK(N,7)*M(9)/(RHOK(N,9)*M(7))+PHI(9,8)*RH   B 129
     1OK(N,8)*M(9)/(RHOK(N,9)*M(8))+PHI(9,10)*RHOK(N,10)*M(9)/(RHOK(N,9)   B 130
     2*M(10))+PHI(9,11)*RHOK(N,11)*M(9)/(RHOK(N,9)*M(11))+PHI(9,12)*RHOK   B 131
     3(N,12)*M(9)/(RHOK(N,9)*M(12))+A)+MU(N)                               B 132
13    CONTINUE                                                             B 133
      IF (MFK(N,10).LT.1.E-5) GO TO 14                                     B 134
      A=1.+PHI(10,1)*RHOK(N,1)*M(10)/(RHOK(N,10)*M(1))+PHI(10,2)*RHOK(N,   B 135
     12)*M(10)/(RHOK(N,10)*M(2))+PHI(10,3)*RHOK(N,3)*M(10)/(RHOK(N,10)*M   B 136
     2(3))+PHI(10,4)*RHOK(N,4)*M(10)/(RHOK(N,10)*M(4))+PHI(10,5)*RHOK(N,   B 137
     35)*M(10)/(RHOK(N,10)*M(5))+PHI(10,6)*RHOK(N,6)*M(10)/(RHOK(N,10)*M   B 138
     4(6))                                                                 B 139
      MU(N)=MUK(10)/(PHI(10,7)*RHOK(N,7)*M(10)/(RHOK(N,10)*M(7))+PHI(10,   B 140
     18)*RHOK(N,8)*M(10)/(RHOK(N,10)*M(8))+PHI(10,9)*RHOK(N,9)*M(10)/(RH   B 141
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     2OK(N,10)*M(9))+PHI(10,11)*RHOK(N,11)*M(10)/(RHOK(N,10)*M(11))+PHI(   B 142
     310,12)*RHOK(N,12)*M(10)/(RHOK(N,10)*M(12))+A)+MU(N)                  B 143
14    CONTINUE                                                             B 144
      IF (MFK(N,11).LT.1.E-5) GO TO 15                                     B 145
      A=1.+PHI(11,1)*RHOK(N,1)*M(11)/(RHOK(N,11)*M(1))+PHI(11,2)*RHOK(N,   B 146
     12)*M(11)/(RHOK(N,11)*M(2))+PHI(11,3)*RHOK(N,3)*M(11)/(RHOK(N,11)*M   B 147
     2(3))+PHI(11,4)*RHOK(N,4)*M(11)/(RHOK(N,11)*M(4))+PHI(11,5)*RHOK(N,   B 148
     35)*M(11)/(RHOK(N,11)*M(5))+PHI(11,6)*RHOK(N,6)*M(11)/(RHOK(N,11)*M   B 149
     4(6))                                                                 B 150
      MU(N)=MUK(11)/(PHI(11,7)*RHOK(N,7)*M(11)/(RHOK(N,11)*M(7))+PHI(11,   B 151
     18)*RHOK(N,8)*M(11)/(RHOK(N,11)*M(8))+PHI(11,9)*RHOK(N,9)*M(11)/(RH   B 152
     2OK(N,11)*M(9))+PHI(11,10)*RHOK(N,10)*M(11)/(RHOK(N,11)*M(10))+PHI(   B 153
     311,12)*RHOK(N,12)*M(11)/(RHOK(N,11)*M(12))+A)+MU(N)                  B 154
15    CONTINUE                                                             B 155
      IF (MFK(N,12).LT.1.E-5) GO TO 16                                     B 156
      A=1.+PHI(12,1)*RHOK(N,1)*M(12)/(RHOK(N,12)*M(1))+PHI(12,2)*RHOK(N,   B 157
     12)*M(12)/(RHOK(N,12)*M(2))+PHI(12,3)*RHOK(N,3)*M(12)/(RHOK(N,12)*M   B 158
     2(3))+PHI(12,4)*RHOK(N,4)*M(12)/(RHOK(N,12)*M(4))+PHI(12,5)*RHOK(N,   B 159
     35)*M(12)/(RHOK(N,12)*M(5))+PHI(12,6)*RHOK(N,6)*M(12)/(RHOK(N,12)*M   B 160
     4(6))                                                                 B 161
      MU(N)=MUK(12)/(PHI(12,7)*RHOK(N,7)*M(12)/(RHOK(N,12)*M(7))+PHI(12,   B 162
     18)*RHOK(N,8)*M(12)/(RHOK(N,12)*M(8))+PHI(12,9)*RHOK(N,9)*M(12)/(RH   B 163
     2OK(N,12)*M(9))+PHI(12,10)*RHOK(N,10)*M(12)/(RHOK(N,12)*M(10))+PHI(   B 164
     312,11)*RHOK(N,11)*M(12)/(RHOK(N,12)*M(11))+A)+MU(N)                  B 165
16    CONTINUE                                                             B 166
      KG=0.                                                                B 167
      IF (MFK(N,1).LT.1.E-5) GO TO 17                                      B 168
      A=(1.+PSI(1,2)*RHOK(N,2)*M(1)/(RHOK(N,1)*M(2))+PSI(1,3)*RHOK(N,3)*   B 169
     1M(1)/(RHOK(N,1)*M(3))+PSI(1,4)*RHOK(N,4)*M(1)/(RHOK(N,1)*M(4))+PSI   B 170
     2(1,5)*RHOK(N,5)*M(1)/(RHOK(N,1)*M(5))+PSI(1,6)*RHOK(N,6)*M(1)/(RHO   B 171
     3K(N,1)*M(6)))                                                        B 172
      KG=KGK(1)/(PSI(1,7)*RHOK(N,7)*M(1)/(RHOK(N,1)*M(7))+PSI(1,8)*RHOK(   B 173
     1N,8)*M(1)/(RHOK(N,1)*M(8))+PSI(1,9)*RHOK(N,9)*M(1)/(RHOK(N,1)*M(9)   B 174
     2)+PSI(1,10)*RHOK(N,10)*M(1)/(RHOK(N,1)*M(10))+PSI(1,11)*RHOK(N,11)   B 175
     3*M(1)/(RHOK(N,1)*M(11))+PSI(1,12)*RHOK(N,12)*M(1)/(RHOK(N,1)*M(12)   B 176
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     4)+A)                                                              B 177
17    CONTINUE                                                          B 178
      IF (MFK(N,2).LT.1.E-5) GO TO 18                                   B 179
      A=(1.+PSI(2,1)*RHOK(N,1)*M(2)/(RHOK(N,2)*M(1))+PSI(2,3)*RHOK(N,3)*  B 180
     1M(2)/(RHOK(N,2)*M(3))+PSI(2,4)*RHOK(N,4)*M(2)/(RHOK(N,2)*M(4))+PSI  B 181
     2(2,5)*RHOK(N,5)*M(2)/(RHOK(N,2)*M(5))+PSI(2,6)*RHOK(N,6)*M(2)/(RHO  B 182
     3K(N,2)*M(6)))                                                     B 183
      KG=KGK(2)/(PSI(2,7)*RHOK(N,7)*M(2)/(RHOK(N,2)*M(7))+PSI(2,8)*RHOK(  B 184
     1N,8)*M(2)/(RHOK(N,2)*M(8))+PSI(2,9)*RHOK(N,9)*M(2)/(RHOK(N,2)*M(9)  B 185
     2)+PSI(2,10)*RHOK(N,10)*M(2)/(RHOK(N,2)*M(10))+PSI(2,11)*RHOK(N,11)  B 186
     3*M(2)/(RHOK(N,2)*M(11))+PSI(2,12)*RHOK(N,12)*M(2)/(RHOK(N,2)*M(12)  B 187
     4)+A)+KG                                                           B 188
18    CONTINUE                                                          B 189
      IF (MFK(N,3).LT.1.E-5) GO TO 19                                   B 190
      A=(1.+PSI(3,1)*RHOK(N,1)*M(3)/(RHOK(N,3)*M(1))+PSI(3,2)*RHOK(N,2)*  B 191
     1M(3)/(RHOK(N,3)*M(2))+PSI(3,4)*RHOK(N,4)*M(3)/(RHOK(N,3)*M(4))+PSI  B 192
     2(3,5)*RHOK(N,5)*M(3)/(RHOK(N,3)*M(5))+PSI(3,6)*RHOK(N,6)*M(3)/(RHO  B 193
     3K(N,3)*M(6)))                                                     B 194
      KG=KGK(3)/(PSI(3,7)*RHOK(N,7)*M(3)/(RHOK(N,3)*M(7))+PSI(3,8)*RHOK(  B 195
     1N,8)*M(3)/(RHOK(N,3)*M(8))+PSI(3,9)*RHOK(N,9)*M(3)/(RHOK(N,3)*M(9)  B 196
     2)+PSI(3,10)*RHOK(N,10)*M(3)/(RHOK(N,3)*M(10))+PSI(3,11)*RHOK(N,11)  B 197
     3*M(3)/(RHOK(N,3)*M(11))+PSI(3,12)*RHOK(N,12)*M(3)/(RHOK(N,3)*M(12)  B 198
     4)+A)+KG                                                           B 199
19    CONTINUE                                                          B 200
      IF (MFK(N,4).LT.1.E-5) GO TO 20                                   B 201
      A=(1.+PSI(4,1)*RHOK(N,1)*M(4)/(RHOK(N,4)*M(1))+PSI(4,2)*RHOK(N,2)*  B 202
     1M(4)/(RHOK(N,4)*M(2))+PSI(4,3)*RHOK(N,3)*M(4)/(RHOK(N,4)*M(3))+PSI  B 203
     2(4,5)*RHOK(N,5)*M(4)/(RHOK(N,4)*M(5))+PSI(4,6)*RHOK(N,6)*M(4)/(RHO  B 204
     3K(N,4)*M(6)))                                                     B 205
      KG=KGK(4)/(PSI(4,7)*RHOK(N,7)*M(4)/(RHOK(N,4)*M(7))+PSI(4,8)*RHOK(  B 206
     1N,8)*M(4)/(RHOK(N,4)*M(8))+PSI(4,9)*RHOK(N,9)*M(4)/(RHOK(N,4)*M(9)  B 207
     2)+PSI(4,10)*RHOK(N,10)*M(4)/(RHOK(N,4)*M(10))+PSI(4,11)*RHOK(N,11)  B 208
     3*M(4)/(RHOK(N,4)*M(11))+PSI(4,12)*RHOK(N,12)*M(4)/(RHOK(N,4)*M(12)  B 209
     4)+A)+KG                                                           B 210
20    CONTINUE                                                          B 211
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```
      IF (MFK(N,5).LT.1.E-5) GO TO 21                                   B 212
      A=(1.+PSI(5,1)*RHOK(N,1)*M(5)/(RHOK(N,5)*M(1))+PSI(5,2)*RHOK(N,2)*  B 213
     1M(5)/(RHOK(N,5)*M(2))+PSI(5,3)*RHOK(N,3)*M(5)/(RHOK(N,5)*M(3))+PSI  B 214
     2(5,4)*RHOK(N,4)*M(5)/(RHOK(N,5)*M(4))+PSI(5,6)*RHOK(N,6)*M(5)/(RHO  B 215
     3K(N,5)*M(6)))                                                     B 216
      KG=KGK(5)/(PSI(5,7)*RHOK(N,7)*M(5)/(RHOK(N,5)*M(7))+PSI(5,8)*RHOK(  B 217
     1N,8)*M(5)/(RHOK(N,5)*M(8))+PSI(5,9)*RHOK(N,9)*M(5)/(RHOK(N,5)*M(9)  B 218
     2)+PSI(5,10)*RHOK(N,10)*M(5)/(RHOK(N,5)*M(10))+PSI(5,11)*RHOK(N,11)  B 219
     3*M(5)/(RHOK(N,5)*M(11))+PSI(5,12)*RHOK(N,12)*M(5)/(RHOK(N,5)*M(12)  B 220
     4)+A)+KG                                                           B 221
21    CONTINUE                                                          B 222
      IF (MFK(N,6).LT.1.E-5) GO TO 22                                   B 223
      A=(1.+PSI(6,1)*RHOK(N,1)*M(6)/(RHOK(N,6)*M(1))+PSI(6,2)*RHOK(N,2)*  B 224
     1M(6)/(RHOK(N,6)*M(2))+PSI(6,3)*RHOK(N,3)*M(6)/(RHOK(N,6)*M(3))+PSI  B 225
     2(6,4)*RHOK(N,4)*M(6)/(RHOK(N,6)*M(4))+PSI(6,5)*RHOK(N,5)*M(6)/(RHO  B 226
     3K(N,6)*M(5)))                                                     B 227
      KG=KGK(6)/(PSI(6,7)*RHOK(N,7)*M(6)/(RHOK(N,6)*M(7))+PSI(6,8)*RHOK(  B 228
     1N,8)*M(6)/(RHOK(N,6)*M(8))+PSI(6,9)*RHOK(N,9)*M(6)/(RHOK(N,6)*M(9)  B 229
     2)+PSI(6,10)*RHOK(N,10)*M(6)/(RHOK(N,6)*M(10))+PSI(6,11)*RHOK(N,11)  B 230
     3*M(6)/(RHOK(N,6)*M(11))+PSI(6,12)*RHOK(N,12)*M(6)/(RHOK(N,6)*M(12)  B 231
     4)+A)+KG                                                           B 232
22    CONTINUE                                                          B 233
      IF (MFK(N,7).LT.1.E-5) GO TO 23                                   B 234
      A=(PSI(7,1)*RHOK(N,1)*M(7)/(RHOK(N,7)*M(1))+PSI(7,2)*RHOK(N,2)*M(7  B 235
     1)/(RHOK(N,7)*M(2))+PSI(7,3)*RHOK(N,3)*M(7)/(RHOK(N,7)*M(3))+PSI(7,  B 236
     24)*RHOK(N,4)*M(7)/(RHOK(N,7)*M(4))+PSI(7,5)*RHOK(N,5)*M(7)/(RHOK(N  B 237
     3,7)*M(5))+PSI(7,6)*RHOK(N,6)*M(7)/(RHOK(N,7)*M(6)))               B 238
      KG=KGK(7)/(1.+PSI(7,8)*RHOK(N,8)*M(7)/(RHOK(N,7)*M(8))+PSI(7,9)*RH  B 239
     1OK(N,9)*M(7)/(RHOK(N,7)*M(9))+PSI(7,10)*RHOK(N,10)*M(7)/(RHOK(N,7)  B 240
     2*M(10))+PSI(7,11)*RHOK(N,11)*M(7)/(RHOK(N,7)*M(11))+PSI(7,12)*RHOK  B 241
     3(N,12)*M(7)/(RHOK(N,7)*M(12))+A)+KG                               B 242
23    CONTINUE                                                          B 243
      IF (MFK(N,8).LT.1.E-5) GO TO 24                                   B 244
      A=(PSI(8,1)*RHOK(N,1)*M(8)/(RHOK(N,8)*M(1))+PSI(8,2)*RHOK(N,2)*M(8  B 245
     1)/(RHOK(N,8)*M(2))+PSI(8,3)*RHOK(N,3)*M(8)/(RHOK(N,8)*M(3))+PSI(8,  B 246
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     24)*RHOK(N,4)*M(8)/(RHOK(N,8)*M(4))+PSI(8,5)*RHOK(N,5)*M(8)/(RHOK(N   B 247
     3,8)*M(5))+PSI(8,6)*RHOK(N,5)*M(8)/(RHOK(N,8)*M(6)))                 B 248
      KG=KGK(8)/(1+PSI(8,7)*RHOK(N,7)*M(8)/(RHOK(N,8)*M(7))+PSI(8,9)*RHO  B 249
     1K(N,9)*M(8)/(RHOK(N,8)*M(9))+PSI(8,10)*RHOK(N,10)*M(8)/(RHOK(N,8)*  B 250
     2M(10))+PSI(8,11)*RHOK(N,11)*M(8)/(RHOK(N,8)*M(11))+PSI(8,12)*RHOK(  B 251
     3N,12)*M(8)/(RHOK(N,8)*M(12))+A)+KG                                  B 252
24    CONTINUE                                                            B 253
      IF (MFK(N,9).LT.1.E-5) GO TO 25                                     B 254
      A=(PSI(9,1)*RHOK(N,1)*M(9)/(RHOK(N,9)*M(1))+PSI(9,2)*RHOK(N,2)*M(9  B 255
     1)/(RHOK(N,9)*M(2))+PSI(9,3)*RHOK(N,3)*M(9)/(RHOK(N,9)*M(3))+PSI(9,  B 256
     24)*RHOK(N,4)*M(9)/(RHOK(N,9)*M(4))+PSI(9,5)*RHOK(N,5)*M(9)/(RHOK(N  B 257
     3,9)*M(5))+PSI(9,6)*RHOK(N,6)*M(9)/(RHOK(N,9)*M(6)))                 B 258
      KG=KGK(9)/(1+PSI(9,7)*RHOK(N,7)*M(9)/(RHOK(N,9)*M(7))+PSI(9,8)*RHO  B 259
     1K(N,8)*M(9)/(RHOK(N,9)*M(8))+PSI(9,10)*RHOK(N,10)*M(9)/(RHOK(N,9)*  B 260
     2M(10))+PSI(9,11)*RHOK(N,11)*M(9)/(RHOK(N,9)*M(11))+PSI(9,12)*RHOK(  B 261
     3N,12)*M(9)/(RHOK(N,9)*M(12))+A)+KG                                  B 262
25    CONTINUE                                                            B 263
      IF (MFK(N,10).LT.1.E-5) GO TO 26                                    B 264
      A=(PSI(10,1)*RHOK(N,1)*M(10)/(RHOK(N,10)*M(1))+PSI(10,2)*RHOK(N,2)  B 265
     1*M(10)/(RHOK(N,10)*M(2))+PSI(10,3)*RHOK(N,3)*M(10)/(RHOK(N,10)*M(3  B 266
     2))+PSI(10,4)*RHOK(N,4)*M(10)/(RHOK(N,10)*M(4))+PSI(10,5)*RHOK(N,5)  B 267
     3*M(10)/(RHOK(N,10)*M(5))+PSI(10,6)*RHOK(N,6)*M(10)/(RHOK(N,10)*M(6  B 268
     4)))                                                                 B 269
      KG=KGK(10)/(1.+PSI(10,7)*RHOK(N,7)*M(10)/(RHOK(N,10)*M(7))+PSI(10,  B 270
     18)*RHOK(N,8)*M(10)/(RHOK(N,10)*M(8))+PSI(10,9)*RHOK(N,9)*M(10)/(RH  B 271
     2OK(N,10)*M(9))+PSI(10,11)*RHOK(N,11)*M(10)/(RHOK(N,10)*M(11))+PSI(  B 272
     310,12)*RHOK(N,12)*M(10)/(RHOK(N,10)*M(12))+A)+KG                    B 273
26    CONTINUE                                                            B 274
      IF (MFK(N,11).LT.1.E-5) GO TO 27                                    B 275
      A=(PSI(11,1)*RHOK(N,1)*M(11)/(RHOK(N,11)*M(1))+PSI(11,2)*RHOK(N,2)  B 276
     1*M(11)/(RHOK(N,11)*M(2))+PSI(11,3)*RHOK(N,3)*M(11)/(RHOK(N,11)*M(3  B 277
     2))+PSI(11,4)*RHOK(N,4)*M(11)/(RHOK(N,11)*M(4))+PSI(11,5)*RHOK(N,5)  B 278
     3*M(11)/(RHOK(N,11)*M(5))+PSI(11,6)*RHOK(N,6)*M(11)/(RHOK(N,11)*M(6  B 279
     4)))                                                                 B 280
      KG=KGK(11)/(1.+PSI(11,7)*RHOK(N,7)*M(11)/(RHOK(N,11)*M(7))+PSI(11,  B 281
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     18)*RHOK(N,8)*M(11)/(RHOK(N,11)*M(8))+PSI(11,9)*RHOK(N,9)*M(11)/(RH   B 282
     2OK(N,11)*M(9))+PSI(11,10)*RHOK(N,10)*M(11)/(RHOK(N,11)*M(10))+PSI(   B 283
     311,12)*RHOK(N,12)*M(11)/(RHOK(N,11)*M(12))+A)+KG                     B 284
27    CONTINUE                                                             B 285
      IF (MFK(N,12).LT.1.E-5) GO TO 28                                     B 286
      A=(PSI(12,1)*RHOK(N,1)*M(12)/(RHOK(N,12)*M(1))+PSI(12,2)*RHOK(N,2)   B 287
     1*M(12)/(RHOK(N,12)*M(2))+PSI(12,3)*RHOK(N,3)*M(12)/(RHOK(N,12)*M(3   B 288
     2))+PSI(12,4)*RHOK(N,4)*M(12)/(RHOK(N,12)*M(4))+PSI(12,5)*RHOK(N,5)   B 289
     3*M(12)/(RHOK(N,12)*M(5))+PSI(12,6)*RHOK(N,6)*M(12)/(RHOK(N,12)*M(6   B 290
     4)))                                                                  B 291
      KG=KGK(12)/(1.+PSI(12,7)*RHOK(N,7)*M(12)/(RHOK(N,12)*M(7))+PSI(12,   B 292
     18)*RHOK(N,8)*M(12)/(RHOK(N,12)*M(8))+PSI(12,9)*RHOK(N,9)*M(12)/(RH   B 293
     2OK(N,12)*M(9))+PSI(12,10)*RHOK(N,10)*M(12)/(RHOK(N,12)*M(10))+PSI(   B 294
     312,11)*RHOK(N,11)*M(12)/(RHOK(N,12)*M(11))+A)+KG                     B 295
28    CONTINUE                                                             B 296
      PR(N)=MU(N)/KG*ROCPM(N)/RHO(N)                                       B 297
      RETURN                                                               B 298
      END                                                                  B 299-
```

```
      SUBROUTINE PDE1 (FS,CRNI)
C     SUBROUTINE FOR SOLVING SECOND ORDER LINEARIZED DIFFERENTIAL EQUA-
C        TIONS FOR TEMPERATURE OF THE CHAR AND UNCHARRED LAYERS.
      DIMENSION AS(110), BS(110), CS(110), DS(110), BP(110), FS(110), GP
     1(110), ALPHB4(110), ALPHA2(110), ALPHB3(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), ALPHP3(110), ALPHP4(110)
      COMMON /DE1DE2/ AS,BS,CS,DS,BP,GP
      COMMON /PDE1/ ALPHI1,ALPHI2,ALPHI3,ALPHI4,ALPHIP1,ALPHIP2,ALPHIP3,
     1ALPHIP4,GAMMI1,GAMMI2,GAMMI4,GAMMIP1,GAMMIP2,GAMMIP3,GAMMIP4,SGMA,
     2DX,ALPHA1,ALPHA2,ALPHP1,ALPHP2,ALPHB3,ALPHB4,DT,L,Q,KS,LP,QPT,KSP1
     3,TSP,DXP,IP,I,IO,IN,IO1,KP,LPP,LPPP,KSPI,KPPI,MGDOT,DHP,MGDOTP,QNE
     4T,QPNET,KPPIP,GAMMI3,IM,EPSS,EPSP,DX1,DXP1,ALPHA4,ALPHP3,ALPHP4,AL
     5PHA3,HTSK,HTSKP,IOPT1,IOPTI,T1BAR,TIBAR
      COMMON /TS/ IP1,IZ1,KPP,GAMIP1,GAMIP2,GAMIP3,GAMIP4,GAMIPP1,GAMIPP
     12,GAMIPP3,GAMIPP4,KAPIP1,KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPIPP2,IL,K
     2APIPP3,KAPIPP4,DXPP,KPPPIP,KPPPIZ,IZ
      DOUBLE PRECISION AS,BS,CS,DS,GSCNST,HSCNST,AISCNST,ZSCNST,YSCNST,X
     1SCNST,AIS,BIS,CIS,DIS,BP,GP,WS,TFS
      REAL KS,KP,L,LP,MGDOT,LPP,LPPP,MGDOTP,KPPI,KSPI,KSP1,KPPIP,KAPIP1,
     1KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPIPP2,KAPIPP3,KAPIPP4,IL,KPPPIZ,KPP
     2PIP,KPP
C     CALCULATE TRI-DIAGONAL MATRIX COEFFICIENTS
      DDX=DX1
      IF (IOPT1.EQ.0) GO TO 1
      IF ((FS(1)-T1BAR).GT.1.E-6) GO TO 2
1     CONTINUE
      BS(1)=CRNI*((ALPHA1(1)-11./(6.*DDX))*L*SGMA*EPSS*FS(1)**3/KS(1)-3.
     1/(2.*DDX**2)+ALPHA2(1))+ALPHB4(1)/DT
      CS(1)=3.*CRNI/(4.*DDX**2)
      GSCNST=CRNI*(3./(2.*DDX**2)-1./(6.*DDX**2))
      HSCNST=-3.*CRNI/(4.*DDX**2)
      AISCNST=CRNI/(6.*DDX**2)
      DS(1)=-ALPHB3(1)+CRNI*(ALPHA1(1)-11./(6.*DDX))*Q*L/KS(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)**3/KSP1-3./(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**   C   37
     42)-1./(6.*DDX**2))*TSP(3)-3./(4.*DDX**2)*TSP(4)+1./(6.*DDX**2)*TSP   C   38
     5(5))                                                                 C   39
      GO TO 3                                                              C   40
2     CONTINUE                                                             C   41
      BS(1)=1.                                                             C   42
      CS(1)=0.                                                             C   43
      GSCNST=0.                                                            C   44
      HSCNST=0.                                                            C   45
      AISCNST=0.                                                           C   46
      DS(1)=T13AR+1.E-4                                                    C   47
3     CONTINUE                                                             C   48
      DO 5 N=2,IM                                                          C   49
      IF (N.NE.20) GO TO 4                                                 C   50
      DDX=DX                                                               C   51
      GO TO 5                                                              C   52
4     AS(N)=CRNI*(1./DDX**2-ALPHA1(N)/(2.*DDX))                            C   53
      BS(N)=CRNI*(ALPHA2(N)-2./DDX**2+ALPHB4(N)/(DT*CRNI))                 C   54
      CS(N)=CRNI*(1./DDX**2+ALPHA1(N)/(2.*DDX))                            C   55
      DS(N)=-ALPHB3(N)-(1-CRNI)*((1./DDX**2-ALPHP1(N)/(2.*DDX))*TSP(N-1)   C   56
     1+(ALPHP2(N)-2./DDX**2-ALPHB4(N)/(DT*(1.-CRNI)))*TSP(N)+(1./DDX**2+   C   57
     2ALPHP1(N)/(2.*DDX))*TSP(N+1))                                        C   58
5     CONTINUE                                                             C   59
      BS(1)=AS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*(C   C   60
     1S(4)*HSCNST-BS(4)*AISCNST))-CS(3)*CS(4)*BS(1)                        C   61
      CS(1)=BS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*(C   C   62
     1S(4)*HSCNST-BS(4)*AISCNST))-CS(1)*CS(3)*CS(4)+AS(3)*(CS(4)*HSCNST-   C   63
     2BS(4)*AISCNST)                                                       C   64
      DS(1)=DS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*(C   C   65
     1S(4)*HSCNST-BS(4)*AISCNST))-CS(3)*CS(4)*DS(1)+CS(3)*DS(4)*AISCNST+   C   66
     2DS(3)*(CS(4)*HSCNST-BS(4)*AISCNST)                                   C   67
      AS(20)=CRNI*(ALPHA1(20)*DX/(DX1*(DX1+DX))-2./(DX1*(DX1+DX)))         C   68
      BS(20)=CRNI*(2./(DX*DX1)-ALPHA2(20)-ALPHA1(20)*(DX-DX1)/(DX1*DX))-   C   69
     1ALPHB4(20)/DT                                                        C   70
      CS(20)=CRNI*(-2./(DX*(DX1+DX))-ALPHA1(20)*DX1/(DX*(DX1+DX)))         C   71
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      DS(20)=-ALPHB3(20)-(1.-CRNI)*(ALPHP1(20)*DX/(DX1*(DX1+DX))-2./(DX1   C   72
     1*(DX1+DX)))*TSP(19)-((1.-CRNI)*(2./(DX*DX1)-ALPHP2(20)-ALPHP1(20)*   C   73
     2(DX-DX1)/(DX1*DX))+ALPHB4(20)/DT)*TSP(20)+(1.-CRNI)*(2./(DX*(DX1+D   C   74
     3X))+ALPHP1(20)*DX1/(DX*(DX1+DX)))*TSP(21)                            C   75
      DDX=DXP1                                                             C   76
      DO 7 N=IN,IO1                                                        C   77
      IF (N.EQ.(I+20)) GO TO 6                                             C   78
      AS(N)=CRNI*(1./DDX**2-ALPHA1(N)/(2.*DDX))                            C   79
      BS(N)=CRNI*(ALPHA2(N)-2./DDX**2+ALPHB4(N)/(DT*CRNI))                 C   80
      CS(N)=CRNI*(1./DDX**2+ALPHA1(N)/(2.*DDX))                            C   81
      DS(N)=-ALPHB3(N)-(1-CRNI)*((1./DDX**2-ALPHP1(N)/(2.*DDX))*TSP(N-1)   C   82
     1+(ALPHP2(N)-2./DDX**2-ALPHB4(N)/(DT*(1.-CRNI)))*TSP(N)+(1./DDX**2+   C   83
     2ALPHP1(N)/(2.*DDX))*TSP(N+1))                                        C   84
      GO TO 7                                                              C   85
6     DDX=DXP                                                              C   86
      AS(N)=CRNI*(ALPHA1(N)*DXP/(DXP1*(DXP+DXP1))-2./(DXP1*(DXP+DXP1)))    C   87
      BS(N)=CRNI*(2./(DXP*DXP1)-ALPHA2(N)-ALPHA1(N)*(DXP-DXP1)/(DXP1*DXP   C   88
     1))-ALPHB4(N)/DT                                                      C   89
      CS(N)=CRNI*(-2./(DXP*(DXP1+DXP))-ALPHA1(N)*DXP1/(DXP*(DXP1+DXP)))    C   90
      DS(N)=-ALPHB3(N)-(1.-CRNI)*(ALPHP1(N)*DXP/(DXP1*(DXP1+DXP))-2./(DX   C   91
     1P1*(DXP1+DXP)))*TSP(N-1)-((1.-CRNI)*(2./(DXP*DXP1)-ALPHP2(N)-ALPHP   C   92
     21(N)*(DXP-DXP1)/(DXP1*DXP))+ALPHB4(N)/DT)*TSP(N)+(1.-CRNI)*(2./(DX   C   93
     3P*(DXP1+DXP))+ALPHP1(N)*DXP1/(DXP*(DXP1+DXP)))*TSP(N+1)              C   94
7     CONTINUE                                                             C   95
      IF (IOPTI.EQ.0) GO TO 8                                              C   96
      IF ((FS(I)-TIBAR).GT.1.E-6) GO TO 9                                  C   97
8     CONTINUE                                                             C   98
      AKSL=DX*KS(I)*ALPHI4/L                                               C   99
      AKPL=DXP1*KP(I)*GAMMI4/LP                                            C  100
      AKAL=CRNI/(AKSL+AKPL)                                                C  101
      AKSLP=DX*KSPI*ALPHIP4/LPP                                            C  102
      AKPLP=DXP1*KPPI*GAMMIP4/LPPP                                         C  103
      AKALP=(1.-CRNI)/(AKSLP+AKPLP)                                        C  104
      ZIS=-AKAL*KS(I)/(6.*DX*L)                                            C  105
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 YIS=AKAL*KS(I)/L*(.75/DX+ALPHI1/3.)                                    C 106
 XIS=-AKAL*KS(I)/L*(4./(3.*DX)+1.5*ALPHI1)                              C 107
 AIS=-AKAL*KS(I)/L*(.75/DX-3.*ALPHI1)                                   C 108
 BIS=AKAL*(KS(I)/L*(1.5/DX-11.*ALPHI1/6.-ALPHI2*DX)+KP(I)/LP*(1.5/D     C 109
1XP1+11.*GAMMI1/6.-GAMMI2*DXP1))-1./DT                                  C 110
 CIS=-AKAL*KP(I)/LP*(.75/DXP1+3.*GAMMI1)                                C 111
 EIS=-AKAL*KP(I)/LP*(4./(3.*DXP1)-1.5*GAMMI1)                           C 112
 FIS=AKAL*KP(I)/LP*(.75/DXP1-GAMMI1/3.)                                 C 113
 GIS=-AKAL*KP(I)/(LP*DXP1*6.)                                           C 114
 DIS=-11.*AKAL/6.*(MGDOT*DHP-6.*ALPHI3/11.*DX*KS(I)/L-6.*GAMMI3*DXP      C 115
11*KP(I)/(11.*LP))-11.*AKALP/6.*(MGDOTP*DHP-6.*ALPHIP3*DX*KSPI/(11.     C 116
2*LPP)-6.*GAMMIP3*DXP1*KPPI/(LPPP*11.))+AKALP*KSPI/LPP*(TSP(I-4)/(6     C 117
3.*DX)-(.75/DX+ALPHIP1/3.)*TSP(I-3)+(4./(3.*DX)+1.5*ALPHIP1)*TSP(I-     C 118
42)+(.75/DX-3.*ALPHIP1)*TSP(I-1))-(AKALP*(KSPI/LPP*(1.5/DX-11.*ALPH     C 119
5IP1/6.-ALPHIP2*DX)+KPPI/LPPP*(1.5/DXP1+11.*GAMMIP1/6.-GAMMIP2*DXP1     C 120
6))+1./DT)*TSP(I)+AKALP*KPPI/LPPP*((.75/DXP1+3.*GAMMIP1)*TSP(I+1)+(     C 121
74./(3.*DXP1)-1.5*GAMMIP1)*TSP(I+2)-(.75/DXP1-GAMMIP1/3.)*TSP(I+3)+     C 122
8TSP(I+4)/(6.*DXP1))                                                    C 123
 AS(I)=-(BS(I-1)*XIS/AS(I-1)-CS(I-3)*BS(I-1)*ZIS/(AS(I-1)*AS(I-3))-      C 124
1BS(I-1)*BS(I-2)*YIS/(AS(I-1)*AS(I-2))+BS(I-1)*BS(I-2)*BS(I-3)*ZIS/     C 125
2(AS(I-1)*AS(I-2)*AS(I-3))-AIS+CS(I-2)*YIS/AS(I-2)-BS(I-3)*CS(I-2)*     C 126
3ZIS/(AS(I-2)*AS(I-3)))                                                 C 127
 BS(I)=-(-BIS+AS(I+1)*EIS/CS(I+1)-AS(I+1)*AS(I+3)*GIS/(CS(I+3)*CS(I      C 128
1+1))-AS(I+1)*BS(I+2)*FIS/(CS(I+1)*CS(I+2))+AS(I+1)*BS(I+2)*BS(I+3)     C 129
2*GIS/(CS(I+1)*CS(I+2)*CS(I+3))+CS(I-1)*XIS/AS(I-1)-CS(I-1)*CS(I-3)     C 130
3*ZIS/(AS(I-1)*AS(I-3))-BS(I-2)*CS(I-1)*YIS/(AS(I-1)*AS(I-2))+BS(I-     C 131
42)*BS(I-3)*CS(I-1)*ZIS/(AS(I-1)*AS(I-2)*AS(I-3)))                      C 132
 CS(I)=-BS(I+1)*EIS/CS(I+1)+AS(I+3)*BS(I+1)*GIS/(CS(I+1)*CS(I+3))+B      C 133
1S(I+1)*BS(I+2)*FIS/(CS(I+1)*CS(I+2))-BS(I+1)*BS(I+2)*BS(I+3)*GIS/(     C 134
2CS(I+1)*CS(I+2)*CS(I+3))+CIS-AS(I+2)*FIS/CS(I+2)+AS(I+2)*BS(I+3)*G     C 135
3IS/(CS(I+2)*CS(I+3))                                                   C 136
 DS(I)=-DS(I+1)*EIS/CS(I+1)+AS(I+3)*DS(I+1)*GIS/(CS(I+1)*CS(I+3))+B      C 137
1S(I+2)*DS(I+1)*FIS/(CS(I+1)*CS(I+2))-BS(I+2)*BS(I+3)*DS(I+1)*GIS/(     C 138
2CS(I+1)*CS(I+2)*CS(I+3))+DIS-DS(I+3)*GIS/CS(I+3)-DS(I+2)*FIS/CS(I+     C 139
33)+BS(I+3)*DS(I+2)*GIS/(CS(I+2)*CS(I+3))+DS(I-1)*CS(I-3)*ZIS/(AS(I     C 140
4-1)*AS(I-3))+BS(I-2)*DS(I-1)*YIS/(AS(I-1)*AS(I-2))-BS(I-2)*BS(I-3)     C 141
```

```
     5*DS(I-1)*ZIS/(AS(I-1)*AS(I-2)*AS(I-3))-DS(I-3)*ZIS/AS(I-3)-DS(I-2)  C 142
     6*YIS/AS(I-2)+BS(I-3)*DS(I-2)*ZIS/(AS(I-2)*AS(I-3))-DS(I-1)*XIS/AS(  C 143
     7I-1)                                                                C 144
      GO TO 10                                                            C 145
9     CONTINUE                                                            C 146
      AS(I)=0.                                                            C 147
      BS(I)=1.                                                            C 148
      CS(I)=0.                                                            C 149
      DS(I)=TIBAR+1.E-4                                                   C 150
10    CONTINUE                                                            C 151
      DO 11 N=IP1,IZ1                                                     C 152
      AS(N)=CRNI*(1./DXPP**2-ALPHA1(N)/(2.*DXPP))                         C 153
      BS(N)=CRNI*(ALPHA2(N)-2./DXPP**2+ALPHB4(N)/(DT*CRNI))               C 154
      CS(N)=CRNI*(1./DXPP**2+ALPHA1(N)/(2.*DXPP))                         C 155
      DS(N)=-ALPHB3(N)-(1.-CRNI)*((1./DXPP**2-ALPHP1(N)/(2.*DXPP))*TSP(N  C 156
     1-1)+(ALPHP2(N)-2./DXPP**2-ALPHB4(N)/(DT*(1.-CRNI)))*TSP(N)+(1./DXP  C 157
     2P**2+ALPHP1(N)/(2.*DXPP))*TSP(N+1))                                 C 158
11    CONTINUE                                                            C 159
      AK=CRNI/(KP(IP)*GAMIP4*DXP/LP+KPP(IP)*KAPIP4*DXPP/IL-HTSK)          C 160
      AKP=(1.-CRNI)/(KPPIP*GAMIPP4*DXP/LPPP+KPPPIP*KAPIPP4*DXPP/IL-HTSK)  C 161
      ZIS=-AK*KP(IP)/(6.*DXP*LP)                                          C 162
      YIS=AK*KP(IP)*(.75/DXP+GAMIP1/3.)/LP                                C 163
      XIS=-AK*KP(IP)*(4./(3.*DXP)+1.5*GAMIP1)/LP                          C 164
      AIS=-AK*KP(IP)*(.75/DXP-3.*GAMIP1)/LP                               C 165
      BIS=-1./DT+AK*(KP(IP)/LP*(1.5/DXP-11.*GAMIP1/6.-GAMIP2*DXP)+KPP(IP  C 166
     1)/IL*(1.5/DXPP+11.*KAPIP1/6.-KAPIP2*DXPP))                          C 167
      CIS=-AK*KPP(IP)*(.75/DXPP+3.*KAPIP1)/IL                             C 168
      EIS=-AK*KPP(IP)*(4./(3.*DXPP)-1.5*KAPIP1)/IL                        C 169
      FIS=AK*KPP(IP)*(.75/DXPP-KAPIP1/3.)/IL                              C 170
      GIS=-AK*KPP(IP)/(6.*DXPP*IL)                                        C 171
      DIS=AK*(KP(IP)*GAMIP3*DXP/LP+KPP(IP)*KAPIP3*DXPP/IL)-AKP*KPPIP/LPP  C 172
     1P*(-TSP(IP-4)/(6.*DXP)+(.75/DXP+GAMIPP1/3.)*TSP(IP-3)-(4./(3.*DXP)  C 173
     2+1.5*GAMIPP1)*TSP(IP-2)-(.75/DXP-3.*GAMIPP1)*TSP(IP-1))-(AKP*(KPPI  C 174
     3P/LPPP*(1.5/DXP-11.*GAMIPP1/6.-GAMIPP2*DXP)+KPPPIP/IL*(1.5/DXPP+11  C 175
     4.*KAPIPP1/6.-KAPIPP2*DXPP))+1./DT)*TSP(IP)+AKP*KPPPIP/IL*((.75/DXP  C 176
```

```
5P+3.*KAPIPP1)*TSP(IP+1)+(4./(3.*DXPP)-1.5*KAPIPP1)*TSP(IP+2)-(.75/
6DXPP-KAPIPP1/3.)*TSP(IP+3)+TSP(IP+4)/(6.*DXPP))+AKP*(KPPIP*GAMIPP3
7*DXP/LPPP+KPPPIP*KAPIPP3*DXPP/IL)
 AS(IP)=-(BS(IP-1)*XIS/AS(IP-1)-CS(IP-3)*BS(IP-1)*ZIS/(AS(IP-1)*AS(
1IP-3))-BS(IP-1)*BS(IP-2)*YIS/(AS(IP-1)*AS(IP-2))+BS(IP-1)*BS(IP-2)
2*BS(IP-3)*ZIS/(AS(IP-1)*AS(IP-2)*AS(IP-3))-AIS+CS(IP-2)*YIS/AS(IP-
32)-BS(IP-3)*CS(IP-2)*ZIS/(AS(IP-2)*AS(IP-3)))
 BS(IP)=-(-BIS+AS(IP+1)*EIS/CS(IP+1)-AS(IP+1)*AS(IP+3)*GIS/(CS(IP+3
1)*CS(IP+1))-AS(IP+1)*BS(IP+2)*FIS/(CS(IP+1)*CS(IP+2))+AS(IP+1)*BS(
2IP+2)*BS(IP+3)*GIS/(CS(IP+1)*CS(IP+2)*CS(IP+3))+CS(IP-1)*XIS/AS(IP
3-1)-CS(IP-1)*CS(IP-3)*ZIS/(AS(IP-1)*AS(IP-3))-BS(IP-2)*CS(IP-1)*YI
4S/(AS(IP-1)*AS(IP-2))+BS(IP-2)*BS(IP-3)*CS(IP-1)*ZIS/(AS(IP-1)*AS(
5IP-2)*AS(IP-3)))
 CS(IP)=-BS(IP+1)*EIS/CS(IP+1)+AS(IP+3)*BS(IP+1)*GIS/(CS(IP+1)*CS(I
1P+3))+BS(IP+1)*BS(IP+2)*FIS/(CS(IP+1)*CS(IP+2))-BS(IP+1)*BS(IP+2)*
2BS(IP+3)*GIS/(CS(IP+1)*CS(IP+2)*CS(IP+3))+CIS-AS(IP+2)*FIS/CS(IP+2
3)+AS(IP+2)*BS(IP+3)*GIS/(CS(IP+2)*CS(IP+3))
 DS(IP)=-DS(IP+1)*EIS/CS(IP+1)+AS(IP+3)*DS(IP+1)*GIS/(CS(IP+1)*CS(I
1P+3))+BS(IP+2)*DS(IP+1)*FIS/(CS(IP+1)*CS(IP+2))-BS(IP+2)*BS(IP+3)*
2DS(IP+1)*GIS/(CS(IP+1)*CS(IP+2)*CS(IP+3))+DIS-DS(IP+3)*GIS/CS(IP+3
3)-DS(IP+2)*FIS/CS(IP+3)+BS(IP+3)*DS(IP+2)*GIS/(CS(IP+2)*CS(IP+3))+
4DS(IP-1)*CS(IP-3)*ZIS/(AS(IP-1)*AS(IP-3))+BS(IP-2)*DS(IP-1)*YIS/(A
5S(IP-1)*AS(IP-2))-BS(IP-2)*BS(IP-3)*DS(IP-1)*ZIS/(AS(IP-1)*AS(IP-2
6)*AS(IP-3))-DS(IP-3)*ZIS/AS(IP-3)-DS(IP-2)*YIS/AS(IP-2)+BS(IP-3)*D
7S(IP-2)*ZIS/(AS(IP-2)*AS(IP-3))-DS(IP-1)*XIS/AS(IP-1)
 ZSCNST=CRNI*KPP(IZ)/(6.*DXPP**2*IL*(HTSKP*(ALPHA1(IZ)+11./(6.*DXPP
1))-ALPHA4(IZ)*KPP(IZ)/IL))
 YSCNST=-4.5*ZSCNST
 XSCNST=8.*ZSCNST
 AS(IZ)=-YSCNST
 BS(IZ)=(6.*DXPP**2*ALPHA2(IZ)-9.)*ZSCNST-CRNI*SGMA*EPSP*FS(IZ)**3*
1(ALPHA1(IZ)+11./(6.*DXPP))/(HTSKP*(ALPHA1(IZ)+11./(6.*DXPP))-ALPHA
24(IZ)*KPP(IZ)/IL)-1./DT
 DS(IZ)=-CRNI*(ALPHA1(IZ)+11./(6.*DXPP))/(HTSKP*(ALPHA1(IZ)+11./(6.
1*DXPP))-ALPHA4(IZ)*KPP(IZ)/IL)*(QNET+ALPHA3(IZ)*KPP(IZ)/(IL*(ALPHA
```

```
     21(IZ)+11./(6.*DXPP))))-(1.-CRNI)*(ALPHP1(IZ)+11./(6.*DXPP))/(HTSKP
     3*(ALPHP1(IZ)+11./(6.*DXPP))-ALPHP4(IZ)*KPPPIZ/IL)*(QPNET+ALPHP3(IZ
     4)*KPPPIZ/(IL*(ALPHP1(IZ)+11./(6.*DXPP)))+KPPPIZ/(IL*(ALPHP1(IZ)+11
     5./(6.*DXPP)))*(TSP(IZ-4)/(6.*DXPP**2)-.75*TSP(IZ-3)/DXPP**2+4.*TSP
     6(IZ-2)/(3.*DXPP**2)+.75*TSP(IZ-1)/DXPP**2-(1.5/DXPP**2-ALPHP2(IZ))
     7*TSP(IZ))-SGMA*EPSP*TSP(IZ)**4)-TSP(IZ)/DT
      AS(IZ)=AS(IZ-2)*BS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-1
     1)*BS(IZ-2)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)+AS(IZ-1)*CS(IZ-2)*(AS
     2(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ)*AS(IZ-1)*AS(IZ-2)*AS(IZ-3)
      BS(IZ)=AS(IZ-2)*CS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-2
     1)*CS(IZ-1)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ-1)*AS(IZ-2)*AS(
     2IZ-3)*BS(IZ)
      DS(IZ)=AS(IZ-2)*DS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-2
     1)*DS(IZ-1)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ-1)*AS(IZ-2)*(AS
     2(IZ-3)*DS(IZ)-DS(IZ-3)*ZSCNST)+AS(IZ-1)*DS(IZ-2)*(AS(IZ-3)*YSCNST-
     3BS(IZ-3)*ZSCNST)
      CS(IZ)=0.
C     SOLVE TRI-DIAGONAL MATRIX FOR TS
      BP(1)=CS(1)/BS(1)
      GP(1)=DS(1)/BS(1)
      DO 12 N=2,IZ
      WS=BS(N)-AS(N)*BP(N-1)
      BP(N)=CS(N)/WS
      GP(N)=(DS(N)-AS(N)*GP(N-1))/WS
12    CONTINUE
      TFS(IZ)=GP(IZ)
      FS(IZ)=TFS(IZ)
      KON=IZ1
      DO 13 N=1,IZ1
      TFS(KON)=GP(KON)-BP(KON)*TFS(KON+1)
      FS(KON)=TFS(KON)
13    KON=KON-1
      RETURN
      END
```

```
      SUBROUTINE PDP (CRNI,DT,L,DX,DX1,MGDOT,MGDOTP,LPP,I,IM,RHO,P,MU,T,
     1TP,RU)
C     SUBROUTINE FOR SOLVING SECOND ORDER LINEARIZED DIFFERENTIAL EQUA-
C        TIONS 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),PWP,PP(50),PM(50),PMU,PPM,PRH
     20(50),ETA(50),ETAP(50),AVGMF(50),AVGMFP(50)
      COMMON /DE1DE2/ AS,BS,CS,DS,BP,GP
      REAL MU,L,MGDOT,LPP,MGDOTP
      DOUBLE PRECISION AS,BS,CS,DS,PX,PY,PZ,PA,PB,PD,BP,GP,W,ZP
C     CALCULATE TRI-DIAGONAL MATRIX COEFFICIENTS
      IN=I-2
      DDX=DX1
      DO 2 N=2,IM
      IF (N.NE.20) GO TO 1
      DDX=DX
      GO TO 2
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))*PP(N-1)**2-
     1(2./DDX**2-PAP2(N)+PAB4(N)/(DT*(1.-CRNI)))*PP(N)**2+(1./DDX**2+PAP
     21(N)/(2.*DDX))*PP(N+1)**2)
2     CONTINUE
      AS(20)=CRNI*(PAL1(20)*DX/(DX1*(DX1+DX))-2./(DX1*(DX1+DX)))
      BS(20)=CRNI*(2./(DX*DX1)-PAL2(20)-PAL1(20)*(DX-DX1)/(DX1*DX))-PAB4
     1(20)/DT
      CS(20)=CRNI*(-2./(DX*(DX1+DX))-PAL1(20)*DX1/(DX*(DX1+DX)))
      DS(20)=-PAB3(20)-(1.-CRNI)*(PAP1(20)*DX/(DX1*(DX1+DX))-2./(DX1*(DX
     11+DX)))*PP(19)**2-((1.-CRNI)*(2./(DX*DX1)-PAP2(20)-PAP1(20)*(DX-DX
     21)/(DX1*DX))+PAB4(20)/DT)*PP(20)**2+(1.-CRNI)*(2./(DX*(DX1+DX))+PA
     3P1(20)*DX1/(DX*(DX1+DX)))*PP(21)**2
      DS(2)=DS(2)-AS(2)*P(1)**2
      AS(2)=0.
```

```
      PX=CRNI/(6.*DX**2)                                                D  37
      PY=-.75*CRNI/DX**2                                                D  38
      PZ=4.*CRNI/(3.*DX**2)                                             D  39
      PA=-PY                                                            D  40
      PB=PAB4(I)/DT+CRNI*(PAL2(I)-3./(2.*DX**2))                        D  41
      PD=-PAB3(I)-(1.-CRNI)*(11./(6.*DX)+PAP1(I))*(2.*PMU*LPP*MGDOTP*RU*  D  42
     1TP(I)/(AVGMFP(I)*PPM))-CRNI*(11./(6.*DX)+PAL1(I))*(2.*MU(I)*L*MGDO  D  43
     2T*RU*T(I)/(AVGMF(I)*PM(I)))-(1.-CRNI)*(PP(I-4)**2/(6.*DX**2)-.75*P  D  44
     3P(I-3)**2/DX**2+4.*PP(I-2)**2/(3.*DX**2)+.75*PP(I-1)**2/DX**2+(PAP  D  45
     42(I)-1.5/DX**2-PAB4(I)/(DT*(1.-CRNI)))*PP(I)**2)                  D  46
      AS(I)=PA-CS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3))-BS(I-1)/AS(I-1)*(  D  47
     1PZ-PX*CS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3)))    D  48
      BS(I)=PB-CS(I-1)/AS(I-1)*(PZ-PX*CS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(P  D  49
     1Y-PX*BS(I-3)/AS(I-3)))                                            D  50
      DS(I)=PD-PX/AS(I-3)*DS(I-3)-DS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3)  D  51
     1)-DS(I-1)/AS(I-1)*(PZ-PX*CS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(PY-PX*BS  D  52
     2(I-3)/AS(I-3)))                                                   D  53
      CS(I)=0.                                                          D  54
C     SOLVE TRI-DIAGONAL MATRIX FOR P                                   D  55
      BP(2)=CS(2)/BS(2)                                                 D  56
      GP(2)=DS(2)/BS(2)                                                 D  57
      DO 3 N=3,I                                                        D  58
      W=BS(N)-AS(N)*BP(N-1)                                             D  59
      BP(N)=CS(N)/W                                                     D  60
      GP(N)=(DS(N)-AS(N)*GP(N-1))/W                                     D  61
3     CONTINUE                                                          D  62
      ZP(I)=DSQRT(GP(I))                                                D  63
      P(I)=ZP(I)                                                        D  64
      KON=IM                                                            D  65
      DO 4 N=1,IN                                                       D  66
      ZP(KON)=DSQRT(GP(KON)-BP(KON)*ZP(KON+1)**2)                       D  67
      P(KON)=ZP(KON)                                                    D  68
4     KON=KON-1                                                         D  69
      RETURN                                                            D  70
      END                                                               D  71-
```

```
      SUBROUTINE PDE2 (BETA1,BETB2,BETB3,BETP1,TP,F,CRNI,DX,DX1,DT,I)
C     SUBROUTINE FOR SOLVING FIRST ORDER LINEARIZED DIFFERENTIAL
C        EQUATIONS GOVERNING PYROLYSIS GAS TEMPERATURE AND FLOW RATE AND
C        CHAR LAYER POROSITY.
      DIMENSION B(50), C(50), D(50), E(50), F(50), TP(50), BETA1(50), BE
     1TB2(50), BETB3(50), BETP1(50), TF(50)
      COMMON /DE1DE2/ B,C,D,E
      DOUBLE PRECISION B,C,D,E,TF
C     CALCULATE TRI-DIAGONAL MATRIX COEFFICIENTS
      IM=I-1
      IN=I-2
      IQ=I-3
      DDX=DX1
      B(19)=BETB3(19)/DT+CRNI*(-(DX**2+2.*DX1*DX)/(DX1*DX*(DX1+DX))+BETA
     11(19))
      C(19)=CRNI*(DX1+DX)/(DX1*DX)
      E(19)=-CRNI*DX1/(DX*(DX1+DX))
      D(19)=-BETB2(19)+(BETB3(19)/DT-(1.-CRNI)*(-(DX**2+2.*DX1*DX)/(DX1*
     1DX*(DX1+DX))+BETP1(19)))*TP(19)-(1.-CRNI)*(DX1+DX)/(DX1*DX)*TP(20)
     2+(1.-CRNI)*DX1/(DX*(DX1+DX))*TP(21)
      DO 2 N=1,IN
      IF (N.NE.19) GO TO 1
      DDX=DX
      GO TO 2
1     CONTINUE
      B(N)=CRNI*(BETA1(N)-1.5/DDX)+BETB3(N)/DT
      C(N)=2.*CRNI/DDX
      E(N)=-.5*CRNI/DDX
      D(N)=-BETB2(N)-((1.-CRNI)*(BETP1(N)-1.5/DDX)-BET33(N)/DT)*TP(N)-(1
     1.-CRNI)*(2.*TP(N+1)/DDX-TP(N+2)/(2.*DDX))
2     CONTINUE
      B(IM)=CRNI*(BETA1(IM)-1./DX)+BETB3(IM)/DT
      C(IM)=CRNI/DX
      E(IM)=0.
      D(IM)=-BETB2(IM)-((1.-CRNI)*(BETP1(IM)-1./DX)-BETB3(IM)/DT)*TP(IM)
     1-(1.-CRNI)/DX*TP(I)
```

```
C       SOLVE TRI-DIAGONAL MATRIX                                        E  37
        TF(I)=F(I)                                                       E  38
        TF(IM)=(D(IM)-C(IM)*TF(I))/B(IM)                                 E  39
        F(IM)=TF(IM)                                                     E  40
        KON=IN                                                           E  41
        DO 3 N=1,IN                                                      E  42
        TF(KON)=(D(KON)-C(KON)*TF(KON+1)-E(KON)*TF(KON+2))/B(KON)        E  43
        F(KON)=TF(KON)                                                   E  44
3       KON=KON-1                                                        E  45
        RETURN                                                           E  46
        END                                                              E  47-
```

```
      SUBROUTINE CHCOM(TIME)                                            F   1
C     SUBROUTINE FOR CALCULATING THE CHEMICAL REACTION RATES OF EACH    F   2
C        SPECIES.                                                       F   3
      COMMON ACEF(12),ACER(12),BCEF(12),BCER(12),CRNI,KUPT(40,12),KUPTV(     4
     140),M(13),MFK(50,12),MNO,NNO,MU(50),MUKT(40,12),MUKTV(40),PR(50),R F   5
     2(50,12),RHO(50),RHOK(50,12),RHOKP(50,12),T(50),TEMP(40),NRCT,KT,RU F   6
     3,NSTEP,ROCPM(50),RS(50),RHR(50,12),RHS(50),DHK(50,12),DHJ(50,12),H F   7
     4RJSUM(50)                                                         F   8
      DIMENSION RMP(9),RMR(9),RJN(9)                                    F   9
      REAL M                                                            F  10
      N=NSTEP                                                           F  11
      RMR(1)=RHOK(N,1)/M(1)                                             F  12
      RMP(1)=1.                                                         F  13
      RMR(2)=RHOK(N,11)/M(11)                                           F  14
      RMP(2)=RHOK(N,3)/M(3)*RHOK(N,2)/M(2)                              F  15
      RMR(3)=RHOK(N,3)/M(3)                                             F  16
      RMP(3)=RHOK(N,4)/M(4)*RHOK(N,2)/M(2)                              F  17
      RMR(4)=(RHOK(N,4)/M(4))**2                                        F  18
      RMP(4)=1.                                                         F  19
      RMR(5)=RHOK(N,12)/M(12)                                           F  20
      RMP(5)=1.                                                         F  21
      RMR(6)=RHOK(N,9)/M(9)                                             F  22
      RMP(6)=1.                                                         F  23
      RMR(7)=RHOK(N,6)/M(6)                                             F  24
      RMP(7)=1.                                                         F  25
      RMR(8)=RHOK(N,7)/M(7)                                             F  26
      RMP(8)=1.                                                         F  27
      RMR(9)=RHOK(N,7)/M(7)                                             F  28
      RMP(9)=1.                                                         F  29
      DO 1 J=1,9                                                        F  30
      AKF=ACEF(J)*EXP(-BCEF(J)/(RU*T(N)))                               F  31
      IF(J.EQ.6)AKF=AKF/T(N)                                            F  32
      AKR=ACER(J)*EXP(-BCER(J)/(RU*T(N)))                               F  33
      RJN(J)= AKF*RMR(J)-AKR*RMP(J)                                     F  34
1     CONTINUE                                                          F  35
      R(N,1)=-RJN(1)                                                    F  36
```

```
 R(N,2)=.5*RJN(1)+RJN(2)+RJN(3)+RJN(4)+3.*RJN(5)+RJN(7)+1.5*RJN(8)+   F   37
1RJN(9)                                                               F   38
 R(N,3)=RJN(2)-RJN(3)                                                 F   39
 R(N,4)=RJN(3)-RJN(4)                                                 F   40
 R(N,5)=2.*RJN(6)+RJN(7)                                              F   41
 R(N,6)=-RJN(7)                                                       F   42
 R(N,7)=-RJN(8)-RJN(9)                                                F   43
 R(N,8)=.5*RJN(8)-RJN(9)                                              F   44
 R(N,9)=-RJN(6)                                                       F   45
 R(N,10)=RJN(9)                                                       F   46
 R(N,11)=.5*RJN(1)-RJN(2)                                             F   47
 R(N,12)=-RJN(5)                                                      F   48
 RS(N)=2.*RJN(4)+6.*RJN(5)                                            F   49
 RHS(N)=-RJN(6)-RJN(7)-RJN(9)                                         F   50
 RHR(N,6)=RJN(6)                                                      F   51
 RHR(N,7)=RJN(7)                                                      F   52
 RHR(N,9)=RJN(9)                                                      F   53
 RETURN                                                               F   54
 END                                                                  F   55-
```

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 $\int_{x(N)}^{1} \left[\frac{\partial}{\partial t} \eta\rho - \eta \sum_i R_{T_i} M_i \right] dx$
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

AKP	Parameter defined in solution of solid temperature equation
AKPL	Parameter defined in solution of solid temperature equation
AKPLP	Parameter defined in solution of solid temperature equation
AKR	Rate of homogeneous chemical reaction in reverse direction, single subscript
AKSL	Parameter defined in solution of solid temperature equation
AKSLP	Parameter defined in solution of solid temperature equation
ALFC	Weighting factor for transpiration effectiveness of char mass loss
ALFP	Weighting factor for transpiration effectiveness of pyrolysis gases
ALPHA	Absorptivity of char surface
ALPHA 1 ALPHA 2 ALPHA 3 ALPHA 4	Coefficients in linearized differential equations for solid temperature evaluated at end of time step, single subscript
ALPHB3 ALPHB4	Coefficients in finite difference equation for solid temperature evaluated at mid point of time step, single subscript
ALPHIP1 ALPHIP2 ALPHIP3 ALPHIP4	Values of ALPHA1, etc. for the char layer at the pyrolysis zone evaluated at the start of the time step
ALPHI1 ALPHI2 ALPHI3 ALPHI4	Values of ALPHA1, etc. for the char layer at the pyrolysis zone evaluated at the end of the time step
ALPHP1 ALPHP2 ALPHP3 ALPHP4	Values of ALPHA1, etc. evaluated at the start of the time step, single subscript

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, AMJ	Dummy parameter defined in computing pyrolysis gas viscosity
AP	Solution of pyrolysis gas pressure equation for previous iteration, single subscript
APR	Dummy parameter defined in computing pyrolysis gas Prandtl number
AP1, ARH	Dummy arrays defined in solution of species continuity equation, single subscript
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	Averag- 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 subject
BCER	Activation temperature for reverse homogeneous chemical reaction involving gaseous species, single subscript

BETA1 BETA2 BETA3	Coefficients in linearized differential equation of pyrolysis gas temperature evaluated at end of time step, single subscript
BETB2 BETB3	Coefficients in finite difference equation for pyrolysis gas temperature evaluated at mid point of time step, single subscript
BETP1 BETP2 BETP3	Values of BETA1, 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 tempe ature, single subscript
CPS	Heat capacity of char layer, single subscript
CPSA11, CPSA12	Dummy parameters defined in computing CPK
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, sinble subscript
DDX	Distance between finite difference stations
DEB2, DEB3	Coefficients in finite difference equation for conservation of species evaluated at mid point of time step, single subscript
DEL1, DEL2, DEL3	Coefficients in linearized differential equation for conservation of species evaluated at end of time step, double subscript
DEN	Denominator defined in solution of first order equations
DEP1, DEP2, DEP3	Values of DEL1, etc. evaluated at start of time step, double subscript
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 layer 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

DXP1	Distance between finite difference stations in uncharred layer in region of the fine grid spacing
DX1	Distance between finite difference stations in char layer in region of fine grid spacing
E	"E" coefficient in matrix formed by first order equations, single subscript
EIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer - insulation layer interface
EPSA1, EPSA2, EPSA3	Coefficients in linearized differential equation for char layer porosity evaluated at end of time step, single subscript
EPSB2, EPSB3	Coefficients in finite difference equation for char layer porosity evaluated at mid point of time step, single subscript
EPSP	Emissivity of radiating heat sink surface behind insulation
EPSP1, EPSP2, EPSP3	Values of EPSA1, etc. evaluated at the start of the time step, single subscript
EPSS	Emissivity of char layer surface
ETA	Porosity of char layer at end of time step, single subscript
ETAP	Porosity of char layer at start of time step, single subscript
F	Dummy array defined in solution of first order differential equations, single subscript
FIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer insulation layer interface
FS	Dummy array defined in solution of solid temperature equations, single subscript
GAMIPP1, GAMIPP2, GAMIPP3, GAMIPP4	Values of ALPHA1, etc. for the uncharred material at the uncharred layer-insulation layer interface evaluated at the start of the time step

GAMIP1 GAMIP2 GAMIP3 GAMIP4	Values of ALPHA1, etc. for the uncharred material at the uncharred layer-insulation layer interface evaluated at the end of the time step
GAMMI1 GAMMI2 GAMMI3 GAMMI4	Values of ALPHA1, etc. for the uncharred material at the pyrolysis zone evaluated at the end of the time step
GIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface
GP	Parameter defined in algorithm for solving set of finite difference equations, single subscript
GSCNST	Coefficient in solid temperature finite difference equation evaluated at the front surface of the char layer
HA	Coefficient of convective heat transfer between char layer and pyrolysis gas, single subscript
HBRKN2	Enthalpy of N_2 at char surface temperature evaluated at end of time step
HBRKO2	Enthalpy of O_2 at char surface temperature evaluated at end of time step
HC	Heat of sublimation of char layer material
HE	Enthalpy of free stream
HK	Enthalpy of gaseous species, double subscript
HKT	Table of gaseous species enthalpy versus temperature, double subscript
HKTV	Dummy array defined for use in table look-up routine for single subscript
HRJSUM HRSUM	Parameters defined in computing coeffcients in pyrolysis gas temperature equation, single subscript
HS	Enthalpy of char layer evaluated at the char temperature, single subscript

HSA11 HSA12	Dummy parameters defined in computing HK
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 $\rho\hat{C}_p\ell$ for heat sink at uncharred layer-insulation layer interface
HTSKP	Value of $\rho\hat{C}_p\ell$ 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 IO IO1	Indices
IP	Total number of finite difference stations in char layer and uncharred material
IPP IP1	Indices
IZ	Total number of finite difference stations in char layer, uncharred material, and insulation layer
IZ1 J	Dummy 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

KAPIPP1 KAPIPP2 KAPIPP3 KAPIPP4	Value of ALPHA1, etc. for the insulation layer at the uncharred layer-insulation layer interface evaluated at the start of the time step
KAPIP1 KAPIP2 KAPIP3 KAPIP4	Value of ALPHA1, 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 KM KON	Dummy indices
KP	Conductivity of uncharred material at end of time step, single subscript
KPP	Conductivity of insulation layer, single subscript
KPPI	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
KSP1	Conductivity of char layer at front surface evaluated at start of time step

KST	Table of char layer conductivity versus temperature, single subscript
KT KTT	Indices
KUPT	Table of gaseous species conductivity versus temperature, double subscript
KUPTV	Dummy array defined for use in table-look-up routine for KGK, single subscript
L	Char layer thickness at end of time step
LAM	Ratio of mass char layer removed to free stream oxygen consumed in first order oxidation of char
LP	Uncharred material thickness at end of time step
LPMIN	Minimum thickness of uncharred layer
LPP	Char layer thickness at start of time step
LPPP	Uncharred material thickness at start of time step
M	Molecular weight of chemical species, single subscript
MCPP	Order of interpolation in obtaining CPP
MFK	Mole fraction of gaseous species, double subscript
MFKI	Mole fraction of gaseous species at pyrolysis zone, single subscript
MGDOT	Rate of pyrolysis of uncharred material at end of time step
MGDOTP	Rate of pyrolysis of uncharred material at start of time step
MKP	Order of interpolation in obtaining KP
MKS	Order of interpolation in obtaining KS
MNO	Order of interpolation in obtaining HS, HST, HK, CPK, HBRKN2, HBRNKO2, MUK, and KGK
MPDOT	Effective mass injection rate at char surface

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 $\dot{m}_g$ = 1.0×10^{-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 $\dot{m}_g = 1.0 \times 10^{-3}$ kg/m^2-sec
NITS	Trigger used in computing CPK and HK
NKP	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, PAB4	Coefficients in finite difference equation for pyrolysis gas pressure evaluated at mid-point of time step, single subscript
PAL1, PAL2, PAL3, PAL4	Coefficients in linearized differential for pyrolysis gas pressure evaluated at end of time step, single subscript
PAMGDOT	Product of chemical species density and velocity at start of time step, double subscript
PAP1, PAP2, PAP3, PAP4	Value of PAL1, etc. evaluated at the start of the time step, single subscript
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_2 at char surface temperature evaluated at start of time step
PHBRKO2	Enthalpy of O_2 at char surface temperature evaluated at start of time step
PHI	Parameter defined in computing viscosity of pyrolysis gas, double subscript

PM	Permeability of char layer at end of time step, single subscript
PMU	Pyrolysis gas viscosity at pyrolysis zone, evaluated at start of time step
PMV	Data input for permeability of char layer
PP	Pyrolysis gas pressure at start of time step, single subscript
PPM	Permeability of char layer at pyrolysis zone, evaluated at start of time step
PR	Prandt number of pyrolysis gas
PRHO	Pyrolysis gas density at start of time step, single subscript
PRINTFQ	Time interval at which output is printed
PROM	Sum of mole density of all chemical species, single subscript
PROPC	Proportionality constant appearing in equation for HA
PSI	Parameter defined in computing conductivity of pyrolysis gas, double subscript
PT	Pyrolysis gas temperature at last table look up of data, single subscript
PTIME	Print time
PTS	Solid temperature at last table-look-up data, single subscript
PW	Dimensionless pressure at surface of char layer
PWP	Dimensional pressure at surface of char layer
PX, PY, PZ	"PX", etc. coefficients in finite difference equation for pyrolysis gas pressure evaluated the pyrolysis zone
Q	Net heat transfer at char surface by conduction at end of time step

QC	Heat transfer to cold, non-ablating body
QCOND	Rate of energy transfer by conduction at char layer surface
QCT	Aerodynamic heat transfer to hot, ablating body
QCTAB	Table of QC versus time, single subscript
QFAC	Parameter define in computation of aerodynamic heat transfer
QNET	Heat transfer to back surface of insulation layer at end of time step
QPNET	Heat transfer to back surface of insulation layer at start of time step
QPT	Net heat transfer at char surface by conduction at start of time step
QRAT	Ratio of set heat transfer at surface by conduction to cold wall, non-ablating heat transfer
QRS	Radiant heat transfer at surface
RAD	Vehicle nose radius
RHO	Pyrolysis gas density at end of time step, single subscript
RHOK	Density of chemical species at end of time step, double subscript
RHOKP	Density of chemical species at start of time step, double subscript
RHOP	Density of uncharred layer at end of time step, single subscript
RHOPP	Density of insulation layer, single subscript
RHOPPV	Data input for insulation density
RHOSO	Density of char layer at front surface
RHOST	Theoretical density of char layer
RHR	Rate of function of chemical species by heterogeneous chemical reactions, double subscript

RHS	Rate of formation of solid by heterogeneous chemical reactions, single subscript
RJN	Rate of reaction of chemical reaction, single subscript
RM	Total mass rate of production, single subscript
RMP	Parameter defined by $\prod_i (\rho_i/M_i)^{v''_i}$, single subscript
RMR	Parameter defined by $\prod_i (\rho_i/M_i)^{v'_i}$, single subscript
ROCPM	Parameter defined by $\sum_i \rho_i C_{P_i}/M_i$, single subscript
ROHM	Parameter defined by $\sum_i \rho_i H_i/M_i$, single subscript
ROM	Total mole density of pyrolysis gas, single subscript
RS	Mole rate of production of solid carbon at end of time step, single subscript
RT	Mole rate of production of chemical species, double subscript
RU	Universal gas constant
S	Trigger for surface removal mechanism
SGMA	Stephan-Boltzmann constant
SP	Trigger for selecting mode of calcualtion of pyrolysis rate of uncharred layer
SPECIES	Identification of gaseous species, single subscript
SQPT	Table of $(PW)^{1/2}$ versus time, single subscript
T	Pyrolysis gas temperature at end of time step, single subscript
TCPP	Temperature table for CPPT, single subscript
TEMP	Temperature table for HSTT, HKT, CPKT, MUKT, and KUPT, single subscript
TF	Pyrolysis gas temperature in double precision, single subscript

TFS	Solid temperature in double precision, single subscript
TIBAR	Maximum temperature at pyrolysis zone
TIME	Time from start of program
TIMET	Time table for QCTAB, single subscript
TKP	Temperature table for KPT, single subscript
TKS	Temperature table for KST, single subscript
TMPRES	Time table for SQPT, single subscript
TP	Pyrolysis gas temperature at start of time step, single subscript
TRAB	Trigger for selecting blocking approximation
TREF	Transpiration effectiveness
TS	Solid temperature at end of time step, single subscript
TSAVE	Parameter used in calculating DHK
TSP	Solid temperature at start of time step, single subscript
T1BAR	Sublimation temperature of char layer
V	Average velocity of gas in char layer, single subscript
VC	Velocity of moring coordinate, single subscript
W	Parameter defined in algorithm for solving finite difference equations for pyrolysis gas pressure
WS	Parameter defined in algorithm for solving finite difference equations for solid temperature
X	Dimensionless char layer coordinate
XIS	Coefficient in solid temperature finite difference equation at the pyrolysis zone and the uncharred layer insulation layer interface
XP	Dimensionless coordinate in uncharred layer

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

VITA

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