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Aerotherm Report No. UM-70-13

USER'S MANUAL
AEROTHERM EQUILIBRIUM SURFACE
THERMOCHEMISTRY COMPUTER PROGRAM,
VERSION 3

Volume I – Program Description and
Sample Problems

April 1970

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Air Force Rocket Propulsion Laboratory
Director of Laboratories
Edwards, California 93523
Air Force Systems Command
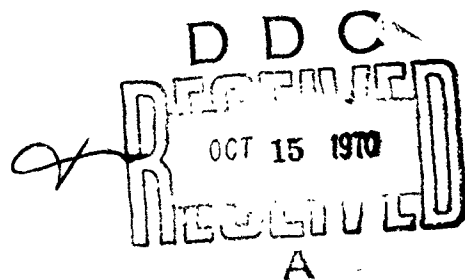United States Air Force

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USER'S MANUAL

AEROTHERM EQUILIBRIUM SURFACE
THERMOCHEMISTRY COMPUTER PROGRAM,
VERSION 3

Volume I - Program Description
and Sample Problems

Prepared Under
the Sponsorship of

Air Force Rocket Propulsion Laboratory
Director of Laboratories
Edwards, California 93523
Air Force Systems Command
United States Air Force

Project Officer, Robert J. Schoner/RPMCH

FOREWORD

This report is one of two computer program user's manuals prepared by Aerotherm Corporation under USAF Contract F04611-70-C-0012. Included herein is Volume I of the manual for Version 3 of the Aerotherm Equilibrium Surface Thermochemistry code. This volume describes the problems solved by the code and presents an input (card format) user's guide and sample problems. The report was first published as Aerotherm Report No. UM-70-13, April 1970. The work was administered under the direction of the Air Force Rocket Propulsion Laboratory, Motor Component Development Branch with Mr. R. J. Schoner as project officer.

Mr. M. R. Wool was program manager and principal investigator. Significant additional assistance was also provided by Dr. C. B. Moyer.

This technical report has been reviewed and is approved.

R. J. Schoner
Project Engineer, AFRPL

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ABSTRACT

A Fortran IV computer code is described which computes the equilibrium or mixed frozen/equilibrium thermodynamic state of general chemical systems. Closed (fixed mass) molecular compositions are evaluated from relative elemental quantities, species thermochemical data and two state properties (pressure and temperature or enthalpy). Open system (diffusive mass flux dependent) states are defined from surface equilibrium considerations utilizing a film coefficient model which accounts for the unequal diffusion of species. The generality of the formulation allows computations for a broad range of environments and surface materials including charring ablators. This computer code is designated Version 3 of the Aerotherm Equilibrium Surface Thermochemistry code (EST3) and provides surface mass balance quantities needed for ablation predictions by the Aerotherm Charring Material Ablation code (CMA).

Volume I of this report, presented herein, contains descriptions of the fundamental physical events modeled, the mathematical equations solved, the information required for input, and the results output by the computer code. An input (card format) user's guide is provided along with sample input and output listings to enable an unfamiliar user to successfully operate the code and understand the results. Volume II of this report contains supplemental information on the specific Fortran IV codings. Included are program listings, flow charts, and definitions of Fortran variables.

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LIST OF SYMBOLS

B'   normalized ablation rate, defined as $\dot{m}/\rho_e u_e C_M$
          (see Eq. (21))

C_H Stanton number for heat transfer

C_M Stanton number for mass transfer

C_{kj} the number of atoms of element k in a molecule
          of species j

D   Fick's law diffusion coefficient

$\bar{D}$ diffusion constant defined by Eq. (37)

$\mathcal{D}_{ij}$ binary diffusion coefficient

$\bar{\tilde{F}}$ ratio of summations defined by Eq. (42)

F_i diffusion factor for species i (see Eq. (37))

H   total enthalpy (sensible + chemical + $u^2/2$)

h   static enthalpy

h   heat transfer coefficient based on temperature
          difference

I   total number of candidate gas phase species in
          the system

j_i diffusional mass flux of species i (e.g.: lbm
          of species i/ft^2sec)

$\tilde{j}_k$ total diffusional mass flux of element k regard-
          less of molecular configuration

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K	total number of chemical elements in the system
K_{pi}	equilibrium constant (see Eq. (3))
K_i	mass fraction of species i
$\tilde{K}_k$	total mass fraction of element k regardless of molecular configuration
L	total number of candidate condensed phase species in the system
Le	Lewis number
$\dot{m}$	mass flux (e.g.: $lbm/ft^2 sec$)
$\mathcal{m}$	molecular weight
N	representing the molecular formula for a species
n	number of equations of the type (9)
P	system pressure
P_i	partial pressure of species i
Pr	Prandtl number
q	heat flux (e.g.: $Btu/ft^2 sec$)
R	universal gas constant
s	entropy
T	temperature

u	velocity
v	velocity normal to surface
X_j	mole fraction of species j
x	streamwise coordinate
y	surface normal coordinate
z_i	unequal diffusion quantity for species i
$\tilde{z}_k$	unequal diffusion quantity for element k regardless of molecular configuration
$\tilde{z}_k^*$	unequal diffusion driving potential quantity for element k regardless of molecular configuration (see Eq. (33))

GREEK

α_{kj}	mass fraction of element k in species j
γ	a mass fraction - Z fraction weighting exponent
ε	emittance
ε	a diffusion factor correlation exponent (see Eq. (38))
μ	dynamic viscosity
ρ	density
σ	Stefan-Boltzmann constant

SUBSCRIPTS

c   denotes the char

e   at the boundary layer edge

g   denotes the pyrolysis gas

i   gas phase species index

j   general species index

k   element index

ℓ condensed phase index

w   adjacent to the surface

o   stagnation value

SUPERSCRIPTS

T_w enthalpy datum temperature   (wall temperature)

*   see $\tilde{Z}_k^*$

* x_i^* denotes the current estimated value of
            the variable x_i during an iterative solution

** x_i^{**} denotes the new estimated value of the
            variable x_i during an iterative solution

SECTION 1

INTRODUCTION

The computer program described in this user's manual
is a revised edition of the Aerotherm Equilibrium Surface Thermo-
chemistry (EST) computer program*. The previous code, EST Version
2, is described in Reference 1. The current program, EST Version
3, solves all problems that earlier versions could solve and pro-
vides additional computational capabilities. The improved program
logic has significantly reduced machine run time and decreased the
complexity of input preparation.

The purpose of Volume I of this user's manual is to
enable an unfamiliar user to effectively utilize Version 3 of the
Aerotherm Equilibrium Surface Thermochemistry computer program.
To this end, this document contains:

- a brief overview of the purpose and capabilities
  of the EST program (this section)

- a non-rigorous discussion of the theoretical
  foundations of the calculation methods (Section 2)

- a brief description of the numerical solution
  procedures and the FORTRAN coding of these
  procedures (Section 3)

- a specification of the meanings and formats of
  the input data deck (Section 4)

- some example problem inputs and outputs
  (Section 5).

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*This manual applies strictly to Version 3 of the EST program (the
current version as of March 1970). Users with earlier or later
versions of the program should contact the authors relative to
differences between their program and this manual.

Part II of this manual contains the following additional program documentation:

- definitions for all Fortran variables used

- listings of Fortran IV source decks

- flow charts of program logic for each Fortran routine.

Three other documents of potential value to a reader desiring a more detailed exposition of the theoretical fundamentals of the EST program are References 2, 3, and 4.

Version 3 of the Equilibrium Surface Thermochemistry program is an extremely versatile code for calculating quantities of importance to a broad variety of thermochemical processes. The thermochemical processes treated may be divided into two categories: closed systems and open systems. Closed systems are those for which the relative amounts of each chemical element in the system is prespecified. Open systems are those for which the relative amounts of chemical elements depend on various mass transfer rates due, for example, to boundary layer convection or solid surface degradation. The EST program can treat both systems in chemical equilibrium and systems for which sets of molecular species may be chemically isolated from other molecules in the system.

The variety of phenomena which may be treated by the EST program can be illustrated by a hypothetical example. Consider an ablative material (at the throat of a rocket nozzle) being exposed to a solid propellant exhaust stream. The situation is depicted in the sketch below. Encircled digits denote some of the types of calculations which may be performed by the EST program. These are discussed briefly below.

1.   The thermodynamic and chemical state at the boundary layer edge may be calculated by specifying the elemental composition (known from the fuel and oxidizer compositions, for example) and two thermodynamic state variables,
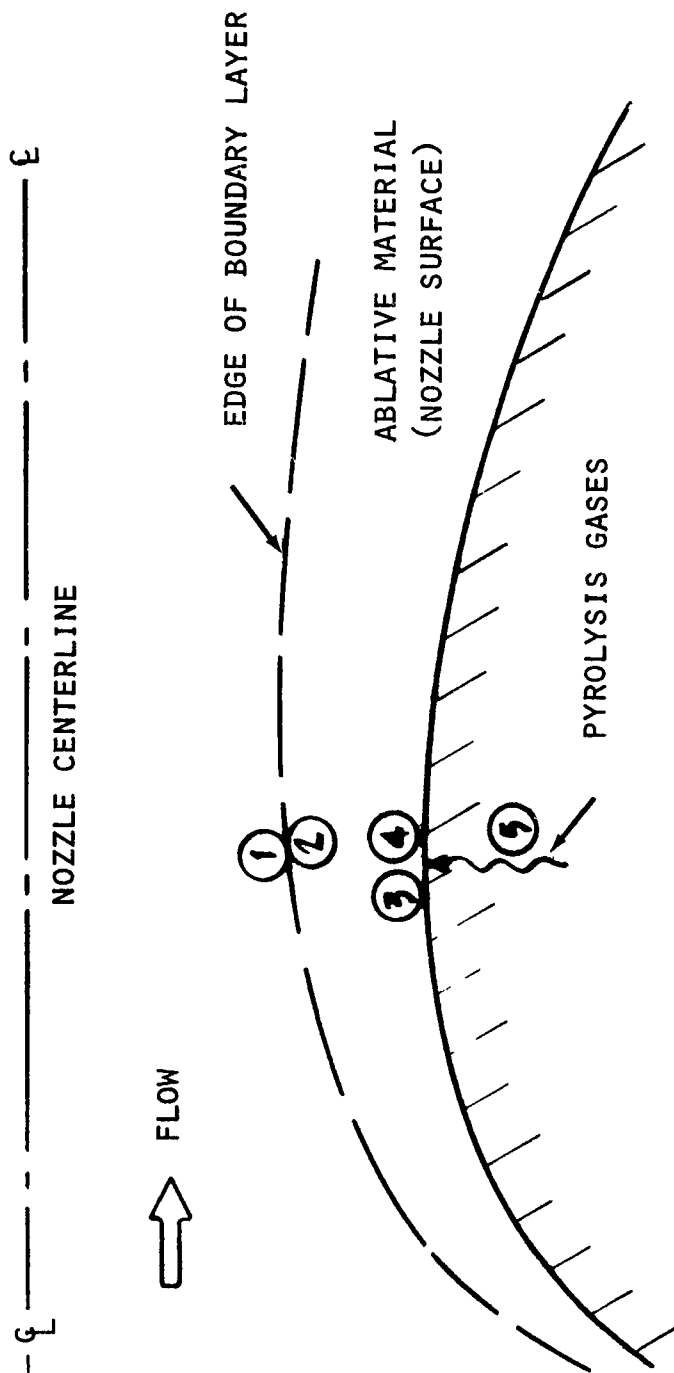
HYPOTHETICAL PROBLEM ILLUSTRATING THE TYPES
OF CALCULATIONS WHICH MAY BE PERFORMED BY
VERSION 3 OF THE EST PROGRAM

one of which must be pressure and the other
may be static enthalpy or static temperature.
This is a closed system calculation.

2.   The variation of enthalpy with temperature
     for the molecular composition of the boundary
     layer edge gases. These calculations often
     called the frozen edge table, are usually
     required in the evaluation of convective
     heat transfer to the ablative surface.

3.   The thermodynamic state of gas in equilibrium
     with the surface of an ablating material may be
     calculated as a function of pyrolysis gas and
     char mass rates normalized by the mass transfer
     coefficients. The effects of equal or unequal
     diffusion coefficient may be accurately accounted
     for in the computation. These are open system
     calculations and the output is usually in the
     form of tables for subsequent input to surface
     energy balance calculations.

4.   The thermodynamic state of gases adjacent to a
     surface but not in equilibrium with that surface
     may be computed by specifying the surface temper-
     ature. Equal or unequal diffusion may be con-
     sidered and normalized transpiration rates may
     be allowed. These are also open system calcula-
     tions.

5.   Equilibrium Mollier diagrams for any real perfect
     gas (such as ablative material pyrolysis gases)
     may be computed. Entropy, density, molecular
     weight, and either enthalpy or temperature are
     calculated as a function of pressure and either
     temperature or enthalpy. Any atomic, molecular
     or ionized species including solids and liquids
     can be considered in this closed system calculation.

Because of the unusual versatility of the EST program, the task of instructing an unfamiliar user in its use is a formidable one. This manual endeavors to fulfill this task through a brief summary of some underlying physical principles, a specification of the input mechanics, and some sample problems. However, regardless of how comprehensive the manual and how well checked out the program, instances will occur in which the program fails to solve a certain problem and the reason for the failure is not apparent from the manual. These cases are best resolved by direct communication with the program or manual authors, and such communication is encouraged.

SECTION 2

THEORY

This section briefly summarizes the theoretical founda-
tions upon which the calculation methods of the EST program are
based. An attempt has been made to present these fundamentals in a
fashion most appropriate to a user unfamiliar with the code. To
this end, and in the interest of brevity, explanations tend to be
nonrigorous and perhaps somewhat heuristic. In discussing each
type of problem treated by the EST program, the pertinent governing
equations are developed and it is shown that these relations are
sufficient to determine the unknown quantities for that particular
problem type. No attempt is made in this section to discuss the
mathematical methods employed to solve these equations. The solu-
tion procedures are very briefly considered in Section 3 which is
concerned primarily with the program coding.

The current version of the EST program is capable of
treating both fully equilibrated chemical systems and those for
which there are mixed groups of isolated systems in individual
equilibrium. The treatment of equilibrium systems is highly gen-
eralized and well checked out. The theoretical fundamentals
relative to a variety of closed and open equilibrium systems are
discussed in Section 2.1. Techniques to obtain the composition
of systems containing isolated species which do not react in equi-
librium with the main system are described in Section 2.2

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*Some judgement is required on the part of the program user relative
to whether chemical equilibrium is an appropriate assumption or if
reaction kinetics are of importance. Unfortunately, there exists
no universally applicable criteria to aid the user in making this
judgement. Within specific classes of problems, however, certain
guidelines may be established from experience. For example, for
the ablation of reinforced phenolic materials, chemical equilibrium
is usually a good assumption for surface temperatures above about
3000°R. For graphitic materials, reaction limiting may be important
up to the onset of graphite sublimation. A computer code which
accounts for heterogeneous graphite reactions in solid propellant
environments has been developed under AF Contract F04611-69-C-0081.

2.1   EQUILIBRIUM SYSTEMS

A variety of problem types, subject to the assumption of chemical equilibrium, are discussed here. Of the many problem options available in the EST program, all fit into one of two categories: closed systems and open systems. For closed systems, the relative amounts of each chemical element is prespecified. In open systems, the relative amounts of chemical elements depend on various mass transfer and material degradation rates. Closed systems are discussed in Section 2.1.1 and open systems are discussed in Section 2.1.2.

2.1.1   Closed Systems in Equilibrium

The discussion of simple closed equilibrium systems in this section is particularly significant because it is here that some equilibrium chemistry relations, which are applicable to all systems subsequently discussed, are first introduced.

Consider K chemical elements introduced into a previously evacuated container in the relative amounts given by N_k. In general, these elements will interact to form a number of chemical species*, N_i (gas phase) and N_ℓ (condensed phases). If enough time has elapsed so that thermodynamic and chemical equilibrium is established, the thermodynamic state of the system, including the relative amounts of chemical species present, is completely determined if two independent thermodynamic variables are known**. Typical variables of this type include temperature, pressure, specific enthalpy and specific entropy.

---

* "Chemical species" as used here includes molecular, atomic, ionic, and electron species.

** Duhem's Theorem.

This condition may be stated mathematically by examining the governing equations for such a system, and showing that the number of independent equations is equal to the number of unknown quantities.

Relations expressing the formation of the gaseous chemical species from the gaseous chemical elements may be written as follows:

$$\sum_{k=1}^{K} C_{ki} N_k \rightarrow N_i \tag{1}$$

Similarly, formation of condensed phase species from the gaseous elements is written:

$$\sum_{k=1}^{K} C_{k\ell} N_k \rightarrow N_\ell \tag{2}$$

In the above, C_{ki} represents the number of atoms of element k in a molecule of species i (gas) or species ℓ (condensed).

If the gas phase species are assumed to individually behave as thermally perfect gases, then the equilibrium relation corresponding to reaction (1) is

$$\frac{P_i}{\prod\limits_{k=1}^{K} P_k^{C_{ki}}} = K_{pi}(T)$$

or

$$\ln P_i - \sum_{k=1}^{K} C_{ki} \ln P_k = \ln K_{pi}(T) \tag{3}$$

where P_k denotes partial pressures and $K_{pi}(T)$ is the equilibrium constant for the formation reaction (1) of species N_i. For each candidate condensed phase species

$$- \sum_{k=1}^{K} C_{k\ell} \ln P_k \overset{\le}{=} \ln K_{p\ell}(T) \tag{4}$$

where

$=$ indicates the existance of the condensed phase species N_ℓ in equilibrium with gas phase species, and

$<$ indicates that the condensed phase species N_ℓ will not be present in equilibrium.

For each chemical element introduced into the system, the conservation of atoms dictates that the amount of any element k in the gas and condensed phases (regardless of molecular configuration) must sum to the total amount of element k in the system. Mathematically, this may be written, for each element k, as

$$\begin{array}{l}\text{Mass fraction}\\\text{of element k}\\\text{input to the}\\\text{system}\end{array} = \frac{m_k}{m P} \sum_{i=1}^{I} C_{ki} P_i + \frac{m_k}{m} \sum_{\ell=1}^{L} C_{k\ell} X_\ell \tag{5}$$

where m is a composite system molecular weight* defined by

$$m = \sum_{i=1}^{I} \frac{P_i}{P} m_i + \sum_{\ell=1}^{L} X_\ell m_\ell \quad \left(\text{units of } \frac{\text{grams of system}}{\text{moles of gas}}\right) \tag{6}$$

---

*This is the molecular weight appropriate to the ideal gas equation of state if condensed phases are present.

and where X_ℓ is a mole fraction of condensed phase species ℓ defined as

$$X_\ell = \frac{\text{molecules of condensed species } \ell}{\text{total gas phase molecules } i} \qquad (7)$$

In addition, for the gas phase species, there exists the requirement that the partial pressures must sum to the total system pressure

$$\sum_{i=1}^{I} P_i = P \qquad (8)$$

Mixture thermodynamic properties, such as specific enthalpy, are related to the species concentrations by equations of the form

$$h = \frac{1}{mP} \sum_{i=1}^{I} P_i h_i + \frac{1}{m} \sum_{\ell=1}^{L} X_\ell h_\ell \qquad (9)$$

Consider now the number of independent equations for the system. The number of gas phase equilibrium relations (3) is equal to the number of gas phase species I minus the number of elements K (because equations (3) are trivial when i=k). In addition, there exists a relation such as (4) for each of the L candidate condensed phase species in the system. Note that the system temperature is contained implicitly in equations (3) and (4) through the temperature dependence of the equilibrium constants. There are K conservation of elements equations (5), one for each atomic element introduced into the system. The requirement that the partial pressures sum to the system pressure (8) contributes one additional equation. For any additional thermodynamic properties of the mixture (enthalpy, entropy, etc.), there exists equations such as (9).

Consider next the variables appropriate to this formulation of the problem. The relative concentrations of the I species

in the gas phase are given by the P_i's and the amounts of the L candidate condensed phase species are given by X_ℓ (most or all of which may be zero). In this formulation, the composite system molecular weight, $\mathcal{m}$, is also a variable. There are one each of the mixture thermodynamic variables T, P, h, s, etc. The number of variables and available independent equations may be summarized as

VARIABLES	NO. OF SUCH VARIABLES	EQUATION NUMBER	NO. OF SUCH EQUATIONS
P_i	I	(3)	I - K
X_ℓ	L	(4)	L
$\mathcal{m}$	1	(5)	K
P	1	(8)	1
T	1		
h, s, ρ, ...	n	of the type (9)	n
total variables	I+L+n+3	total equations	I+L+n+1

Thus, there are two less equations than there are variables, and so if two independent variables are specified (e.g., P and T) in addition to the elemental composition, then closure is obtained and the chemical and thermodynamic state of the system may, in principal, be determined.

The EST program performs this determination. That is, to determine the equilibrium thermodynamic and chemical state of any closed system, one needs only to furnish the EST program with the elemental composition, the candidate gaseous and condensed phase

species,* and two thermodynamic properties. One of these properties must be pressure, and the other may be either temperature or enthalpy. Given this information, the EST program will calculate and output the mole fractions of each candidate species, the temperature, enthalpy, entropy, density, effective molecular weight, equilibrium and frozen specific heats, the isentropic exponent, and a few other quantities of potential interest. Where appropriate, these properties are output for the gas phase, condensed phase, and composite system. The exact convention for inputting data to the program is specified in Section 4, and some example problems of this type are presented in Section 5.

2.1.2   Open Systems in Equilibrium

The previous sections were concerned with systems for which the relative quantities of each chemical element were prespecified. These were termed closed systems. In many circumstances of engineering interest, however, the relative amounts of chemical elements are not known a priori. Such systems are called open systems. For example, the gases adjacent to an ablating surface (e.g., a reentry body or a rocket nozzle throat insert) constitute an open system because the elemental composition of these gases depend on boundary layer transport events, material pyrolysis rates, material char rates, etc. The EST program is capable of treating this type of open system in a particularly convenient fashion.

As will be discussed in more detail subsequently, the EST program relates the surface state (T_w, h_w, etc.) to the ablation rate(s). The surface state and ablation rate(s) are also related by surface energy balance considerations which depend on the rate of

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*The EST program must be supplied certain basic thermodynamic data (described in Section 4) for each candidate species to be considered in a given system. This data is contained in a three card set, one set for each species. A certain amount of judgement is required on the part of the user relative to which candidate species should be included in a given system. Frequently this judgement is avoided by simply inputting data for all species containing combinations of the input elements.

heat conduction into the solid. Thus, the particular ablation rate, surface temperature, etc., is calculated by combining these two relations: surface thermochemistry + in-depth heat conduction. In addition, the boundary layer heat and mass transfer coefficients must, of course, be specified. Computationally, the surface thermo-chemistry relations are usually generated by the EST program in the form of tables (card sets) for subsequent input to transient heat conduction and ablation programs such as the CMA (Charring Material Ablation - Reference 5) program, the SCRIMP (Silica Carbon Reactions Including Melting Phenomena - Reference 6) program, or the ASTHMA (Axisymmetric Transient Heating and Material Ablation - Reference 7) program. The information flow for a complete transient ablation prediction may be illustrated diagramatically as:

```
                        ┌─────────────────────┐
                        │ thermochemistry     │
                        │ calculations        │
                        │ (EST program)       │
                        └──────────┬──────────┘
                                   │
surface (and perhaps B.L.          │        C_H and C_M - B.L. heat and
edge) thermochemistry              │        mass transfer coefficient
tables                             ▼        distributions and histories
                        ┌────────────────────────────────────┐
                        │ in-depth transient heat conduction and │
                        │ ablation calculations               │
                        │ (CMA, SCRIMP, or ASTHMA programs)   │
                        └──────────┬─────────────────────────┘
                                   │
                                   ▼
                        surface temperature and recession
                        history, in-depth temperature
                        distribution history, etc.
```
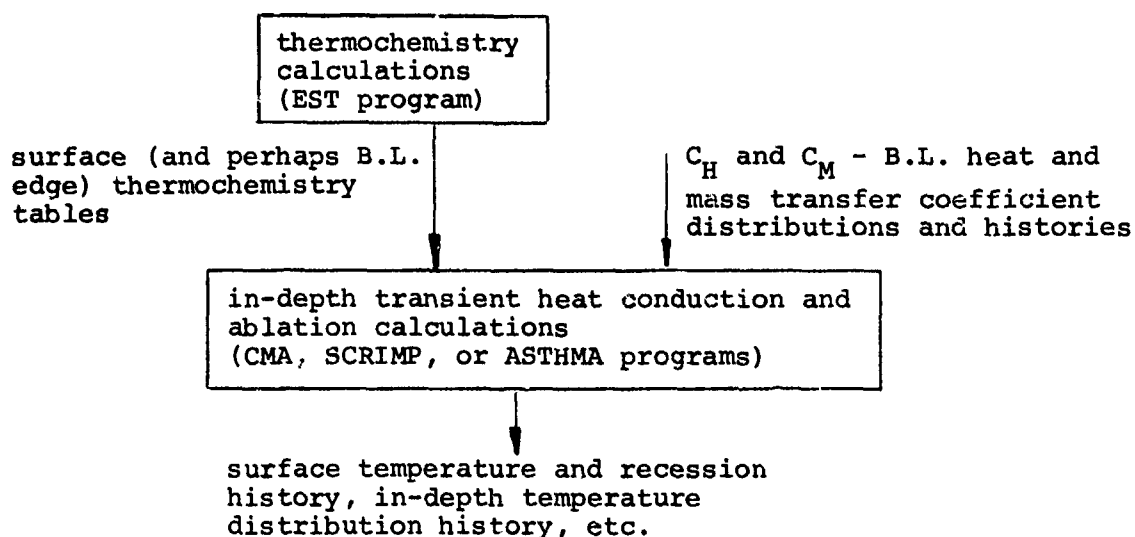
The preparation of the input for these ablation calcula-tions is discussed in Section 4 for the EST program and in References 5, 6, and 7 for CMA, SCRIMP, and ASTHMA programs, respectively. The fundamentals underlying open system thermochemistry are briefly summarized here. Open system calculations, subject to a few simpli-fying assumptions to more clearly illustrate the basic theory, are discussed first in Section 2.1.2.1. These considerations are exten-ded to more general systems in Section 2.1.2.2.

2.1.2.1   Open Systems in Equilibrium - Simplified Case

The basic theory underlying the treatment of open systems
may best be illustrated by examining the equations expressing the
conservation of chemical elements and energy at the ablating surface.
If the boundary layer is characterized by equal diffusion coefficients,
unity Prandtl number, and unity Lewis number, and if no material is
removed from the surface in a condensed phase (i.e., no mechanical
erosion or liquid layer removal), then these equations take on a
particularly simple form for equilibrium systems. This simplified
situation will be considered in this section and these considerations
will be extended to more generalized cases in Section 2.1.2.2.

Consider first the fluxes of chemical elements (k)
entering and leaving a control surface affixed to the ablating
surface. The solid material may be visualized as moving into this
surface at a rate $\dot{s}$. If it is assumed that no material is being
removed in a condensed phase, then the surface and the fluxes of
the kth chemical element may be illustrated as follows:

boundary
layer edge

$$\tilde{j}_{k_w} \qquad (\rho v)_w \tilde{K}_{k_w}$$

ablating
surface $\dot{s}$

$$\dot{m}_g \tilde{K}_{k_g} \qquad \dot{m}_c \tilde{K}_{k_c}$$
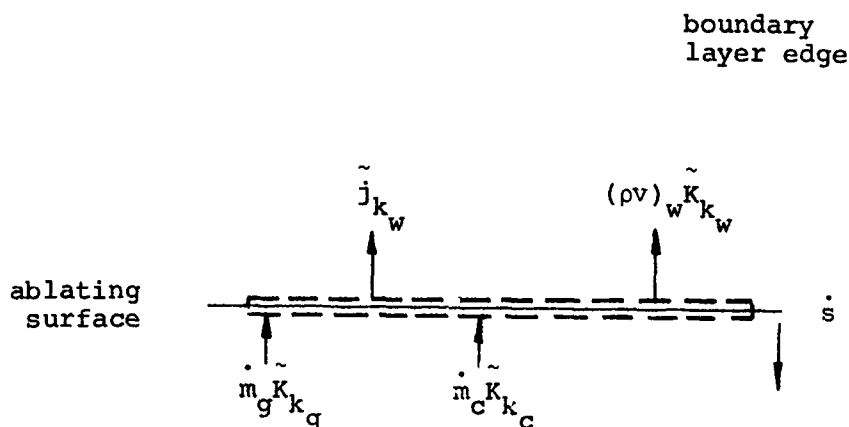
Terms superscripted by a tilde (~) represent the total mass fraction or flux of element k, independent of molecular configuration. Thus

$$\tilde{K}_{k_w} = \sum_{i=1}^{I} \alpha_{k_i} K_{i_w} \tag{10}$$

$$\tilde{j}_{k_w} = \sum_{i=1}^{I} \alpha_{k_i} j_{i_w} \tag{11}$$

where k pertains to element k, i pertains to species i, and α_{k_i} is the mass fraction of element k in species i. Fluxes of element k away from the surface consist of boundary layer diffusion and gross motion of the fluid adjacent to the surface due to injection fluxes $\dot{m}_g$ (pyrolysis gas rate) and $\dot{m}_c$ (char rate).

From the above sketch, it is seen that conservation of chemical elements requires that

$$\tilde{j}_{k_w} + (\rho V)_w \tilde{K}_{k_w} = \dot{m}_g \tilde{K}_{k_g} + \dot{m}_c \tilde{K}_{k_c} \tag{12}$$

Summing Equation (12) over all elements k yields the total mass continuity equation (for the case when there is no condensed phase material removal)

$$(\rho V)_w = \dot{m}_g + \dot{m}_c \tag{13}$$

An important fundamental of the present mathematical modeling of the ablation process is the expression of the diffusive heat and mass fluxes in terms of a transfer coefficient formulation. This formulation will be discussed briefly in the following paragraphs, and more detailed treatments are given in References 8, 9, and 10.

Heat and Mass Transfer Coefficients - Simplified Case

For low speed flow of an incompressible, constant property, non-reacting fluid, the boundary layer

energy equation may be written in the form

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2} \tag{14}$$

and solutions to this equation have historically been correlated in terms of a heat transfer coefficient h where

$$q = h(T_e - T_w) \tag{15}$$

For high speed chemically reacting boundary layers (as are of interest in ablation problems), the energy equation can be written in the following form if diffusion coefficients are equal and if the Prandtl and Lewis numbers are unity (e.g., Reference 8)

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y} \left(\mu \frac{\partial H}{\partial y} \right) \tag{16}$$

where H is the total (sensible + chemical + $u^2/2$) **enthalpy.** By analogy to Equations (14) and (15), solutions to (16) are conveniently expressed in terms of a dimensionless heat transfer coefficient C_H where

$$q = \rho_e u_e C_H (H_e - H_w) \tag{17}$$

Corresponding formulations for non-unity Prandtl and Lewis number cases will be considered in Section 2.1.2.2.

Consider now the equation for mass transfer diffusion in the boundary layer. If the diffusion coefficients for all chemical species are equal (Fick's Law), then an appropriate summation (Reference 8) of the boundary layer species conservation equation yields the following equation for each element k

$$u \frac{\partial \tilde{K}_k}{\partial x} + \rho v \frac{\partial \tilde{K}_k}{\partial y} = \frac{\partial}{\partial y} \left(\rho D \frac{\partial \tilde{K}_k}{\partial y} \right) \tag{18}$$

Again, by analogy, solutions to this equation may be correlated in terms of a dimensionless mass transfer coefficient C_M where

$$-\tilde{j}_{k_w} = \rho_e u_e C_M (\tilde{K}_{k_e} - \tilde{K}_{k_w}) \tag{19}$$

And for the unity Prandtl and Lewis numbers case under consideration, the similarity of Equations (16) and (18) indicates that if the corresponding boundary conditions are also similar, then $C_M = C_H$.

Utilizing this transfer coefficient formulation (19) for the diffusion flux in the elemental balance Equation (12) yields

$$\rho_e u_e C_M (\tilde{K}_{k_w} - \tilde{K}_{k_e}) + (\rho v)_w \tilde{K}_{k_w} = \dot{m}_g \tilde{K}_{k_g} + \dot{m}_c \tilde{K}_{k_c} \tag{20}$$

defining dimensionless pyrolysis and char rates as

$$B_g' \equiv \frac{\dot{m}_g}{\rho_e u_e C_M} , \qquad B_c' \equiv \frac{\dot{m}_c}{\rho_e u_e C_M} \qquad \text{and} \qquad B' \equiv \frac{(\rho v)_w}{\rho_e u_e C_M} \tag{21}$$

and solving (20) for the total mass fraction of element k at the wall yields (for equal diffusion coefficients, Pr = Le = 1.0, and no condensed phase material removal)

$$\tilde{K}_{k_w} = \frac{B_g' \tilde{K}_{k_g} + B_c' \tilde{K}_{k_c} + \tilde{K}_{k_e}}{1 + B'} \tag{22}$$

Given the relative amounts of chemical elements specified by (22), the chemical and thermodynamic state of the gases adjacent to the ablating surface may be calculated from equilibrium relations similar to those discussed in Section 2.1.1.

Since the gases are in equilibrium with the ablating surface

$$- \sum_{k=1}^{K} C_{k\ell} \, \ell n \, P_k = \ell n \, K_{p\ell}(T) \qquad (23)$$

if ℓ represents the surface species, and

$$- \sum_{k=1}^{K} C_{k\ell} \, \ell n \, P_k < \ell n \, K_{p\ell}(T) \qquad (24)$$

for all other candidate condensed phase species. In the present for-
mulation, (24) may be thought of as being used to identify surface
species ℓ for which (23) applies. The equilibrium relations for gas
phase species is again (see Section 2.1.1) of the form

$$\ell n \, P_i - \sum_{k=1}^{K} C_{ki} \, \ell n \, P_k = \ell n \, K_{pi}(T) \qquad (25)$$

and the partial pressures must obey the relation

$$\sum_{i=1}^{I} P_i = P \qquad (26)$$

The elemental mass fractions adjacent to the surface, $\tilde{K}_{k_w}$, of (22)
are related to the species partial pressures, P_i, by relations such
as (5) (except that no condensed phase is being considered here)

$$\tilde{K}_{k_w} = \frac{m_k}{Pm} \sum_{i=1}^{I} C_{ki} P_i \qquad (27)$$

Thus, if P is known and B'_g and B'_c are specified (these may be varied
parametrically as will be discussed subsequently), and if T_w and P_i
are unknowns, then the number of unknowns and equations available
may be summarized as

UNKNOWNS	NO. OF SUCH UNKNOWNS	EQUATION NO.	NO. OF SUCH EQUATIONS AVAILABLE
P_i	I	(25)	I-K
$\widetilde{K}_{k_w}$	K	(23)	1
$\mathcal{M}$	1	(22)	K
T_w	1	(26)	1
		(27)	K
Total Unknowns	I+K+2	Total Equations	I+K+2

Thus, closure is obtained and, in principal, the temperature and chemical composition of the gases adjacent to the surface may be determined if P, B_g', and B_c' are specified. From the pressure, temperature, and chemical composition, the calculation of other thermodynamic properties (enthalpy, etc.) is straightforward.

The EST program has the capability to determine the chemical and thermodynamic state of the gases adjacent to an ablating surface in a fashion similar to that discussed here. Indeed, the EST program is capable of treating more complex ablation situations, and these are discussed in Section 2.1.2.2. In general, the pressure P and a matrix of B_g' and B_c' values are input. This is usually most convenient since T_w is usually single valued with respect to B_c' and B_g' as illustrated by a typical example

B_g' and P constant
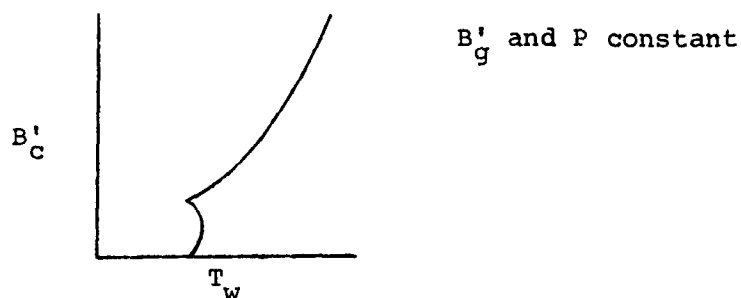
Clearly, calculating B_c' from input T_w would not be appropriate for this case. For other cases such as

B'_g and P constant

B'_c

T_w
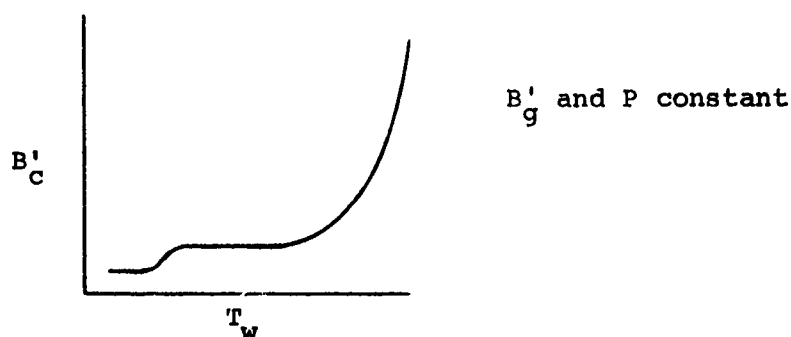
the program possesses some special "fill-in" options (discussed in
Section 4). For open systems, the EST output consists of card sets
(in addition to regular printed output) referred to as surface
thermochemistry tables. Each card contains information relative to
one surface state (i.e., one P, T_w, B'_g, B'_c,..., combination). As
previously discussed, this surface thermochemistry data alone is
insufficient to solve an ablation problem; it must be combined with
in-depth heat conduction and surface energy balance considerations.
In order to more clearly demonstrate this interdependence, the
relation of the surface thermochemistry to the surface energy balance
is discussed briefly in the following paragraphs.

Relation to Surface Energy Balance - Consider the fluxes
of energy entering and leaving a control surface affixed
to the ablating surface. For the unity Prandtl number,
unity Lewis number, no condensed phase removal ablation
case being considered, these fluxes may be illustrated as

boundary
layer edge

q_{conv} $(\rho v)H_w$ $q_{rad\ in}$ $\sigma \epsilon T_w^4$

ablating
surface

q_{cond} $\dot{m}_g H_g$ $\dot{m}_c H_c$
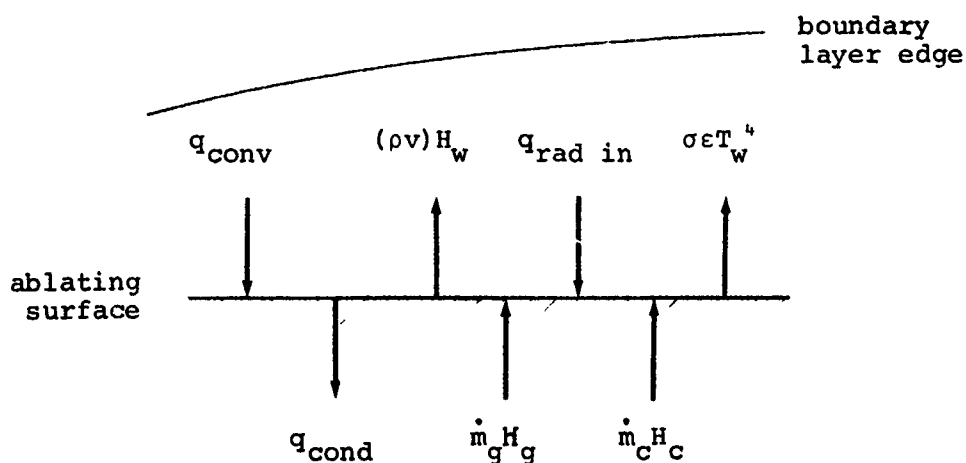
where:

q_{conv} is the energy convected to the surface as a result of boundary layer transport events. This term includes effects of both heat conduction due to a temperature gradient in the gas adjacent to the surface, and energy transport due to endothermic or exothermic chemical reactions at the surface. For the equal diffusion coefficient, $Pr = Le = 1.0$ case under consideration here, the previously discussed transfer coefficient form of this term is (17)

$$q_{conv} = \rho_e u_e C_H (H_e - H_w) \, . \qquad (17)$$

$(\rho v)_w H_w$ is the energy flux leaving the surface with the "blowing" flux $(\rho v)_w$.

$q_{rad\ in}$ is the incident radiation flux.

$\sigma \epsilon T_w^4$ is the surface re-radiation flux.

q_{cond} is the heat flux conducted into the solid material, $q_{cond} = - k \left. \frac{\partial T}{\partial y} \right)_{w,solid}$

$\dot{m}_g H_g$ and

$\dot{m}_c H_c$ are the energy fluxes entering the surface associated with the pyrolysis gas and char respectively.

Conservation of energy at the surface requires that

$$\rho_e u_e C_H (H_e - H_w) + \dot{m}_g H_g + \dot{m}_c H_c - (\rho v)_w H_w + q_{rad\ in} -$$
$$\sigma \epsilon T_w^4 = q_{cond}$$

or, utilizing (21)

$$H_e - (1+B')H_w + B'_g H_g + B'_c H_c + \frac{q_{rad~in}}{\rho_e u_e C_H} -$$

$$\frac{\sigma \varepsilon}{\rho_e u_e C_H} T_w^4 = \frac{q_{cond}}{\rho_e u_e C_H} \qquad (28)$$

For most problems, H_e is known, $\rho_e u_e C_H$ is independently determined from boundary layer calculations, ε is known, q_{rad} is known (frequently zero), and H_g and H_c are known functions of T_w. Additionally, B'_c and H_w are related to T_w through the surface thermochemistry tables generated by the EST program as previously discussed. Based on considerations thus far, all quantities in (28) except q_{cond} and B'_g are determined for a given T_w. The in-depth heat conduction term, q_{cond}, depends only on previous heat conduction events and the current T_w. The pyrolysis gas rate, B'_g, is given by a decomposition law (Reference 9) which depends on in-depth temperature which, through heat conduction considerations, depends on T_w. Thus, it is seen that in general there exists only one value of T_w which satisfies (28). This T_w is usually determined in an iterative fashion by a heat conduction and ablation program (e.g., References 6 or 7) which utilizes the surface thermochemistry tables as boundary conditions. Once T_w is known for a given time in a transient solution, B'_c, B'_g, surface recession rate, in-depth temperature distributions, and other quantities of interest follow directly.

The above has been a brief discussion indicating the interdependence of the surface thermochemistry solution and the in-depth heat conduction solution for a somewhat simplified case. It should be pointed out that similar considerations apply for situations when unequal species diffusion effects are significant and when $Pr \neq 0 \neq 1.0$. The EST program is able to treat these effects and details relative to the treatment of them will be considered in Section 2.1.2.2

2.1.2.2   Open Systems in Equilibrium - Nonunity Prandtl and
           Lewis Numbers, Unequal Diffusion Coefficients

         The discussion of the previous section was limited
to open systems with unity Prandtl and Lewis numbers, equal
species diffusion coefficients, and no removal of surface mat-
erial in the condensed phase. These simplifications were made
in order to render the basic theory easier to explain. While
this simple model is reasonably accurate for many ablation sit-
uations, these assumptions are inappropriate for others. The
equal diffusion coefficient, $Pr = Le = 1.0$ simplifications per-
tain to boundary layer mass, energy, and momentum transport
events, and the effects of the relaxation of these assumptions
on the problem formulation and solution procedure will be briefly
discussed in this section.

         $\underline{Pr \neq Le \neq 1.0}$ - For nonunity Prandtl and Lewis num-
bers, the transfer coefficient formulation for the boundary
layer energy flux is not as straightforward as that discussed in
the previous section. This is because the boundary layer energy
equation is no longer of the similar form and thus a transfer
coefficient formulation cannot be justified purely by analogy.
A detailed discussion of boundary layer transport models for the
$Pr \neq Le \neq 1.0$ case is beyond the scope of this manual (see, e.g.,
References 9 and 10) and only a few of the results as they relate
to film transfer coefficient formulations will be discussed here.

         When the Prandtl number is not unity, the viscous
dissipation and heat conduction terms in the boundary layer energy
equation cannot be combined thus rendering the equation inhomo-
geneous. Solutions to this equation indicate that the driving
potential in the transfer coefficient expression for the surface
heat flux should be defined in terms of a recovery enthalpy (e.g.,
Reference 11) in place of the actual boundary layer edge enthalpy.

Thus, nonunity Prandtl number has no influence on EST calculations and the primary practical implication is that the recovery enthalpy, rather than the boundary edge enthalpy, should be input to the heat conduction and ablation solution.

When the Lewis number is not unity, the terms in the boundary layer energy equation representing energy transfer by heat conduction and chemical species diffusion cannot be combined, again rendering the equation inhomogeneous. The energy flux to the surface is given by

$$q_w = k \left. \frac{\partial T}{\partial y} \right)_w - \sum_{i=1}^{I} j_{iw} h_i^o = \left. \frac{k}{c_p} \frac{\partial h}{\partial y} \right)_w + \sum_{i=1}^{I} h_i^o \rho D \left. \frac{\partial K_i}{\partial y} \right)_w$$

(29)

where the first term characterizes the heat conducted to the surface as a result of the temperature gradient in the gas adjacent to the surface, and the second term represents the effect of endothermic and exothermic chemical reactions at the surface. The appropriate transfer coefficient form of (29) is not firmly established at this time. However, Reference 9 suggests the form

$$q_w = \rho_e u_e C_H \left(H_r - h_w \right)_{\substack{frozen \\ edge\ gas}} + \rho_e u_e C_M \sum_{i=1}^{I} \left(K_{i_e} - K_{i_w} \right) h_i^{T_w}$$

(30)

and this is the form employed in Aerotherm ablation programs. In (30), the driving potential in the first term is the recovery enthalpy at the boundary layer edge minus the enthalpy of the boundary layer edge gases frozen at the edge composition and at the surface temperature, and $h_i^{T_w}$ represent the enthalpy of chemical species i with respect to a base temperature equal to the surface temperature. It can be shown (Reference 9) that for Le = 1.0 and $C_M = C_H$, (30) collapses

to (17) as expected. However, where Le $\neq$ 1.0, the heat and mass transfer coefficients are generally unequal and a correlation frequently employed (Reference 12) is

$$\frac{C_M}{C_H} = Le^{2/3} \tag{31}$$

It is apparent from (30) that, in addition to surface thermochemical data, boundary layer edge thermochemical data are also required when Le $\neq$ 1.0 in order to specify the quantity

$$h_{w \text{ frozen} \atop \text{edge gas}} = \sum_{i=1}^{I} K_{i_e} h_i^{T_w}$$

This quantity is also calculated by the EST program for subsequent input to heat conduction and ablation programs. The calculation of these frozen edge tables is usually accomplished by performing a closed system equilibrium calculation at the boundary layer edge temperature and elemental composition (as discussed in Section 2.1.1) and then performing closed system calculations frozen at this composition for an array of temperatures spanning the expected wall temperature range. The program input for frozen composition calculations is discussed in Section 4. Thus, for problems with $C_M \neq C_H$, frozen edge tables, as well as surface thermochemistry tables, are prepared by the EST program for input to the CMA (Reference 5), ASTHMA (Reference 7), or related heat conduction and ablation programs.

Unequal Diffusion Coefficients - A significant simplification of the boundary layer energy and mass diffusion equations results if all binary diffusion coefficients for a given species i are assumed to be equal (e.g., Reference 11) and all considerations up to this point have been predicated on this assumption. However, for many chemical systems of interest in ablation problems (e.g., when there is a significant difference between the molecular weights of the major species present) this assumption is a severe compromise

with reality. Based upon an accurate approximation for binary diffusion coefficients, Reference 3 presents simplified equations for a multicomponent boundary layer with unequal diffusion coefficients for all species. The application of similarity arguments to these equations suggests the following form for the transfer coefficient formulation for the diffusion flux of element k at the surface

$$\tilde{j}_{k_w} = \rho_e u_e C_M (\tilde{z}^*_{k_w} - \tilde{z}^*_{k_e}) \tag{33}$$

In (33), $\tilde{z}^*_k$ is, in effect, a weighted average of the mole and mass fractions of element k. The $\tilde{z}^*_k$ are defined by

$$\tilde{z}^*_k = \sum_{i=1}^{I} C_{ki} z^*_i \tag{34}$$

$$z^*_i = \frac{z_i^{\gamma} K_i^{1-\gamma}}{\sum_{i=1}^{I} z_i^{\gamma} K_i^{1-\gamma}} \qquad \begin{array}{l}(\gamma \simeq 2/3, \text{ see} \\ \text{Reference 2})\end{array} \tag{35}$$

$$z_i = \frac{K_i/F_i}{\sum_{i=1}^{I} K_i/F_i} \tag{36}$$

where the F_i are diffusion factors defined by the following relation for the binary diffusion coefficients

$$\mathcal{D}_{ij} = \frac{\bar{D}}{F_i F_j} \tag{37}$$

where $\bar{D}$ is a constant for a given temperature and pressure and the F_i depend weakly on temperature. The $\mathcal{D}_{ij}$ must obey (37) in order for the boundary layer species diffusion equations to reduce to a form from which (33) can be inferred by similarity arguments. Reference 3 demonstrates that the binary diffusion coefficients for a

variety of chemical systems are accurately correlated by (37). This reference also shows the reasonably good correlation equation for the F_i is

$$F_i \approx \left(\frac{\mathcal{m}_i}{\mathcal{m}_{ref}} \right)^{\varepsilon} \qquad \text{where} \qquad \mathcal{m}_{ref} \approx 23.4 \qquad \text{and} \qquad \varepsilon \approx 0.431 \qquad (38)$$

when $\bar{D}$ is taken as the self-diffusion coefficient of O_2.

Consideration of unequal diffusion coefficients affects the surface elemental balance relationships which are needed to determine the equilibrium thermochemical state at the surface. Substituting (33) into (12) yields

$$\rho_e u_e C_M (\tilde{z}_{k_w}^* - \tilde{z}_{k_e}^*) + (\rho v)_w \tilde{K}_{k_w} = \dot{m}_g \tilde{K}_{k_g} + \dot{m}_c \tilde{K}_{k_c} \qquad (39)$$

and the unknowns here are $\tilde{K}_{k_w}$ and $\tilde{z}_{k_w}^*$, each of which may be expressed in terms of the species partial pressures

$$\tilde{K}_k = \mathcal{m}_k \frac{\displaystyle\sum_{i=1}^{I} C_{ki} P_i}{\displaystyle\sum_{i=1}^{I} \mathcal{m}_i P_i} = \frac{\mathcal{m}_k}{P \mathcal{m}_g} \sum_{i=1}^{I} C_{ki} P_i \qquad (40)$$

and

$$\tilde{z}_k^* = \mathcal{m}_k \frac{\displaystyle\sum_{i=1}^{I} C_{ki} P_i / F_i^{\gamma}}{\displaystyle\sum_{i=1}^{I} \mathcal{m}_i P_i / F_i^{\gamma}} = \frac{\mathcal{m}_k \bar{F}}{P \mathcal{m}_g} \sum_{i=1}^{I} C_{ki} P_i / F_i^{\gamma} \qquad (41)$$

where $\mathcal{M}_g$ is the mean molecular weight of the gas phase and $\bar{F}$ is a mean F_i^γ defined as

$$\bar{F} \equiv \frac{\displaystyle\sum_{i=1}^{I} \mathcal{M}_i P_i}{\displaystyle\sum_{i=1}^{I} \mathcal{M}_i P_i / F_i^\gamma} \tag{42}$$

Substituting these expressions into (39) and utilizing (21) yields an expression for the species partial pressures at the surface in terms of quantities at the boundary layer edge and in the material

$$B' \sum_{i=1}^{I} C_{ki} P_{iw} + \bar{F} \sum_{i=1}^{I} C_{ki} P_{iw} / F_i^\gamma = \frac{P \mathcal{M}_g}{\mathcal{M}_k} (\tilde{z}_{k_e}^* + B_g' \tilde{K}_{k_g} + B_c' \tilde{K}_{k_c}) \tag{43}$$

Note that (43) reduces to (22) when the diffusion coefficients are equal.

When performing unequal diffusion coefficient open system calculations, the EST program utilizes (43) rather than (22) as the elemental mass balance equations. Other than this, the solution philosophy is essentially as discussed in Section 2.1.2.1. The diffusion factors utilized in the EST program may be calculated in three ways, at the user's option

a. diffusion factors F_i may be input individually for each species i

b. diffusion factors may be calculated according to (38) with the user specifying the reference molecular weight, $\mathcal{M}_{ref}$, and the exponent ϵ

c. if neither of the above options are utilized the program will calculate F_i according to (38) with $\mathcal{M}_{ref} = 23.4$ and $\epsilon = 0.431$.

The actual program input for these alternatives will be discussed in Section 4.

For unequal diffusion coefficients, the transfer coefficient formulation for the surface energy flux has the following form (Reference 9)

$$q_w = \rho_e u_e C_H (H_r - h_w)_{\substack{frozen \\ edge \ gas}} + \rho_e u_e C_M \sum_{i=1}^{I} (Z^*_{i_e} - Z^*_{i_w}) h_i^{T_w}$$

(44)

Note that for equal diffusion coefficients, $Z^*_i = K_i$ and (44) reduces to (30) as expected. Consistent with (44), for unequal diffusion coefficient problems, the surface thermochemistry tables prepared by the EST program contain the quantity

$$\sum_{i=1}^{I} Z^*_{i_w} h_i^{T_w}$$

in addition to the quantities previously discussed. Note again, that for equal diffusion coefficients

$$\sum_{i=1}^{I} Z^*_{i_w} h_i^{T_w} = \sum_{i=1}^{I} K_{i_w} h_i^{T_w} = h_w$$

(45)

Similarly, the previously discussed frozen edge table must contain the quantity

$$\sum_{i=1}^{I} Z^*_{i_e} h_i^{T_w}$$

in addition to

$$h_w \qquad \text{frozen} \atop \text{edge gas}$$

The EST program input arrangement for the preparation of these
surface and edge thermochemistry tables, for equal or unequal dif-
fusion coefficients, is specified in Section 4.

2.2   NON-FULLY EQUILIBRATED SYSTEMS

         To calculate the equilibrium state of a chemical system,
information relative to all chemical reactions is not needed. This
fact permits a significant simplification in the problem formulation,
and those options of the EST program discussed thus far take advan-
tage of these simplifications. For some systems of interest, how-
ever, the effects of reaction kinetics may not be neglected. A
general solution of complex problems for which reaction kinetics
effects are important is potentially difficult for at least two rea-
sons: a) there are significant computational and bookkeeping problems
associated with the analytical treatment of mixed equilibrium and non-
equilibrium systems, and b) for many systems of engineering interest,
the rate controlling reactions are not well known and/or rate con-
stants for these reactions are unavailable. Difficulties of these
types frequently preempt any exact analytical treatment. In these
cases, various approximate treatments can often yield useful informa-
tion. These approximate treatments essentially consist of not allow-
ing certain species, or groups of species, to react with an otherwise
equilibrated system. A few examples of this sort of approximate
treatment will be discussed in the following paragraphs.

         Completely Frozen Systems - The EST program contains a
provision for performing thermodynamic state calculations for sys-
tems with frozen chemical compositions. The calculations are carried
out by performing an equilibrium calculation at one temperature and
pressure, freezing the chemical composition, and then performing

thermodynamic state calculations at other temperatures and pressures but at this frozen chemical composition. This type of calculation was previously discussed in reference to frozen boundary layer edge tables (in Section 2.1.2.2). Program input details relative to this type of calculation are discussed in Section 4.

Removal of Selected Species from the System - the simplest, and perhaps the crudest, way to approximate certain kinetic effects is to simply remove from the equilibrium system those species whose formation is, in reality, suppressed by reaction kinetic effects. Computationally, these species are removed merely by removing the thermochemical data cards for that molecule from the species thermochemical data deck. See Section 4.

Isolated Species - Certain chemical species may be frozen individually at any given concentration. This treatment is sometimes useful for species which are relatively nonreactive because of chemical kinetic effects. For example, consider the flow of of a C-O-H gas over a relatively low temperature ablating carbon surface. Isolation of H_2O at its boundary layer edge concentration would provide a more realistic surface thermochemistry table than if full equilibrium were assumed (since the water-gas reaction at the surface is relatively slow at lower temperatures). In the EST program, this isolation of species is achieved by treating that particular species as an atomic element, an element with a fictitious atomic number so that it cannot react chemically with any other members of the chemical systems. Computationally, this requires specification of the input of the appropriate quantity of this "element" (accompanied by appropriate reductions in the amounts of other actual elements), and the alteration of the species thermochemistry data card set for that species so that it contains only one "atom" of the fictitious "element".

Isolated Subgroups of Elements - In some practical applications, there exists a subgroup of elements which are in equilibrium with each other, but the subgroup is not in chemical equilibrium with

the system as a whole. For example, there are indications (Reference 13) that for some ablative plastics, the pyrolysis gases do not come into chemical equilibrium with the boundary layer gases. This effect may be studied by performing a solution with the pyrolysis gases isolated from the rest of the system. The isolation of a subgroup of elements can be achieved by considering these elements to be different "elements" with properties the same as, but with atomic numbers different from, the corresponding actual elements (e.g., add 100 to the atomic numbers of the elements in the isolated subgroup). For this type of calculation, the subgroup to be isolated is considered to be one component, and the composition of this component is specified as the actual relative elemental composition of the subgroup to be isolated, but in terms of the altered elements. In order that these altered elements may equilibrate with each other, the species thermochemical data card set must contain a set of species which may be formed from these altered elements, i.e., species with the same atomic number convention.

Low Temperature Surface Equilibrium Suppression - As previously discussed, equilibrium is an increasingly poor assumption at low surface temperatures (e.g., below 2000°R) in some ablation problems. However, when generating surface thermochemistry tables with the EST program (Section 2.1.2.2), lower temperature ranges are usually only of minor interest (e.g., during a very short initial period of a transient ablation problem). Nontheless, the surface tables must frequently extend to these lower temperatures in order to be compatible with the subsequent heat conduction and ablation solution. For these cases, the EST program contains an option by which, for each pyrolysis gas rate and at the lowest specified char rate, surface equilibrium will be suppressed and a series of specified temperature solutions will be performed (at 500°K intervals) to fill the table out down to 500°K. For many cases, surface thermochemistry tables generated in this fashion are closer to reality than full equilibrium solutions down to 500°K. The input convention for implementing this option is discussed in Section 4.

SECTION 3

CODING

This section presents some details relative to the
FORTRAN coding of the EST program. A brief description of the
numerical solution procedure, which includes a discussion of the
"base species" concept, is presented first in Section 3.1. Each
subroutine making up the EST program is identified and briefly
discussed in Section 3.2. Definitions of several diffusion factor
dependent properties appearing on the program output are given in
Section 3.3. Some miscellaneous program details are documented in
Section 3.4. These include storage requirements, tape requirements,
operator controls, dumps and diagnostics, and run time.

3.1   COMPUTATIONAL PROCEDURE

The computational procedure employed in the EST program
to solve the equations set forth in Section 2 is briefly discussed
here. Considerably greater detail is presented in Reference 4 and
in particular Table 1 of that reference.

3.1.1   Basic Solution Technique

The basic solution technique may be illustrated by con-
sidering, for example, an open system with unequal diffusion
coefficients (i.e., as discussed in Section 2.1.2.2). For this
system, the basic equations defining the problem are the elemental
conservation equations (43), the total pressure equation (26), the
reaction equilibrium equations (25), and one heterogeneous vapor
pressure relation (23). The table of Section 2.1.2.1 shows that
there are as many knowns as unknowns in these equations so closure
is obtained.

Summarizing these equations,

$$B' \sum_{i=1}^{I} C_{ki} P_i + \bar{F} \sum_{i=1}^{I} C_{ki} P_i / F_i^{\gamma} - \frac{P \tilde{m}_g}{\tilde{m}_k} (\tilde{z}_{k_e}^{*} + B_g' \tilde{K}_{k_g} + B_c' \tilde{K}_{k_c}) = 0 \qquad (46)$$

$$\sum_{i=1}^{I} P_i - P = 0 \qquad (47)$$

$$\ln P_i - \sum_{k=1}^{K} C_{ki} \ln P_k - \ln K_{pi}(T_w) = 0 \qquad (48)$$

$$- \sum_{k=1}^{K} C_{k\ell} \ln P_k - \ln K_{p\ell}(T_w) = 0 \qquad (49)$$

The number of unknowns could immediately be reduced by I-K through the direct substitution of (48), as solved for P_i, into the other relations. It proves advantageous, however, to continue to treat the full set of equations, and to subsequently utilize this substitution during the iterative convergence procedure. The solution of these simultaneous nonlinear algebraic equations is based on Newton-Raphson iteration. Since this procedure is accelerated by casting the equations into a more linear form (via transformations, substitutions, etc.) it is well to examine the set of equations above. With the boundary layer edge, char and pyrolysis gas composition given as well as the B', (46) and (47) are linear relations between the P_i and $\tilde{m}_g$ providing that $\bar{F}$ is reasonably constant. In contrast, (48) and (49) are linear relations between the $\ln P_i$, $\ln P_k$ and $\ln K_{pi}$, the latter variable being approximately linear in 1/T.

The EST program takes advantage of this situation by treating those species which are significant in the mass and pressure

balances (46) and (47) in terms of P_i and the less significant species in terms of their $\ln P_i$.

The Newton-Raphson procedure, as applied by the EST program, can be summarized by considering a set of equations of the general form

$$f_j(x_1, x_2, \ldots, x_i, \ldots) = 0$$

At any point in the solution procedure there exists a set of estimates, x_i^*, for all the variables which will in general not satisfy all of the relations and will lead to a non-zero value of the f_j, namely, ε_j. The Newton-Raphson method proceeds to "drive" these errors toward zero by evaluating the change in each unknown variable, Δx_i, which would reduce all the errors to zero if the functions, f_j, were linear. The linear approximation is based on the current values of the unknown variables and the corresponding array of values of the partial derivatives $\partial f_j / \partial x_i$. Thus

$$df_j = \sum \frac{\partial f_j}{\partial x_i} dx_i \tag{50}$$

which is locally correct and is integrated to

$$(\Delta f_j)^* \approx \sum \left(\frac{\partial f_j}{\partial x_i}\right)^* (\Delta x_i)^* \tag{51}$$

in the linear approximation. The solution of (50) is

$$dx_i = \sum \frac{\partial x_i}{\partial f_j} df_j \tag{52}$$

where the array of partial derivatives appearing in (52) is simply the matrix inverse of the array in (50). In the EST program the

formulation of the partial derivatives uses the variables, $\ln P_i$,* $\ln T$ and $\ln \mathcal{M}$ and (52) yields, for example,

$$d(\ln P_i) = \sum \frac{\partial \ln P_i}{\partial f_j} df_j \tag{53}$$

which if taken as linear all the way to solution yields

$$\ln \frac{P_i^{**}}{P_i^*} = (\Delta \ln P_i)^* \approx \sum \left(\frac{\partial \ln P_i}{\partial f_j}\right)^* (-\varepsilon_j)^* \tag{54}$$

since the desired change in the functions is simply the negative of the error. An equally _exact_ relation obtained from (53) is

$$dP_i = P_i \sum \frac{\partial \ln P_i}{\partial f_j} df_j \tag{55}$$

which if taken as linear all the way to solution yields

$$P_i^{**} - P_i^* = \Delta P_i^* \approx P_i^* \sum \left(\frac{\partial \ln P_i}{\partial f_j}\right)^* (-\varepsilon_j^*) \tag{56}$$

The EST program uses (56) for all species significant in mass balances and (54) for the others.

3.1.2 Restriction on Corrections

The set of correction $(\Delta x_i)^*$ can be thought of as a vector in the space of the independent variables which is added to the current vector approximation x_i^* to yield a new estimate x_i^{**}.

---

*The choice of $\ln P_i$ permits a matrix reduction by the use of the simple algebraic substitution, previously mentioned after (49), prior to matrix inversion.

Experience has shown that it is frequently unwise to proceed along this correction vector the full amount indicated by (54) or (56). Rather, it is better to proceed a limited way, although preserving the same direction. At other times, it is expedient to depart from this vector, and seek another based on freezing the value of some variable and eliminating a corresponding equation.

The scaling of the correction vector is such as to limit changes in the partial pressures of major species to increases of one order of magnitude and decreases of three orders of magnitude, and changes of temperature to approximately 20 percent.

Molecular weight, temperature and condensed phase concentration corrections are frozen and a new correction vector generated if the initial set of corrections indicate excessive temperature or molecular weight excursions, a contradictory temperature change, or negative corrections on newly introduced condensed species.

The formulation of these and other scaling and freezing criteria is an essential feature of the EST program. Because of these features, convergence is virtually assured for well formulated, physically unique problems.

3.1.3   Base Species

The discussion of Section 2 described the equilibrium reaction equations as equations giving the formation of a species from atomic elements. Thus the reactants are elements and the products are usually molecules. This scheme has the advantage of formal simplicity, since the stoichiometric coefficients needed in the equilibrium equations are given directly by the product species chemical formula. This scheme can have computational disadvantages, however, since the atomic elements are frequently not present to any great extent in the equilibrium system. This in itself results in no disadvantage. If, however, a molecule (e.g., CO) dominates more than one mass balance (e.g., C and O) loss of significant figures can slow or defeat convergence.

It is more desirable to write the equilibrium reactions (1) and (2) as well as the mass balances in terms of reactant species which are actually present in appreciable amounts. These species are termed "base species" (from Ref. 20) since all other species are taken to be formed from them.

The EST program selects the base species from the candidate species thermochemical data which are input as specified in Section 4. The program automatically selects as base species the first set of species satisfying the requirement that (1) all other species may be formed from this base species set and (2) that no balanced reaction can be written involving only base species. One base species may be considered to represent each element. Thus, the base species are established by the order in which the user inputs the candidate species thermochemical data. The calculation of the stoichiometric coefficients and equilibrium constants appropriate to any set of base species is handled automatically by the program.

While the selection of base species is not usually critical, certain computational economies may be realized if the base species are those species which occur in relatively high concentrations in the system. Thus, the user is advised to place at the head of the species thermochemistry data card set (Section 4) a group of species which are expected to occur in high concentrations.

3.2   FORTRAN ROUTINES

In order to permit an understanding of the actual solu-
tion mechanics and their relation to the FORTRAN source program, a
brief description of each of the subroutines are provided in
this section. For convenience the routines have been grouped,
where possible, under more general headings. The calling of these
routines and the principal iterative loop is controlled by the main-
line program. All routines except SQUEE and ETIMEF are called by
the mainline program.

3.2.1   Thermodynamic Data Input Routines

IMELM: Reads elemental data information and normalizes
elemental composition information.

INPUT: Reads species thermochemical data, selects base
species, determines stoichiometric coefficients
of formation reactions of all other species from
the base species, flags condensed species, sets
up first guesses, reads diffusion factor and
fail temperature data $(KR(3) \neq 9)$*. and calculates
species molecular weights.

BELCH: Establishes a base species-element correspon-
dence table which is required if an input
element is temporarily omitted from the chem-
ical system being analyzed.

3.2.2   Problem Setup and Initiation

ZIPIN: Reads control card, relative mass or ablation
rate data, and (if requested) title information;
controls logic for temperature fill-in opera-
tions $(KR(10))$; and initializes and sets various
control flags.

---

* $KR(I)$ refers to elements of an input array which controls most of
the program options - see Section 4.

ALPST: Reads diffusion factor values if KR(3) = 7,
8 or 9; sets diffusion factors based on expo-
nential approximation or input values using
information from INPUT and ALPST; determines
which elements are absent from the system and
flags corresponding molecular species and, in
particular, corresponding base species (see
BELCH); reinitializes species omitted from the
prior solution and zeros those to be omitted
from current solution; evaluates conserved
quantity parameters entering mass balances.

3.2.3   Calculation of Errors and Error Derivatives Used Within
Newton Raphson Iteration

THERM: On first iteration and after every change of
system temperature this routine is called to
evaluate molecular thermodynamic properties
(e.g., enthalpy, entropy, free energy, specific
heat) and the equilibrium constants appropriate
to each formation reaction. On the first iter-
ation certain reinitializations are performed
including assigning temperature to 3000°K if the
nonconvergent flag has been set and certain key
summations are evaluated. Subsequently these
summations are determined in CRECT. (The rea-
son for these functions inclusion in THERM
relates to the overlaying of subroutines and
molecular species data in an IBM 1130 version
of this program.)

MAT1:   Initializes mass balance error equations and
determines contribution of base species to
these errors. Initializes matrix of partial
derivatives of mass balance errors with respect
to log of base species partial pressures and

introduces base species contributions to these coefficients. Commences search for surface species. On first iteration normalizes gas phase partial pressures.

MAT2: Evaluates errors in formation reaction equilibrium relation for non-base species. Introduces contribution of non-base species to mass balance equations. For gases the contribution of the partial derivatives of the mass balance errors with respect to the non-base species log partial pressure is related to base species log partial pressure via the equilibrium equation and introduced into the array initialized in MAT1. For each condensed species which has been previously introduced into the system an additional equilibrium relation is added to the mass balance equations. One additional condensed species relation is accepted if equilibrium indicates a positive formation potential (see AFMAT relative to this species). Completes search for surface species.

MAT3: Completes formulation of mass balance errors and their derivatives. Checks for convergence of mass and equilibrium equations.

3.2.4   Calculation of Variable Corrections

Upon inversion of the matrix of error derivatives and its multiplication of the errors (see RERAY) a set of corrections are obtained for temperature, pressure-molecular weight product, log partial pressure of the base species and the relative moles of condensed species. Before these constraints can be applied, however, a significant amount of messaging is required.

AFMAT: Immediately after the inversion, performs a
series of tests on the corrections and if
necessary imposes constraints on equations and
repeats inversion. Examples include: the newly
introduced condensed species with zero concentra-
tion has a calculated negative correction - the
corresponding equilibrium equation is removed
and the correction set to zero; if the tempera-
ture is currently equal to a minimum or maximum
value dictated by phase change or other discon-
tinuous phenomena and if a contrary temperature
correction is predicted - the temperature con-
straint is removed and the temperature frozen -
if an excessive negative change in the pressure-
molecular weight product is predicted - the
pressure constraint is removed and pressure
frozen. Certain temperature minima and maxima
are also set to control the convergence on sur-
face equilibrium calculations.

SCALE: From basic corrections, corrections to log partial
pressures of non-base species are calculated.
Scans all corrections and determines maximum
damping factor which will permit all corrections
to satisfy certain constraints. These include
one order of magnitude increase and three orders
of magnitude decrease in partial pressures of
significant species, and less restrictive con-
straints on less important species. The scale
factor generated by this routine will subsequently
be applied to all corrections. Performs correc-
tion of temperature and pressure-molecular weight
product.

CRECT: Performs all corrections according to scale fac-
tors calculated in SCALE. Makes corrections

based either on linearization of mass balances
(delta of mole fractions) or of equilibrium equa-
tions (delta of log of mole fractions) depending
on relative importance in mass balances. Evalu-
ates set of summations previously discussed rela-
tive to THERM in Section 3.2.3.

3.2.5   Calculation of Output Quantities

PROPS: Determines certain derivative properties from
the inverse matrix of error derivatives includ-
ing the equilibrium specific heat and the isen-
tropic exponent; calculates quantities using
diffusion factor model and outputs calculated
quantities.

OUTPUT: Generates and outputs all additional terms re-
quired for output as displayed in Section 5.

3.2.6   Utility Routines

RERAY: Linear equation solver and inversion routine.
Call list is

    N = number of rows in C
    C = coefficient array
   NN = number of columns in C minus N
    D = set of column vectors of length N
  NNN = number of column vectors
   LS = column rearrangement flag (zero implies
       no rearrangement)
   IS = Flag, -2 at call results in before and
       after display of arrays, <0 at return
       implies singularity encountered at row-IS.
   Returns with left N x N square of C inverted
   and this inverse multiplied by remaining
   columns of C (if any) and D.

SWAP: Replaces one array and vector with another set, call list is

         A   array 1 (16 x 16 in current listing)
         B   vector 1 (16 in length currently)
    SLA   array 2
    SLB   vector 2

Returns with A and B replaced by SLA and SLB, respectively. SLA and SLB are unchanged.

SQUEE: Prepares integer and alphanumeric information from real variables for compressed card output. Call list is

         A   real variable to be converted
         I   first of three storage locations for results
    IDEE   presumed decimal location in result

Returns with I(1) an integer, I(2) the sign of the exponent (alphanumeric), I(3) the exponent, such that

$$A = \frac{I(1)}{10^{IDEE}} \cdot 10^{\pm I(3)}$$

ETIMEF
and
ETIME: System time routines available on Univac 1108 systems tape. For other systems a conversion or dummy routine is required. Call of ETIME sets zero time in clock. Subsequent call of ETIMEF(X) retunrs time in seconds from last call of ETIME as real variable X.

3.3   DEFINITIONS OF SEVERAL OUTPUT QUANTITIES

Several quantities appear on the standard program output under abbreviated names. In this section, these variables are more accurately defined. The derivative property output gives the following:

$$\text{CP-FROZEN} = \sum_{i=1}^{I} K_i \frac{\partial h_i}{\partial T} \text{ , the frozen constant}$$

pressure specific heat capacity
(Btu/lbm°R or Cal/gm°K)

$$\text{CP-EQUIL} = \frac{\partial h}{\partial T}\bigg)_p = \sum_{i=1}^{I} h_i \frac{\partial k_i}{\partial T}\bigg)_p + \sum_{i=1}^{I} k_i \frac{\partial h_i}{\partial T}\bigg)_p \text{ ,}$$

the equilibrium constant pressure
specific heat capacity
(Btu/lbm°R or Cal/gm°K)

$$\text{DLNM/DLNT} = \frac{\partial \ln \mathscr{m}}{\partial \ln T}\bigg)_p \qquad \text{(unitless)}$$

$$\text{DLNM/DLNP} = \frac{\partial \ln \mathscr{m}}{\partial \ln P}\bigg)_T \qquad \text{(unitless)}$$

$$\text{GAMMA} = \frac{\partial \ln P}{\partial \ln \rho}\bigg)_s = C_p/C_v \text{ , for an ideal gas}$$

(unitless)

Other property output includes:

$$\text{MU1} = \mu_1 = \sum_j X_j F_j \text{ , a gas mixture}$$

property which reduces to unity
for assumed equal diffusion coef-
ficients $F_j = \overline{F} = 1.0$ (unitless)

MU2 $= \mu_2 = \sum \mathcal{m}_j X_j / F_j$, a gas mixture property which reduces to the mixture molecular weight, $\mathcal{m}$, for assumed equal diffusion coefficient $F_j = \overline{F} = 1.0$ (grams of system/mole of gas)

MØL.WT = $\mathcal{m}$, the composite mixture molecular weight (see Equation 6, page 2-4) (grams system/moles of gas)

HTIL = $\tilde{h} = \sum_{j=1}^{I} Z_i h_i$, a property of the gas mixture which reduces to the static enthalpy, h, for assumed equal diffusion coefficients. Z_i is defined by Equation 36, page 2-21. (Btu/lbm)

CPTIL = $\tilde{C}_p = \sum_{i=1}^{I} Z_i \dfrac{\partial h_i}{\partial T}\Big|_p$, a property of the gas mixture which reduces to the frozen specific heat capacity for assumed equal diffusion coefficients. Z_i is defined by Equation 36, page 2-21 (Btu/lbm°R or Cal/gm°K)

HTIL* = h* $= \sum_{i=1}^{I} Z_i^* h_i$, a property of the gas mixture which reduces to HTIL when GAMEX (the unequal diffusion exponent) = 1.0, and reduces to static enthalpy, h, for assumed equal diffusion coefficients. Z_i^* is defined by Equation 35, page 2-21. (Btu/lbm)

GAMEX = γ, the weight factor exponent between K and Z mass fractions used to obtain the Z_i^* values in Equation 35, page 2-21. (unitless)

ELEMENTAL K MASS FRACTIONS = $\tilde{K}_k$, usual definition of mass fraction for element K in the system, see Equation 10, page 2-10. (gm of k/gm system).

ELEMENTAL Z MASS FRACTIONS = $\tilde{Z}_k^*$, elemental F_i^γ weighted mass fraction of element K in the system, defined by Equation 34, page 2-21. (gm of K/gm system).

All of the above properties are calculated and output for each problem solution using the current values of Γ_i and GAMEX, even though the particular option being computed does not require these values. An important example is the equal diffusion surface equilibrium option. Even though the HTIL* value is computed and printed for a GAMEX value of 0.667, the value of HTIL* punched on output cards (for input to a heat conduction program) will be static enthalpy, h, as it should be.

Additional descriptions of the variables computed and output by the EST code are given in References 2, 3, and 4.

3.4   PROGRAM OPERATION DETAILS

3.4.1   Program Storage Requirements

The current version of the EST program allows 149 chemical species, 10 elements, a total of up to 16 simultaneous equations (1 pressure balance, 10 mass balances, 4 present condensed species, and 1 enthalpy, temperature or surface equilibrium condition), 50 B_g' and B_c' entries, and 50 entries in the diffusion factor tables. With these limits approximately 25,000 (decimal) words of storage are required.

3.4.2   Tape Requirements

All input and output tape designations are set at the beginning of the main program with one exception. The designations are

KIN	System input	(=5)
KOUT	System output	(=6)
JAN	Scratch (or save)	(=18)
	tape, see KR(3)	

In RERAY, KOUT is also set to the system output tape (=6 currently).

3.4.3   Operator Controls

No operator intervention control switches exist. All controls are set at the initiation of execution of each problem with the corresponding control card (see Section 4).

3.4.4   Dumps and Diagnostics

Control column 7 (KR(7)) controls the output of requested diagnostic data. The interpretation of this data is not always obvious and users should consult with the program authors if interpretation is mandatory. This same data will automatically be obtained if more than 67 iterations are required for convergence and will continue through the 70th and last iteration. Other diagnostic complaints may be self-explanatory. The failure to obtain convergence is usually related to physical situations for which no unique solution exists. For example specification of a graphite B' less than about 0.09 in equilibrium with air results in the program flailing about the program minimum temperature (300°K) since the CO_2 plateau represents the minimum equilibrium B'.

3.4.5   Program Running Time

Program run time is most conveniently measured in terms of the number of solutions, and time per solution, required for a

given problem. Time per solution is conveniently measured in terms of the number of iterations, and time per iteration, required for a converged solution. Thus, the run time for a given problem may be estimated as:

$$\text{Run Time} = \text{No. of Solutions} \times \frac{\text{Iterations}}{\text{Solutions}} \times \frac{\text{Time}}{\text{Iteration}}$$

The number of solutions required for a given problem is determined by the user (except when one of the fill-in options are used, in which case the exact number of inserted or appended solutions is not known a priori). For example, for simple closed system problems, the number of solutions is equal to the number of times card set 1 (Section 4) is repeated, and for surface equilibrium open system problems, the number of solutions is equal to the number of elements in the input $B_g' \times B_c'$ matrix.

The number of iterations required for a converged solution is, of course, a function of the type of problem being solved. The sample problems, Section 5, should provide some guidance in estimating this quantity. Roughly, most solutions, other than the initial solution, converge in about 5 to 15 iterations.

The time required per iteration is a function of the computing machine as well as the problem type. Machines in the speed range of the Univac 1108 or CDC 6600 require on the order of 10 to 60 milliseconds per iteration. Again, the sample problems in Section 4 (which were run on a Univac 1108) should provide some guidance here.

SECTION 4

INPUT PREPARATION

This section defines the format and significance of each field of the input data card deck for Version 3 of the Aerotherm Equilibrium Surface Thermochemistry (EST) program. The input consists of six card sets. These are:

1. CONTROL CARD
2. TITLE INFORMATION
3. SURFACE FLUXES
4. ELEMENTAL COMPOSITION DATA
5. DIFFUSION FACTOR DATA
6. SPECIES THERMOCHEMICAL EQUILIBRIUM DATA

Card Set 1 is a control card which contains a 10-element array, $KR(I)$. This array controls most of the program options and tells the program what to expect from the remaining card sets. Few problems require all card sets. The card sets are described in detail in this section.

CARD SET 1 - CONTROL CARD (1 Card)

FIELD 1   (Columns 1-10, Format 10I1)   this is the variable
           array KR(I) which is used to control the various
           program options.

COLUMN 1 -- STATE OPTION

0	Assigned temperature
1	Surface equilibrium
2	Assigned enthalpy
3	Assigned temperature supressing surface equilibrium
8	Stop Program Execution

COLUMN 2 -- ELEMENTAL COMPOSITION

0	Accept the resident values (i.e., those used in the previous solution)
1	Input new elemental compositions for the system components (card set 4)

COLUMN 3 -- SPECIES THERMOCHEMICAL DATA

0	9	Accept the resident values for species thermochemistry data (i.e., those used in the previous solution)
1234		Read from cards new species thermochemistry data (card set 6) and, if provided, data on diffusion factors (card set 5)
34		Store all species data including diffusion factors read above from card sets 5 and 6 on tape
5678		Read all species data from tape as last stored
789		Update values of diffusion factors (card set 5)
2 4 6 8		Print out the thermochemistry data for all species read or stored which may be formed from the elements input (card set 4)

COLUMN 4 -- MASS BALANCE OPTIONS

0	Closed system mass balance
1234	Open system mass balances
1	Equal diffusion coefficients. This flag overrides the use of all unequal diffusion coefficient equations.

COLUMN 4 -- MASS BALANCE OPTIONS (Continued)

	Hence, no corrections to F_i values or GAMEX are required.
234	Unequal diffusion coefficients (requires boundary layer edge composition)
2	No change from previously saved boundary layer edge composition
3	Use the prior solution as the boundary layer edge composition
4	Determine the boundary layer edge composition , in terms of Z mass fractions, from the elemental data cards (card set 4) as last read.

COLUMN 5 -- TITLE INFORMATION OPTION

| 0 | No effect |
| 1 | Read three cards and print contents on the top of problem output. |

COLUMN 6 -- Not used

COLUMN 7 -- DIAGNOSTIC OUTPUT CONTROL

0	No diagnostic output
1	Output a single line of diagnostic information per iteration
j	(where j is a digit greater than one) Output full diagnostic information for 5(j-1) iterations and output a single line of diagnostic information for subsequent iterations.

COLUMN 8 -- PUNCHED CARD OUTPUT FORMAT
(implemented only if KR(10) $\neq$ 0)

0	Format appropriate to input the CMA program
1	Format appropriate to input the ASTHMA program
2	Output cards in both of the above formats

COLUMN 9 -- Not used

COLUMN 10 --- OPEN SYSTEM SOLUTION CONTROL AND PUNCHED CARD OUTPUT OPTIONS (used to provide punched card output for input to energy balance programs)

0	No effect
123456789	For each convergent solution, output a card or cards of data appropriate to energy balance calculations (see KR(8))
2345	Input an array of pyrolysis gas (component 2) and char (component 3) fluxes (card set 2). For each pyrolysis gas flux, obtain a solution for all char fluxes (valid only for KR(1) = 1)
6789	Using last input arrays, obtain solutions as above (valid only for KR(1) = 1)
2 4 6 8	For each pyrolysis gas rate, append a sequence of assigned temperature solutions (suppressing surface equilibrium) at the last char flux commencing at the next 500°K multiple below the last surface equilibrium temperature and, after a succession of 500°K decrements, terminate at 500°K
45 89	For each pyrolysis gas rate, insert up to ten additional char fluxes between each pair of tabular char flux entries as required to limit temperature gaps between solutions to less than 500°K

FIELD 2 (Columns 11-20, Format F10.5) The thermodynamic state variable, Z

If $KR(1) = 0, 1, 3$, and $Z \neq 0$: Z is assigned to temperature (°K)

If $KR(1) = 2$ and $Z \neq 0$: Z is assigned to enthalpy (cal/gm)

If $Z = 0$: resident values of temperature or enthalpy (whichever is consistent with the KR(1) specification) will be used

A negative temperature entry results in a frozen composition of the system (as previously calculated) and the calculation of properties of this system at the absolute value of the assigned temperature

If $KR(1) = 1$, the temperature assignment serves only as a first guess supplanting the resident temperature (on the first solution or after completing solutions for an array of pyrolysis gas and char rates, the first guess temperature is taken as 3000°K)

FIELD 3 (Columns 21-30, Format F10.5) Pressure variable, PR

If PR $\neq$ 0, PR is assigned to the system pressure (atmospheres)

If PR = 0, the resident value of pressure will be used

Field 4 (columns 31-40, Format F10.5) the Z mass fraction weighting factor exponent, GAMER

If GAMER $\neq$ 0, GAMER is assigned to GAMEX which is the weighting factor exponent for the mass transfer driving potential fractions (Z*) in terms of the mass and Z fractions where

$$Z* \propto Z^{GAMEX} K^{1-GAMEX}$$

If GAMER = 0, no change will be made in the weighting factor exponent GAMEX. GAMEX is set equal to 2/3 prior to the first solution, and this value is appropriate for most calculations

Field 5 (Columns 41-70, Format 3F10.5) Relative component mass variables WR(1), WR(2), WR(3)

If any of these three variables is non-zero, these variables are assigned to W(1), W(2), W(3), the relative masses of components 1, 2, and 3 respectively.

For surface mass balances, the relative masses are the relative mass fluxes normalized by $\rho_e u_e C_M$ and:

> W(1) = boundary layer edge gas
>
> W(2) = pyrolysis gas
>
> W(3) = char

If KR(10) > 1, this field will be ignored.

If all WR are zero, resident values of W are used (prior to the first solution, W(1) = 1.0, W(2) = 0, and W(3) = 0).

Field 6 (Columns 71-80, Format 2A4, A2) Input a title, job name, etc., which will appear on all printed and punched output.

CARD SET 2 - TITLE INFORMATION (3 cards)

IF KR(5) = 0 skip this card set

> Cards 1, 2, and 3 (Columns 1-80, Format 20A4)
> Enter any 80 alphanumeric characters on each card.

CARD SET 3 - SURFACE FLUXES (number of cards = 3 + 1/8 x (no. of
B_g''s -1) + 1/8 x (no. of B_c''s -1)

If KR(10) $\neq$ 2,3,4 or 5, skip this card set

If KR(10) = 2,3,4, or 5, the normalized pyrolysis gas and char
fluxes are input here. These fluxes are normalized with respect
to the mass transfer coefficient as per:

$$\frac{\text{pyrolysis gas surface mass flux}}{\rho_e u_e C_M} = B_g'$$

$$\frac{\text{char surface mass flux}}{\rho_e u_e C_M} \cdot B_c'$$

CARD 1

FIELD 1 (Columns 1-3, Format I3) Number of B_g''s to be read
from the next card(s)

FIELD 2 (Columns 4-6, Format I3) Number of B_c''s to be read
from subsequent card(s)

CARD(S) 2 (Columns 1-80, Format 8F10.) Enter values of B_g''s, eight
to a card, to a maximum of 50

For convenience of subsequent energy balance input
(using card output from this program), the B_g''s should
be ordered in either ascending or descending sequence

CARD(S) 3 (Columns 1-80, Format 8F10.) Enter values of B_c''s, eight
to a card

These values should be in descending sequence

NOTE: Care should be taken to avoid zero entries if
by so doing elements are not available from
which condensable species may be formed. If
edge gas is air, simultaneous zero assignments
for pyrolysis gas and char flux reduces the
the system to nitrogen and oxygen; i.e., no
condensables. Note that from inert pyrolysis
gases, no condensables are available.

CARD SET 4 - ELEMENTAL COMPOSITION DATA (Number of cards = number of elements + 1)

If KR(2) = 0, skip this card set

CARD 1 (Columns 1-3, Format I3) The number of elements in the system (in ionized systems, the electron is counted as an additional element)

CARD 2,3,4 . . . . . (one such card for each element)

FIELD 1 (Columns 1-3, Format I3) the atomic number identifier of the element (the electron which must be included for ionized closed system calculations must have identifier 99. Any non-zero identifier may be used for other elements in this list but thermochemical species formed from this element must have an identical identifier)

FIELD 2 (Columns 4-15, Format 3A4) the name of the element (for output identification only)

FIELD 3 (Columns 16-25, Format F10.) the atomic weight of the element

FIELD 4 (Columns 26-55, Format 3F10.) the relative amounts of the element in components 1, 2, and 3, respectively (see field 5 of card set 1)

Positive values are in relative gram-atomic-weights (or moles)

Negative values are in relative masses

If KR(4) = 4 (column 4 of card set 1), columns 26-35 should vontain the Z mass fraction of the element in che boundary layer edge gas. They must be entered with a minus. These values are most conveniently obtained from a prior solution where they are output corresponding to the relevant atomic numbers. Identical diffusion factors must be used to insure meaningful results.

If elements are added to, deleted from, or rearranged with respect to a prior input, it is necessary to re-read card set 6 either directly or from the tape.

FIELD 4   (Continued)

A typical example of Field 4 input is as
follows: If component 3 consists of 50%
mass of C and 50% mass of SiO_2, or equiva-
lently, 60.06 gm of C for each 60.06 gm of
SiO_2 (1 mole of SiO_2), or finally 60.06 gm
of C for each 1. gram-atomic-weight of Si
and 2 gram-atomic-weight of 0, it would be
most convenient to input -60.06, 2.0, and
1.0 into columns of 36-45 of the cards for
the elements C, 0, and Si.

CARD SET 5 - DIFFUSION FACTOR DATA (number of cards = 1/4 x (7 + no. of data items, viz., diffusion factors, reference molecular weight, diffusion exponent)

If KR(3) = 5 or 6, this card set must be skipped

If KR(3) = 1,2,3 or 4, this card set may be skipped

If KR(3) = 7,8 or 9, this card set must not be skipped

CARD 1 (Columns 1-3, Format I3) the total number of data items (viz., diffusion factors, reference molecular weight, diffusion exponent) to be entered

Diffusion factors may be specified for any or all species individually and/or diffusion factors may be calculated via the

$$\text{Diffusion Factor} = \left(\frac{\text{Molec.Wt.}}{\text{REFM}}\right)^{\text{FFA}}$$

where REFM and FFA may be specified here. For species for which diffusion factors are not specified individually, diffusion factors will be calculated via the above correlation, and if REFM and FFA are not specified, diffusion factors will be calculated from the above with **REFM = 23.4** and **FFA = 0.431**, assigned internally.

CARD(S) 2

FIELDS 1,3,5,7 (Columns 1-8, 21-28, 41-48, 61-68, each format 2A4)

The chemical symbol of the species for which data is to be provided, <u>exactly</u> as it appears in columns 73-80 of the first card of the 3 thermochemical data cards (card set 6) for that species. To specify values of REFM or FFA in the next field, enter the alpha characters "REFM" of "FFA" respectively here.

FIELDS 2,4,6,8 (Columns 9-20, 29-40, 49-60, 69-80, each format E12.4)

If the name of a chemical species was entered in the preceding field: the number in this field is presumed to be a diffusion factor.

If the name REFM or FFA was entered in the preceding field: enter the desired values of REFM or FFA respectively in this field.

The diffusion factors introduced into the solution in this fashion supplant the values set automatically via the above correlation, with REFM = 23.4 and FFA = 0.431, respectively) every time species thermochemical data are read from cards or tape (i.e., for KR(3) between 1 and 8 inclusive).

This card set data is not saved in core. However, this card set will be stored on tape together with the current card set 6 if KR(3) = 3 or 4, and thus will be introduced automatically if the tape is subsequently read with KR(3) = 5 or 6. If KR(3) = 7 or 8, an additional card set 5 is expected and will be temporarily appended to any card set 5 stored on tape. If this composite set contains competing data for the same species, the latter entry will be chosen. Latter entries of REFM and FFA will be chosen. If KR(3) = 9, only those species indicated on the card set will be modified.

CARD SET 6 - SPECIES THERMOCHEMICAL EQUILIBRIUM DATA (Number of
           cards = 1 + 3 x number of species)

If KR(3) = 0,5,6,7,8 or 9, skip this card set

There are three of these cards for each molecular, atomic, condensed,
ionic, or electron species. The end of this card set is signaled by
a blank card (see reference 3 for additional discussion relative to
this card set)

        CARDS 1,4,7 . . . Describe the elemental composition of the
                          species and establish its name designation

            FIELDS 1,3,5,...,13. (one for each element in the species)
                                 (Columns 1-3,7-9,13-15,...,37-39,
                                 each format F3.0)

                                 The number of atoms (of atomic number
                                 given in the following field) in a
                                 molecule of this species

                                 (If field 1 is zero, this card is pre-
                                 sumed to represent the end of card
                                 set 6)

            FIELDS 2,4,6,...,14. (one for each element in the species)
                                 (Columns 4-6,10-12,16-18,...,40-42,
                                 each format I3)

                                 The atomic number identifiers (cor-
                                 responding to Card Set 4) of the ele-
                                 ments in the molecule (the number of
                                 atoms of which was given in the pre-
                                 vious field)

                                 (If field 2 is zero, this card is pre-
                                 sumed to be the first card of card set 5)

        Ionized species are described by the addition or sub-
    traction of an electron (atomic number 99). For example,
    NO^+ would be described in fields 1 through 6 as
    bb1bb7bb1bb8b-1b99.

        FIELD 15 (Columns 43-72, Format 7A4A2) the source and date
                 of the thermochemical data for this specie. Used
                 for output only

        FIELD 16 (Columns 73-80, Format 2A4) the name designation of
                 this species (e.g., AL203). This variable is used
                 for output and as a means of identifying data en-
                 tered in card set 5. Typically the species chemical
                 symbol

CARDS 2,5,8...Lower temperature range thermochemical data

FIELDS 1,2,3,4,5 and 6 (Columns 1-54, Format 6E9.6) Input the 5 constants (F1,F2,F3,F4,F5,F6) appropriate to the lower temperature range of the thermodynamic data for this species. These constants are defined as follows, where T is in ^{O}K:

F1 = the heat of formation of the species at 298°K from the JANAF base state (elements in most natural form at 298°K) in cal/mole

F2 = the enthalpy change of the species from 298°K to 3000°K in cal/mole

F3,F4 and F5 are defined by a curve fit to the heat capacity at constant pressure of the form:

$$C_p = F3 + F4\ T + \frac{F5}{T^2} \quad \text{in cal/mole } ^OK$$

F6 = the entropy of the species at 3000°K in cal/mole ^{O}K

FIELD 7 (Columns 61-66, Format F6.0) the upper limit of the lower temperature range in ^{O}K

FIELD 8 (Column 67, Format I1) the phase specification:

1 signifies gaseous species
2 signifies solid species
3 signifies liquid species

The only phase combination allowed in one three card set is solid-liquid in which case a 2 and 3 would appear in fields 8 of cards 2 and 3, respectively.

CARDS 3,6,9...Upper temperature range thermochemical data

> These cards are the same as cards 2,5,8... except use constants for the upper temperature range and field 7 is ignored

LAST CARD OF CARD SET 6 MUST BE BLANK

The end of the species thermochemical data is signified by a blank card. Hence, the last card of card set 6 _must_ be a blank card.

The arrangement of these three card sets is, mathematically, unimportant for equilibrium solutions. In fact if no condensed phase species exist within the system the convergence path should be identical. Numerically this is not always true. A single species can dominate more than one mass equation, which in turn can lead to singular arrays. This can be avoided by placing these dominate species at the front of the deck.

The program automatically selects as "base species" the first set of species satisfying the requirement that (1) all other species may be formed from this base species set and (2) that no balanced reaction can be written involving only base species. One base species may be considered to represent each element. In the numerics of the program, the base species actually become the "elements" of the mass balances. The means of establishing whether one species may be formed from another are the specifications given in fields 1 to 14 of cards 1,4,7,.... Any reaction which can occur based on these specifications will be considered equilibriated in the system under study. To suppress equilibrium it is thus required to change names (i.e., atomic numbers) of certain elements and to introduce new "elements."

STOP OR CONTINUE

The program normally expects problems or cases to be stacked.
An 8 punch in column 1 signifies the end of an input data deck.
Thus, if the program is to exit in a graceful fashion, the last
card in the input data deck should have an 8 punch in column 1.

SECTION 5

SAMPLE PROBLEMS

Presented in this section are five sample problems which were run on a Univac 1108. These problems are relatively simple but do exercise most of the EST program options. The table on the following page gives a brief discussion of the nature of each sample problem. In addition, for each sample problem, the following is presented:

- A listing of the input data deck

- A few typical pages of the program output

DESCRIPTION OF EST
SAMPLE PROBLEMS

Sample Problem	Description	Comment
No. 1	Closed system calculations of the thermochemical states of two octane-air ratios ("Stoichiometric" and "110% theoretical air), at one pressure (10 atm) and four temperatures (3000, 2500, 2000, 500°K). 119 different molecular species are considered, including condensed carbon (C*).	This problem demonstrates the use of two component input for a closed system calculation. Air is input as component 1 (mass fractions of oxygen and nitrogen), and octane (C_8H_{18}) is input as component 2. Relative mass of each component is input on card set 1. Note that blanks imply reuse of previous data.
No. 2	Closed system calculation of the thermochemical states of an aluminized solid rocket propellant. The propellant consists of 70.4 percent ammonium perchlorate (component 1), 9.6 percent butadiene binder (component 2) and 20 percent aluminum (component 3). Specified enthalpy calculations were performed at two conditions (-777.4 cal/gm, 68 atm and -1369.1 cal/gm, 2.0 atm).	Three components are used to define the elemental quantities in this problem. Condensed phase alumina (Al_2O_3*) is found to be present in the system and the resultant output format is shown. For the -1369.1 cal/gm, 2.0 atm calculation, the program determined that 25.452 percent of the condensed Al_2O_3* was liquid. The option to read and print out three lines of title information is also demonstrated in this problem.
No. 3	Closed system calculation of the thermochemical states of air at one pressure (1.0 atm) and five temperatures (2000, 4000, 6000, 10,000°K). Elemental composition includes nitrogen, oxygen, argon, and the electron.	This problem demonstrates the computation of the thermochemical states of disassociated and ionized species. The output of species thermochemical data is also shown in this sample problem.
No. 4	Open system calculation of the equilibrium surface thermochemical response of carbon exposed to air. Equal diffusion coefficients are employed and an array of B'_{char} values (2.0, 1.0, 0.5, 0.2, 0.18, and 0.17) is input. The same B'_{char} values are utilized for three pressures (1.0, 10.0 and 100.0 atm) and the option to insert up to 10 B'_{char} values is employed.	This problem demonstrates the calculation of an equal diffusion, equilibrium surface thermochemistry table. Several B'_{char} values were inserted between the specified values to limit the maximum temperature gap in the table to less than 500°K. The typical output is from the 10 atm table. Also shown is the CMA format punched card output (also written on printed output).
No. 5	Closed and open system calculations of the surface response of carbon (or graphite) phenolic to air. An assigned temperature closed system edge calculation (5530°K, 0.1 atm) defines the edge gas composition, a frozen edge gas table is generated (7 temperatures), and two sets of matrices are input.	This problem shows the typical techniques used to generate a matrix of B'_{gas} and B'_{char} values suitable for input to the CMA code. The effects of unequal diffusion coefficients (defined internally) are accounted for and nonablating table entries are appended to the end of the final set of B'_{char} values. Note that this does not represent a complete surface thermochemical matrix.

```
0110000000    3000.    10.0                  15.1       1.0              OCT/AIR
    4
    1 HYDROGEN      1.008                  1A.
    6 CARBON       12.011                   8.
    7 NITROGEN     14.008    -0.767
    8 OXYGEN       16.000    -0.233
    1   6   2   8   0   0   0   0   0   0   0   0   0JANAF 03/61          CO2
-940540+5 365350+5 144559+2 210386-3-182392+7 798480+2  500. 3000.1    0.CO2
-940540+5 365350+5 156451+2-381561-4-602768+7 798480+2 3000. 5000.1    0.CO2
    2   1   1   8   0   0   0   0   0   0   0   0   0JANAF 03/61          H2O
-577980+5 302010+5 112254+2 811397-3-260800+7 684210+2  500. 3000.1    0.H2O
-577980+5 302010+5 15727R+2-191548-3-173599+8 684210+2 3000. 5000.1    0.H2O
    2   7   0   0   0   0   0   0   0   0   0   0   0JANAF 03/61          N2
 000000-0 221650+5 862699+1 116090-3-103715+7 637650+2  500. 3000.1    0.N2
 000000-0 221650+5 984175+1-116232-3-612728+7 637650+2 3000. 5000.1    0.N2
    1   6   1   0   0   0   0   0   0   0   0   0   0JANAF 03/61          CO
-264170+5 223570+5 865040+1 117021-3-898211+6 653700+2  500. 3000.1    0.CO
-264170+5 223570+5 115496+2-424139-3-131563+8 653700+2 3000. 5000.1    0.CO
    1   7   1   8   0   0   0   0   0   0   0   0   0JANAF 06/63          NO
 215800+5 227000+5 877623+1 899031-4-789656+6 688490+2  500. 3000.1    0.NO
 215800+5 227000+5 916260+1 657885-5-212519+7 688490+2 3000. 5000.1    0.NO
    1   7   2   8   0   0   0   0   0   0   0   0   0JANAF 06/63          NO2
 801100+4 345800+5 137819+2 315611-4-133765+7 848890+2  500. 3000.1    0.NO2
 801100+4 345800+5 130154+2 172586-3 175340+7 848890+2 3000. 5000.1    0.NO2
    1   7   3   8   0   0   0   0   0   0   0   0   0JANAF 12/64          NO3
 170000+5 498219+5 192301+2 191161-3-112129+7 998970+2  500. 3000.1    0.NO3
 170000+5 498219+5 198709+2 577142-7-172913+7 998970+2 3000. 5000.1    0.NO3
    2   7   1   8   0   0   0   0   0   0   0   0   0JANAF 12/60          N2O
 195000+5 365450+5 144686+2 120489-3-153478+7 815900+2  500. 3000.1    0.N2O
 195000+5 365450+5 123036+2 459018-3 942382+7 815900+2 3000. 5000.1    0.N2O
    2   7   3   8   0   0   0   0   0   0   0   0   0JANAF 12/64          N2O3
 197999+5 617799+5 272121+2 477580-3-124103+7 123217+3  500. 3000.1    0.N2O3
 197999+5 617799+5 248304+2 102872-5-293892+7 123217+3 3000. 5000.1    0.N2O3
    2   7   4   8   0   0   0   0   0   0   0   0   0JANAF 9/64           N2O4
 216999+4 785969+5 297734+2 594431-3-178833+7 134908+3  500. 3000.1    0.N2O4
 216999+4 785969+5 317815+2 175630-5-385969+7 134908+3 3000. 5000.1    0.N2O4
    2   7   5   8   0   0   0   0   0   0   0   0   0JANAF 12/64          N2O5
 216999+4 915759+5 353051+2 147295-3-163850+7 156719+3  500. 3000.1    0.N2O5
 216999+4 915759+5 357365+2 624545-5-171267+7 156719+3 3000. 5000.1    0.N2O5
    1   1   1   6   0   0   0   0   0   0   0   0   0JANAF 03/61          CH
 142006+6 221300+5 826079+1 302211-3-100184+7 616120+2  500. 3000.1    0.CH
 142006+6 221300+5 707091+1 463281-3 552860+7 616120+2 3000. 5000.1    0.CH
    2   1   1   6   0   0   0   0   0   0   0   0   0JANAF 12/62          CH2
 950000+5 329960+5 132894+2 413822-3-290273+7 684940+2  500. 3000.1    0.CH2
 950000+5 329960+5 140728+2 132150-3-239493+7 684940+2 3000. 5000.1    0.CH2
    3   1   1   6   0   0   0   0   0   0   0   0   0JANAF 12/62          CH3
 319400+5 434190+5 182763+2 401025-3-461203+7 786040+2  500. 3000.1    0.CH3
 319400+5 434190+5 204899+2-108028-3-114692+8 786040+2 3000. 5000.1    0.CH3
    4   1   1   6   0   0   0   0   0   0   0   0   0JANAF 03/61          CH4
-178950+5 530790+5 230948+2 677896-3-755061+7 825970+2  500. 3000.1    0.CH4
-178950+5 530790+5 236053+2 374323-3-368234+7 825970+2 3000. 5000.1    0.CH4
    1   1   2   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C2H
 117395+6 349620+5 134210+2 469100-3-187509+7 781140+2  500. 3000.1    0.C2H
 117395+6 349620+5 148516+2 109402-3-503862+7 781140+2 3000. 5000.1    0.C2H
    2   1   2   6   0   0   0   0   0   0   0   0   0JANAF 03/61          C2H2
 541900+5 482570+5 189960+2 769044-3-409039+7 849690+2  500. 3000.1    0.C2H2
 541900+5 482570+5 203952+2 389062-3-645297+7 849690+2 3000. 5000.1    0.C2H2
    3   1   2   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C2H3
 659250+5 562430+5 230065+2 691322-3-499095+7 965150+2  500. 3000.1    0.C2H3
 659250+5 562430+5 239033+2 331771-3-335425+7 965150+2 3000. 5000.1    0.C2H3
    4   1   2   6   0   0   0   0   0   0   0   0   0JANAF 12/60          C2H4
 124960+5 676830+5 294887+2 526568-3-865313+7 101790+3  500. 3000.1    0.C2H4
 124960+5 676830+5 313872+2 616238-4-131858+8 101790+3 3000. 5000.1    0.C2H4
    6   1   2   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C2H6
-203200+5 892710+5 484236+2-169721-2-193680+8 119447+3  500. 3000.1    0.C2H6
-203200+5 892710+5 393119+2 764877-3-383891+7 119447+3 3000. 5000.1    0.C2H6
    1   1   3   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C3H
 127703+6 489620+5 194464+2 508379-3-311933+7 928820+2  500. 3000.1    0.C3H
 127703+6 489620+5 199582+2 245687-3-632514+6 928820+2 3000. 5000.1    0.C3H
    2   1   3   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C3H2
 106522+6 635170+5 247444+2 992918-3-437596+7 104666+3  500. 3000.1    0.C3H2
 106522+6 635170+5 266623+2 364767-3-467730+7 104666+3 3000. 5000.1    0.C3H2
    3   1   3   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C3H3
 764850+5 709520+5 286929+2 766031-3-548098+7 113604+3  500. 3000.1    0.C3H3
 764850+5 709520+5 291672+2 456238-3-138601+7 113604+3 3000. 5000.1    0.C3H3
    4   1   3   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C3H4
 442940+5 822470+5 372219+2-528861-4-101994+8 120293+3  500. 3000.1    0.C3H4A
 442940+5 822470+5 344271+2 578173-3-208515+7 120293+3 3000. 5000.1    0.C3H4A
    5   1   3   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C3H5
 324310+5 946210+5 397325+2 958555-3-904683+7 141759+3  500. 3000.1    0.C3H5
 324310+5 946210+5 395073+2 733720-3-949766+6 141759+3 3000. 5000.1    0.C3H5
    1   1   4   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C4H
 155196+6 645030+5 252172+2 574336-3-339547+7 113166+3  500. 3000.1    0.C4H
 155196+6 645030+5 249358+2 402513-3 377676+7 113166+3 3000. 5000.1    0.C4H
    2   1   4   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C4H2
 111715+6 763230+5 298897+2 735927-3-430646+7 119311+3  500. 3000.1    0.C4H2
 111715+6 763230+5 301707+2 456896-3 698124+6 119311+3 3000. 5000.1    0.C4H2
    3   1   4   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C4H3
 101975+6 851450+5 343217+2 855861-3-624935+7 130072+3  500. 3000.1    0.C4H3
 101975+6 851450+5 345194+2 564141-3-151557+6 130072+3 3000. 5000.1    0.C4H3
    4   1   4   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C4H4
 737050+5 971240+5 398132+2 961427-3-792442+7 139440+3  500. 3000.1    0.C4H4A
 737050+5 971240+5 395899+2 720956-3 577880+6 139440+3 3000. 5000.1    0.C4H4A
    1   1   5   6   0   0   0   0   0   0   0   0   0DUFF BAUER 6/61      C5H
 185980+6 776470+5 299470+2 946114-3-430591+7 121859+3  500. 3000.1    0.C5H
 185980+6 776470+5 291522+2 690014-3 976229+7 121859+3 3000. 5000.1    0.C5H
```

Sample Problem Number 1
Listing of Input

```
2  1  5  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C5H2
165230+6 933660+5 369008+2 965961-3-583890+7 137191+3  500. 3000.1             0.C5H2
165230+6 933660+5 370815+2 638028-3 137088+7 137191+3 3000. 5000.1             0.C5H2
3  1  5  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C5H3
135414+6 100517+6 405377+2 799736-3-675863+7 147599+3  500. 3000.1             0.C5H3
135414+6 100517+6 396951+2 706570-3 334017+7 147599+3 3000. 5000.1             0.C5H3
1  1  6  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C6H
213164+6 942310+5 374677+2 420482-3-474514+7 148238+3  500. 3000.1             0.C6H
213164+6 942310+5 351470+2 661760+3 962699+7 148238+3 3000. 5000.1             0.C6H
2  1  6  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C6H2
169683+6 105052+6 412157+2 896814-3-569006+7 153063+3  500. 3000.1             0.C6H2
169683+6 105052+6 409176+2 665591-3 323615+7 153063+3 3000. 5000.1             0.C6H2
3  1  6  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C6H3
158461+6 114839+6 461927+2 874250-3-738470+7 164599+3  500. 3000.1             0.C6H3
158461+6 114839+6 450580+2 812263-3 450167+7 164599+3 3000. 5000.1             0.C6H3
6  1  6  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C6H6
197700+5 147317+6 626122+2 117808-2-139277+8 172317+3  500. 3000.1             0.C6H6
197700+5 147317+6 595572+2 140760-2 737034+7 172317+3 3000. 5000.1             0.C6H6
1  1  7  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C7H
241752+6 108509+6 434324+2 412328-3-559294+7 160749+3  500. 3000.1             0.C7H
241752+6 108509+6 402025+2 823782-3 123670+8 160749+3 3000. 5000.1             0.C7H
2  1  7  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C7H2
220830+6 119871+6 479372+2 119639-2-828438+7 166034+3  500. 3000.1             0.C7H2
220830+6 119871+6 479388+2 825569-3 171374+7 166034+3 3000. 5000.1             0.C7H2
1  1  8  5  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C8H
288875+6 122402+6 489887+2 527442-3-644448+7 174023+3  500. 3000.1             0.C8H
288875+6 122402+6 454317+2 953953-3 140527+8 174023+3 3000. 5000.1             0.C8H
2  1  8  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C8H2
226156+6 133849+6 528472+2 975801-3-710651+7 180289+3  500. 3000.1             0.C8H2
226156+6 133849+6 511890+2 960081-3 821940+7 180289+3 3000. 5000.1             0.C8H2
1  1  9  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C9H
293122+6 137308+6 546536+2 609606-3-683518+7 189983+3  500. 3000.1             0.C9H
293122+6 137308+6 507642+2 106604-2 158457+8 189983+3 3000. 5000.1             0.C9H
2  1  9  6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C9H2
272220+6 148147+6 592585+2 135861-2-988554+7 194630+3  500. 3000.1             0.C9H2
272220+6 148147+6 585236+2 106325-2 470277+7 194630+3 3000. 5000.1             0.C9H2
1  1  10 6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C10H
346750+6 151795+6 605449+2 627977-3-760351+7 208392+3  500. 3000.1             0.C10H
346750+6 151795+6 562113+2 115764-2 170972+8 208392+3 3000. 5000.1             0.C10H
2  1  10 6  0  0   0  0  0   0  0  0  0  0DUFF BAUER 6/61                          C10H2
284031+6 163084+6 643258+2 109715-2-831845+7 214369+3  500. 3000.1             0.C10H2
284031+6 163084+6 620020+2 115832-2 109441+8 214369+3 3000. 5000.1             0.C10H2
1  1  1  6  1  8   0  0  0   0  0  0  0  0JANAF 03/61                              CHO
-290000+4 323670+5 128033+2 300638-2-201721+7 789830+2  500. 3000.1             0.CHO
-290000+4 323670+5 103028+2 633312-3 121615+8 789830+2 3000. 5000.1             0.CHO
2  1  1  6  1  8   0  0  0   0  0  0  0  0JANAF 03/61                              CH2O
-277000+5 437910+5 184022+2 379921-3-431982+7 848880+2  500. 3000.1             0.CH2O
-277000+5 437910+5 184628+2 161963-3-372770+7 848880+2 3000. 5000.1             0.CH2O
4  1  2  6  1  8   0  0  0   0  0  0  0  0JANAF 12/60                              C2H4O
-121900+5 813210+5 353747+2 546144-3-966936+7 117211+3  500. 3000.1             0.C2H4O
-121900+5 813210+5 373112+2 690621-4-141968+8 117211+3 3000. 5000.1             0.C2H4O
1  1  1  6  1  7   0  0  0   0  0  0  0  0JANAF 03/61                              CHN
312000+5 355930+5 137023+2 552243-3-228955+7 758620+2  500. 3000.1             0.CHN
312000+5 355930+5 178895+2-295052-3-183671+8 758620+2 3000. 5000.1             0.CHN
1  1  1  6  1  7   1  8  0   0  0  0  0  0JANAF 12/60                              CHNO
-279000+5 461930+5 179701+2 469024-3-200904+7 928990+2  500. 3000.1             0.CHNO
-279000+5 461930+5 210167+2-229915-2-105568+8 928990+2 3000. 5000.1             0.CHNO
1  1  0  0  0  0   0  0  0   0  0  0  0  0JANAF 12/60                              H
521020+5 134230+5 480223+1 555469-4 173095+6 388628+2  500. 3000.1             0.H
521020+5 134230+5 308752+1 315025-3 929744+7 388628+2 3000. 5000.1             0.H
1  7  0  0  0  0   0  0  0   0  0  0  0  0JANAF 03/61                              N
112965+6 134370+5 486944+1 383516-4 958460+5 480900+2  500. 3000.1             0.N
112965+6 134370+5 428957+1 240844-3-417273+6 480900+2 3000. 5000.1             0.N
1  8  0  0  0  0   0  0  0   0  0  0  0  0JANAF 06/62                              O
595590+5 135220+5 497228+1 380768-5 154749+5 500960+2  500. 3000.1             0.O
595590+5 135220+5 657489+1-224268-3-891782+7 500960+2 3000. 5000.1             0.O
2  8  0  0  0  0   0  0  0   0  0  0  0  0JANAF 03/61                              O2
000000-0 234460+5 804370+1 510872-3-152718+6 679730+2  500. 3000.1             0.O2
000000-0 234460+5 103071+2 290991-4-783079+7 679730+2 3000. 5000.1             0.O2
3  8  0  0  0  0   0  0  0   0  0  0  0  0JANAF 6/61                               O3
341030+5 360230+5 135311+2 238739-3-606511+7 860919+2  500. 3000.1             0.O3
341000+5 360230+5 139121+2 125613-3-980654+6 860919+2 3000. 5000.1             0.O3
1  1  1  7  0  0   0  0  0   0  0  0  0  0JANAF 12/60                              HN
792000+5 217660+5 829133+1 281555-3-126896+7 609290+2  500. 3000.1             0.HN
792000+5 217660+5 765457+1 359853-3 180778+7 609290+2 3000. 5000.1             0.HN
1  1  1  7  1  8   0  0  0   0  0  0  0  0JANAF 12/60                              HNO
238000+5 327550+5 133820+2 122061-3-232403+7 783850+2  500. 3000.1             0.HNO
238000+5 327550+5 141523+2-470424-4-469135+7 783850+2 3000. 5000.1             0.HNO
1  1  1  7  2  8   0  0  0   0  0  0  0  0JANAF 06/63                              HNO2
-183400+5 468800+5 190278+2 189744-3-308752+7 962310+2  500. 3000.1             0.HNO2
-183400+5 468800+5 210284+2-229017-3-978618+7 962310+2 3000. 5000.1             0.HNO2
1  1  1  7  3  8   0  0  0   0  0  0  0  0JANAF 06/63                              HNO3
-321000+5 609120+5 253548+2 608154-4-450532+7 110851+3  500. 3000.1             0.HNO3
-321000+5 609120+5 266283+2-145785-3-102656+8 110851+3 3000. 5000.1             0.HNO3
1  1  1  8  0  0   0  0  0   0  0  0  0  0JANAF 12/60                              HO
933000+4 214040+5 773193+1 394386-3-973561+6 613820+2  500. 3000.1             0.HO
933000+4 214040+5 965144+1-44352R-4-686115+7 613820+2 3000. 5000.1             0.HO
1  1  2  8  0  0   0  0  0   0  0  0  0  0JANAF 03/64                       111    HO2
500000+4 325340+5 127161+2 292770-3-172279+7 799790+2 1000. 3000.1             0.HO2     1
500000+4 325340+5 138028+2 147068-4-399551+7 799790+2 3000. 5000.1             0.HO2     1
2  1  0  0  0  0   0  0  0   0  0  0  0  0JANAF 03/61                              H2
000000-0 212100+5 711963+1 621950-3-712694+6 484650+2  500. 3000.1             0.H2
000000-0 212100+5 681794+1 589854-3 265186+7 484650+2 3000. 5000.1             0.H2
2  1  1  7  0  0   0  0  0   0  0  0  0  0JANAF 12/65                              H2N
400999+5 305799+5 975862+1 114401-2-518970+6 701580+2  500. 3000.1             0.H2N
400999+5 305799+5 117419+2 229493-4-610024+7 701580+2 3000. 5000.1             0.H2N
```

Sample Problem Number 1
Listing of Input, Continued

```
 3  1  1  7  0  0  0  0  0  0  0  0  0  0 0JANAF 09/65                      H3N
-109700+5 416309+5 125186+2 219670-2-978531+6 769080+2  500. 3006.1       0.H3N
-109700+5 416309+5 166320+2 923148-3-361337+7 769080+2 3000. 5000.1       0.H3N
 4  1  2  7  0  0  0  0  0  0  0  0  0  0 0JANAF 12/65                      H4N2
 227899+5 685359+5 229856+2 241933-2-195931+7 108099+3  500. 3000.1       0.H4N2
 227899+5 685359+5 314319+2 487945-4-139705+8 108099+3 3000. 5000.1       0.H4N2
 3  6  2  8  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                      C3O2
-830000+4 652120+5 263775+2 103904-3-350368+7 112723+3  500. 3000.1       0.C3O2
-830000+4 652120+5 263543+2 882201-4-287091+7 112723+3 3000. 5000.1       0.C3O2
 1  6  1  7  0  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      CN
 109000+6 232490+5 655906+1 115326-2 479517+6 669760+2  500. 3000.1       0.CN
 109000+6 232490+5 988013+1 313855-3-649453+7 669760+2 3000. 5000.1       0.CN
 2  6  2  7  0  0  0  0  0  0  0  0  0  0 0JANAF 3/61                       C2N2
 738699+5 511070+5 188740+2 559856-3-896873+6 985479+2  500. 3000.1       0.C2N2
 738699+5 511070+5 208204+2 630229-5-346865+7 985479+2 3000. 5000.1       0.C2N2
 4  6  2  7  0  0  0  0  0  0  0  0  0  0 0JANAF 3/61                       C4N2
 127500+6 801239+5 297490+2 856052-3-152255+7 133063+3  500. 3000.1       0.C4N2
 127500+6 801239+5 327212+2 952999-5-541654+7 133063+3 3000. 5000.1       0.C4N2
 1  6  0  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      C
 170886+6 135500+5 444433+1 228125-3 409830+6 492870+2  500. 3000.1       0.C
 170886+6 135500+5 412212+1 261908-3 262886+7 492870+2 3000. 5000.1       0.C
 2  6  0  0  0  0  0  0  0  0  0  0  0  0 0JANAF 9/61                       C2
 198999+6 246990+5 776612+1 696081-3 185649+6 685519+2  500. 3000.1       0.C2
 198999+6 246990+5 104162+2 566841-4-649205+7 685519+2 3000. 5000.1       0.C2
 3  6  0  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                      C3
 189670+6 366220+5 146441+2 622536-4-168227+7 798410+2  500. 3000.1       0.C3
 189670+6 366220+5 144782+2 792232-4-646877+6 798410+2 3000. 5000.1       0.C3
 4  6  0  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                      C4
 242321+6 511230+5 205903+2 623436-4-257703+7 986760+2  500. 3000.1       0.C4
 242321+6 511230+5 210714+2-434895-4-404939+7 986760+2 3000. 5000.1       0.C4
 5  6  0  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                      C5
 242374+6 656230+5 264706+2 806528-4-337125+7 111641+3  500. 3000.1       0.C5
 242374+6 656230+5 271156+2-580271-4-543183+7 111641+3 3000. 5000.1       0.C5
 6  6  0  0  0  0  0  0  0  0  0  0  0  0 0DUFF BAUER 6/61                  C6
 291342+6 772700+5 303965+2 607305-3-475660+7 128958+3  500. 3000.1       0.C6
 291342+6 772700+5 308488+2 643430-4 583350+7 128958+3 3000. 5000.1       0.C6
 7  6  0  0  0  0  0  0  0  0  0  0  0  0 0DUFF BAUER 6/61                  C7
 292116+6 909770+5 359795+2 669838-3-579638+7 140555+3  500. 3000.1       0.C7
 292116+6 909770+5 355785+2 210202-3 102222+8 140555+3 3000. 5000.1       0.C7
 8  6  0  0  0  0  0  0  0  0  0  0  0  0 0DUFF BAUER 6/61                  C8
 344891+6 104684+6 415594+2 733634-3-683462+7 159275+3  500. 3000.1       0.C8
 344891+6 104684+6 402894+2 359448-3 146984+8 159275+3 3000. 5000.1       0.C8
 9  6  0  0  0  0  0  0  0  0  0  0  0  0 0DUFF BAUER 6/61                  C9
 340665+6 118391+6 471410+2 796582-3-787328+7 170872+3  500. 3000.1       0.C9
 340665+6 118391+6 450207+2 505033-3 190813+8 170872+3 3000. 5000.1       0.C9
10  6  0  0  0  0  0  0  0  0  0  0  0  0 0DUFF BAUER 6/61                  C10
 400439+6 132098+6 527202+2 860613-3-891076+7 189592+3  500. 3000.1       0.C10
 400439+6 132098+6 497439+2 651908-3 235109+8 189592+3 3000. 5000.1       0.C10
 1  6  0  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      C*
 000000-0 144120+5 586075+1 953976-4-766621+6 121290+2  500. 3000.2 100.C*
 000000-0 144120+5 485134+1 291605-3 307202+7 121290+2 3000. 5000.2 100.C*
```

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               2500.                                              OCT/AIR
               2000.                                              OCT/AIR
                500.                                              OCT/AIR
               3000.                            16.5      1.0     OCT/AIR
               2500.                                              OCT/AIR
               2000.                                              OCT/AIR
                500.                                              OCT/AIR
     8
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Sample Problem Number 1

Listing of Input, Concluded

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY JOB   OCT/AIR   0110000000

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	COMPONENT 1	COMPONENT 2	COMPONENT 3
1	HYDROGEN	1.00800	.0000000	.1575741	-.0000000
6	CARBON	12.01100	.0000000	.0700329	-.0000000
7	NITROGEN	14.00800	.0547544	.0000000	-.0000000
8	OXYGEN	16.00000	.0145625	.0000000	-.0000000

ELEMENT	HYDROGEN	CARBON	NITROGEN	OXYGEN
BASE SP	H2O	CO2	N2	CO

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   OCT/AIR

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM DLNT	DLNM/DLNP	GAMMA
.35365-00	.81113-00	-.28037-00	.12870-01	.11543+01

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.10598+01	.25361+02	.27406+02	.83312+03	.37038-00	.77823+03

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)

1	6	7	8
.98655-02	.52246-01	.71936-00	.21853-00
.12351-01	.48658-01	.72005-00	.21894-00

SOLUTION TIMES
    ITERATIONS = 46   MACHINE TIME = 3.631 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT
    RELATIVE MASSES OF COMPONENTS 1,2, AND 3.   .15100+02   .10000+01 -.00000

THERMODYNAMIC STATE

PRESSURE (ATMOSPHERES) =	10.0000	TEMPERATURE (DEG K) =	3000.000
(LBF/IN2-ABS) =	146.9600	(DEG R) =	5400.000
DENSITY (GM/CM3) =	.1113-02	ENTHALPY (CAL/GM) =	394.848
(LBM/FT3) =	.6949-01	(BTU/LBM) =	710.726
MOLECULAR WEIGHT =	27.4063	ENTROPY (BTU/LBM-R) =	.2295+01

CHEMICAL STATE
    MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.68344-01	H2O	.11107+00	N2	.69661+00	CO	.50869-01	NO	.14174-01
NO2	.70668-05	NO3	.27093-10	N2O	.21844-05	N2O3	.51878-12	N2O4	.25019-16
N2O5	.19441-19	CH	.36906-12	CH2	.51277-13	CH3	.57583-12	CH4	.36782-13
C2H	.12183-15	C2H2	.16826-15	C2H3	.20809-19	C2H4	.34354-20	C2H6	.16763-25
C3H	.39459-22	C3H2	.45716-24	C3H3	.18447-25	C3H4	.18026-27	C3H5	.82435-28
C4H	.88682-29	C4H2	.40108-30	C4H3	.10658-32	C4H4	.18523-34	C5H	.50215-38
C5H2	.00000	C5H3	.00000	C6H	.00000	C6H2	.00000	C6H3	.00000
C6H6	.00000	C7H	.00000	C7H2	.00000	C8H	.00000	C8H2	.00000
C9H	.00000	C9H2	.00000	C10H	.00000	C10H2	.00000	CHO	.17564-05
CH2O	.32759-08	C2H4O	.60298-23	CHN	.10823-07	CHNO	.22941-07	H	.53175-02
N	.36473-05	O	.49424-02	O2	.19343-01	O3	.82171-08	HN	.16865-05
HNO	.22230-05	HNO2	.22778-06	HNO3	.39993-10	HO	.17850-01	HO2	.77581-05
H2	.11453-01	H2N	.28597-06	H3N	.71272-07	H4N2	.32820-15	C3O2	.61663-18
CN	.20774-09	C2N2	.11532-15	C4N2	.49147-30	C	.24470-11	C2	.62000-18
C3	.13318-23	C4	.25244-32	C5	.16951-38	C6	.00000	C7	.00000
C8	.00000	C9	.00000	C10	.00000	C*	.00000		

Sample Problem Number 1

Sample Output

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY JOB OCT/AIR   **********

DERIVATIVE PROPERTY OUTPUT
CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.35035-00	.79342-00	-.27215-00	.12526-01	.11553+01

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.10637+01	.25473+02	.275 5+02	.86527+03	.36474-00	.81653+03

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .567)
1	6	7	8
.90763-02	.48067-01	.72317-00	.21969-00
.11243-01	.44563-01	.72461-00	.21958-00

SOLUTION TIMES
     ITERATIONS = 12   MACHINE TIME =   .611 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT
     RELATIVE MASSES OF COMPONENTS 1,2, AND 3.   .16500+02   .10000+01 -.00000

     THERMODYNAMIC STATE
          PRESSURE (ATMOSPHERES) =   10.0000   TEMPERATURE (DEG K) =   3000.000
                    (LBF/IN2-ABS) =   146.9600   (DEG R) =   5400.000

          DENSITY (GM/CM3)   =   .1120-02   ENTHALPY (CAL/GM)   =   419.191
                   (LBM/FT3)   =   .6992-01   (BTU/LBM) =   754.543

          MOLECULAR WEIGHT   =   27.5750   ENTROPY (BTU/LBM-R) =   .2282+01

     CHEMICAL STATE
          MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.67964-01	H2O	.10344+00	N2	.70328-00	CO	.42387-01	NO	.16995-01
NO2	.10113-04	NO3	.46272-10	N2O	.26319-05	N2O3	.89026-12	N2O4	.51240-16
N2O5	.47517-19	CH	.22763-12	CH2	.27939-13	CH3	.27715-12	CH4	.15639-13
C2H	.52467-16	C2H2	.64009-16	C2H3	.69929-20	C2H4	.10199-20	C2H6	.38833-26
C3H	.11864-22	C3H2	.12143-24	C3H3	.43283-26	C3H4	.37363-28	C3H5	.15094-28
C4H	.18617-29	C4H2	.74381-31	C4H3	.17460-33	C4H4	.26806-35	C5H	.00000
C5H2	.00000	C5H3	.00000	C6H	.00000	C6H2	.00000	C6H3	.00000
C6H6	.00000	C7H	.00000	C7H2	.00000	C8H	.00000	C8H2	.00000
C9H	.00000	C9H2	.00000	C10H	.00000	C10H2	.00000	CHO	.12929-05
CH2O	.21301-08	C2H4O	.21363-23	CHN	.67071-08	CHNO	.16968-07	H	.46974-02
N	.36647-05	O	.58984-02	O2	.27550-01	O3	.13967-07	HN	.14970-05
HNO	.23548-05	HNO2	.28796-06	HNO3	.60339-10	HO	.18818-01	HO2	.97611-05
H2	.89376-02	H2N	.22423-06	H3N	.49366-07	H4N2	.20177-15	C3O2	.29893-18
CN	.14574-09	C2N2	.56756-16	C4N2	.11792-30	C	.17085-11	C2	.30224-18
C3	.45329-24	C4	.59992-33	C5	.00000	C6	.00000	C7	.00000
C8	.00000	C9	.00000	C10	.00000	C*	.00000		

Sample Problem Number 1
Sample Output, Concluded

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211 1 1      -777.4    68.                    .704      .096      .20   AL PROPLNT
COMPOSITION OF THE BOUNDARY LAYER EDGE FLOW IN A SOLID PROPELLANT ROCKET MOTOR
      PROPELLANT IS 70.4 PCT AMMONIUM PERCHLORATE, 9.6 PCT BUTADIENE BINDER,
      AND 20.0 PCT ALUMINUM POWDER.  PRESSURE IS 68. ATM, ENTHALPY IS -777. CAL/GM
    6
    1 HYDROGEN       1.008      4.0        6.0
    6 CARBON        12.011                 4.0
    7 NITROGEN      14.008      1.0
    8 OXYGEN        16.000      4.0
   13 ALUMINUM      26.970                            1.0
   17 CHLORINE      35.457      1.0
    1  1  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                        H
    521020+5 134230+5 480223+1 555469-4 173095+6 388620+2  500. 3000.1    0.H
    521020+5 134230+5 308752+1 315025-3 929744+7 388620+2 3000. 5000.1    0.H
    1  6  1  8  0  0  0  0  0  0  0  0  0 0JANAF 03/61                       CO
   -264170+5 223570+5 865040+1 117021-3-898211+6 653700+2  500. 3000.1    0.CO
   -264170+5 223570+5 115496+2-424139-3-131563+8 653700+2 3000. 5000.1    0.CO
    1  7  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                        N
    112965+6 134370+5 486944+1 383516-4 958460+5 480900+2  500. 3000.1    0.N
    112965+6 134370+5 428957+1 240844-3-417273+6 480900+2 3000. 5000.1    0.N
    1  8  0  0  0  0  0  0  0  0  0  0  0 0JANAF 06/62                        O
    595590+5 135220+5 497228+1 380768-3 154749+5 500960+2  500. 3000.1    0.O
    595590+5 135220+5 657489+1-224268-3-891782+7 500960+2 3000. 5000.1    0.O
    1 13  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                        A1
    780000+5 134610+5 492905+1 113634-4 706967+5 508440+2  500. 3000.1    0.AL
    780000+5 134610+5 395674+1 204094-3 361777+7 508440+2 3000. 5000.1    0.AL
    1001 01 17                            JANAF 03/61                       CLH
   -219700+5 218640+5 839693+1 214828-3-125475+7 623640+2  500. 3000.1    0.CLH
   -219700+5 218640+5 837177+1 103261-3-446002+6 623640+2 3000. 5000.1    0.CLH
    1  6  1 13  0  0  0  0  0  0  0  0  0 0JANAF 12/60                       ALC
    209958+6 240440+5 896909+1-757687-5-752532+5 746650+2  500. 3000.1    0.ALC
    209958+6 240440+5 961609+1-128042-3-264567+7 746650+2 3000. 5000.1    0.ALC
    1 13  1 17  0  0  0  0  0  0  0  0  0 0JANAF 06/61                       ALCL
   -116200+5 244690+5 895305+1 115091-3-929251+5 750380+2  500. 3000.1    0.ALCL
   -116200+5 244690+5 951089+1 835189-5-223156+7 750380+2 3000. 5000.1    0.ALCL
    1 13  2 17  0  0  0  0  0  0  0  0  0 0JANAF 06/61                       ALCL2
   -780000+5 371170+5 138896+2 586012-5-137329+6 106813+3  500. 3000.1    0.ALCL2
   -780000+5 371170+5 136493+2 486738-4 869684+6 100813+3 3000. 5000.1    0.ALCL2
    1  8  2 13  0  0  0  0  0  0  0  0  0 0JANAF 09/61                       AL2O
   -314400+5 359700+5 138891+2 485413-5-663265+6 912000+2  500. 3000.1    0.AL2O
   -314400+5 359700+5 144656+2-108570-3-278920+7 912000+2 3000. 5000.1    0.AL2O
    1  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                         C
    170886+6 135500+5 444433+1 228125-3 409830+6 492870+2  500. 3000.1    0.C
    170886+6 135500+5 412212+1 261908-3 262886+7 492870+2 3000. 5000.1    0.C
    4  1  1  6  0  0  0  0  0  0  0  0  0 0JANAF 03/61                       CH4
   -178950+5 530790+5 230948+2 677896-3-755061+7 825970+2  500. 3000.1    0.CH4
   -178950+5 530790+5 236053+2 374323-3-368234+7 825970+2 3000. 5000.1    0.CH4
    1  6  2  8  0  0  0  0  0  0  0  0  0 0JANAF 03/61                       CO2
   -940540+5 365350+5 144559+2 210386-3-182392+7 798480+2  500. 3000.1    0.CO2
   -940540+5 365350+5 156451+2-381561-4-602768+7 798480+2 3000. 5000.1    0.CO2
    2  1  2  6  0  0  0  0  0  0  0  0  0 0JANAF 03/61                       C2H2
    541900+5 482570+5 189960+2 769044-3-409039+7 849690+2  500. 3000.1    0.C2H2
    541900+5 482570+5 203952+2 389062-3-645297+7 849690+2 3000. 5000.1    0.C2H2
    3  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                        C3
    189670+6 366220+5 146441+2 622536-4-168227+7 798410+2  500. 3000.1    0.C3
    189670+6 366220+5 144782+2 792232-4-646877+6 798410+2 3000. 5000.1    0.C3
    1 17  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                        CL
    289220+5 140280+5 508338+1-272037-4 290013+6 516230+2  500. 3000.1    0.CL
    289220+5 140280+5 539251+1-770696-4-114573+7 516230+2 3000. 5000.1    0.CL
    2 17  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                       CL2
    000000-0 244290+5 852234+1 273227-3 287718+6 737600+2  500. 3000.1    0.CL2
    000000-0 244290+5 100329+2-141907-4-554731+7 737600+2 3000. 5000.1    0.CL2
    1  1  1  8  0  0  0  0  0  0  0  0  0 0JANAF 12/60                        HO
    933000+4 214040+5 773193+1 394386-3-973561+6 613820+2  500. 3000.1    0.HO
    933000+4 214040+5 965144+1-443528-4-686115+7 613820+2 3000. 5000.1    0.HO
    2  1  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                        H2
    000000-0 212100+5 711963+1 621950-3-712694+6 484650+2  500. 3000.1    0.H2
    000000-0 212100+5 681794+1 589854-3 265106+7 484650+2 3000. 5000.1    0.H2
    2  1  1  8  0  0  0  0  0  0  0  0  0 0JANAF 03/61                       H2O
   -577980+5 302010+5 112254+2 811397-3-260800+7 684210+2  500. 3000.1    0.H2O
   -577980+5 302010+5 157278+2-191548-3-173599+8 684210+2 3000. 5000.1    0.H2O
    1  7  1  8  0  0  0  0  0  0  0  0  0 0JANAF 06/63                        NO
    215800+5 227000+5 877623+1 899031-4-789656+6 688490+2  500. 3000.1    0.NO
    215800+5 227000+5 916260+1 657885-5-212519+7 688490+2 3000. 5000.1    0.NO
    2  7  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                        N2
    000000-0 221650+5 862699+1 116090-3-103715+7 637650+2  500. 3000.1    0.N2
    000000-0 221650+5 984175+1-116232-3-612728+7 637650+2 3000. 5000.1    0.N2
    2  8  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                        O2
    000000-0 234460+5 804370+1 510872-3-152718+6 679730+2  500. 3000.1    0.O2
    000000-0 234460+5 103071+2 290991-4-783079+7 679730+2 3000. 5000.1    0.O2
    3  8  2 13  0  0  0  0  0  0  0  0  0 0JANAF 09/61                       AL2O3*
   -400400+6 811817+5 319699+2 120451-4-217514+7 772577+2  500. 2318.2 100.AL2O3*
   -366770+6 759318+5 351153+2-192777-4-555942+6 893107+2 2319. 5000.3 100.AL2O3*
    1  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                        C*
    000000-0 144120+5 586075+1 953976-4-766621+6 121290+2  500. 3000.2 100.C*
    000000-0 144120+5 485134+1 291605-3 307202+7 121290+2 3000. 5000.2 100.C*

    2         -1369.1    2.00
    8
```

Sample Problem Number 2

Listing of Input

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY JOB AL PROPLNT   211*1*1***
COMPOSITION OF THE BOUNDARY LAYER EDGE FLOW IN A SOLID PROPELLANT ROCKET MOTOR
   PROPELLANT IS 70.4 PCT AMMONIUM PERCHLORATE, 9.6 PCT BUTADIENE BINDER,
   AND 20.0 PCT ALUMINUM POWDER. PRESSURE IS 68. ATM, ENTHALPY IS -777. CAL/GM

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	COMPONENT 1	COMPONENT 2	COMPONENT 3
1	HYDROGEN	1.00800	.0340434	.1109221	.0000000
6	CARBON	12.01100	.0000000	.0739481	.0000000
7	NITROGEN	14.00800	.0085109	.0000000	.0000000
8	OXYGEN	16.00000	.0340434	.0000000	.0000000
13	ALUMINUM	26.97000	.0000000	.0000000	.0370782
17	CHLORINE	35.45700	.0085109	.00C0000	.0000000

ELEMENT	HYDROGEN	CARBON	NITROGEN	OXYGEN	ALUMINUM	CHLORINE
BASE SP	H	CO	N	O	AL	CLH

ITS	TEMP	PRES*MWT	EQUIL ER	MASBAL ER	SCALE	1 MASBAL	2 MASBAL	3 MASBAL	4 MASBAL	5 MASBAL	6 MASBAL
1	3000.00	.136+04	.608+02	.259+01	.000	.212+02	-.199+02	-.368+01	.229+02	-.765+01	-.125+02
2	3297.98	.130+04	.506+02	.276+01	.189-00	.172+02	-.161+02	-.297+01	.186+02	-.620+01	-.102+02
3	3493.82	.128+04	.362+02	.340+01	.174-00	.142+02	-.133+02	-.246+01	.154+02	-.512+01	-.840+01
4	3582.42	.129+04	.282+02	.518+01	.136-00	.123+02	-.115+02	-.212+01	.133+02	-.442+01	-.726+01
5	3603.64	.133+04	.203+02	.449+01	.702-01	.115+02	-.107+02	-.197+01	.124+02	-.411+01	-.675+01
6	3631.40	.140+04	.185+02	.316+01	.850+01	.105+02	-.979+01	-.179+01	.114+02	-.374+01	-.616+01
7	3667.30	.151+04	.162+02	.142+01	.126-00	.933+01	-.852+01	-.154+01	.'00+02	-.324+01	-.536+01
8	3703.21	.167+04	.128+02	.796-00	.202-00	.767+01	-.675+01	-.118+01	.811+01	-.253+01	-.423+01
9	3705.44	.186+04	.840+01	.437-00	.312-00	.557+01	-.457+01	-.754-00	.575+01	-.167+01	-.285+01
10	3622.98	.201+04	.555+01	.203-00	.369-00	.356+01	-.276+01	-.428-00	.361+01	-.978-00	-.171+01
11	3432.79	.218+04	.807+01	.265-01	.862-00	.695-00	-.332-00	-.171-01	.619-00	-.833-01	-.195-00
12	3346.96	.219+04	.328+01	.595-05	.100+01	.230-03	.565-04	.497-04	.135-03	.594-04	.481-04
13	3343.00	.219+04	.204+01	.887-06	.100+01	.238-06	-.834-07	.358-06	-.477-06	-.238-06	-.917-08
14	3339.87	.219+04	.945-00	.212-05	.100+01	.119-05	.156-06	.358-06	.477-06	.238-06	.185-06
15	3335.78	.219+04	.263-00	.652-06	.100+01	.143-05	.218-06	.477-06	.715-06	.119-06	.401-06
16	3333.63	.218+04	.262-01	.142-05	.100+01	-.715-06	-.790-07	-.238-06	-.715-06	-.119-06	-.209-06
17	3333.36	.218+04	.288-03	.256-06	.100+01	.000	-.109-06	-.238-06	.238-06	-.119-06	-.114-06
-1	3333.36	.218+04	.131-05	.725-06	.100+01	-.238-06	-.183-06	-.119-06	-.477-06	-.238-06	-.515-07

Sample Problem Number 2

Sample Output

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY JOB   2*********

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.40311-00	.65782+05	-.38964-01	.16232-02	.99838-00

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.85586-00	.19801+02	.32790+02	.44478+03	.70115-00	.61272+02

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)

1	6	7	8	13	17
.34892-01	.85266-01	.83931-01	.38347-00	.20000-00	.21245-00
.89480-01	.13246-00	.13184-00	.33675-00	.39238-03	.30908-00

SOLUTION TIMES
    ITERATIONS = 11   MACHINE TIME = .411 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT
    RELATIVE MASSES OF COMPONENTS 1,2, AND 3.   .70400-00   .96000-01   .20000-00

   MASS CONDENSED/MASS GAS =   .60593-00

   THERMODYNAMIC STATE

PRESSURE (ATMOSPHERES) =	2.0000	TEMPERATURE (DEG K) =	2318.000
(LBF/IN2-ABS) =	29.3920	(DEG R) =	4172.400

	GAS	CONDENSED	COMPOSITE
DENSITY (LBM/FT3) =	.1340-01		.2152-01
(GM/CM3) =	.2147-03		.3447-03
ENTHALPY (BTU/LBM) =	-.3822+03	-.5901+04	-.2464+04
(CAL/GM) =	-.2123+03	-.3278+04	-.1369+04
ENTROPY (BTU/LB DEG-R) =	.2923+01	.7057-00	.2087+01
MOLECULAR WEIGHT =	.2042+02	.1019+03	.3279+02

   CHEMICAL STATE
    MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H	.40973-02	CO	.21165-00	N	.10438-07
O	.34960-05	AL	.30759-07	CLH	.19368-00
ALC	.26533-21	ALCL	.34785-04	ALCL2	.39536-03
AL2O	.38314-09	C	.18188-12	CH4	.99444-09
CO2	.21122-01	C2H2	.14737-11	C3	.22070-21
CL	.19541-02	CL2	.16914-05	HO	.39032-03
H2	.30096-00	H2O	.16746-00	NO	.11954-04
N2	.98226-01	O2	.81884-06	AL2O3*	.12136+00
C*	.00000				

    AL2O3* IS .25452 LIQUID AND .74548 SOLID BY MASS.

Sample Problem Number 2

Sample Output, Concluded

```
0120000000 2000.    1.0                        1.0                    AIR PROP
004
    7 NITROGEN     14.008    0.7811
    8 OXYGEN       16.000    0.2095
   18 ARGON        39.948    0.0094
   99 ELECTRON      0.00055
    1  7  0  0  0  0  0  0  0  0  0  0  0  0JANAF 03/61            N
  112965+6 134370+5 486944+1 383516-4 958460+5 480900+2  500. 3000.1  0.N
  112965+6 134370-5 428957+1 240844-3-417273+6 480900+2 3000. 5000.1  0.N
    1  8  0  0  0  0  0  0  0  0  0  0  0  0JANAF 06/62            O
  595590+5 135220+5 497228+1 380768-5 154749+5 500960+2  500. 3000.1  0.O
  595590+5 135220+5 657489+1-224768-3-891782+7 500960+2 3000. 5000.1  0.O
    1 18  0  0  0  0  0  0  0  0  0  0  0  0CONVAIR 2PH-122 12/61  A
  000000+0+149400+5+418099+1+122960-4+371200+7+484619+22000. 10000.1  A
  000000+0+149400+5+418099+1+122960-4+371200+7+484619+22000. 10000.1  A
    2  7  0  0  0  0  0  0  0  0  0  0  0  0JANAF 03/61            N2
  000000-0 221650+5 862699+1 116090-3-103715+7 637650+2  500. 3000.1  0.N2
  000000-0 221650+5 984175+1-116232-3-612728+7 637650+2 3000. 5000.1  0.N2
    2  8  0  0  0  0  0  0  0  0  0  0  0  0JANAF 03/61            O2
  000000-0 234460+5 804370+1 510872-3-152718+6 679730+2  500. 3000.1  0.O2
  000000-0 234460+5 103071+2 290991-4-783079+7 679730+2 3000. 5000.1  0.O2
    1  7  1  8  0  0  0  0  0  0  0  0  0  0JANAF 06/63            NO
  215800+5 227000+5 877623+1 899031-4-789656+6 688490+2  500. 3000.1  0.NO
  215800+5 227000+5 916260+1 657885-5-212519+7 688490+2 3000. 5000.1  0.NO
    2  7  1  8  0  0  0  0  0  0  0  0  0  0JANAF 12/60            N2O
  195000+5 365450+5 144686+2 120489-3-153478+7 815900+2  500. 3000.1  0.N2O
  195000+5 365450+5 123036+2 459018-3 942382+7 815900+2 3000. 5000.1  0.N2O
    1 99  0  0  0  0  0  0  0  0  0  0  0  0CONVAIR 2PH-122 12/61  E-
            +149010+5+498851+1-272800-5-135900+6+164558+22000. 10000.1  E-
            +149010+5+498851+1-272800-5-135900+6+164558+22000. 10000.1  E-
    1 18 -1 99  0  0  0  0  0  0  0  0  0  0CONVAIR 2PH-122 12/61  A+
  363437+6+157330+5+486079+1+211800-4+165300+7+519257+22000. 10000.1  A+
  363437+6+157330+5+486079+1+211800-4+165300+7+519257+22000. 10000.1  A+
    1  7 -1 99  0  0  0  0  0  0  0  0  0  0CONVAIR 2PH-122 12/61  N+
  +446641+6+151310+5+501751+1+617100-4-184100+7+496847+22000. 10000.1  N+
  +446641+6+151310+5+501751+1+617100-4-184100+7+496847+22000. 10000.1  N+
    1  7  1  8 -1 99  0  0  0  0  0  0  0  0CONVAIR 2PH-122 12/61  NO+
  +232919+6+241970+5+910216+1+277400-4-316600+7+654379+22000. 10000.1  NO+
  +232919+6+241970+5+910216+1+277400-4-316600+7+654379+22000. 10000.1  NO+
    1  8 -1 99  0  0  0  0  0  0  0  0  0  0CONVAIR 2PH-122 12/61  O+
  +371999+6+149290+5+336271+1+306710-3+590200+7+484849+22000. 10000.1  O+
  +371999+6+149290+5+336271+1+306710-3+590200+7+484849+22000. 10000.1  O+

         4000.                                                 AIR PROP
         6000.                                                 AIR PROP
         8000.                                                 AIR PROP
        10000.                                                 AIR PROP
  8
```

Sample Problem Number 3

Listing of Input

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY JOB AIR PROP   01200000C0

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	COMPONENT 1	COMPONENT 2	COMPONENT 3
7	NITROGEN	14.00800	.0532478	-.0000000	-.0000000
8	OXYGEN	16.00000	.0142817	-.0000000	-.0000000
18	ARGON	39.94800	.0006408	-.0000000	-.0000000
99	ELECTRON	.00055	.0000000	-.0000000	-.0000000

```
1.  7 0.  0 0.   0 0.   0 0.   0 0.   0 0.  0JANAF 53/61                N
    .11296+06  .13437+05  .48694+01  .38352-04  .95846+05  .48090+02 3000.0000 1
    .11296+06  .13437+05  .42896+01  .24064-03 -.41727+06  .48090+02 5000.0000 1  .8016
1.  8 0.  0 0.   0 0.   0 0.   0 0.   0 0.  0JANAF 06/62                O
    .59559+05  .13522+05  .49723+01  .38077-05  .15475+05  .50096+02 3000.0000 1
    .59559+05  .13522+05  .65749+01 -.22427-03 -.89178+07  .50096+02 5000.0000 1  .8489
1. 18 0.  0 0.   0 0.   0 0.   0 0.   0 0.  0CONVAIR 2PH-122 12/61      A
    .00000     .14940+05  .41810+01  .12296-04  .37120+07  .48462+0210000.0000 1
    .00000     .14940+05  .41810+01  .12296-04  .37120+07  .48462+0210000.0000 1 1.2593
2.  7 0.  0 0.   0 0.   0 0.   0 0.   0 0.  0JANAF 03/61                N2
    .00000     .22165+05  .86270+01  .11609-03 -.10372+07  .63765+02 3000.0000 1
    .00000     .22165+05  .98417+01 -.11623-03 -.61273+07  .63765+02 5000.0000 1 1.0807
2.  8 0.  0 0.   0 0.   0 0.   0 0.   0 0.  0JANAF 03/61                O2
    .00000     .23446+05  .80437+01  .51087-03 -.15272+06  .67973+02 3000.0000 1
    .00000     .23446+05  .10307+02  .29099-04 -.78308+07  .67973+02 5000.0000 1 1.1444
1.  7 1.  8 0.   0 0.   0 0.   0 0.   0 0.  0JANAF 06/63                NO
    .21580+05  .22700+05  .87762+01  .89903-04 -.78966+06  .68849+02 3000.0000 1
    .21580+05  .22700+05  .91626+01  .65788-05 -.21252+07  .68849+02 5000.0000 1    132
2.  7 1.  8 0.   0 0.   0 0.   0 0.   0 0.  0JANAF 12/60                N2O
    .19500+05  .36545+05  .14469+02  .12049-03 -.15348+07  .81590+02 3000.0000 1
    .19500+05  .36545+05  .12304+02  .45902-03  .94238+07  .81590+02 5000.0000 1    130
1. 99 0.  0 0.   0 0.   0 0.   0 0.   0 0.  0CONVAIR 2PH-122 12/61      E-
   -.00000     .14901+05  .49885+01 -.27280-05 -.13590+06  .16456+0210000.0000 1
   -.00000     .14901+05  .49885+01 -.27280-05 -.13590+06  .16456+0210000.0000 1* *****
```

ELEMENT	NITROGEN	OXYGEN	ARGON	ELECTRON
BASE SP	N	O	A	E-

```
1. 18-1. 99 0.   0 0.   0 0.   0 0.   0 0.  0CONVAIR 2PH-122 12/61      A+
    .36344+06  .15733+05  .48608+01  .21180-04  .16530+07  .51926+0210000.0000 1
    .36344+06  .15733+05  .48608+01  .21180-04  .16530+07  .51926+0210000.0000 1 1.2592
1.  7-1. 99 0.   0 0.   0 0.   0 0.   0 0.  0CONVAIR 2PH-122 12/61      N+
    .44664+06  .15131+05  .50175+01  .61710-04 -.18410+07  .49685+0210000.0000 1
    .44664+06  .15131+05  .50175+01  .61710-04 -.18410+07  .49685+0210000.0000 1  .8016
1.  7 1.  8-1. 99 0.   0 0.   0 0.  0CONVAIR 2PH-122 12/61      NO+
    .23292+06  .24197+05  .91022+01  .27740-04 -.31660+07  .65438+0210000.0000 1
    .23292+06  .24197+05  .91022+01  .27740-04 -.31660+07  .65438+0210000.0000 1 1.1132
1.  8-1. 99 0.   0 0.   0 0.   0 0.  0CONVAIR 2PH-122 12/61      O+
    .37200+06  .14929+05  .33627+01  .30671-03  .59020+07  .48485+0210000.0000 1
    .37200+06  .14929+05  .33627+01  .30671-03  .59020+07  .48485+0210000.0000 1  .8489
```

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   AIR PROP

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.29670-00	.31731-00	-.22871-02	.74834-04	.12761+01

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.10972+01	.26453+02	.29061+02	.85054+03	.29751-00	.84985+03

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)

7	8	18	99
.74589-00	.22851-00	.25599-01	.00000
.75412-00	.22250-00	.23375-01	.00000

SOLUTION TIMES
    ITERATIONS = 22   MACHINE TIME = .677 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT
  RELATIVE MASSES OF COMPONENTS 1,2, AND 3.   .10000+01 -.00000   -.00000

  THERMODYNAMIC STATE

PRESSURE (ATMOSPHERES) =	1.0000		TEMPERATURE (DEG K) =	2000.000	
(LBF/IN2-ABS) =	14.6960		(DEG R) =	3600.000	
DENSITY (GM/CM3) =	.1771-03		ENTHALPY (CAL/GM) =	471.348	
(LBM/FT3) =	.1105-01		(BTU/LBM) =	848.426	
MOLECULAR WEIGHT =	29.0608		ENTROPY (BTU/LBM-R) =	.2136+01	

  CHEMICAL STATE
    MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
N	.78499-09	O	.29907-03	A	.18622-01
E-	.95365-12	N2	.76976-00	O2	.20341-00
NO	.79086-02	N2O	.40650-06	A+	.20913-26
N+	.47971-31	NO+	.95365-12	O+	.82434-24

Sample Problem Number 3

Sample Output

```
1121000005              1.0                                          C* IN AIR
  1  6
  0.
  2.0        1.0        0.5        0.2       0.18       0.17
003
  6 CARBON       12.011                        -1.0
  7 NITROGEN     14.008     -0.767
  8 OXYGEN       16.000     -0.233
  3  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60               C3
189670+6 366220+5 146441+2 622536-4-168227+7 798410+2  500. 3000.1  0.C3
189670+6 366220+5 144782+2 792232-4-646877+6 798410+2 3000. 5000.1  0.C3
  1  6  1  8  0  0  0  0  0  0  0  0  0 0JANAF 03/61               CO
-264170+5 223570+5 865040+1 117021-3-898211+6 653700+2  500. 3000.1  0.CO
-264170+5 223570+5 115496+2-424139-3-131563+8 653700+2 3000. 5000.1  0.CO
  2  7  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61               N2
000000-0 221650+5 862699+1 116090-3-103715+7 637650+2  500. 3000.1  0.N2
000000-0 221650+5 984175+1-116232-3-612728+7 637650+2 3000. 5000.1  0.N2
  1  6  0  0  0  0  0  0  0  0  0- 0  0 0JANAF 03/61               C
170886+6 135500+5 444433+1 228125-3 409830+6 492870+2  500. 3000.1  0.C
170886+6 135500+5 412212+1 261908-3 262886+7 492870+2 3000. 5000.1  0.C
  2  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 9/61                C2
198999+6 246990+5 776612+1 696081-3 185649+6 685519+2  500. 3000.1  0.C2
198999+6 246990+5 104162+2 556841-4-640205+7 685519+2 3000. 5000.1  0.C2
  4  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60               C4
242321+6 511230+5 205903+2 623436-4-257703+7 986760+2  500. 3000.1  0.C4
242321+6 511230+5 210714+2-434895-4-404939+7 986760+2 3000. 5000.1  0.C4
  5  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60               C5
242374+6 656230+5 264706+2 806528-4-337125+7 111641+3  500. 3000.1  0.C5
242374+6 656230+5 271156+2-580271-4-543183+7 111641+3 3000. 5000.1  0.C5
  1  8  0  0  0  0  0  0  0  0  0  0  0 0JANAF 06/62               O
595590+5 135220+5 497228+1 380763-5 154749+5 500960+2  500. 3000.1  0.O
595590+5 135220+5 657489+1-224265-3-891782+7 500960+2 3000. 5000.1  0.O
  2  8  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61               O2
000000-0 234460+5 804370+1 510872-3-152718+6 679730+2  500. 3000.1  0.O2
000000-0 234460+5 103071+2 290991-4-783079+7 679730+2 3000. 5000.1  0.O2
  3  8  0  0  0  0  0  0  0  0  0  0  0 0JANAF 6/61                O3
341000+5 360230+5 135311+2 238739-3-606511+6 860919+2  500. 3000.1  0.O3
341000+5 360230+5 139121+2 125613-3-980654+6 860919+2 3000. 5000.1  0.O3
  1  7  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61               N
112965+6 134370+5 486944+1 383516-4 958460+5 480900+2  500. 3000.1  0.N
112965+6 134370+5 428957+1 240844-3-417273+6 480900+2 3000. 5000.1  0.N
  1  6  2  8  0  0  0  0  0  0  0  0  0 0JANAF 03/61               CO2
-940540+5 365350+5 144559+2 210386-3-182392+7 798480+2  500. 3000.1  0.CO2
-940540+5 365350+5 156451+2-391561-4-602768+7 798480+2 3000. 5000.1  0.CO2
  3  6  2  8  0  0  0  0  0  0  0  0  0 0JANAF 12/60               C3O2
-830000+4 652120+5 263775+2 103904-3-350368+7 112723+3  500. 3000.1  0.C3O2
-830000+4 652120+5 263543+2 882201-4-287091+7 112723+3 3000. 5000.1  0.C3O2
  1  6  1  7  0  0  0  0  0  0  0  0  0 0JANAF 12/66               CN
111000+6 232490+5 655906+1 115326-2 479517+6 669760+2  500. 3000.1  0.CN
111000+6 232490+5 988013+1 313855-3-649453+7 669760+2 3000. 5000.1  0.CN
  2  6  2  7  0  0  0  0  0  0  0  0  0 0JANAF 3/61                C2N2
738699+5 511070+5 188740+2 559856-3-896873+6 985479+2  500. 3000.1  0.C2N2
738699+5 511070+5 208204+2 630229-5-346865+7 985479+2 3000. 5000.1  0.C2N2
  4  6  2  7  0  0  0  0  0  0  0  0  0 0JANAF 3/61                C4N2
127500+6 801239+5 297490+2 856052-3-152255+7 133063+3  500. 3000.1  0.C4N2
127500+6 801239+5 327212+2 952999-5-541654+7 133063+3 3000. 5000.1  0.C4N2
  1  7  1  8  0  0  0  0  0  0  0  0  0 0JANAF 06/63               NO
215800+5 227000+5 877623+1 899031-4-789656+6 688490+2  500. 3000.1  0.NO
215800+5 227000+5 916260+1 657885-5-212519+7 688490+2 3000. 5000.1  0.NO
  1  7  2  8  0  0  0  0  0  0  0  0  0 0JANAF 06/63               NO2
801100+4 345800+5 137819+2 315611-4-133765+7 848890+2  500. 3000.1  0.NO2
801100+4 345800+5 130154+2 172586-3 175340+7 848890+2 3000. 5000.1  0.NO2
  2  7  1  8  0  0  0  0  0  0  0  0  0 0JANAF 12/60               N2O
195000+5 365450+5 144686+2 128489-3-153478+7 815900+2  500. 3000.1  0.N2O
195000+5 365450+5 123036+2 459018-3 942382+7 815900+2 3000. 5000.1  0.N2O
  1  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61               C*
000000-0 144120+5 586075+1 953976-4-766621+6 121290+2  500. 3000.2 100.C*
000000-0 144120+5 485134+1 291605-3 307202+7 121290+2 3000. 5000.2 100.C*

1001000009              10.0                                        C IN AIR
1001000009             100.0                                        C IN AIR
8
```

Sample Problem Number 4

Listing of Input

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   C* IN AIR

DERIVATIVE PROPERTY OUTPUT
```
  CP-FROZEN    CP-EQUIL    DLNM/DLNT    DLNM/DLNP    GAMMA
  .38619-00   .19303+01   -.12929+01    .76738-01   .11104+01
```

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
```
    MU1         MU2        MOL.WT       HTIL        CPTIL        HTIL*
  .11120+01   .27018+02   .30715+02   .92709+04   .38476-00   .92126+04
```

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =   .667)
```
     6           7           8
  .66667-00   .25567-00   .77667-01
  .65033-00   .26319-00   .80483-01
```

SOLUTION TIMES
    ITERATIONS = 15   MACHINE TIME =   .998 SEC.

OPEN SYSTEM OUTPUT (SURFACE EQUILIBRIUM=
  BPRIME PYROLYSIS GAS =   .00000   BPRIME CHAR =   .20000+01

  SURFACE SPECIES IS C*

  THERMODYNAMIC STATE ADJACENT TO THE SURFACE
      PRESSURE (ATMOSPHERES) =   10.0000   TEMPERATURE (DEG K) =   4458.747
                (LBF/IN2-ABS) =   146.9600   (DEG R) =   8025.745

      DENSITY (GM/CM3)   =   .8394-03   ENTHALPY (CAL/GM)   =   5073.854
              (LBM/FT3)   =   .5240-01   (BTU/LBM) =   9132.938

      MOLECULAR WEIGHT   =   30.7146   ENTROPY (BTU/LBM-R) =   .2458+01

  CHEMICAL STATE ADJACENT TO THE SURFACE
      MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

```
      SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
      C3        .29431-00     CO        .14909-00     N2        .22837-00
      C         .59404-01     C2        .12460+00     C4        .22153-01
      C5        .32923-01     O         .10743-05     O2        .10733-11
      O3        .22862-22     N         .11973-02     CO2       .43431-07
      C3O2      .20517-09     CN        .73254-01     C2N2      .10539-01
      C4N2      .41560-02     NO        .19430-06     NO2       .34433-15
      N2O       .18584-10     C*        .00000
```

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(10.0000   .00000 2.000004458.7474 .000 5073.854 5073.854 1 C*   C* IN AIR   )

Sample Problem Number 4

Sample Output

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   C* IN AIR

DERIVATIVE PROPERTY OUTPUT
```
  CP-FROZEN    CP-EQUIL    DLNM/DLNT   DLNM/DLNP    GAMMA
  .31142-00    .31145-00  -.94537-05   .74059-05   .12949+01
```

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
```
    MU1         MU2        MOL.WT       HTIL        CPTIL       HTIL*
  .10807+01   .25924+02   .28015+02   .46021+03   .31142-00   .46023+03
```

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)
```
     6           7           8
  .14888-00   .65281-00   .19831-00
  .14888-00   .65280-00   .19832-00
```

SOLUTION TIMES
     ITERATIONS = 15   MACHINE TIME =   .344 SEC.

OPEN SYSTEM OUTPUT (SURFACE EQUILIBRIUM=
     BPRIME PYROLYSIS GAS =   .00000   BPRIME CHAR =   .17492-00

     SURFACE SPECIES IS C*

     THERMODYNAMIC STATE ADJACENT TO THE SURFACE
         PRESSURE (ATMOSPHERES) =   10.0000   TEMPERATURE (DEG K) =   2330.186
                  (LBF/IN2-ABS) =   146.9600   (DEG R) =   4194.335

         DENSITY (GM/CM3)   =   .1465-02   ENTHALPY (CAL/GM)   =   255.699
                 (LBM/FT3)   =   .9145-01   (BTU/LBM) =   460.258

         MOLECULAR WEIGHT   =   28.0147   ENTROPY (BTU/LBM-R) =   .2099+01

     CHEMICAL STATE ADJACENT TO THE SURFACE
         MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

```
         SPECIES    MOLE FR.      SPECIES    MOLE FR.      SPECIES    MOLE FR.
         C3         .19978-08     CO         .34721-00     N2         .65276-00
         C          .14669-08     C2         .24225-09     C4         .65724-12
         C5         .96775-12     O          .19122-09     O2         .10660-13
         O3         .62259-27     N          .13712-07     CO2        .82019-05
         C3O2       .57861-11     CN         .16625-05     C2N2       .14820-04
         C4N2       .22952-07     NO         .36033-08     NO2        .25489-17
         N2O        .53188-12     C*         .00000
```

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(10.0000   .00000   .174922330.1860 .000   255.699   255.699 1 C*   C* IN AIR   )

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   C* IN AIR

DERIVATIVE PROPERTY OUTPUT
```
  CP-FROZEN    CP-EQUIL   DLNM/DLNT    DLNM/DLNP    GAMMA
  .29132-00    .29132-00  -.11726-07   -.14901-07   .13194+01
```

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
```
    MU1        MU2        MOL.WT       HTIL      CPTIL       HTIL*
  .10829+01  .25998+02    .28172+02  -.14616+03  .29128-00  -.14390+03
```

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =   .667)
```
      6           7           8
   .14530-00   .65556-00   .19915-00
   .14506-00   .65677-00   .19816-00
```

SOLUTION TIMES
    ITERATIONS = 28   MACHINE TIME =   .582 SEC.

OPEN SYSTEM OUTPUT (SURFACE EQUILIBRIUM*
    BPRIME PYROLYSIS GAS =   .00000   BPRIME CHAR =   .17000-00

    SURFACE SPECIES IS C*

    THERMODYNAMIC STATE ADJACENT TO THE SURFACE
        PRESSURE (ATMOSPHERES) =   10.0000   TEMPERATURE (DEG K) =   1256.736
                 (LBF/IN2-ABS) =   146.9600   (DEG R) =   2262.125

        DENSITY (GM/CM3)   = .2731-02   ENTHALPY (CAL/GM)   =   -86.071
                (LBM/FT3)   = .1705-00   (BTU/LBM) =   -154.927

        MOLECULAR WEIGHT   =   28.1718   ENTROPY (BTU/LBM-R) =   .1907+01

    CHEMICAL STATE ADJACENT TO THE SURFACE
        MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES
```
    SPECIES   MOLE FR.    SPECIES   MOLE FR.    SPECIES   MOLE FR.
    C3        .19193-23   CO        .33096-00   N2        .65920-00
    C         .28371-22   C2        .32717-25   C4        .36105-31
    C5        .49770-31   O         .14266-16   O2        .33387-18
    O3        .17990-36   N         .92697-17   CO2       .98435-02
    C3O2      .84722-15   CN        .25748-14   C2N2      .15504-10
    C4N2      .10583-17   NO        .37487-12   NO2       .18318-22
    N2O       .66687-16   C*        .00000
```

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(10.0000   .00000 .170001256.7362 .000 -86.071 -86.071 1 C*   C* IN AIR   )

```
0110      5530.      .1                    1.0        0.        0.     CMA INPUT
 5
  1 HYDROGEN      1.008              -.0930
  6 CARBON       12.011              -.5470     -.488
  7 NITROGEN     14.008    -.7650    -.0190
  8 OXYGEN       16.000    -.2350    -.3410     -.273
 14 SILICON      28.090                        -.239
  1  1  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                      H
 521020+5 134230+5 480223+1 555469-4 173095+6 388620+2  500. 3000.1    0.H
 521020+5 134230+5 308752+1 315025-3 929744+7 388620+2 3000. 5000.1    0.H
  1  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      C
 170886+6 135500+5 444433+1 228125-3 409830+6 492870+2  500. 3000.1    0.C
 170886+6 135500+5 412212+1 261908-3 262886+7 492970+2 3000. 5000.1    0.C
  2  7  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      N2
 000000-0 221650+5 862699+1 116090-3-103715+7 637650+2  300. 3000.1    0.N2
 000000-0 221650+5 984175+1-116232-3-612728+7 637650+2 3000. 5000.1    0.N2
  1  6  1  8  0  0  0  0  0  0  0 70  0 0JANAF 03/61                      CO
-264170+5 223570+5 865040+1 117021-3-898211+6 653700+2  500. 3000.1    0.CO
-264170+5 223570+5 115496+2-424139-3-131563+8 653700+2 3000. 5000.1    0.CO
  1 14  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      SI
 106000+6 140180+5 457930+1 301346-3 142859+6 519920+2  500. 3000.1    0.SI
 106000+6 140180+5 457930+1 301346-3 142859+6 519920+2  500. 3000.1    0.SI
 106000+6 140180+5 478318+1 141019-3 259988+7 519920+2 3000. 5000.1    0.SI
  3  1  1  6  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      CH3
 319400+5 434190+5 182763+2 401025-3-461203+7 786040+2  500. 3000.1    0.CH3
 319400+5 434190+5 204899+2-108028-3-114692+8 786040+2 3000. 5000.1    0.CH3
  1  8  0  0  0  0  0  0  0  0  0  0  0 0JANAF 06/62                      O
 595590+5 135220+5 497228+1 380768-5 154749+5 500960+2  500. 3000.1    0.0
 595590+5 135220+5 657489+1-224268-3-891782+7 500960+2 3000. 5000.1    0.0
  2  8  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      O2
 000000-0 234460+5 804370+1 510872-3-152718+6 679730+2  500. 3000.1    0.02
 000000-0 234460+5 103071+2 290991-4-783079+7 679730+2 3000. 5000.1    0.02
  1  8  1 14  0  0  0  0  0  0  0  0  0 0JANAF 09/63                      OSI
-242000+5 233590+5 891444+1 545951-4-452091+6 697470+2  500. 3000.1    0.0SI
-242000+5 233590+5 850773+1 132710-3 104918+7 697470+2 3000. 5000.1    0.0SI
  1  1  1  6  1  7  0  0  0  0  0  0  0 0JANAF 03/61                      CHN
 312000+5 355930+5 137023+2 552243-3-228955+7 758620+2  500. 3000.1    0.CHN
 312000+5 355930+5 178895+2-295052-3-183671+8 758620+2 3000. 5000.1    0.CHN
  1  6  1  7  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      CN
 109000+6 232490+5 655986+1 115376-2 479517+6 669760+2  500. 3000.1    0.CN
 109000+6 232490+5 988013+1 313135-3-649453+7 669760+2 3000. 5000.1    0.CN
  2  1  2  6  0  '  0  0  0  0  0  0  0 0JANAF 03/61                      C2H2
 541900+5 482570+5 189960+2 749034-3-409039+2 849690+2  500. 3000.1    0.C2H2
 541900+5 482570+5 203577+2 389052-3-645297+7 849690+2 3000. 5000.1    0.C2H2
  2  6  2  7  0  0  0  0  0  0  0  0  0 0JANAF 3/61                       C2N2
 738699+5 511070+5 188740+2 535056-3-896873+6 985479+2  500. 3000.1    0.C2N2
 738699+5 511070+5 208204+2 630229-5-346865+7 985479+2 3000. 5000.1    0.C2N2
  2  1  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      H2
 008000-0 212100+5 711963+1 621950-3-712694+6 484650+2  500. 3000.1    0.H2
 000000-0 212100+5 681794+1 589854-3 265106+7 484650+2 3000. 5000.1    0.H2
  1  1  2  6  0  0  0  0  0  0  0  0  0 0DUFF BAUER 6/61                  C2H
 117395+6 349620+5 134210+2 469100-3-187309+7 781140+2  500. 3000.1    0.C2H
 117395+6 349620+5 148516+2 109402-3-503862+7 781140+2 3000. 5000.1    0.C2H
  2  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 9/61                       C2
 198999+6 246990+5 776612+1 696081-3 185649+6 685519+2  500. 3000.1    0.C2
 198999+6 246990+5 104162+2 566841-4-640205+7 685519+2 3000. 5000.1    0.C2
  1  1  1  6  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      CM
 142006+6 221300+5 826079+1 302211-3-100184+7 616120+2  500. 3000.1    0.CM
 142006+6 221300+5 707091+1 463281-3 552860+7 616120+2 3000. 5000.1    0.CH
  1  1  1 14  0  0  0  0  0  0  0  0  0 0JANAF 12/60                      HSI
 114000+6 230100+5 879959+1 194499-3-972082+6 659960+2  500. 3000.1    0.HSI
 114000+6 230100+5 995466+1-335662-4-521070+7 659960+2 3000. 5000.1    0.HSI
  3  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/60                      C3
 189670+6 366220+5 146441+2 622536-4-168227+7 798410+2  500. 3000.1    0.C3
 189670+6 366220+5 144782+2 792232-4-646877+6 798410+2 3000. 5000.1    0.C3
  1  1  3  6  0  0  0  0  0  0  0  0  0 0DUFF BAUER 6/61                  C3H
 127703+6 489620+5 194464+2 508379-3-311933+7 928820+2  500. 3000.1    0.C3H
 127703+6 489620+5 199582+2 245687-3-632514+6 928820+2 3000. 5000.1    0.C3H
  2 14  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      SI2
 130900+6 243430+5 891154+1 102582-3-354376+5 753940+2  500. 3000.1    0.SI2
 130900+6 243430+5 106398+2-190701-3-845149+7 753940+2 3000. 5000.1    0.SI2
  1  6  0  0  0  0  0  0  0  0  0  0  0 0JANAF 03/61                      C*
 000000-0 144120+5 586075+1 953976-4-766621+6 121290+2  500. 3000.2 100.C*
 000000-0 144120+5 485134+1 291685-3 307202+7 121290+2 3000. 5000.2 100.C*
  1  6  1 14  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      CSI*
-206400+5 334219+5 152771+2-222607-3-503627+7 296828+2  500. 2773.2 100.CSI*
-756200+4 348054+5 152568+2-219419-4-170023+7 348989+2 2773. 5000.3 100.CSI*
  2  8  1 14  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      O2SI*
-217500+6 468950+5 176582+2 549817-3-236409+7 473990+2  500. 1883.2 100.O2SI*
-215948+6 507890+5 217500+2-193988-4-282763+6 499160+2 1883. 5000.3 100.O2SI*
  1 14  0  0  0  0  0  0  0  0  0  0  0 0JANAF 12/62                      SI*
 000000-0 172470+5 652874+1 838825-4-322164+6 185450+2  500. 1685.2 100.SI*
 120920+5 165620+5 600789+1 234623-4 356236+6 254280+2 1685. 5000.3 100.SI*

            1  -6000.                                            CMA INPUT
            1  -4500.                                            CMA INPUT
            1  -3000.                                            CMA INPUT
            1  -2000.                                            CMA INPUT
            1  -1500.                                            CMA INPUT
            1  -1000.                                            CMA INPUT
            1  - 500.                                            CMA INPUT
  1003000003                                                     CMA INPUT
     2  2
     20.0        .1
       .65        .3
  1002000002                                                     CMA INPUT
     1  4
       .0
       .65        .3        .1        .001
   8
```

Sample Problem Number 5

Listing of Input

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY JOB CMA INPUT   *********1

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.31821-00	.31890-00	-.79270-03	.76815-04	.13549+01

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.99964-00	.23450+02	.23815-02	.50594+04	.31780-00	.49511+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)

1	6	7	8	14
.00000	.00000	.76500-00	.23500-00	.00000
.00000	.00000	.73486-00	.26514-00	.00000

SOLUTION TIMES
ITERATIONS = 9   MACHINE TIME = .048 SEC.

CLOSED SYSTEM FROZEN COMPOSITION OUTPUT
RELATIVE MASSES OF COMPONENTS 1, 2, AND 3.   .10000+01   .00000   .00000

THERMODYNAMIC STATE

PRESSURE (ATMOSPHERES) =	.1000	TEMPERATURE (DEG K) =	6000.000
(LBF/IN2-ABS) =	1.4696	(DEG R) =	10800.000

DENSITY (GM/CM3) =	.4836-05	ENTHALPY (CAL/GM) =	2637.101
(LBM/FT3) =	.3019-03	(BTU/LBM) =	4746.782

MOLECULAR WEIGHT = 23.8151   ENTROPY (BTU/LBM-R) = .2944+01

CHEMICAL STATE
MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H	.00000	C	.00000	N2	.65029-00
CO	.00000	SI	.00000	CH3	.00000
O	.34963-00	O2	.76810-04	OSI	.00000
CHN	.00000	CN	.00000	C2H2	.00000
C2N2	.00000	H2	.00000	C2H	.00000
C2	.00000	CH	.00000	HSI	.00000
C3	.00000	C3H	.03000	SI2	.00000
C*	.00000	CSI*	.00000	O2SI*	.00000
SI*	.00000				

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(.1000 .00000 .000005999.9999 .667 2750.638 2637.101-1 CHAR   CMA INPUT)

Sample Problem Number 5

Sample Output

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   CMA INPUT

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.31979-00	.32059-00	-.86084-03	.76696-04	.13525+01

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.99964-00	.23450+02	.23815-02	.47898+04	.31951-00	.46814+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)

1	6	7	8	14
.00000	.00000	.76500-00	.23500-00	.00000
.00000	.00000	.73486-00	.26514-00	.00000

SOLUTION TIMES
ITERATIONS = 9   MACHINE TIME = .545 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT
RELATIVE MASSES OF COMPONENTS 1, 2, AND 3.   .10000+01   .00000   .00000

THERMODYNAMIC STATE

PRESSURE (ATMOSPHERES) =	.1000	TEMPERATURE (DEG K) =	5530.000
(LBF/IN2-ABS) =	1.4696	(DEG R) =	9954.000

DENSITY (GM/CM3) =	.5248-05	ENTHALPY (CAL/GM) =	2487.157
(LBM/FT3) =	.3276-03	(BTU/LBM) =	4476.883

MOLECULAR WEIGHT = 23.8151   ENTROPY (BTU/LBM-R) = .2918+01

CHEMICAL STATE
MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H	.00000	C	.00000	N2	.65029-00
CO	.00000	SI	.00000	CH3	.00000
O	.34963-00	O2	.76810-04	OSI	.00000
CHN	.00000	CN	.00000	C2H2	.00000
C2N2	.00000	H2	.00000	C2H	.00000
C2	.00000	CH	.00000	HSI	.00000
C3	.00000	C3H	.00000	SI2	.00000
C*	.00890	CSI*	.00000	O2SI*	.00000
SI*	.00000				

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   CMA INPUT

DERIVATIVE PROPERTY OUTPUT
CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.18324-00	.18324-00	.40069-06	.29802-07	.15971+01

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.10965+01	.26628-02	.29002+02	.10394+03	.18237-00	.10378+03

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)
1	6	7	8	14
.00000	.48250-03	.72661-00	.27264-00	.26917-03
.00000	.48752-03	.73413-00	.26514-00	.23873-03

SOLUTION TIMES
ITERATIONS = 4   MACHINE TIME = .114 SEC.

OPEN SYSTEM OUTPUT (ASSIGNED TEMPERATURE SUPPRESSING SURFACE EQUILIBRIUM)
BPRIME PYROLYSIS GAS = .00000   BPRIME CHAR = .10000-02

THERMODYNAMIC STATE ADJACENT TO THE SURFACE
PRESSURE (ATMOSPHERES) = .1000   TEMPERATURE (DEG K) = 500.000
         (LBF/IN2-ABS) = 1.4696   (DEG R) = 900.000

DENSITY (GM/CM3) = .7068-04   ENTHALPY (CAL/GM) = 57.4469
        (LBM/FT3) = .4412-02   (BTU/LBM) = 103.444

MOLECULAR WEIGHT = 29.0020   ENTROPY (BTU/LBM-R) = .1944+01

CHEMICAL STATE ADJACENT TO THE SURFACE
MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H	.00000	C	.00000	N2	.75219-00
CO	.11651-02	SI	.00000	CH3	.00000
O	.17558-22	CN	.24637-00	OSI	.27791-03
CHN	.00000	H2	.00000	C2H2	.00000
C2N2	.00000	CH	.00000	C2H	.00000
C2	.00000	C3H	.00000	HSI	.00000
C3	.00000	CSI*	.00000	SI2	.00000
C*	.00000			O2SI*	.00000
SI*	.00000				

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(.1000 .00000 .00100 500.0000 .667 57.469 0 CHAR   CMA INPUT)

Sample Problem Number 5
Sample Output, Concluded

AEROTHERM EQUILIBRIUM SURFACE THERMOCHEMISTRY SOLUTION   CMA INPUT

DERIVATIVE PROPERTY OUTPUT
CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.31705-00	.55273-00	-.13240-00	.57901-02	.11938+01

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.10501+01	.25165+02	.27422+02	.97957+03	.35273-00	.81120+03

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .667)
1	6	7		14
.35318-02	.14291-00	.52360-00	.27411-00	.55838-01
.78873-02	.14393-00	.52732-00	.27150-00	.49365-01

SOLUTION TIMES
ITERATIONS = 22   MACHINE TIME = .763 SEC.

OPEN SYSTEM OUTPUT (SURFACE EQUILIBRIUM)
BPRIME PYROLYSIS GAS = .10000+20   BPRIME CHAR = .30000-00

SURFACE SPECIES IS O2SI*

THERMODYNAMIC STATE ADJACENT TO THE SURFACE
PRESSURE (ATMOSPHERES) = .1000   TEMPERATURE (DEG K) = 2530.932
         (LBF/IN2-ABS) = 1.4696   (DEG R) = 4555.677

DENSITY (GM/CM3) = .1320-04   ENTHALPY (CAL/GM) = 349.066
        (LBM/FT3) = .8242-03   (BTU/LBM) = 628.319

MOLECULAR WEIGHT = 27.4215   ENTROPY (BTU/LBM-R) = .2522+01

CHEMICAL STATE ADJACENT TO THE SURFACE
MOLE FR. = MOLECULES / TOTAL GAS PHASE MOLECULES

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H	.17892-01	C	.51249-00	N2	.21967-12
CO	.32658+00	SI	.26146-13	CH3	.10992-07
O	.10470-01	O2	.54510-01	OSI	.39265-01
CHN	.11811-08	CN	.35876-17	C2H2	.11468-10
C2N2	.27026-18	H2	.21134-17	C2H	.39093-01
C2	.45423-20	CH	.11162-21	HSI	.15934-13
C3	.24943-26	C3H	.14135-15	SI2	.89862-25
C*	.00000	CSI*	.00000	O2SI*	.00000
SI*	.00000				

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(.1000 .10000 .30000 2530.9320 .667 450.669 349.066 1 O2SI* CMA INPUT)

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13 ABSTRACT   A Fortran IV computer code is described which computes the equilibrium or mixed frozen/equilibrium thermodynamic state of general chemical systems. Closed (fixed mass) molecular compositions are evaluated from relative elemental quantities, species thermochemical data and two state properties (pressure and temperature or enthalpy). Open system (diffusive mass flux dependent) states are defined from surface equilibrium considerations utilizing a film coefficient model which accounts for the unequal diffusion of species. The generality of the formulation allows computations for a broad range of environments and surface materials including charring ablators. This computer code is designated Version 3 of the Aerotherm Equilibrium Surface Thermochemistry code (EST3) and provides surface mass balance quantities needed for ablation predictions by the Aerotherm Charring Material Ablation code (CMA).

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Ablation						
Boundary layer heat and mass transfer						
Charring ablators						
Chemical Equilibrium						
Chemistry						
Corrosivity						
Equilibrium computer codes						
Fortran computer program						
Heat transfer						
Heterogeneous chemistry						
Resin degradation						
Rocket nozzle analysis						
Solid propellant						
Surface Reactions						
Thermal Decomposition						
Thermal response						
Thermochemistry						
User's Manual (Computer Code)						