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USER'S MANUAL

AEROTHERM GRAPHITE SURFACE KINETICS COMPUTER PROGRAM

Volume I - Program Description and Sample Problems

January 1972

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

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AEROTHERM GRAPHITE SURFACE KINETICS COMPUTER PROGRAM

VOLUME I

PROGRAM DESCRIPTION AND SAMPLE PROBLEMS

Prepared under the Sponsorship of

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FOREWORD

This report is one of two computer program user's manuals prepared by Aerotherm Division of Acurex Corporation under USAF Contract F04611-69-C-0081. Included herein is Volume I of the manual for the Aerotherm Graphite Surface Kinetics (GASKET) computer code. This volume describes the problems solved by the code and presents an input (card format) user's guide and sample problems. The work was administered under the direction of the Air Force Rocket Propulsion Laboratory with Mr. Robert J. Schoner as the Project Officer.

Mr. John W. Schaefer was the Program Manager and Mr. Mitchell R. Wool was Program Engineer. The GASKET code was developed by Dr. Kimble J. Clark.

This technical report has been reviewed and is approved.

A. D. Brown, Jr., Lt. Col., USAF
Chief, Technology Division

ABSTRACT

A Fortran IV computer code is described which computes thermochemical ablation rates of pyrolytic graphite surfaces, as a function of surface temperature and pressure, assuming all heterogeneous reactions at the surface are kinetically controlled. The calculation of the chemical state at the surface utilizes a film coefficient model which accounts for the unequal diffusion of species. All homogeneous reactions between gas-phase species adjacent to the surface are assumed to be in equilibrium. The specific surface reactions which are taken to be kinetically controlled include the reactions of condensed-phase carbon with water vapor, carbon dioxide, and hydrogen. Several options are available for computation of the boundary-layer edge state required in the diffusion model, including isentropic expansion or compression and normal or oblique shock wave calculation procedures.

This computer code is designated as the Aerotherm Graphite Surface Kinetics (GASKET) program and provides surface mass balance quantities needed for ablation predictions by the Aerotherm Charring Material Ablation (CMA) code or the Aerotherm Axisymmetric Transient Heating and Material Ablation (ASTHMA) code.

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 routines. Included are program listings, flow charts, and definitions of Fortran variables.

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LIST OF SYMBOLS

A	area
A^*_{ii}	a ratio of collision integrals based on a Lennard-Jones intermolecular potential (see Ref. 3)
a	sound speed
B'	normalized ablation rate, defined as $\dot{m}_s/\rho_e u_e C_M$ (see Eq. (24))
B_m	pre-exponential factor for kinetic reaction m (see Eq. (46))
C_H	Stanton number for heat transfer
C_M	Stanton number for mass transfer
C_p	specific heat capacity at constant pressure
$\tilde{C}_p$	Z_i averaged heat capacity (see Eq. (62))
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. (36)
$\mathcal{D}_{ij}$	binary diffusion coefficient
E_m	activation energy for kinetic reaction m
$\bar{F}$	ratio of summations defined by Eq. (39)

F_i	diffusion factor for species i (see Eq. (36))
F_{jm}	inhibiting species partial pressure coefficient for jth base specie and mth reaction (see Eq. (47))
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 regardless of molecular configuration
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
k	thermal conductivity
k_{Fm}	forward reaction rate constant for kinetic reaction m (see Eq. (44))
L	total number of candidate condensed phase species in the system
Le	Lewis number
M	Mach number

$\dot{m}$	mass flux (e.g.: lbm/ft^{2}sec)
$\mathcal{m}$	molecular weight
N	representing the molecular formula for a species
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
R_m	net forward rate of reaction m (see Eq. (44))
Sc	Schmidt number
s	entropy
T	temperature
u	velocity
v	velocity normal to surface
w	mass flow rate (e.g.: lbm/sec)
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. (35))

GREEK

α	thermal diffusivity
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. (37))
θ	angle between velocity vector and a line normal to a shock
μ	dynamic viscosity
μ_{jm}	stoichiometric coefficient for species j of kinetic reaction m (see Eq. (45))
μ_1, μ_2, μ_3	quantities defined by Eqs. (51), (52), and (61), respectively
ρ	density
σ	Stefan-Boltzmann constant
ϕ_m	temperature exponent in the rate coefficient for kinetic reaction m (see Eq. (46))
ψ_{jm}	inhibiting species partial pressure coefficient for jth base specie and mth reaction (see Eq. (47))

SUBSCRIPTS

e	at the boundary layer edge
i	gas phase species index
j	general species index
k	element index

ℓ	condensed phase index
m	kinetic reaction index
s	denotes the surface material
w	adjacent to the surface
o	stagnation value
1	upstream of shock
2	downstream of shock

SUPERSCRIPTS

P	reaction products
R	reaction reactants
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 Aerotherm Graphite Surface Kinetics (GASKET) computer program is described in this user's manual. This program was designed specifically for calculating graphite surface thermochemical ablation rates assuming the heterogeneous reactions of the condensed-phase surface carbon with water vapor, carbon dioxide, and hydrogen to be kinetically controlled. The GASKET code was developed from the Aerotherm Equilibrium Surface Thermochemistry (EST) computer program. As described in Reference 1, the EST program is extremely versatile (although it excludes kinetics) and, as a result, the preparation of input data decks is rather complex. In contrast, the GASKET code solves a much more restricted class of problems and accepts a much more simplified form of input data, thereby reducing considerably the amount of work required of the program user.

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

- a brief overview of the purpose and capabilities of the GASKET 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 their FORTRAN coding (Section 3)
- a specification of the definitions and formats of the input data deck (Section 4)
- several examples of computer program input decks and printed output (Section 5)

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

- definitions for all FORTRAN variables used
- listing of FORTRAN IV source decks
- flow charts of program logic for each FORTRAN routine

Other documents of potential value to the reader requiring a more detailed description of the theoretical fundamentals of the GASKET program are References 2 and 3.

The Graphite Surface Kinetics program computes graphite surface ablation rates under the assumption that the condensed-phase carbon at the surface is consumed according to the following kinetically-controlled reactions:

$$C^* + H_2O \rightleftarrows CO + H_2$$

$$C^* + CO_2 \rightleftarrows 2CO$$

$$2C^* + H_2 \rightleftarrows C_2H_2$$

where * denotes the condensed phase species.

All other heterogeneous reactions between the surface carbon and gas-phase species in the boundary layer are assumed to be unimportant, and all homogeneous reactions involving only gas-phase species adjacent to the surface are assumed to be in equilibrium. In some problems the elements H and/or O are not present in the edge gas, in which case one or more of the above reactions cannot occur. GASKET automatically determines which of the three reactions are possible in a given problem.

The GASKET program contains a number of options which can be used to specify the boundary layer edge state. In most cases the program of interest is the chemical response of graphite nozzle surfaces or graphite ablative models exposed to high-temperature propellant combustion products. The sketch below indicates the various possible edge state definitions:

1. From a specified chamber state, a one-dimensional, real gas, isentropic expansion through the nozzle may be performed. The edge gas state at amy downstream station, e g., the nozzle throat, is thus determined.
2. By utilizing the solution obtained in 1. and specifying a shock angle (0° for a normal shock, as is the case here), the static conditions behind a shock may be calculated.
3. By utilizing the solution obtained in 1. and specifying the shock angle, the isentropic stagnation conditions behind a shock may be calculated.

Inherent in the edge state calculations described above is the assumption of chemical equilibrium. Once the boundary layer edge state is determined, the GASKET program proceeds to compute graphite surface ablation rates for a range of surface temperatures.

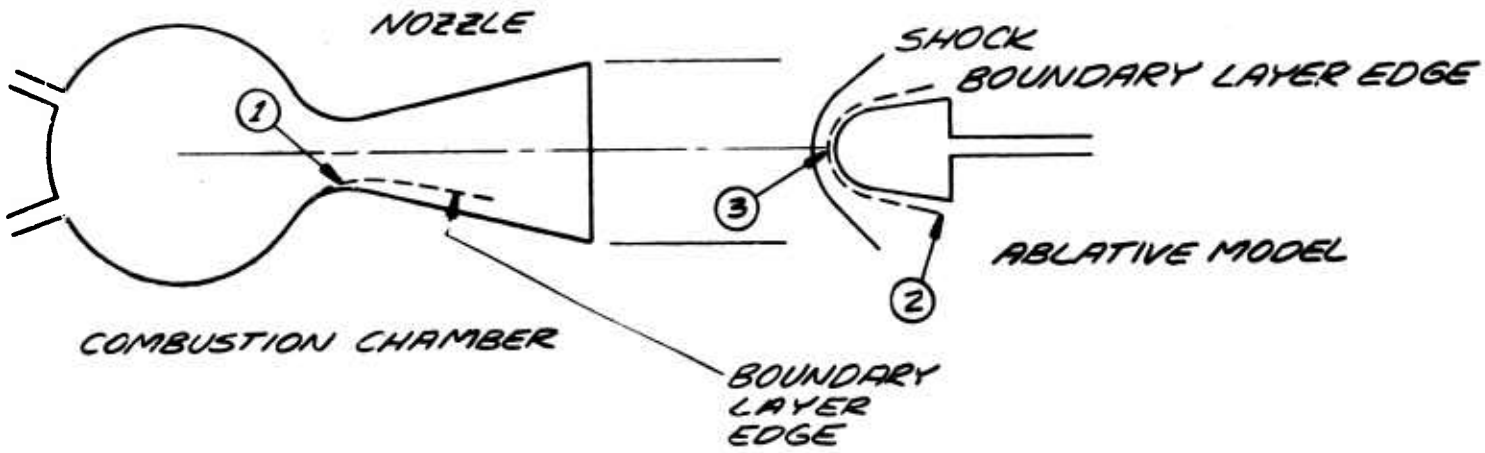

FIGURE SKETCH OF ROCKET NOZZLE ILLUSTRATING VARIOUS OPTIONS AVAILABLE IN GASKET FOR DETERMINING THE BOUNDARY LAYER EDGE STATE.

This manual attempts to acquaint the unfamiliar user with the GASKET program by providing a brief summary of underlying physical principles, a specification of the input mechanics, and some sample problems. It will be seen that utilization of the GASKET code is quite straightforward. However, instances will occur in which the program fails to solve a certain problem and the reason for the failure will not be 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 theory upon which the calculation methods of the GASKET program are based. An attempt has been made to present these fundamentals in a fashion most appropriate to a user unfamiliar with the code. For this reason, and in the interest of brevity, explanations tend to be nonvrigorous and perhaps somewhat heuristic. No attempt is made in this section to discuss the mathematical methods employed to solve these equations. The solution procedures are very briefly considered in Section 3 which is concerned primarily with the program coding.

As already mentioned in Section 1, the GASKET code is designed specifically for calculating thermochemical ablation rates for graphite surfaces in the presence of certain kinetically-controlled chemical reactions. Such calculations are inherently open system calculations, since the relative amounts of chemical elements at the surface depend upon various mass transfer and material degradation rates. In general, to perform these ablation calculations the thermochemical state of the gases at the boundary layer edge must be specified so that the driving potential for elemental mass diffusion to the surface can be established. This determination of the edge state is a closed system calculation, since the relative amounts of each chemical element are prespecified (for example, by specifying the propellant elemental composition). Furthermore, in performing such closed system calculations the assumption of chemical equilibrium is invoked. As mentioned in Section 1, the GASKET code has several options for determination of the boundary layer edge state, including real-gas isentropic expansion or compression and normal or oblique shock wave calculations.

It is apparent, then, that the GASKET program performs calculations for two basic types of systems: 1.) equilibrium closed systems, and 2.) mixed equilibrium-nonequilibrium open systems. The former are discussed in Section 2.1 and latter are discussed in Section 2.2. In addition to calculating the chemical and thermodynamic states of the two basic systems, the GASKET program also calculates and prints out transport properties (e.g., viscosity, thermal conductivity, etc.) appropriate to those states. The methods employed by the program to calculate these transport properties are briefly discussed in Section 2.3.

2.1 CLOSED SYSTEMS IN EQUILIBRIUM

Closed systems have been defined as those for which the relative amounts of chemical elements are prespecified. In the following, closed systems are (somewhat artificially) subgrouped into static and flowing closed systems. The discussion of simple static closed equilibrium systems, Section 2.1.1, is particularly significant because it is here that equilibrium chemistry relations, which are applicable to all systems subsequently discussed, are first introduced. Flowing closed systems include isentropic expansions or compressions (Section 2.1.2) and flows with normal or oblique shock waves (Section 2.1.3).

2.1.1 Static Closed Systems in Equilibrium

Consider K chemical elements, N_k, introduced into a previously evacuated container. 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**. 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:

$$\sum_{k=1}^{K} C_{ki}\, N_k \rightarrow N_i \qquad (1)$$

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

$$\sum_{k=1}^{K} C_{k\ell}\, N_k \rightarrow N_\ell \qquad (2)$$

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

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

**Duhem's Theorem.

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

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

or

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

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

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

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

$$\text{Mass fraction of element k input to the system} = \frac{m_k}{m_P} \sum_{i=1}^{I} C_{ki} P_i + \frac{m_k}{m} \sum_{\ell=1}^{L} C_{k\ell} X_\ell \qquad (5)$$

where $\mathcal{M}$ is a composite system molecular weight* defined by

$$\mathcal{M} = \sum_{i=1}^{I} \frac{P_i}{P} \mathcal{M}_i + \sum_{\ell=1}^{L} X_\ell \mathcal{M}_\ell \qquad \left(\text{units of } \frac{\text{grams of system}}{\text{moles of gas}}\right)$$

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

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

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

$$\sum_{i=1}^{I} P_i = P \tag{6}$$

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

$$h = \frac{1}{\mathcal{M}P} \sum_{i=1}^{I} P_i h_i + \frac{1}{\mathcal{M}} \sum_{\ell=1}^{L} X_\ell h_\ell \tag{7}$$

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 trival 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 (6) contributes one additional equation. For any additional thermodynamic properties of the mixture (enthalpy, entropy, etc), there exists equations such as (7).

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

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

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	(6)	1
T	1		
h,s,ρ,...	n	of the type (7)	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 principle, be determined.

The GASKET program performs this determination. That is, to determine the equilibrium thermodynamic and chemical state at the boundary layer edge, one needs only to furnish the GASKET program with the elemental composition, the candidate gaseous and condensed phase species,* and two thermodymanic properties. One of these properties must be pressure, and the otenr may be either temperature, enthalpy, or entropy. Given this information, the GASKET program

*In order to perform thermochemical calculations, certain basic thermodynamic data (described in Section 4) must be provided for each candidate species. As one of the options of the GASKET program, the user must decide whether or not he wishes to use the thermodynamic data built into the program. If not, he must input this data in the form of three-card sets, one set for each species. A certain amount of judgment is required on the part of the user relative to which candidate species should be included in a given system. Frequently this judgment is avoided by simply inputting data for all species containing combinations of the input elements.

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. Also output are some transport properties which will be discussed in Section 2.3. The exact convention for inputting data to the program is specified in Section 4, and some example proglems of this type are presented in Section 5.

2.1.2 Equilibrium Isentropic Flow

The relations discussed in the previous section for static equilibrium may be applied to calculate the states of a flowing fluid if local thermodynamic and chemical equilibrium is assumed. The treatment of equilibrium isentropic flows is discussed in this section, and the calculation of the state downstream of a shock wave is discussed in Section 2.1.3.

For adiabatic flows, the conservation of energy requires that

$$h + \frac{1}{2} u^2 = h_o \qquad (8)$$

and if such flows are in equilibrium (or if they are fully frozen), they are isentropic

$$s = \text{constant} \qquad (9)$$

The application of these relations in calculating the states of a flowing chemically reacting gas may be demonstrated by considering the expansion of a gas from a plenum chamber through a nozzle. In the plenum chamber, a closed system static equilibrium solution (discussed in the previous section) may be performed to obtain the stagnation conditions (s, h_o) for the subsequent isentropic expansion. Consider next the state at some point in the nozzle. Recall that in Section 2.1.1 it was shown that the thermodynamic and chemical state of a closed equilibrium system is determined by two independent state variables. In the present case, one of these is given since the flow is isentropic (9). Thus, the thermodynamic and chemical state of the fluid may be completely determined by specifying only one property, conveniently the state pressure, P. Once the state is known, the local velocity may be calculated from (8).

The local Mach number is the ratio of the local velocity and sound speed where the local sound speed is given by

$$a = \sqrt{\left(\frac{\partial P}{\partial \rho}\right)_s} \tag{10}$$

For simple one-dimensional internal flow, continuity requires that

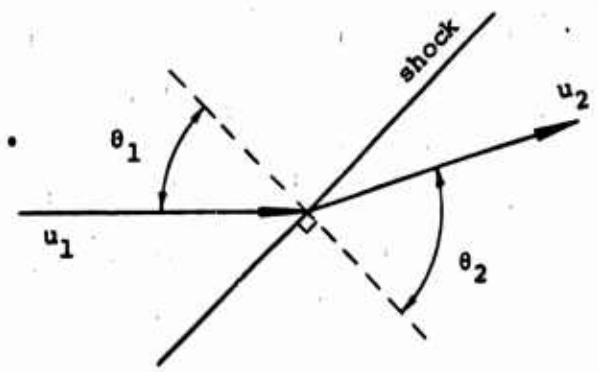
$$\frac{W}{A} = \rho u \tag{11}$$

In (10) and (11), ρ is the total system density, i.e., the mass of gaseous and condensed phases per unit volume. When performing isentropic flow calculations, the GASKET program prints out (in addition to the local thermodynamic and chemical state) the local velocity (8) Mach number (10), and mass flux (11). The appropriate input for isentropic flow calculations is specified in Section 4, and some related example problems are presented in Section 5.

2.1.3 Shock Waves

In addition to equilibrium isentropic flows (discussed in the previous section), the GASKET program can calculate the equilibrium state downstream of a normal or oblique shock wave. The basis for these calculations is discussed in this section.

To illustrate, consider flow through an oblique shock wave with upstream conditions known and downstream conditions unknown.



Equations expressing the conservation of mass, energy, and momentum (independent of events "in" the shock) may be written as follows:

Mass

$$\rho_2 u_2 \cos\theta_2 = \rho_1 u_1 \cos\theta_1 \tag{12}$$

Energy

$$h_2 + \tfrac{1}{2} u_2^2 = h_1 + \tfrac{1}{2} u_1^2 \tag{13}$$

Normal Momentum

$$P_2 + \rho_2 u_2^2 \cos^2\theta_2 = P_1 + \rho_1 u_1^2 \cos^2\theta_1 \tag{14}$$

Tangential Momentum

$$\rho_2 u_2^2 \cos\theta_2 \sin\theta_2 = \rho_1 u_1^2 \cos\theta_1 \sin\theta_1 \tag{15}$$

The four conservation equations, as written above, involve five unknowns: θ_2, u_2, P_2, ρ_2, h_2. However, the thermodynamic variables on the downstream side of the shock are related by the chemical equilibrium and thermodynamic state relations discussed in Section 2.1.1. Recall that these relations were sufficient to completely define the thermodynamic and chemical state of a system given the elemental composition and any two independent thermodynamic state variables (e.g., ρ_2 as a function of P_2 and h_2).

Thus, the chemical equilibrium and thermodynamic state relations, plus the four conservation equations (12) through (15) are sufficient to determine the conditions downstream of a shock wave if all upstream conditions are known. The GASKET program performs this determination as part of the normal or oblique shock option. The conditions upstream of the shock may be specified directly, or they may be carried over from a previous isentropic flow solution (Section 2.1.2). The calculated conditions downstream of the shock include all thermodynamic state variables, chemical species concentrations, θ_2, u_2, M_2, etc. The

setup of the program input for performing a shock solution is discussed in Section 4 and some related example problems are presented in Section 5.

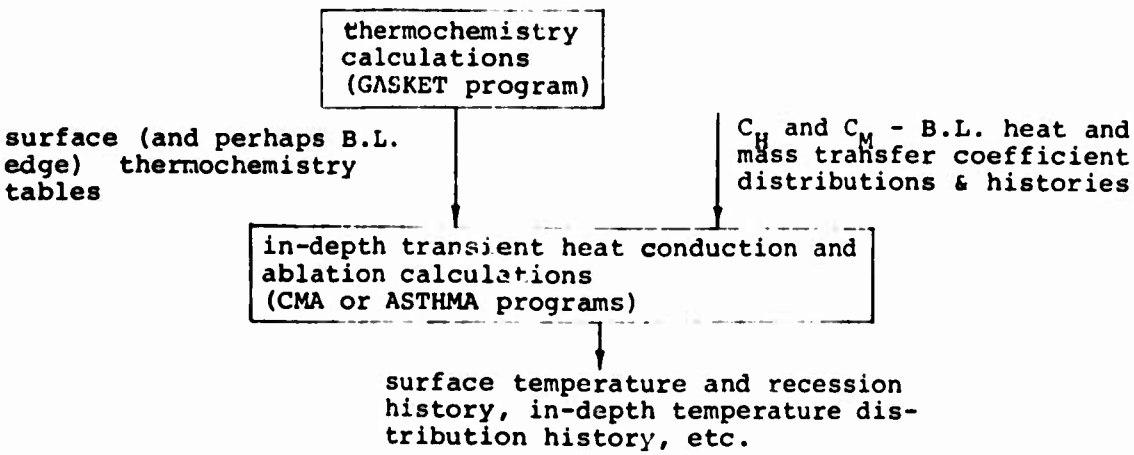
2.2 MIXED EQUILIBRIUM - NONEQUILIBRIUM OPEN SYSTEMS

The theory upon which the surface ablation calculations are based is best described by considering a sequence of physical models of increasing complexity. Thus, in Section 2.2.1 both simplified and more refined models for open systems in equilibrium are discussed. Then, in Section 2.2.2, further refinements to the open-system model to account for chemical kinetics are considered.

2.2.1 Open Systems in Equilibrium

An open system model must be used to treat thermochemical ablation of carbon surfaces, because the elemental composition in a control volume attached to the surface depends upon boundary layer transport events and the rate of surface material degradation. The GASKET program uses a reasonably sophisticated approach for the treatment of such problems.

As will be discussed in more detail subsequently, the GASKET program relates the surface state (T_w, h_w, etc.) to the ablation rate. The surface state and ablation rate are also related by surface energy balance considerations which depend on the rate of 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 be specified. Computationally, the surface thermochemistry relations are usually generated by the GASKET 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 - Ref. 4) program or the ASTHMA (Axisymmetric Transient Heating and Material Ablation - Ref. 5) program. The information flow for a complete transient ablation prediction may be illustrated diagramatically as:

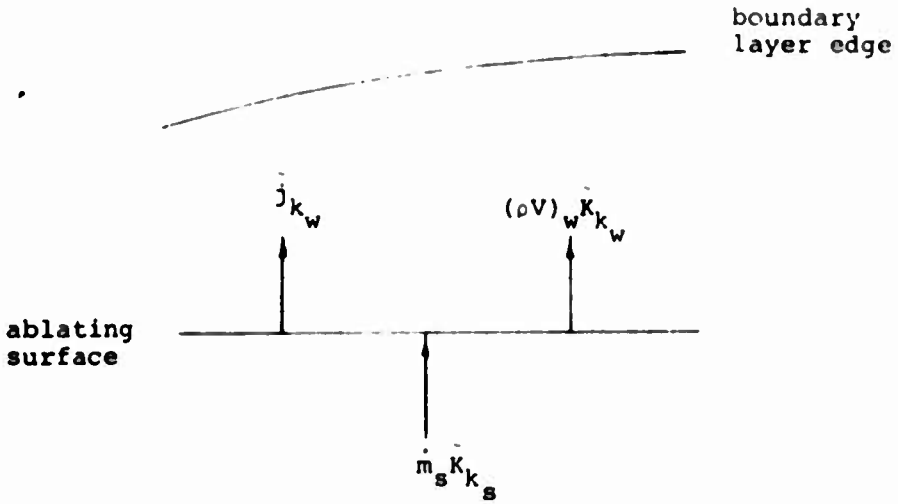


The preparation of the input for these ablation calculations is discussed in Section 4 for the GASKET program and in References 4 and 5 for the CMA and ASTHMA programs. The fundamentals underlying open system thermochemistry are briefly summarized here. Open system calculations, subject to a few simplifying assumptions to more clearly illustrate the basic theory, are discussed first in Section 2.2.1.1. These considerations are extended to more general systems in Section 2.2.1.2.

2.2.1.1 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), then these equations take on a particularly simple form for equilibrium systems.

Consider first the fluxes of chemical elements (k) entering and leaving a control surface affixed to the ablating surface. The graphite surface 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 k^{th} chemical element may be illustrated as



Terms superscripted by a tilde (~) represent the total mass fraction or flux of element k, independent of molecular configuration. Thus

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

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

where k pertains to element k, i pertains to species i, and α_{ki} 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 the injection flux $\dot{m}_s$. Note that for graphite surfaces the quantity $\tilde{K}_{k_s}$ is unity for k = C and zero for k ≠ C (where C represents the element carbon).

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

$$\tilde{j}_{k_w} + (\rho V)_w \tilde{K}_{k_w} = \dot{m}_s \tilde{K}_{k_s}$$

Summing Equation (16) over all elements k yields the total mass continuity equation (for the case when there is no condensed phase material removal)

$$(\rho V)_w = \dot{m}_s \qquad (16)$$

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 6, 7, and 8.

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

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2} \tag{17}$$

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

$$q = h(T_e - T_w) \tag{18}$$

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., Ref. 6)

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y}\left(\mu \frac{\partial H}{\partial y}\right) \tag{19}$$

where H is the total (sensible + chemical + $u^2/2$) enthalpy. By analogy to Equations (17) and (18), solutions to (19) are conveniently expressed in terms of a dimensionless heat transfer coefficient C_H where

$$q = \rho_e u_e C_H (H_e - H_w) \tag{20}$$

Corresponding formulations for non-unity Prandtl and Lewis number cases will be considered in Section 2.2.1.2

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 (Ref. 6) of the

boundary layer species conservation equation yields the following equation for each element k

$$u \frac{\partial \tilde{K}_k}{\partial x} + \rho v \frac{\partial \tilde{K}_k}{\partial y} = \frac{\partial}{\partial y} \left(\rho D \frac{\partial \tilde{K}_k}{\partial y} \right) \tag{21}$$

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

$$-\tilde{j}_{k_w} = \rho_e u_e C_M (\tilde{K}_{k_e} - \tilde{K}_{k_w}) \tag{22}$$

And for the unity Pradtl and Lewis number case under consideration, the similarity of Equations (19) and (21) indicates that if the corresponding boundary conditions are also similar, then $C_m = C_H$.

Utilizing this transfer coefficient formulation (22) for the diffusion flux in the elemental balance Equation (16) yields

$$\rho_e u_e C_M (\tilde{K}_{k_w} - \tilde{K}_{k_e}) + (\rho v)_w \tilde{K}_{k_w} = \dot{m}_s \tilde{K}_{k_s} \tag{23}$$

defining a dimensionless ablation rate as

$$B'_g \equiv \frac{\dot{m}_g}{\rho_e u_e C_M}, \qquad B'_c \equiv \frac{\dot{m}_c}{\rho_e u_e C_M} \qquad \text{and} \qquad B' \equiv \frac{(\rho v)_w}{\rho_e u_e C_M} \equiv \frac{\dot{m}_s}{\rho_e u_e C_M} \tag{24}$$

and solving (23) 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)

$$\tilde{K}_{k_w} = \frac{B' \tilde{K}_{k_s} + \tilde{K}_{k_e}}{1 + B'} \tag{25}$$

Given the relative amounts of chemical elements specified by (25), 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. If the gases are in equilibrium with the ablating surface

$$-\sum_{k=1}^{K} C_{k\ell} \ln P_k = \ln K_{p\ell}(T) \tag{26}$$

if ℓ represents the surface species, and

$$-\sum_{k=1}^{K} C_{k\ell} \ln P_k < \ln K_{p\ell}(T) \tag{27}$$

for all other candidate condensed phase species. For a graphite surface, however, it is assumed that the only possible surface species is condensed-phase carbon and, further, that the surface is kinetically isolated from the edge gases. Consequently, GASKET uses rate equations in place of equations (26) and (27). The equilibrium relations for gas phase species is again (see Section 2.1.1 of the form

$$\ln P_i - \sum_{k=1}^{K} C_{ki} \ln P_k = \ln K_{pi}(T) \tag{28}$$

and the partial pressures must obey the relation

$$\sum_{i=1}^{I} P_i = P \tag{29}$$

The elemental mass fractions adjacent to the surface, $\tilde{K}_{k_w}$, of (25) are related to the species partial pressures, P_i, by relations such as (5) (except that no condensed phase is being considered here)

$$\tilde{K}_{k_w} = \frac{m_k}{P\bar{m}} \sum_{i=1}^{I} C_{ki} P_i \tag{30}$$

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

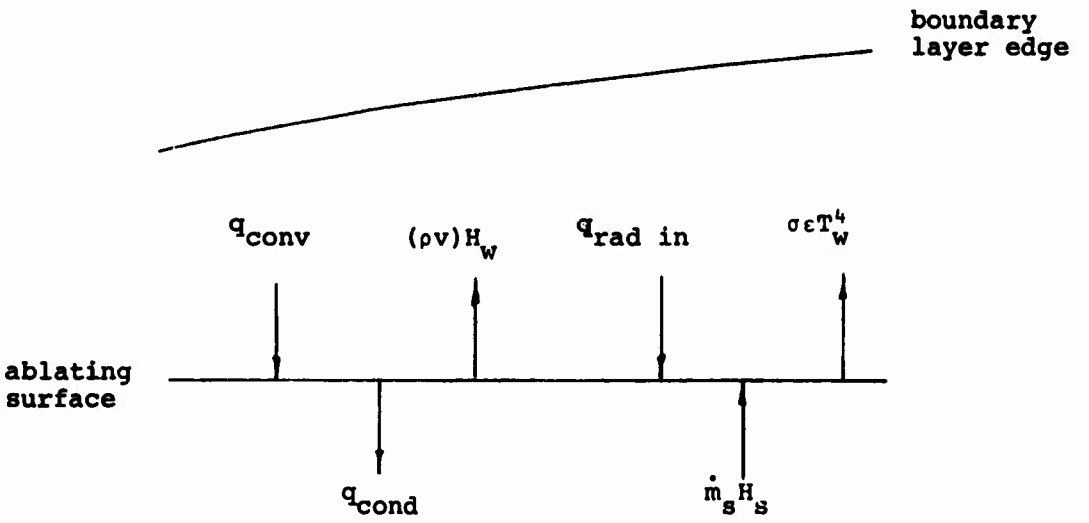
UNKNOWNS	NO. OF SUCH UNKNOWNS	EQUATION NO.	NO. OF SUCH EQUATIONS AVAILABLE
P_i	I	(28)	I-K
$\tilde{K}_{k_w}$	K	(26)	1
$\bar{m}$	1	(25)	K
B'	1	(29)	1
		(30)	K
Total Unknowns	I+K+2	Total Equations	I+K+2

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

The GASKET 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. For open systems, the GASKET 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'..., 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



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 (20)

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

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

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

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

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

$\dot{m}_s H_s$ is the energy flux intering the surface associated with the surface ablation

Conservation of energy at the surface requires that

$$\rho_e u_e C_H (H_e - H_w) + \dot{m}_s H_s - (\rho v)_w H_w + q_{rad\ in} - \sigma\varepsilon T_w^4 = q_{cond}$$

or, utilizing (24)

$$H_e - (1+B')H_w + B'H_s + \frac{q_{rad\ in}}{\rho_e u_e C_H} - \frac{\sigma\varepsilon}{\rho_e u_e C_H} T_w^4 = \frac{q_{cond}}{\rho_e u_e C_H} \qquad (31)$$

For the 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_s is a known function of T_w. Additionally, B' and H_w are related to T_w through the surface thermochemistry tables generated by the GASKET program as previously discussed. Based on considerations thus far, all quantities in (31) except q_{cond} 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. Thus, it is seen that in general there exists only one value of T_w which satisfies (31). This T_w is usually determined in an iterative fashion by a heat conduction and ablation program (e.g., Refs. 4 or 5) which utilizes the surface thermochemistry tables as boundary conditions. Once T_w is known for a given time in a transient solution, B', 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 ≠ Le ≠ 1.0. The GASKET program is able to treat all of these effects and details relative to the treatment of some of these will be considered in Section 2.2.1.2.

2.2.1.2 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 material 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 situations, these assumptions are inappropriate for others. For this reason, calculations performed by the GASKET program (and the CMA and ASTHMA programs) are not restricted to any of these simplifications.

The equal diffusion coefficient, Pr = Le = 1.0 simplifications pertain 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.

Pr ≠ Le ≠ 1.0 - For nonunity Prandtl and Lewis numbers, 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 ≠ Le ≠ 1.0 case is beyond the scope of this manual (see, e.g., Refs. 7 and 8) 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 inhomogeneous. 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., Ref. 9) in place of the actual boundary layer edge enthalpy. Thus, nonunity Prandtl number has no influence on GASKET calculations and the primary practical implication is that the recovery enthalpy, rather than the boundary layer 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

$$q_w = k \frac{\partial T}{\partial y}\Big)_w - \sum_{i=1}^{I} j_{iw} h_i^o = \frac{k}{C_p} \frac{\partial h}{\partial y}\Big)_w + \sum_{i=1}^{I} h_i^o \rho D \frac{\partial K_i}{\partial y}\Big)_w \qquad (32)$$

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 (32) is not firmly established at this time. However, Reference 7 suggests the form

$$q_w = \rho_e u_e C_H \Big(H_r - h_w\Big)_{\substack{\text{frozen} \\ \text{edge gas}}} + \rho_e u_e C_M \sum_{i=1}^{I} \Big(K_{i_e} - K_{i_w}\Big) h_i^{T_w} \qquad (33)$$

and this is the form employed in Aerotherm ablation programs. In (33), 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 $h_i^{T_w}$ represents the enthalpy of chemical species i with respect to a base temperature equal to the surface temperature. It can be shown (Ref. 7) that for Le = 1.0 and $C_M = C_H$, (33) collapses to (20) as expected. However, where Le $\neq$ 1.0, the heat and mass transfer coefficients are generally unequal and a correlation frequently employed (Ref. 10) is

$$\frac{C_M}{C_H} = Le^{2/3} \qquad (34)$$

It is apparent from (33) 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

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

This quantity is also calculated by the GASKET 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 GASKET program for input to the CMA (Ref. 4), ASTHMA (Ref. 5), 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., Ref. 9), 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

$$\tilde{j}_{k_w} = \rho_e u_e C_M (\tilde{z}^*_{k_w} - \tilde{z}^*_{k_e}) \qquad (35)$$

In (35), $\tilde{z}^*_k$ is, in effect, a weighted average of the mole and mass fractions of element k. The z^*_k are defined by

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

$$z_i^* = \frac{z_i^{\gamma} K_i^{1-\gamma}}{\sum_{i=1}^{I} z_i^{\gamma} K_i^{1-\gamma}} \qquad (\gamma \simeq 2/3, \text{ see Reference 2})$$

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

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

$$\mathcal{D}_{ij} = \frac{\bar{D}}{F_i F_j} \tag{36}$$

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 (36) in order for the boundary layer species diffusion equations to reduce to a form from which (35) can be inferred by similarity arguments. Reference 3 demonstrates that the binary diffusion coefficients for a varity of chemical systems are accurately correlated by (36). This reference also shows that a reasonably good correlation equation for the F_i is

$$F_i = \left(\frac{m_i}{m_{ref}}\right)^{\varepsilon} \quad \text{where} \quad m_{ref} \approx 23.4 \quad \text{and} \quad \varepsilon \approx 0.431 \tag{37}$$

when $\bar{D}$ is taken as the self-diffusion coefficient of O_2. Additional discussion relative to this unequal diffusion coefficient formulation is contained in Section 2.3.

Consideration of unequal diffusion coefficients affects the surface elemental balance relationships which are needed to determine the equilibrium state

at the surface. Substituting (35) into (16) yields

$$\rho_e u_e C_M (\tilde{z}^*_{k_w} - \tilde{z}^*_{k_e}) + (\rho v)_w \tilde{K}_{k_w} = \dot{m}_s \tilde{K}_{k_s} \tag{38}$$

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

$$\tilde{K}_k = \mathcal{M}_k \frac{\sum_{i=1}^{I} C_{ki} P_i}{\sum_{i=1}^{I} \mathcal{M}_i P_i} = \frac{\mathcal{M}_k}{P \mathcal{M}_g} \sum_{i=1}^{I} C_{ki} P_i$$

and

$$\tilde{z}^*_k = \mathcal{M}_k \frac{\sum_{i=1}^{I} C_{ki} P_i / F_i^{\gamma}}{\sum_{i=1}^{I} \mathcal{M}_i P_i / F_i^{\gamma}} = \frac{\mathcal{M}_k \bar{F}}{P \mathcal{M}_g} \sum_{i=1}^{I} C_{ki} P_i / F_i^{\gamma}$$

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

$$\bar{F} \equiv \frac{\sum_{i=1}^{I} \mathcal{M}_i P_i}{\sum_{i=1}^{I} \mathcal{M}_i P_i / F_i^{\gamma}} \tag{39}$$

Substituting these expressions into (38) and utilizing (24) yields an expression for the species partial pressures at the surface in terms of quantities at the boundary layer edge and in the material

$$B' \sum_{i=1}^{I} C_{ki} P_{iw} + \bar{F} \sum_{i=1}^{I} C_{ki} P_{iw} / F_i^{\gamma} = \frac{P \mathcal{M}_g}{\mathcal{M}_k} (\tilde{z}^*_{k_e} + B' \tilde{K}_{k_s}) \tag{40}$$

Note that (40) reduces to (25) when the diffusion coefficients are equal.

When performing unequal diffusion coefficient open system calculations, the GASKET program utilizes (40) rather than (25) as the elemental mass balance equations. Other than this, the solution philosophy is essentially as discussed in Section 2.2.1.1. The diffusion factors utilized in the GASKET 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 (37) with the user specifying the reference molecular weight, $\mathcal{M}_{ref}$, and the exponent ε

c. if the user does nothing special, the program will calculate F_i according to (37), with $\mathcal{M}_{ref} = 23.4$ and $\varepsilon = 0.431$.

The actual program input for these alternatives will be discussed in Section 4. It should also be pointed out that the diffusion factors have an effect on the other transport properties calculated and printed out by the GASKET program, and these will be briefly discussed in Section 2.3.

For unequal diffusion coefficients, the transfer coefficient formulation for the surface energy flux has the form (Ref. 7)

$$q_w = \rho_e u_e C_H (H_r - h_w)_{\substack{\text{frozen} \\ \text{edge gas}}} + \rho_e u_e C_M \sum_{i=1}^{I} (Z_{i_e}^* - Z_{i_w}^*) h_i^{T_w} \qquad (41)$$

Note that for equal diffusion coefficients, $Z_i^* = K_i$ and (41) reduces to (33) as expected. Consistent with (41), for unequal diffusion coefficient problems, the surface thermochemistry tables prepared by the GASKET 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

$$\sum_{i=1}^{I} z^*_{i_w} h_i^{T_w} = \sum_{i=1}^{I} K_{i_w} h_i^{T_w} = h_w \qquad (42)$$

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

$$\sum_{i=1}^{I} z^*_{i_e} h_i^{T_w} \qquad (43)$$

in addition to

$$h_w \begin{matrix} \text{frozen} \\ \text{edge gas} \end{matrix}$$

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

2.2.2 Open Systems With Kinetically - Controlled Reactions

To calculate the equilibrium state of a chemical system, detailed atomic data for each possible chemical reaction is not needed. This fact permits a significant simplification in the problem formulation, and the theory briefly outlined in Section 2.2.1 takes advantage of these simplifications. For the graphite ablation problem, however, it has been shown that the most important reactions involving the condensed-phase surface carbon and gas-phase species near the surface do not satisfy the requirements of chemical equilibrium (see Ref. 11). Thus, an accurate treatment of the thermochemical ablation of graphite requires an open system model which accounts for both equilibrium and nonequilibrium chemical reactions.

A general solution of chemistry problems for which reaction kinetics effects are important is potentially difficult for at least two reasons: a) there are significant computational and bookkeeping problems associated with the analytical treatment of mixed equilibrium and nonequilibrium systems, and b) for many systems of engineering interest, the rate controlling reactions are not well known and/or rate constants for these reactions are unavailable. The GASKET program effectively surmounts the first of these problems as discussed in Reference 4 and summarized below. With regard to difficulties falling into the second

category, experimental and analytical studies conducted at Aerotherm have resulted in values of the reaction rate constants for graphite kinetics which are the most accurate available to date (References 11 and 12).

In the remainder of this section the GASKET methodology for the treatment of chemical kinetics is briefly summarized. In Section 2.2.2.1 reaction kinetics in general are discussed, and in Section 2.2.2.2 the specific models used in the code for graphite surface kinetics are outlined.

2.2.2.1 Reaction Kinetics in General

The inclusion of kinetically controlled chemical reactions is accomplished by removing equilibrium relations such as equation (3) from the set of equations for certain species participating in reactions that are to be kinetically controlled. These equations are replaced by kinetic rate equations for each kinetically controlled reaction. This is accomplished, first, by identifying the primary reactive species in the reactions which are to be kinetically controlled and, second, by allowing these species to be created or destroyed only via the kinetic rate equations. This approach is performed by a relabeling of species to be considered in the kinetically controlled reactions. These species are called pseudo-elements since they behave like elements except that they may be created or destroyed at rates specified by the reaction rate equations.

Computationally, the inclusion of kinetics results in the addition of a rate-of-creation or destruction term to the elemental balance equations for these pseudo-elements. This adds additional unknowns to the system equal in number to the number of species whose concentrations are kinetically controlled, i.e., the pseudo-elements. The relative creation and destruction rates of all pseudo-elements in a given reaction are related by stoichiometry, however, so the number of additional unknowns remaining is equal to the number of kinetically controlled reactions. The reaction rates, from which the pseudo-element creation or destruction rates derive, are given by

$$R_m = k_{Fm}\left[\prod_j p_j^{\mu^R_{jm}} - \frac{1}{K_{pm}}\prod_j p_j^{\mu^P_{jm}}\right] \qquad (44)$$

for each kinetically controlled reaction m of the form

$$\sum_j \mu_{jm}^R N_j \rightarrow \sum_j \mu_{jm}^P N_j \qquad (45)$$

where the sums and products are over the species and pseudo-elements N_j, μ are the stoichiometric coefficients, and superscripts R and P denote reactants and products respectively. In (44), K_{pm} is the equilibrium constant for reaction (45) and k_{Fm} is the forward rate constant. In the present formulation, k_{Fm} is represented by an Arrhenius type function

$$k_{Fm} = B_m T^{\phi_m} \exp\ (-E_m/RT) \qquad (46)$$

where E_m is the activation energy, ϕ_m is the temperature exponent, and B_m is factor representing a multitude of phenomena. These quantities are generally based on experimental data. The uncertainty in, or unavailability of, these data for many chemical systems of interest in ablation problems frequently represent a significant constraint on the application of a kinetics model to these problems.

When certain chemical reactions are taken to be kinetically controlled, the arrangement of the thermodynamic data for all candidate species must be modified. This requirement is related to the fact that all species involved in kinetically-controlled reactions are relabeled and designated as pseudo-elements. Section 3.1.3 presents a more complete discussion of this modeling subtlely in the GASKET program.

2.2.2.2 Kinetics of Hetergogeneous Reactions at a Graphite Surface

As already mentioned in Section 1, in the graphite ablation problem the condensed-phase surface carbon is kinetically isolated from all species in the boundary layer adjacent to the surface. That is, only three species are allowed to react with the graphite surface material, and the corresponding reactions are kinetically controlled. The three allowed species are water gas, carbon dioxide, and hydrogen, and the stoichiometric equations for the three reactions are as follows:

1) $C^* + H_2O \rightleftarrows CO + H_2$

2) $C^* + CO_2 \rightleftarrows 2\ CO$

3) $2C^* + H_2 \rightleftarrows C_2H_2$

The detailed development of the graphite kinetics model used by GASKET can be found in Reference 12. Only the final results are summarized here.

In the study described in Reference 12, it was found that the effects of reaction inhibition should be included in the graphite ablation model. That is, experimental evidence indicates that the kinetics of the heterogeneous surface reactions can be most accurately modeled by accounting for the fact that the presence of certain species near the surface tend to inhibit the forward rates of the three reactions. The method of Langmuir (e.g., Reference 13) was used in the development of this heterogeneous inhibition kinetics model. The effects of reaction inhibition are formally treated by modifiying the pre-exponential factor in Equation (46):

$$\dot{B}_m = B'_m \left(\frac{1}{1 + \sum_j \psi_{jm} P_j} \right) \left(\frac{1}{1 + \sum_j F_{jm} P_j} \right) \qquad (47)$$

In equation (47) B'_m, ψ_{jm} and F_{jm} are constants for the Mth reaction and P_j is the partial pressure of the j species. The first term in brackets accounts for the inhibition effects due to any species which is also involved in any of the three reactions above; thus the summation is over the species C*, H_2O, CO, H_2, CO_2 and C_2H_2. The second term in brackets accounts for the inhibition effects due to all other base species not involved in the three kinetically controlled reactions. At present, the quantity K_{jm} is non-zero only for the species HCl and HF. The kinetics model comprised of Equations (46) and (47)is referred to as the "Arrhenius/Langmiur" model.

The ψ_{jm} inhibition effects are assumed to be the same for layer-oriented, edge-oriented, and bulk pyrolytic graphite. The matrix of ψ_{jm} values is summarized as follows:

ψ_{jm}, atm^{-1}

m \ j	H_2O	CO	H_2	CO_2	C_2H_2	C*
1	1	1	1	1	0	0
2	1	1	1	1	0	0
3	1	1	0	1	0	0

The F_{jm} inhibition effects depend upon the type of graphite surface; they are the same for bulk and edge-oriented graphite and different for layer-oriented graphite. The matrix of K_{jm} values is summarized as follows:

$$F_{jm} = 3\ atm^{-1};\quad m = 1,2,\ j = HCl,\ HF$$

$$F_{jm} = 0\ ;\quad m = 1,2,\ j = \text{all species other than HCl and HF}$$

$$m = 3,\quad j = \text{all species}$$

The other constants in the Arrhenius/Langmiur model which are built into GASKET are summarized as follows:

Surface	lb mole reaction/ft²sec			cal/gm mole			unitless		
	B'_1	B'_2	B'_3	E_1	E_2	E_3	ϕ_1	ϕ_2	ϕ_3
Layer	12.5	12.5	0.77	46,000	46,000	55,500	0	0	0
Edge	1.65×10^{4}	1.65×10^{4}	4.12×10^{6}	65,500	65,500	129,500	0	0	0
Bulk	1.98×10^{5}	1.98×10^{5}	4.94×10^{7}	65,500	65,500	129,500	0	0	0

These latter constants were also determined from experimental data, as described in Reference 12.

2.3 TRANSPORT PROPERTIES

In addition to the thermochemical state properties discussed in previous sections, the GASKET program calculates and outputs mixture transport properties. These include the mixture viscosity, thermal conductivity, and species diffusion quantities. The Prandtl and Schmidt numbers are also output. These transport properties are calculated from expressions which derive from simple kinetic theory and the particular multicomponent diffusion representation previously discussed in Section 2.2.1.2. The development of these expressions is discussed in detail in Reference 3. A brief summary of this development, and the resulting expressions, are presented in this section.

Diffusion Coefficients - In Section 2.2.1.2 a bifurcation approximation for binary diffusion coefficients was mentioned which characterized multicomponent diffusion phenomena with reasonable accuracy without unduly complicating the system of equations to be solved. This simplification is achieved through a correlation for binary diffusion coefficients of the form

$$\mathcal{D}_{ij} = \frac{\bar{D}}{F_i F_j} \tag{48}$$

where $\bar{D}$ is a reference diffusion coefficient and the F_i are diffusion factors. These quantities are discussed in detail in Reference 3. The incorporation of (48) in the Stefan-Maxwell relation for mass diffusion fluxes indicates that the diffusion flux of species i may be written in terms of only properties of species i and global system properties. Subject to a few simplifying assumptions (Ref. 3), this expression for j_i may be written

$$j_i = \frac{\rho \bar{D} \mu_2}{\mathcal{M} \mu_1} \frac{\partial z_i}{\partial y} \tag{49}$$

where

$$z_i = \mathcal{M}_i x_i / F_i \mu_2 \tag{50}$$

$$\mu_1 = \sum_j x_j F_j \tag{51}$$

$$\mu_2 = \sum_j \mathcal{M}_j x_j / F_j \tag{52}$$

The accuracy of this formulation is examined in Reference 3 for a variety of chemical systems. It is shcwn that the $\mathcal{D}_{ij}$ calculated by (36) represent a very substantial improvement over equal diffusion coefficients when compared to exact values calculated directly from kinetic theory. The calculation of the mixture viscosity and thermal conductivity is based on the diffusion factors given by (48), and these will be discussed in the following paragraphs.

Mixture Viscosity - The expression employed by the GASKET program to calculate the mixture viscosity derives from rigorous first order kinetic theory (Ref. 14), subject to a few simplifying assumptions, as discussed in Reference 3.

$$\mu_{mix} = \sum_{i=1}^{I} \left[\frac{x_i \mu_i}{x_i + 1.385 \frac{RT\mu_i}{P\mathcal{M}_i} \sum_{\substack{j=1 \\ j \neq i}}^{I} \frac{x_j}{\mathcal{D}_{ij}}} \right] \tag{53}$$

where μ_i is the viscosity of the pure species i. The μ_i may be expressed in terms of the self diffusion coefficients $\mathcal{D}_{ii}$

$$\mu_i = \frac{5}{6A^*_{ii}} \rho_i \mathcal{D}_{ii} \tag{54}$$

where A^*_{ii} is a ratio of collision integrals based on a Lennard-Jones intermolecular potential. Substituting (48) and (54) into (53) results in the following expression for the viscosity of the multicomponent mixture.

$$\mu_{mix} = \frac{\rho \bar{D}}{\mu_1} \sum_{i=1}^{I} \left[\frac{\frac{x_i \mathcal{M}_i}{F_i \mathcal{M}}}{1.385 + \frac{x_i F_i}{\mu_1} \left(\frac{6A^*_{ii}}{5} - 1.385 \right)} \right] \tag{55}$$

and this is the expression utilized to calculate the mixture viscosity output by the GASKET program.

Mixture Thermal Conductivity - The thermal conductivity in a polyatomic gas mixture may be represented by (Ref. 14)

$$k_{mix} = k_{mono\text{-}mix} + k_{int} \tag{56}$$

where $k_{mono\text{-}mix}$ is the thermal conductivity in a mixture computed neglecting all internal degrees of freedom and k_{int} is the contribution to the thermal conductivity of the mixture due to the internal degrees of freedom of the molecules. A simplified expression for the mono-mixture thermal conductivity can be derived in a manner similar to the procedure previously discussed for the mixture viscosity. This simplified expression is (from Ref. 3)

$$k_{mono\text{-}mix} = \sum_{i=1}^{I} \left[\frac{x_i k_{i\ mono}}{x_i + 1.475 \frac{RT\mu_i}{P\mathcal{M}_i} \sum_{\substack{j=1 \\ j\neq i}}^{I} \frac{x_j}{\mathcal{D}_{ij}}} \right] \tag{57}$$

where $k_{i\ mono}$ is the thermal conductivity of the pure species i neglecting all internal degrees of freedom of the molecule. The $k_{i\ mono}$ may be expressed in terms of the μ_i as per

$$k_{i\ mono} = \frac{15}{4} \frac{R}{\mathcal{M}_i} \mu_i \tag{58}$$

The contribution to the thermal conductivity from the internal degrees of freedom may be expressed as (from Ref. 3)

$$k_{int} = \sum_{i=1}^{I} \frac{\rho x_i \frac{\mathcal{M}_i}{\mathcal{M}} \left(C_{pi} - \frac{5}{2} \frac{R}{\mathcal{M}_i} \right)}{\sum_{j=1}^{I} \frac{x_j}{\mathcal{D}_{ij}}} \tag{59}$$

By combining (48) with (56) through (59), the mixture thermal conductivity may be written as

$$k_{mix} = \frac{\rho \bar{D}}{\mu_1} \left\{ \sum_{i=1}^{I} \left[\frac{\frac{15}{4} \frac{x_i}{F_i} \frac{R}{\mathcal{M}}}{1.475 + \frac{x_i F_i}{\mu_1} \left(\frac{6A^*_{ii}}{5} - 1.475 \right)} \right] + \frac{\mu_2}{\mathcal{M}} \left[\tilde{C}_p - \frac{5}{2} R\mu_2 \right] \right\} \tag{60}$$

where μ_1 and μ_2 are given by (51) and (52) respectively, and

$$\mu_3 = \sum_{i=1}^{I} \frac{z_i}{\mathcal{M}_i} = \frac{1}{\mu_2} \sum_{i=1}^{I} \frac{x_i}{F_i} \tag{61}$$

$$\tilde{C}_p = \sum_{i=1}^{I} z_i C_{pi} \tag{62}$$

Thus, (60) is the expression utilized to calculate the mixture thermal conductivity output by the GASKET program.

Also calculated and output by the GASKET program are the Prandtl and Schmidt numbers which are defined here as

$$Pr = \frac{\mu}{k} C_{p\text{-frozen}} \tag{63}$$

$$Sc = \frac{\mu_1}{\mu_2} \frac{\mathcal{M}_\mu}{\rho \bar{\mathcal{D}}} \tag{64}$$

The transport properties calculated by the GASKET program are all based on the bifurcation approximation for the binary diffusion coefficients expressed in (48). This is so even for closed system calculations (in which case diffusion phenomena need not be considered to calculate the chemical and thermodynamic state of the system) and for open system calculations for which equal diffusion coefficients are assumed (Section 2.2.1.1). From the equations presented, it may be observed that the properties calculated are highly dependent on the diffusion factors, F_i. Three alternate methods for prescribing the F_i were discussed Section 2.2.1.2. The use of the diffusion factor correlation (48) with resident values of $\mathcal{M}_{ref}$ and ε (which were derived primarily from consideration of species diffusion coefficients) should result in reasonably accurate values of other transport properties. Alternately, the correlation (48) may be used with values of $\mathcal{M}_{ref}$ and ε derived by correlating available transport property data for the particular system of interest. If transport properties of maximum accuracy are to be calculated, then the diffusion factors should be input individually for each species. These data may be obtained from tabulations such as Reference 14.

SECTION 3

CODING

This section presents some details relative to the FORTRAN coding of the GASKET 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 GASKET program is identified and briefly discussed in Section 3.2, and definitions of several output quantities are provided 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 procedures employed in the GASKET program to solve the equations set forth in Section 2 are briefly discussed here. Considerably greater detail is presented in Reference 2 and in particular Table I of that reference.

3.1.1 Basic Solution Technique

The basic solution technique may be illustrated by considering, for example, an open system with unequal diffusion coefficients, no condensed phase material removal, and no kinetics (i.e., as discussed in Section 2.2.1.2). For this system, the basic equations defining the problem are the elemental conservation equations (40), the total pressure equation (29), the reaction equilibrium equations (28), and one heterogeneous vapor pressure relation (26). The table of Section 2.2.1.1 shows that there are many knowns as unknowns in these equations so closure is obtained.

Summarizing these equations,

$$B'\sum_{i=1}^{I} C_{ki} P_i + \bar{F}\sum_{i=1}^{I} C_{ki} P_i / F_i^{\gamma} - \frac{P\dot{m}_g}{\dot{m}_k}\left(\tilde{z}^*_{k_e} + B'\tilde{K}_{k_s}\right) = 0 \qquad (65)$$

$$\sum_{i=1}^{I} P_i - P = 0 \qquad (66)$$

$$\ell n\, P_i - \sum_{k=1}^{K} C_{ki}\, \ell n\, P_k - \ell n\, K_{pi}(T_w) = 0 \qquad (67)$$

$$-\sum_{k=1}^{K} C_{k\ell}\, \ell n\, P_k - \ell n\, K_{p\ell}(T_w) = 0 \qquad (68)$$

The number of unknowns could immediately be reduced by I-K through the direct substitution of (67), 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', (65) and (66) are linear relations between the P_i and $\dot{m}_g$ providing that $\bar{F}$ is reasonably constant. In contrast, (67) and (68) are linear relations between the $\ell n\, P_i$, $\ell n\, P_k$ and $\ell n\, K_{pi}$, the latter variable being approximately linear in 1/T.

The GASKET program takes advantage of this situation by treating those species which are significant in the mass and pressure balances (65) and (66) in terms of P_i and the less significant species in terms of their $\ell n\, P_i$.

The Newton-Raphson procedure, as applied by the GASKET 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

$$df_j = \sum \frac{\partial f_j}{\partial x_i} dx_i \tag{69}$$

which is locally correct and is integrated to

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

in the linear approximation. The solution of (69) is

$$dx_i = \sum \frac{\partial x_i}{\partial f_j} df_j \tag{70}$$

where the array of partial derivatives appearing in (70) is simply the matrix inverse of the array in (69). In the GASKET program the formulation of the partial derivatives uses the variables, $\ell n\ P_i$,* $\ell n\ T$ and $\ell n \mathcal{M}$, and (70) yields, for example,

$$d(\ell n\ P_i) = \sum \frac{\partial\ \ell n\ P_i}{\partial f_j} df_j \tag{71}$$

which if taken as linear all the way to solution yields

$$\ln \frac{P_i^{**}}{P_i^*} = (\Delta \ln P_i)^* \approx \sum \left(\frac{\partial \ln P_i}{\partial f_j} \right)^* (-\varepsilon_j)^* \qquad (72)$$

since the desired change in the functions is simply the negative of the error. An equally exact relation obtained from (71) is

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

which if taken as linear all the way to solution yields

$$P_i^{**} - P_i^* = \Delta P_i^* \approx P_i^* \sum \left(\frac{\partial \ln P_i}{\partial f_j} \right)^* (-\varepsilon_j^*) \qquad (73)$$

The GASKET program uses (73) for all species significant in mass balances and (72) 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^{**}. Experience has shown that it is frequently unwise to proceed along this correction vector the full amount indicated by (72) or (73). 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.

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*The choice of $\ln P_i$ permits a matrix reduction by the use of the simple algebraic substitution, previously mentioned after (68), prior to matrix inversion.

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 GASKET 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 equlibrium 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. 15) since all other species are taken to be formed from them.

The GASKET program selects the base species from the candidate species thermochemical data. 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 of 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.

As mentioned in Section 2.2.2.1, when chemical kinetics are considered the arrangement of the candidate species thermochemical data must be modified, because all species involved in kinetically controlled reactions are identified as pseudo-elements. The treatment of chemical kinetics in GASKET requires that each of the species involved in kinetically controlled reactions also be identified as a base specie. Therefore, the thermochemical data must be arranged so that the species C^*, H_2O, CO, H_2, CO_2, and C_2H_2 appear at the top of the list and, thus, can be selected as base species when required. The thermochemical data built into GASKET is arranged in this required order.

Another subtle aspect of the base specie selection procedure occurs when chemical kinetics is considered. For certain edge-gas compositions the number of elements involved is fewer in number than the number of species present in the three kinetically-controlled reactions. When this occurs, additional "elements" must be created in order that the number of corresponding base species is large enough to include all species in the reactions. An example will serve to illustrate. Suppose that the edge gas contains H, C, and O. If only these elements are considered, then only three base species are possible and, therefore, only three of the species C^*, H_2O, CO, H_2, CO_2, and C_2H_2 appearing in the kinetically-controlled reactions can possibly be base species. This situation is remedied by taking two steps. First, GASKET defines two new "elements C^* and CO_2, identified by fictitious atomic numbers, whose corresponding base species are C^* and CO_2, respectively. These new "elements" are added to the set comprised of H, C, and O. Then, GASKET reinterprets the kinetically controlled reaction 3) as

$$2C^* + H_2 \overset{k}{\rightleftharpoons} C_2H_2 \rightleftharpoons 2CO + 3H_2 - 2H_2O$$

That is, the products of a kinetically controlled reaction can be replaced by their equilibrium base species in stoichiometrically correct proportions. Thus, with the "elemental" set comprised of H, C, O, CO_2, and C^*, five base species are possible. And, with the thermochemical data in the correct order, the five base species selected will be H_2, CO, H_2O, CO_2, and C^*.

Finally, one subtlety remains to be considered. In the previous paragraph it was mentioned that the "element" C^* was defined and assigned a fictitious atomic number. It follows that C^* can communicate with the remainder of the chemical system only through the three kinetically-controlled reactions. With this in mind, consider the second fictitious "element" CO_2. In reality, it is possible that CO_2 can be in equilibrium with many other gas phase species while simultaneously reacting with the graphite surface. The only way this can be accomplished is to introduce explicitly a kinetically-controlled reaction

involving CO_2 and other gas phase species and then allow the rate of this reaction to approach infinity, i.e., chemical equilibrium. GASKET does, indeed, perform this operation automatically by considering explicitly a fourth reaction

$$H_2O + CO \rightleftharpoons CO_2 + H_2$$

to be in equilibrium. This is the so-called water gas shift reaction.

In conclusion, it should be reiterated that the complexities involved in the selection of base species for mixed equilibrium - nonequilibrium systems are handled automatically by GASKET whenever the user selects all program options which utilize data built into the program. In this case, the user needs to input only the actual edge gas composition (see Section 4). However, if the user chooses to input his own kinetic and thermochemical data, then he must carefully follow the procedure prescribed in Section 4 so that GASKET will select the proper base species and kinetic reactions.

3.2 FORTRAN ROUTINES

In order to permit an understanding of the actual solution mechanics and their relation to the FORTRAN source program, a brief description of each of the subroutines will be 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 mainline program. With the exception of KININ, SQUEE, and ETIMEF all routines are called only by the mainline program.

3.2.1 Thermodynamic Data Input Routines

IMELM: Reads elemental data information and normalizes elemental composition information; creates fictitious "elements" when necessary.

INPUT: Reads species thermochemical data from DATX or input cards 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 molecular weights.

BELCH: Establishes a base species-element correspondence table which is required if an input element is temporily omitted from the chemical system being analyzed.

DATX: Contains built-in JANAF thermochemical data deck (see Volume II).

3.2.2 Problem Setup and Initiation

SIPIN: Initializes and sets various internal control flags and reads shock data.

KININ: Reads control card and optional frozen edge and surface temperature arrays; generates an array of internal control integers to define sequence of subsequent calculations.

ALPST: Reads diffusion factor values if KRK(3) = 9; sets diffusion factors based on exponential approximation or input values; 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 iteration certain reinitializations are performed including assigning temperature to 3000°K if the nonconvergent flag has been set. Also on first iteration, certain kinetic rate data are read or generated by this routine and certain key summations are determined in CRECT. (The reason for these functions inclusion in THERM relates to the overlaying of subroutines and molecular species data in an IBM 1130 version of this program).

MATL: 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. Introduces condensed species coefficients into their error equations. Determines if redundancy exists amongst condensed species equilibria. Removes any redundancy by eliminating either newly introduced species (see MAT2) or previously present species, based on equilibrium errors. In latter case mass of eliminated condensed species is distributed amongst other condensed species in order to preserve mass balances.

KINET: Generates certain kinetic rate data, adds kinetic rate terms to mass balance equations, and evaluates and introduces error derivatives into derivative matrix. Rearranges mass balances so that controlling reactions influence only one mass balance. Modifies coefficients if controlling reaction is approaching equilibrium so as to achieve linearity of equation.

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 concentration has a calculated negative correction - the corresponding equilibrium equation is removed and the correction set to zero; if the temperature is currently equal to a minimum or maximum value dictated by phase change or other discontinuous phenomena and if a contrary temperature correction is predicted - the temperature constraint is removed and the temperature frozen; if the surface equilibrium error and the temperature correction are of conflicting signs - the temperature constraint is removed and 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 surface equilibrium calculations.

SCALE: From basic corrections, corrections to log partial pressure 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 order of magnitude decrease in partial pressures of significant species, and less restrictive constraints on less important species. The scale factor generated by this routine will subsequently be applied to all corrections. Performs correction of temperature and pressure-molecular weight product.

CRECT: Performs all corrections according to scale factors calculated in SCALE. Makes corrections based either on linearization of mass balances (delta of mole fractions) or of equilibrium equations (delta of log of mole fractions) depending on relative importance in mass balances. Evaluates set of summations previously discussed relative 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 including the equilibrium specific heat and the isentropic exponent; calculates transport properties using model based on diffusion factors. Calculates Mach number in shock stagnation calculation, evaluates next pressure in iteration and assesses convergence at stagnation solution; outputs calculated quantities.

OUTPT: Generates and outputs all additional terms required for output as displayed in Section 5. Initiates iteration for shock stagnation solution.

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 NXN 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) returns 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:

$$\text{CP-FROZEN} = \sum_{i=1}^{I} K_i \frac{\partial h_i}{\partial T}$$, the frozen constant pressure specific heat capacity (Btu/lbm°R or Cal/gm°K)

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

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

$$\text{DLNM/DLNT} = \frac{\partial \ell n \mathcal{M}}{\partial \ell n T}\Big)_p \qquad \text{(unitless)}$$

$$\text{DLNM/DLNP} = \frac{\partial \ell n \mathcal{M}}{\partial \ell n P}\Big)_T \qquad \text{(unitless)}$$

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

(unitless)

Other property output includes:

MU1 = $\mu_1 = \sum_j X_j F_j$, a gas mixture property which reduces to unity for assumed equal diffusion coefficients $F_j = \bar{F} = 1.0$ (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 $F_j = \bar{F} = 1.0$ (grams of system/mole of gas)

MØL.WT = $\mathcal{M}$, the composite mixture molecular weight (see Equation 5, (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. (Btu/lbm)

CPTIL = $\tilde{C}_p = \sum_{i=1}^{I} Z_i \frac{\partial h_i}{\partial T}_p$, a property of the gas mixture which reduces to the frozen specific heat capacity for assumed equal diffusion coefficients. (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 tc static enthalpy, h, for assumed equal diffusion coefficients. (Btu/lbm)

GAMEX = γ, the weight factor exponent between K and Z mass fractions used to obtain the Z_i^* values. (unitless)

ELEMENTAL K MASS FRACTIONS = K_k, usual definition of mass fraction for element K in the system. (gm of-k/gm system).

ELEMENTAL Z MASS FRACTIONS = Z_k^*, elemental F_i^γ weighted mass fraction of element K in the system. (gm of K/gm-system).

All of the above properties are calculated and output for each problem solution using the current values of F_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 GASKET code are given in References 2 and 3.

3.4 PROGRAM OPERATION DETAILS

3.4.1 Program Storage Requirements

The current version of the GASKET program allows 179 chemical species 10 elements, 8 entries in the frozen edge temperature table, 15 entries in the surface temperature table, and 50 entries in the diffusion factor table. With these limits approximately 43,000 (decimal) words of storage are required. However, roughly 13,600 (decimal) words of this storage are occupied by the thermochemical data contained in the routine DATX.

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) tape, see KR(3)	(=18)

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 10 (KRK(10)) 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.

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:

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

The number of solutions depends upon the type of problem being solved. For example, when the isentropic expansion option is used to calculate the edge state and the edge elemental composition includes both H and O, three solutions are required t obtain the final form of the edge solution. Then, if the built-in frozen edge and surface temperature arrays are utilized, 17 additional solutions are provided, making a total of 20 solutions in this particular problem.

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 (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 the Aerotherm Graphite Surface Kinetics (GASKET) program. In the most general case, the input consists of eight card sets. These are:

1. CONTROL CARD
2. FROZEN-EDGE TEMPERATURE ARRAY
3. SURFACE TEMPERATURE ARRAY
4. ELEMENTAL COMPOSITION
5. DIFFUSION FACTOR DATA
6. SPECIES THERMOCHEMICAL EQUILIBRIUM DATA
7. OBLIQUE OR NORMAL SHOCK DATA
8. REACTION RATE DATA

Card Set 1 is a control card which contains a 10-element array, KRK(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 since, in most cases, the user will wish to utilize the data built into the GASKET program to replace card sets 2, 3, 5, 6, and 8. The card sets are described in detail in this section.

CARD SET 1 - CONTROL CARD (1 Card)

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

COLUMN 1 -- EDGE THERMODYNAMIC STATE

0	Input
1	Static state behind shock, upstream conditions input (card set 7)
2	Same as 1, except stagnation state behind shock
3	Isentropic expansion from input chamber conditions
4	Static state behind shock, upstream conditions calculated via isentropic expansion from input chamber conditions (card set 7)
5	Same as 4, except stagnation state behind shock

COLUMN 2 -- STATE OPTION (pertains to Z, cols. 11-20 of this card)

0	Assigned temperature
2	Assigned enthalpy
3	Assigned entropy

COLUMN 3 -- SPECIES THERMOCHEMICAL DATA

0 9	Use built-in JANAF data
0	Use built-in diffusion factor data
1234	Read from cards new JANAF data and, if provided, diffusion factor data
2 4	Print out thermochemistry for allowable species
34	Store all JANAF data and diffusion factors read from from cards on tape (must be requested if KRK (8) = 4)
9	Update diffusion factor data

COLUMN 4 -- PYROLYTIC GRAPHITE SURFACE SPECIFICATION

1	Layer-oriented
2	Edge-oriented
3	Bulk

COLUMN 5 -- FROZEN - EDGE TEMPERATURE ARRAY

0	Bypass this calculation
1	Use built-in temperature array
2	Read the temperature array from cards (card set 2)

COLUMN 6 -- SURFACE TEMPERATURE ARRAY

0	Bypass this calculation
1	Use built-in temperature array
2	Read the temperature array from cards (card set 3)

NOTE: When KRK(6) $\geq$ 1, GASKET automatically provides two equilibrium surface calculations, for 500°K and 1000°K, with the restriction of zero ablation; this is done in order to provide tables for CMA and/or ASTHMA which facilitate smooth interpolation.

COLUMN 7 -- KINETIC CONSTANTS

0	Use built-in Arrhenius/Langmuir model (see Section 2.2.2.2)
1 3	Read from cards the pre-exponential factor, B'_m (lb mole reaction/ft^{2}sec), activation energy, E_m (cal/gm mole), and temperature exponent, ϕ_m
23	Read from cards the partial pressure multiplicative factors, x_{jm} and K_{jm} (atm^{-1})

COLUMN 8 -- EDGE GAS ELEMENTAL COMPOSITION

1	e.g. does not contain H or O (Kinetically inert surface)
2	e.g. does not contain H (reaction 2. only)
3	e.g. does not contain O (reaction 3. only)
4	e.g. contains both H and O (reactions 1., 2., and 3.)

COLUMN 9 -- PUNCHED CARD OUTPUT

0	No punched card output
1 3	Punch a card appropriate to CMA input for each convergent frozen edge or surface solution
23	Punch a card appropriate to ASTHMA input for each convergent frozen edge or surface solution

COLUMN 10 -- 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.

FIELD 2 (Columns 11-20, Format F10.5) Thermodynamic State Variable, Z

1) a) If KRK(2) = 0, Z is assigned to temperature, °K
   b) If KRK(2) = 2, Z is assigned to enthalpy, cal/gm
   c) If KRK(2) = 3, Z is assigned to entropy, cal/gm°K

2) a) If KRK(1) = 0, Z pertains to the edge state
   b) If KRK(1) = 1 or 2, Z pertains to the thermodynamic state upstream of a shock wave
   c) If KRK(1) > 3, Z pertains to the chamber thermodynamic state
      i) If PC = 0, Z pertains to the actual chamber state
      ii) If PC ≠ 0, Z pertains to the ideal chamber state (see PC, Cols. 41-50 of this card)

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

1) If KRK(1) = 0, PR pertains to the edge thermodynamic state
2) If KRK(1) ≠ 0, PR pertains to the actual chamber thermodynamic state or to the thermodynamic state upstream of a shock wave

FIELD 4 (Columns 31-40, Format F10.5) Edge or Shock Upstream Thermodynamic State, ZE

1) IF KRK(1) $\leq$ 2, this field is ignored

2) a) If ZE > 0, it is assigned as the pressure, atm, at either the edge (KRK (1) = 3), or the upstream side of a shock wave (KRK(1) = 4 or 5)
   b) If ZE < 0, it is assigned as the Mach number at either the edge (KRK (1) = 3) or the upstream side of a shock wave (KRK(1) = 4 or 5)

FIELD 5 (Columns 41-50, Format F10.5) Ideal Chamber Pressure, PC atm

FIELD 6 (Columns 51-60, Format F10.5) Mass Transfer Coefficient, ROUCM $lbm/ft^2 sec$

FIELD 7 (Columns 61-70, Format F10.5) Diffusion Coefficient Exponent for Unequal Diffusion Coefficient Model, GAMER

1) If GAMER = 0.0, it is automatically set to 2/3 (this value is appropriate for most calculations)

2) If GAMER = 10^{-5}, the diffusion model reduces to equal diffusion coefficients

FIELD 8 (Columns 71-80, Format 2A4,A2) Job Title, Tile (3)

CARD SET 2 - FROZEN-EDGE TEMPERATURE ARRAY TFA(I) (number of cards = no. of temperatures + 1)

1) If KRK(5) = 0 or 1, skip this card set

2) If KRK(5) = 2, read in an array of no more than eight temperatures, TFA(I) °K

CARD(S) 1,2,... (Columns 1-10, Format F10.5) one temperature per card

FINAL CARD blank

NOTE: The TFA(I) array built into GASKET contains temperatures from 500 to 4000°K in 500°K increments

CARD SET 3 - SURFACE TEMPERATURE ARRAY TSA(I) (number of cards = no. of temperatures + 1)

1) If KRK(6) = 0 or 1, skip this card set

2) If KRK(6) = 2, read in an array of no more than fifteen temperatures, TSA(I) °K

CARD(S) 1,2.... (Columns 1-10, Format F10.5) one temperature per card

FINAL CARD blank

NOTE: The TSA(I) array built into GASKET contains temperatures from 1200 to 4000°K in 2000°K increments. Also, whenever KRK(6) $\geq$ 1 two surface equilibrium, zero-ablation calculations are performed for surface temperatures of 500 and 1000°K.

CARD SET 4 - ELEMENTAL COMPOSITION (number of cards = no. of elements +1)

CARD 1 (Columns 1-3, Format I3) the number of elements in the system

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

FIELD 1 (Columns 1-3, Format I3) the atomic number of the element

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

FIELD 3 (Columns 16-25, Format F10.5) the atomic weight of the element

FIELD 4 (Columns 26-35, Format F10.5) the relative amount of the element in the edge gas (this is the same as the relative amount of the element in the chamber or at the upstream side of a shock wave, since elements are conserved)

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

2) Negative values are in relative masses

FIELD 5 (Columns 46-55, Format F10.5) the relative amount of the element in the surface material (the present version of GASKET allows the surface to be comprised of carbon only; hence, the quantity 1.0 must be entered in this field for the element carbon)

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

1) If KRK(3) = 0, this card set must be skipped

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

3) If KRK(3) = 9, this card set must not be skipped

CARD 1 (Columns 1-3, Format I3) the total number of data items (e.g., 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

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

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.

CARD(S) 2,3,. . .

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

The "name" of the species for which data is to be provided, exactly 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" or "FFA" respectively here.

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

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

2) 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 manner replace either the values set automatically (see card 1 above) if the species thermochemical data are read from cards or tape, or the values built into the GASKET program (see Volume II).

NOTE: If KRK(3) = 9 and KRK(1) = 1,2,4, or 5, this card set must follow the OBLIQUE OR NORMAL SHOCK DATA card set; if KRK(3) = 1,2,3, or 4 this card set, if used, precedes the SPECIES THERMOCHEMICAL EQUILIBRIUM DATA card set.

CARD SET 6 - SPECIES THERMOCHEMICAL EQUILIBRIUM DATA (number of cards = 1 + 3 x no. of species)

1) If KRK(3) = 0 or 9, skip this card set

2) If KRK(3) = 1,2,3, or 4, read in this card set; there are three of these cards for each molecular, atomic, or condensed species; the end of this card set is signaled by a blank card

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 specie) (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 presumed 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 numbers of the elements in the molecule (the number of atoms of which was given in the previous field)

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

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 entered in card set 5

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 is in °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:

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

F5 = the entropy of the species at 3000°K in cal/mole °K

FIELD 7 (Columns 61-66, Format F6.0) the upper limit of the lower temperature range in °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.

See Section 3.1.3 for additional comments on the ordering of the species thermochemical data and the selection of base species.

NOTE: If this data is read in on cards, the species at the top of the deck must be in the following order: CO_2, H_2, H_2O, CO, C*, C_2H_2, HCl, HF, ... Furthermore, the atomic number of C* must be 106, rather than the actual value of 6. Finally, all condensed phase species (except C*) must follow the gas phase species.

CARD SET 7 - OBLIQUE OR NORMAL SHOCK DATA (1 card)

1) If KRK(1) = 0 or 3, skip this card set

2) If KRK(1) = 1,2,4, or 5, this card set must be read in

FIELD 1 (Column 1, Format I1) Input the variable KVH which determines how the velocity ahead of the shock, the static enthalpy ahead of the shock, and the total enthalpy are calculated (since total enthalpy = static enthalpy + 1/2 velocity^2)

If KVH = 1, velocity is calculated from specified total and static enthalpy

If KVH = 2, total enthalpy is calculated from specified static enthalpy and velocity

If KVH = 3, static enthalpy is calculated from specified total enthalpy and velocity

FIELD 2 (Columns 2-10, Format F9.4) The velocity variable, UR (this field is ignored if KVH = 1)

If UR ≠ -9999, then UR is assigned to SVL, the velocity upstream of the shock in ft/sec

If UR = -9999, the velocity calculated in the prior solution is assigned to SVL

FIELD 3 (Columns 11-20, Format F10.4) The total enthalpy variable, HTR (this field is ignored if KVH = 2)

If HTR ≠ 0, then HTR is assigned to HCH, the total enthalpy of the system in BTU/lbm
If HTR = 0, HCH is unchanged

FIELD 4 (Columns 21-30, Format F10.4) the static enthalpy variable, HSR (this field is ignored if KVH = 3)

If HSR ≠ -9999, then HSR is assigned to SH1, the static enthalpy upstream of the shock in BTU/lbm

If HSR = -9999., the static enthalpy calculated in the prior solution is assigned to SH1

FIELD 5 (Columns 41-50, Format F10.4) the shock angle (0.0 for a normal shock) in degrees

CARD SET 8 - REACTION RATE DATA (number of cards = 5 x MT at maximum)

1) If KRK(7) = 0, skip this card set

2) If KRK(7) = 1 or 3, the first subset of this card set must be read in

3) If KRK(7) = 2 or 3, the second subset of this card set must be read in

First Subset: MT cards

CARDS 1,2, . . ., MT

FIELD 1 (Columns 1-10, Format E10.4), FKF(M) the pre-exponential factor for the Mth reaction, lb mole/ft^{2}sec atm

FIELD 2 (Columns 11-20, Format E10.4), EAK(M), the activation energy for the Mth forward reaction, cal/gm mole

FIELD 3 (Columns 21-30, Format E10.4), EXK(M), the temperature exponent for the Mth reaction

Second Subset: 4 x MT cards (for maximum of 10 base species)

CARDS MT + 1, MT + 2; MT + 5, MT + 6;. . . 5 x MT - 3, 5 x MT - 2;

FIELDS 1-IS (Columns 1-10 x IS, Format 8F10.6, will require 2 cards if IS > 8) inhibiting specie partial pressure coefficient, PSI (J,M), J = 1, IS, atm^{-1} (see Section 2.2.2.2)

CARDS MT + 3, MT + 4; MT + 7, MT + 8; . . . 5 x MT - 1, 5 x MT

FIELDS 1-IS (Columns 1-10 x IS, Format 8F10.6, will require 2 cards if IS > 8) inhibiting specie partial pressure coefficient FKK(J,M), J = 1, IS, atm^{-1} (see Section 2.2.2.2)

NOTE: MT = no. of reactions

1) IF KRK(8) = 1, MT = 0, kinetics ignored

2) If KRK(8) = 2, MT = 1

M = 1 $C^* + CO_2 \rightleftarrows 2CO$

3) If KRK(8) = 3, MT = 1

M = 1 $2C^* + H_2 \rightleftarrows C_2H_2$

4) If KRK(8) = 4, MT = 4

M = 1 $C^* + H_2O \rightleftarrows CO + H_2$

M = 2 $C^* + CO_2 \rightleftarrows 2CO$

M = 3 $2C^* + H_2 \rightleftarrows C_2H_2$

M = 4 $H_2O + CO \rightleftarrows CO_2 + H_2$

IS = no. of base species

1) If KRK(8) = 1, kinetics ignored

2) If KRK(8) = 2, J = 1 CO_2

J = 2 CO

J = 3 C*

J $\geq$ 4 remaining base species

3) If KRK(8) = 3, J = 1 H_2

J = 2 C*

J = 3 C_2H_2

J $\geq$ 4 remaining base species

4) If KRK(8) = 4, J = 1 CO_2

J = 2 H_2

J = 3 H_2O

J = 4 CO

J = 5 C*

J = 6 HCl or HF

J $\geq$ 7 remaining base species

TO TERMINATE A JOB KRK(1) = 8 on final card

MULTIPLE JOBS

1) Several jobs may be loaded back to back, with a control card signifying the start of each new job:

```
CONTROL CARD #1
   :
ELEMENTAL COMPOSITION #1
   :
additional data as required for job #1
   :
CONTROL CARD #2
   :
ELEMENTAL COMPOSITION # 2
   :
additional data as required for job #2
   :
KRK(1) = 8
```

2) If jobs following the first job have the same elemental composition as the first job, Card Set #4 (ELEMENTAL COMPOSITION) may be replaced by a single blank card for all jobs after the first:

```
CONTROL CARD #1
   :
ELEMENTAL COMPOSITION #1
   :
additional data as required for job #1
   :
CONTROL CARD #2
   :
blank card
   :
additional data as required for job #2
   :
KRK(1) = 8
```

SECTION 5

SAMPLE PROBLEMS

Presented in this section are five sample problems which were run on a Univac 1108 digital computer. An attempt was made to utilize almost all of the options available in the GASKET program. For each sample problem, the following is presented:

- A brief description of the nature of the problem and solution
- A listing of the input data deck
- A few typical pages of the program output

Sample Problem 1

In this problem, ablation rates at the throat of a rocket nozzle are calculated. The propellant gases are comprised of seven elements, including both hydrogen and oxygen. The program options which utilize built-in physical data are selected; hence, only nine cards of input data are required for the complete sequence of calculations. The ideal chamber conditions (propellant flame temperature of 3764°K, ideal pressure of 68.07 atm) are input. After redefining the elemental set to include the fictitious element "GRAPHITE", subsequent calculations performed by the program include determination of the actual chamber state (54.42 atm) and an isentropic expansion to the throat (unity Mach no.). The boundary layer edge state at the throat is then recomputed with a redfined elemental set which includes the fictitious element "HOT DRY ICE"; this is done for the purpose of the subsequent surface kinetics calculations. The frozen edge state is computed for the built-in array of eight temperatures, and the surface ablation rate is computed for the built-in array of fifteen surface temperatures. Also, a punched card, with format appropriate for CMA input, is output for each of the frozen edge and surface solutions. Molecules whose concentrations are smaller than machine capacity appear with zero mole fractions in the output.

```
3001110410 1764.      54.42      -1.0      68.02      0.949      0.          PR 8. 1
  7
  1 HYDROGEN    1.008      3.3192
  4 BERYLLIUM   9.012      1.4265
  6 CARBON     12.011      0.9236              1.0
  7 NITROGEN   14.007      0.8352
  8 OXYGEN     16.0        1.9161
  9 FLUORINE   19.0        0.8680
 17 CHLORINE   35.453      0.4012
```

Sample Problem 1
Listing of Input

GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 0110000000

RELATIVE ELEMENTAL COMPOSITIONS. ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	EDGE GAS	SURFACE
1	HYDROGEN	1.00800	.0330707	.0000000
4	BERYLLIUM	9.01200	.0142129	.0000000
6	CARBON	12.01100	.0092023	.0000000
7	NITROGEN	14.00700	.0083215	.0000000
8	OXYGEN	16.00000	.0190910	.0000000
9	FLUORINE	19.00000	.0086483	.0000000
17	CHLORINE	35.45300	.0039973	.0000000
106	GRAPHITE	12.01100	.0000000	.0832570

ELEMENTS HYDROGEN BERYLLIUM CARBON NITROGEN OXYGEN
FLUORINE CHLORINE GRAPHITE

BASE SPECIES H2 BE CO2 CCLN H2O
FH CLH C. F

UPDATE OF DIFFUSION FACTORS

SPECIES	DIFFUSION FACTOR
CO2	1.24950
H2	.28302
H2O	.77040
CO	1.01720
C	.68950
CHN	1.14730
CH4	.95030
CN	1.03330
H	.19396
HO	.74210
N	.75530
O	.70630
N2	1.02750
O2	.95530

Sample Problem 1
Sample Output

GRAPHITE SURFACE KINETICS (GASKET) SOLUTION PROB. 1

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.49545-00	.12580+01	-.57602-00	.35229-01	.11338+01

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

TEMP	VISC	COND	DBAR	PR	SC
.67752+04	.60817-04	.74711-04	.23259-03	.81218-00	.72427-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.78138-00	.20521+02	.25599+02	.43715+04	.87678-00	.24336+04

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

1	4	6	7	8	9	17	106
.33335-01	.12809-00	.11053+00	.11656+00	.30546-00	.16432-00	.14172-00	.00000
.90344-01	.68015-01	.13745-00	.14421-00	.24135-00	.17505-00	.14359-00	.00000

SOLUTION TIMES
ITERATIONS = 29 TIME = 5.989 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .21215-00
TEMP = 6775.1499 DEG R. = 3764.0000 DEG K. PRESS = 68.02000 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.28931+03	-.58624+04	-.78736+03
ENTROPY - BTU/LBM DEG R	.28060+01	.15349+01	.25835+01
DENSITY - LBM/FT3	.29030-00		.35189-00
MOLECULAR WEIGHT	21.1184	25.0120	25.5986

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	.28681-02	H2	.31374-00	H2O	.32153-01	C* F	.00000	CLM	.39942-01
FM	.26427-01	BE	.37865-02	CCLN	.88120-07	CO	.23259-00	C2H2	.31456-07
C	.12442-06	C2	.66065-10	C3	.21189-12	C4	.84802-18	C F	.00000
C2 F	.00000	C3 F	.00000	C4 F	.00000	C2BE	.74619-09	BECL	.37108-02
BECLF	.36218-01	BECL2	.82985-02	BEF	.43163-01	BEF2	.40630-01	BEMO	.66279-02
BEH2	.19498-03	BEH2O2	.38210-02	HEO	.25368-03	BE2CL4	.35485-07	BE2O2	.27032-03
BE3O3	.24759-03	BE4O4	.85632-04	BE5O5	.31054-05	BE6O6	.20125-06	CCL	.36754-08
CCLFO	.58481-09	CCLF3	.79560-17	CCL2O	.24220-09	CCL3F	.43880-17	CCL4	.12540-17
CF	.21656-07	CFN	.44796-08	CF2	.12010-09	CF2O	.42082-09	CF3	.70361-14
CF4	.41132-17	CH	.10493-06	CHCLF2	.96051-14	CHCL2F	.86893-14	CHCL3	.47037-14
CHFO	.79573-07	CHF3	.43854-14	CHN	.51285-04	CHNO	.95549-06	CHO	.45571-04
CH2	.57841-07	CH2CLF	.28644-11	CH2CL2	.37433-11	CH2F2	.10232-11	CH2O	.27401-05
CH3	.44354-06	CH3CL	.10870-08	CH3F	.23177-09	CH4	.97096-07	CN	.24543-05
C2F2	.18879-15	C2F4	.28364-22	C2H4	.23420-10	C2H4O	.19663-14	C2N2	.24840-09
C3O2	.41003-10	C4N2	.75546-17	CL	.58432-02	CLF	.84859-07	CLFO3	.60026-24
CLF3	.87612-21	CLNO	.17413-05	CLNO	.18005-07	CLO	.15244-05	CLO2	.89297-11
CL2O	.95230-11	F	.11110-03	FHO	.13168-07	FN	.68111-08	FNO	.10759-08
FO	.39431-08	F2O	.32961-15	F3N	.24553-19	H	.69679-01	HN	.40321-04
HO	.38114-02	H2N	.29586-04	H2O2	.53788-07	H3N	.18218-04	H4N2	.45197-11
N	.27902-04	NO	.38568-03	NO2	.94106-08	N2O	.58770-07	N2O3	.10572-15
N2O4	.28330-11	N2O5	.17632-25	O	.48951-03	O3	.22818-11	CCL2F2	.72649-17
CCLO	.51757-0	CFO	.14886-06	C2F6	.68667-30	FNO2	.41704-14	CLNO2	.41138-13
F2N	.62872-13	FNO3	.19497-20	HNO	.83023-06	BEN	.17155-04	HNO2	.20359-08
HNO3	.18560-13	BE2O	.10082-02	F4N2	.16499-32	HO2	.12061-06	NO3	.47547-14
CF4O	.84379-23	CCL2	.82626-10	CCL3	.16171-13	F2N2	.42902-17	H2N2	.28485-08
BE2F2O	.17103-01	CN2	.88852-09	C2O	.24566-07	CLF5	.11751-36	BEM	.65591-15
FO2	.24159-11	C2H	.12374-07	C2N	.95277-09	C2CL4	.12864-20	C2CL6	.28053-30
C2HF	.67411-11	C2CL2	.17562-17	C2HCL	.15177-09	CHCL	.40746-08	CHF	.35808-0H
C2F3N	.17597-19	F3NO	.14489-24	F2	.31940-10	CL2	.30764-05	N2	.10623+00
O2	.19692-04	CNO	.14311-06	N3	.83700-09	CLM4N*	.00000	CLM4NO4*	.00000
BEH2O2*	.00000	BE*	.00000	HEO*	.17912-00	CBE2*	.00000	BE3N2*	.00000
HECL2*	.00000	HEF2*	.00000						

GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 2060200000

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.49506-00	.13039+01	-.60504-00	.36699-01	.11327+01

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

TEMP	VISC	COND	DBAR	PR	SC
.67212+04	.60485-04	.74235-04	.28089-03	.51243-00	.72426-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.78030-00	.20491+02	.25514+02	.44188+04	.87594-00	.24568+04

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

1	4	6	7	8	9	17	106
.33335-01	.12809-00	.11053+00	.11656+00	.30546-00	.16432-00	.14172-00	.00000
.96270-01	.68304-01	.13725-00	.14400-00	.24157-00	.17506-00	.14355-00	.00000

SOLUTION TIMES

ITERATIONS = 3 TIME = .942 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .21135-00

TEMP = 6721.2491 DEG R. = 3734.0273 DEG K. PRESS = 54.42000 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.29254+03	-.58969+04	-.78736+03
ENTROPY - BTU/LBM DEG R	.28272+01	.15297+01	.26009+01
DENSITY - LBM/FT3	.23351-00		.26286-00
MOLECULAR WEIGHT	21.0627	25.0120	25.5143

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	.29183-02	H2	.31040-00	H2O	.32357-01	C* F	.00000	CLM	.44019-01
FM	.26414-01	HE	.40393-02	CCLN	.67381-07	CO	.23178-00	C2H2	.19238-07
C	.10485-06	C2	.43830-10	C3	.11548-12	C4	.35696-18	C F	.00000
C2 F	.00000	C3 F	.00000	C4 F	.00000	C2BE	.49368-09	BECL	.37336-02
BECLF	.35728-01	BECL2	.81426-02	BEF	.44298-01	BEF2	.40404-01	BEMO	.67278-02
BEM2	.17333-03	BEM2O2	.37582-02	BEO	.27204-03	BE2CL4	.27308-07	BE2O2	.29386-03
BE3O3	.27990-03	BE4O4	.97477-04	BESO5	.35546-05	BE6O6	.23314-06	CCL	.28819-08
CCLFO	.46249-09	CCLF3	.44421-17	CCL2O	.19074-09	CCL3F	.26988-17	CCL4	.77082-18
CF	.17226-07	CFN	.33543-08	CF2	.89380-10	CF2O	.33469-09	CF3	.47004-14
CF4	.25784-17	CH	.81195-07	CHCLF2	.60000-14	CHCL2F	.54184-14	CHCL3	.29411-14
CHFO	.63030-07	CHF3	.27583-14	CHN	.39842-04	CHNO	.75218-06	CHO	.38830-04
CH2	.42021-07	CH2CLF	.15030-11	CH2CL2	.23708-11	CH2F2	.64383-12	CH2O	.21617-05
CH3	.30546-06	CH3CL	.09674-09	CH3F	.14695-09	CH4	.62909-07	CN	.19863-05
C2F2	.10752-15	C2F4	.13398-22	C2H4	.11879-10	C2H4O	.97335-15	C2N2	.14962-09
C3O2	.25279-10	C4H2	.28097-17	CL	.62048-02	CLF	.79011-07	CLFO3	.47634-24
CLF3	.58376-21	CLHO	.15640-05	CLNO	.16559-07	CLO	.15549-05	CLO2	.86633-11
CL2O	.76640-11	F	.11359-03	FHO	.12099-07	FN	.59609-08	FNO	.97331-09
FO	.37907-08	F2O	.93454-15	F3N	.16507-19	H	.73024-01	HN	.34700-04
HO	.40034-02	H2N	.25088-04	H2O2	.50038-07	H3N	.14492-04	H4N2	.27351-11
N	.27506-04	NO	.38019-03	NO2	.94616-08	N2O	.54463-07	N2O3	.88768-16
N2O4	.22938-21	N2O5	.13586-25	O	.54582-03	O3	.23779-11	CCL2F2	.44826-17
CCLO	.44727-05	CFO	.12597-05	C2F6	.26883-30	FNO2	.36221-14	CLNO2	.36384-13
F2N	.48535-13	FNO3	.15578-20	HNO	.76653-06	HEN	.15949-04	HNO2	.18689-08
HNO3	.16414-13	HE2O	.11155-02	F4N2	.79529-33	HO2	.12142-06	NO3	.44898-14
CF4O	.48137-23	CCL2	.60609-10	CCL3	.10865-13	F2N2	.29146-17	H2N2	.21249-08
HE2F2O	.16646-01	CN2	.83231-09	C2O	.17837-07	CLFS	.55392-37	BEM	.50405-15
FO2	.22864-11	C2H	.81306-08	C2N	.60477-09	C2CL4	.62617-21	C2CL6	.10766-30
C2HF	.39915-11	C2CL2	.10515-12	C2HCL	.92043-10	CHCL	.29571-08	CHF	.26186-08
C2F3N	.85521-20	F3NO	.11894-24	F2	.27915-10	CL2	.29698-05	N2	.10589+00
O2	.22352-04	CNO	.12322-06	N3	.66632-09	CLM4N*	.00000	CLM4NO4*	.00000
HEM2O2*	.00000	HE*	.00000	BEO*	.17796-00	CHE2*	.00000	BE3N2*	.00000
BECL2*	.00000	BEF2*	.00000						

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        GRAPHITE SURFACE KINETICS (GASKET) PROB. 1          3000100000

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNM/DLNT   DLNM/DLNP      GAMMA
  .49587-00    .12511+01   -.54367-00   .31934-01    .11302+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP         VISC         COND         DBAR          PR           SC
  .03793+04    .58468-04    .71940-04    .45482-03    .38744+00    .72433-00
     MU1          MU2        MOL.WT         MTIL         CPTIL        HTIL
  .77932-00    .20471+02    .25806+02    .30538+04    .87804-00    .21147+04

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA =  .667)
      1            6            8            7            8            9           17          106
   .33335-01    .12809-00    .11853+00    .11656+00    .30540-00    .16432-00    .14172-00    .00000
   .91602-01    .04916-01    .13895-00    .14577-00    .23695-00    .17659-00    .14517-00    .00000

SOLUTION TIMES
        ITERATIONS =    6                       TIME =     1.753 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

  MASS CONDENSED/MASS GAS =     .22523-00
  TEMP =  6379.3011 DEG R.  =  3544.0562 DEG K.      PRESS =      31.47833 ATM

                                GAS            CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM          .72629+02       -.01156+04        -.10649+04
  ENTROPY - BTU/LBM DEG R     .28496+01        .14963-01         .20089+01
  DENSITY - LBM/FT3           .14230-00                          .17436-00
  MOLECULAR WEIGHT           23.0621          25.0120           25.8059

 ABOVE ARE STATIC PROPERTIES                R-KINETIC =     .27759+03 BTU/LBM
  VEL. =      .3728+04 FT/SEC    FLUX =     .04995+03 LBM/FT2SEC   MACH =    1.00004

 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       .27318-02     H2        .32262-00     H2O       .30269-01     C* F      .00000        CLN       .41121-01
   FH        .26684-01     UE        .29798-02     CCLN      .36302-07     CO        .23664-00     C2H2      .88519-08
   C         .42832-07     C2        .12001-10     C3        .28176-13     C4        .51448-19     C F       .00000
   C2 F      .00000        C3 F      .00000        C4 F      .00000        C2BE      .10436-09     BECL      .28718-02
   BECLF     .37213-01     BECL2     .81873-02     HEF       .38901-01     BEF2      .44398-01     BEHO      .48529-02
   BEH2      .10969-03     BEH2O2    .30026-02     BEO       .16679-03     BE2CL4    .15897-07     BE2O2     .19662-03
   BE3O3     .24291-03     BE4O4     .88307-04     BESOS     .33307-05     BE6O6     .23615-06     CCL       .11208-08
   CCLFO     .23637-09     CCLF3     .14908-17     CCL2O     .94859-10     CCL3F     .75761-18     CCL4      .21509-18
   CF        .73673-08     CF2       .13668-08     CF3       .17757-10     CF2O      .17754-09     CF3       .14843-14
   CF4       .82069-18     CH        .31811-07     CHCLF2    .20569-14     CHCL2F    .18378-14     CHCL3     .18163-14
   CHFO      .35848-07     CHF3      .98948-15     CHN       .26279-04     CHNO      .43530-06     CHO       .23341-04
   CH2       .18336-07     CH2CLF    .71700-12     CH2CL2    .98335-12     CH2F2     .25524-12     CH2O      .13182-05
   CH3       .15837-06     CH3CL     .34490-09     CH3F      .67572-10     CH4       .36065-07     CN        .10136-05
   C2F2      .25143-14     C2H4      .21301-23     C2H6      .44983-11     C2H4O     .25138-15     C2N2      .57502-10
   C3O2      .91601-11     C4N2      .47399-14     CL        .55665-02     CLF       .44978-07     CLFO3     .47939-25
   CLF3      .83535-22     CLHO      .99412-06     CLNO      .73927-08     CLO       .84982-06     CLO2      .27128-11
   CL2O      .27719-11     F         .78547-04     FHO       .53668-08     FN        .23788-08     FNO       .38823-09
   FO        .14624-04     F2O       .90912-16     F3N       .26001-20     H         .65694-01     HN        .20948-04
   HO        .29339-02     H2N       .15136-04     H2O2      .22176-07     H3N       .97000-05     H4N2      .81192-12
   N         .15777-04     NO        .23032-03     NO2       .39910-08     N2O       .27127-07     N2O3      .14671-16
   N2O4      .23865-22     N2O5      .81268-27     O         .35128-03     O3        .92527-12     CCL2F2    .12848-17
   CCLO      .26961-05     CFO       .65594-07     C2F6      .28888-31     FNO2      .88244-15     CLNO2     .10023-13
   F2N       .12818-13     FNO3      .17391-21     HNO       .38644-06     HEN       .76398-05     HNO2      .72831-09
   HNO3      .39992-14     HE2O      .70920-03     F4N2      .34641-34     HO2       .53635-07     NO3       .99771-15
   CF4O      .65870-24     CCL2      .23277-10     CCL3      .35736-14     F2N2      .53440-18     H2N2      .88777-09
   BE2F2O    .15761-01     CN2       .22542-04     C2O       .71944-08     CLF3      .18459-38     BEH       .69606-16
   FO2       .60519-12     C2H       .31928-08     C2N       .20159-03     C2CL4     .12229-21     C2CL6     .10169-31
   C2HF      .13129-11     C2CL2     .36356-13     C2HCL     .36300-10     CHCL      .11634-08     CHO       .18842-08
   C2F3N     .16821-20     F3NO      .11447-25     F2        .10373-10     CL2       .21574-05     N2        .18720-00
   O2        .13016-04     CNO       .36336-07     N3        .24375-09     CLHNO*    .00000        CLHNO2*   .00000
   BEH2O2*   .00000        BE*       .00000        HEO*      .18965-09     CBE2*     .00000        BEJN2*    .00000
   BECL2*    .00000        BEF2*     .00000
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GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 0110000000

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	EDGE GAS	SURFACE
1	HYDROGEN	1.00800	.0330707	.0000000
4	BERYLLIUM	9.01200	.0142129	.0000000
6	CARBON	12.01100	.0090964	.0000000
7	NITROGEN	14.00700	.0083215	.0000000
8	OXYGEN	16.00000	.0188793	.0000000
9	FLUORINE	19.00000	.0086483	.0000000
17	CHLORINE	35.45300	.0039973	.0000000
106	GRAPHITE	12.01100	.0032570	.0032570
44	HOT DRY ICE	44.01100	.0001054	.0000000

ELEMENTS	HYDROGEN	BERYLLIUM	CARBON	NITROGEN	OXYGEN
	FLUORINE	CHLORINE	GRAPHITE	HOT DRY ICE	
BASE SPECIES	H2	BE	CO	CCLN	H2O
	FH	CLH	C2F	CO2	

UPDATE OF DIFFUSION FACTORS

SPECIES	DIFFUSION FACTOR
CO2	1.24950
H2	.26302
H2O	.77040
CO	1.01720
C	.68950
CHN	1.14730
CH4	.95030
CN	1.03330
H	.19396
HO	.74210
N	.75530
O	.70630
N2	1.02750
O2	.95530

Sample Problem 1
Sample Output, Continued

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.49587-00	.12479+01	-.54134-00	.31302-01	.11303+01

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

TEMP	VISC	COND	DBAR	PR	SC
.63793+04	.58468-04	.71948-04	.45482-03	.30744-00	.72033-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.77932-00	.20471+02	.25800+02	.3953E+04	.67804-00	.21147+04

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

1	4	6	7	8	9	17	106	44
.33335-01	.12809-00	.10926+00	.11656+00	.30207-00	.16432-00	.14172-00	.00000	.44509-02
.91602-01	.04916-01	.13756-00	.14577-00	.23323-00	.17659-00	.14517-00	.00000	.51141-02

SOLUTION TIMES

ITERATIONS = 26 TIME = 6.254 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .22523-00

TEMP = 6379.3011 DEG R. = 3544.0562 DEG K. PRESS = 31.47833 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.72630+02	-.61156+04	-.18649+04
ENTROPY - BTU/LBM DEG R	.28496+01	.14963+01	.26009+01
DENSITY - LBM/FT3	.14230-00		.17436-00
MOLECULAR WEIGHT	21.0621	25.0120	25.8059

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	.27318-02	H2	.32262-00	H2O	.30269-01	CO	.23469-00	C* F	.00000
CLH	.41120-01	FH	.20684-01	BE	.29798-02	CCLN	.36302-07	C2H2	.00519-00
C	.42832-07	C2	.12001-10	C3	.28174-13	C4	.51448-19	C F	.00000
C2 F	.00000	C3 F	.00000	C4 F	.00000	C2BE	.16436-09	BECL	.28718-02
BECLF	.37213-01	BECL2	.01873-02	BEF	.38901-01	BEF2	.44398-01	BEHO	.00529-02
BEH2	.10869-03	BEH2O2	.00026-02	BEO	.16679-03	BE2CL4	.15897-07	BE2O2	.19662-03
BE3O3	.24291-03	BE4O4	.00307-04	BE5O5	.33307-05	BE6O6	.23613-06	CCL	.11200-08
CCLFO	.23637-09	CCLF3	.14808-17	CCL2O	.94859-10	CCL3F	.75741-18	CCL4	.21569-18
CF	.73673-08	CFH	.15668-08	CF2	.37757-10	CF2O	.17754-09	CF3	.14843-14
CF4	.02069-18	CH	.31811-07	CHCLF2	.20564-14	CHCL2F	.18370-14	CHCL3	.10163-14
CHFO	.35848-07	CHF3	.98968-15	CHN	.26279-04	CHNO	.43530-06	CHO	.23341-04
CH2	.18336-07	CH2CLF	.71700-12	CH2CL2	.98335-12	CH2F2	.25524-12	CH2O	.13102-05
CH3	.15837-06	CH3CL	.34490-09	CH3F	.67572-10	CH4	.36865-07	CN	.10136-05
C2F2	.25193-16	C2F4	.21301-23	C2H4	.44983-11	C2H4O	.25130-15	C2N2	.57502-10
C3O2	.91461-11	C4N2	.47399-18	CL	.55665-02	CLF	.44978-07	CLFO3	.47909-25
CLF3	.03535-22	CLHO	.99812-06	CLNO	.73927-08	CLO	.84982-06	CLO2	.27128-11
CL2O	.27719-11	F	.78548-04	FHO	.55668-08	FN	.23708-08	FNO	.38823-09
FO	.14624-08	F2O	.90911-15	FJN	.26001-20	H	.65694-01	HN	.20948-06
HO	.29339-02	HFN	.15136-04	H2O2	.22176-07	H3N	.97008-05	H4N2	.81192-12
N	.15777-04	NO	.25032-03	NO2	.39910-08	N2O	.27127-07	N2O3	.14671-16
N2O4	.23865-22	N2O5	.81268-27	O	.35128-03	O3	.62527-12	CCL2F2	.12848-17
CCLO	.26841-05	CFO	.55594-07	C2F6	.28887-31	FNO2	.88244-15	CLNO2	.10023-13
F2N	.12818-13	FNO3	.17391-21	HNO	.38649-06	HFN	.76398-05	HNO2	.72831-09
HNO3	.39992-14	HF2O	.70920-03	F4N2	.34641-34	HO2	.53635-07	NO3	.99771-15
CF4O	.65870-24	CCL2	.23277-10	CCL3	.35738-14	F2N2	.53440-18	H2N2	.88777-09
HF2F2O	.15761-31	CH2	.22592-09	C2O	.71998-08	CLF5	.18459-38	BEM	.09606-16
FO2	.80519-12	C2H	.31928-08	C2N	.20159-09	C2CL4	.12229-21	C2CL6	.10169-31
C2HF	.13129-11	C2CL2	.34554-13	C2HCL	.38300-10	CHCL	.11634-08	CHF	.10862-08
C2F3O	.16821-26	F3NO	.11447-25	F2	.10373-10	CL2	.21579-05	N2	.10720+00
O2	.13015-04	CNO	.58038-07	N3	.24375-09	CLH4NO	.00000	CLH4NO4	.00000
BEH2O2	.00000	BEO	.00000	BE3O	.18966-00	CHE2O	.00000	BE3N2O	.00000
HECL2O	.00000	HEF2O	.00000						

GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 0000000001

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.36603+00	.49695+02	-.43916+01	.49080-01	.99538+00

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

TEMP	VISC	COND	DBAR	PR	SC
.90000+03	.10085-04	.15701-04	.17053-04	.30511+00	.72433+00
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.77932-00	.20471+02	.25806+02	-.45437+03	.69384+00	-.13337+04

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

1	4	6	7	8	9	17	106	44
.33335-01	.12809+00	.10926+00	.11656+00	.30207+00	.16432+00	.14172+00	.00000	.46589-02
.91662-01	.64916-01	.13756+00	.14577+00	.23323+00	.17659+00	.14517+00	.00000	.51141-02

SOLUTION TIMES
ITERATIONS = 26 TIME = .326 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000
TEMP = 900.0000 DEG R. = 500.0000 DEG K. PRESS = 31.47833 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.22911+04	.00000	-.37409+04
ENTROPY - BTU/LBM DEG R	.20345+01	.00000	.17153+01
DENSITY - LBM/FT3	.10087+01		.12359+01
MOLECULAR WEIGHT	21.0621	.0000	25.8059

Sample Problem 1
Sample Output, Continued

5-6

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(31.4783 .00000 .00000 500.0000 .667 -740.922-1272.832-1 CHAR .000)

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	.27318-02	H2	.32262-00	H2O	.30269-01	CO	.23469+00	C* F	.00000
CLH	.41120-01	FH	.26684-01	BE	.29798-02	CCLN	.36302-07	C2H2	.88519-08
C	.42832-07	C2	.12001-10	C3	.28174-13	C4	.51448-19	C F	.00000
C2 F	.00000	C3 F	.00000	C4 F	.00000	C2BE	.16436-09	BECL	.28718-02
BECLF	.37213-01	BECL2	.01873-02	BEF	.38901-01	BEF2	.44390-01	BEHO	.48529-02
BEH2	.10869-03	BEH2O2	.30026-02	BEO	.16679-03	BE2CL4	.15897-07	BE2O2	.19662-03
BE3O3	.24291-03	BE4O4	.08307-04	BE5O5	.33307-05	BE6O6	.23613-06	CCL	.11200-08
CCLFO	.23637-09	CCLF3	.14808-17	CCL2O	.94859-10	CCL3F	.75741-18	CCL4	.21569-18
CF	.73673-08	CFN	.15668-08	CF2	.37757-10	CF2O	.17754-09	CF3	.14843-14
CF4	.82069-18	CH	.31811-07	CHCLF2	.20569-14	CHCL2F	.18370-14	CHCL3	.10163-14
CHFO	.35848-07	CHF3	.98948-15	CHN	.26279-04	CHNO	.43530-06	CHO	.23341-04
CH2	.18336-07	CH2CLF	.71700-12	CH2CL2	.98335+12	CH2F2	.25524-12	CH2O	.13182-05
CH3	.15837-06	CH3CL	.34490-09	CH3F	.67572-10	CH4	.36865-07	CN	.10136-05
C2F2	.25193-16	C2F4	.21301-23	C2H4	.44983-11	C2H4O	.25130-15	C2N2	.57502-10
C3O2	.91461-11	C4N2	.47399-18	CL	.55665-02	CLF	.44978-07	CLFO3	.47909-25
CLF3	.83535-22	CLHO	.99812-06	CLNO	.73927-08	CLO	.84982-06	CLO2	.27128-11
CL2O	.27719-11	F	.78548-04	FHO	.55668-08	FN	.23708-08	FNO	.38823-09
FO	.14624-08	F2O	.90911-16	F3N	.26601-20	H	.65694-01	HN	.20948-04
HO	.29339-02	H2N	.15136-04	H2O2	.22176-07	H3N	.97080-05	H4N2	.81192-12
N	.15777-04	NO	.23032-03	NO2	.39910-08	N2O	.27127-07	N2O3	.14671-16
N2O4	.23865-22	N2O5	.01208-27	O	.35128-03	O3	.62527-12	CCL2F2	.12848-17
CCLO	.24841-05	CFO	.05594-07	C2F6	.28887-31	FNO2	.88244-15	CLNO2	.10023-13
F2N	.12818-13	FNO3	.17391-21	HNO	.38649-06	BEN	.76398-05	HNO2	.72831-09
HNO3	.39992-14	HE2O	.70920-03	F4N2	.34641-34	HO2	.53635-07	NO3	.99771-15
CF4O	.65870-24	CCL2	.23277-10	CCL3	.3573d-14	F2N2	.53440-18	H2N2	.88777-09
BE2F2O	.15761-01	CN2	.22592-09	C2O	.71998-08	CLF5	.18459-38	BEH	.69609-16
FO2	.60519-12	C2H	.31928-08	C2N	.20159-09	C2CL4	.12229-21	C2CL6	.10169-31
C2HF	.13129-11	C2CL2	.34554-13	C2HCL	.36300-10	CHCL	.11634-08	CHF	.10842-08
C2F3N	.16821-20	F3NO	.11497-25	F2	.10373-10	CL2	.21579-05	N2	.10720+00
O2	.13016-04	CNO	.98038-07	N3	.24375-09	CLH4NO	.00000	CLH4NO4*	.00000
BEH2O2*	.00000	BE*	.00000	BEO*	.18966-00	CBE2*	.00000	BE3N2*	.00000
BECL2*	.00000	BEF2*	.00000						

GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 0000000001

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.49957-00	.10754+01	-.47532-00	.31302-01	.11422+01

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

TEMP	VISC	COND	UBAR	PR	SC
.72000+04	.63322-04	.79012-04	.55595-03	.38013-00	.72433-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.77932-00	.20471+02	.25806+02	.46796+04	.89062-00	.26797+04

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX = .6667)

1	6	6	7	8	9	17	106	44
.33335-01	.12809-00	.10926+00	.11656+00	.30207-00	.10432-00	.14172-00	.00000	.46589-02
.91602-01	.64916-01	.13756-00	.14577-00	.23323-00	.17659-00	.14517-00	.00000	.51141-02

SOLUTION TIMES

ITERATIONS = 26 TIME = .319 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 7199.9999 DEG R. = 4000.0000 DEG K. PRESS = 31.47833 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY = BTU/LBM	.45489+03	.00000	-.65045+03
ENTROPY = BTU/LBM DEG R	.29060+01	.00000	.26611+01
DENSITY = LBM/FT3	.12608-00		.15448-00
MOLECULAR WEIGHT	21.0621	.0000	25.8059

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .

(31.4783 .00000 .000004000.0000 .667 1488.700 252.716-1 CHAR .000 1

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	.27318-02	H2	.32262-00	H2O	.30264-01	CO	.23469-00	C* F	.00000
CLH	.41120-01	FH	.66684-01	HE	.29798-02	CCLN	.36302-07	C2H2	.00519-00
C	.42832-07	C2	.12001-10	C3	.28174-13	C4	.51448-19	C F	.00000
C2 F	.00000	C3 F	.00000	C4 F	.00000	C2BE	.16436-09	BECL	.28718-02
BECLF	.37213-01	BECL2	.61873-02	BEF	.38901-01	BEF2	.44390-01	BEHO	.48529-02
BEH2	.10869-03	BEH2O2	.30028-02	BEO	.16679-03	BE2CL4	.15897-07	BE2O2	.19662-03
BE3O3	.24291-03	BE4O4	.88307-04	BE5O5	.33307-05	BE6O6	.23613-06	CCL	.11200-08
CCLFO	.23437-09	CCLF3	.14808-17	CCL2O	.94859-10	CCL3F	.75741-18	CCL4	.21569-18
CF	.73673-08	CFN	.15668-08	CF2	.37757-10	CF2O	.17754-09	CF3	.14843-14
CF4	.82069-18	CH	.31811-07	CHCLF2	.20569-14	CHCL2F	.18378-14	CHCL3	.10163-14
CHFO	.35848-07	CHF3	.98948-15	CHN	.26279-04	CHNO	.43530-06	CHO	.23341-04
CH2	.18336-07	CH2CLF	.71700-12	CH2CL2	.98335-12	CH2F2	.25524-12	CH2O	.13182-05
CH3	.15837-06	CH3CL	.34490-09	CH3F	.67572-10	CH4	.30865-07	CN	.10136-05
C2F2	.25193-16	C2F4	.21301-23	C2H4	.44983-11	C2H4O	.25130-15	C2N2	.57502-10
C3O2	.91461-11	C4N2	.47399-18	CL	.55665-02	CLF	.44976-07	CLFO3	.47909-25
CLF3	.83535-22	CLNO	.99812-06	CLNO	.73927-08	CLO	.84982-06	CLO2	.27128-11
CL2O	.27719-11	F	.78548-04	FHO	.55666-08	FN	.23708-08	FNO	.38823-09
FO	.14624-08	F2O	.90911-16	F3N	.26601-20	H	.65696-01	HN	.20948-04
HO	.29339-02	H2N	.15136-04	H2O2	.22176-07	H3N	.97000-05	H4N2	.81192-12
N	.15777-04	NO	.25032-03	NO2	.39910-08	N2O	.27127-07	N2O3	.14671-16
N2O4	.23865-22	N2O5	.81264-27	O	.35128-03	O3	.62527-12	CCL2F2	.12848-17
CCLO	.26841-05	CFO	.05594-07	C2F6	.28887-31	FNO2	.88244-15	CLNO2	.10023-13
F2N	.12814-13	FNO3	.17391-21	HNO	.38649-06	HFN	.76398-05	HNO2	.72831-09
HNO3	.39992-14	HF2O	.70920-03	F4N2	.34641-34	HO2	.53635-07	NO3	.99771-15
CF4O	.65870-24	CCL2	.63277-10	CCL3	.35738-14	F2N2	.53440-18	H2N2	.88777-09
HF2FO	.15701-01	CH2	.22542-09	C2O	.71998-08	C2CL4	.18459-38	BFM	.69606-16
FO2	.90514-12	C2H	.31428-08	C2N	.20159-09	C2CL6	.12229-21	C2CL6	.10169-31
C2HF	.13129-11	C2CL2	.34554-13	C2HCL	.38300-10	CHCL	.11634-08	CNN	.10842-08
C2F3N	.18421-20	F3NO	.11497-25	F2	.10373-10	CL2	.21579-05	N2	.10720-00
O2	.13016-04	CFO	.58034-07	N3	.24375-09	CLH4NO	.00000	CLH4NO4*	.00000
HBH2O2*	.00000	BE*	.00000	HFO*	.18966-00	CHE2*	.00000	BE3N2*	.00000
HECL2*	.00000	HBF2*	.00000						

GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 0003000001

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.37125-00	.63883-00	-.70841-01	.61789-02	.11498+01

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

TEMP	VISC	COND	DBAR	PR	SC
.90000+03	.15054-04	.91906-05	.17953-04	.60811-00	.72460-00
MU1	MU2	MOL.WT	MTIL	CPTIL	HTIL*
.98048-00	.24096+02	.26136+02	-.36088+04	.43507-00	-.37705+04

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

1	4	6	7	8	9	17	106	44
.74878-01	.84611-01	.12401+00	.13638-00	.21593-00	.20247-00	.15556-00	.11511-18	.55602-02
.91662-01	.64916-01	.13756-00	.14577-00	.23323-00	.17659-00	.14517-00	.10000-18	.51141-02

SOLUTION TIMES
ITERATIONS = 44 TIME = 8.984 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
MASS TRANSFER COEFFICIENT ROUCM = .94400-00
RHO V WALL/RHOE UE CM = .10000-18 BPRIME = .10300-18

STATE ADJACENT TO THE SURFACE . . . .
TEMP = 900.0000 DEG R = 500.0000 DEG K PRESS = 31.47833 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.40089+04	.00000	-.40089+04
ENTROPY - BTU/LBM DEG R	.18305+01	.00000	.00000
DENSITY - LBM/FT3	.12517+01		.12517+01
MOLECULAR WEIGHT	26.1362	.0000	26.1362

PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
(31.4783 .00000 .00000 500.0000 .667-2094.749-2227.164 0 CHAR .000)

CHEMICAL STATE ADJACENT TO THE SURFACE
(MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES)
(MOLE FR FOR CONDENSED = BPRIME CONDENSED). . . .

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.33019-02	H2	.38535-01	H2O	.24874-00	CO	.31879-10	C* F	.00000
CLH	.10979+00	FH	.26262-03	BE	.00000	CCLN	.73794-27	C2H2	.14257-27
C	.00000	C2	.00000	C3	.00000	C4	.00000	C F	.00000
C2 F	.00000	C3 F	.10609-20	C4 F	.61827-19	C2BE	.00000	BECL	.16784-33
BECLF	.43058-02	BECL2	.29201-03	HEF	.75311-27	HEF2	.13681-00	BEHO	.24826-31
BEH2	.11101-33	BE2O2	.16684-03	BEO	.00000	BE2CL4	.11414-08	BE2O2	.00000
BE3O3	.61125-25	BE4O4	.68055-17	BE5O5	.20299-10	BE6O6	.17247-01	CCL	.00000
CCLFO	.56123-25	CCLF3	.00000	CCL2O	.20480-25	CCL3F	.00000	CCL4	.00000
CF	.00000	CF2	.14533-37	CF2	.00000	CF2O	.14640-24	CF3	.00000
CF4	.00000	CH	.00000	CHCLF2	.40093-31	CHCL2F	.2072E-30	CHCL3	.26268-28
CHFO	.13878-19	CHF3	.15[illegible]-30	CHN	.39571-16	CHNO	.41014-17	CHO	.3N684-28
CH2	.00000	CH2CLF	.6[illegible]-22	CH2CL2	.31696-18	CH2F2	.60042-24	CH2O	.29408-15
CH3	.15713-19	CH3CL	.74805-09	CH3F	.90969-15	CH4	.27115-00	CN	.00000
C2F2	.00000	C2F4	.00000	C2H4	.37511-15	C2H4O	.13956-30	C2N2	.67054-37
C3O2	.00000	C4N2	.00000	CL	.89263-21	CLF	.1912E-36	CLFO3	.00000
CLF3	.00000	CLHO	.45599-26	CLNO	.00000	CLO	.00000	CLO2	.00000
CL2O	.00000	F	.17517-37	FHO	.00000	FN	.00000	FNO	.00000
FO	.00000	F2O	.00000	F3N	.00000	H	.29885-21	HN	.34161-35
HO	.11507-26	H2	.59951-20	H2O2	.11511-36	H3N	.43981-01	H4N2	.15961-21
N	.00000	NO	.33632-32	NO2	.00000	N2O	.20371-35	N2O3	.00000
N2O4	.00000	N2O5	.00000	O	.00000	O3	.00000	CLL2F2	.00000
CCLO	.32890-27	CFO	.14686-37	C2F6	.00000	FNO2	.00000	CLNO2	.00000
F2N	.00000	FNO3	.00000	HNO	.87978-36	HEN	.00000	HNO2	.00000
HNO3	.00000	HE2O	.00000	F4N2	.00000	HO2	.00000	NO3	.00000
CF4O	.00000	CCL2	.00000	CCL3	.00000	F2N2	.00000	H2N2	.31282-28
BE2F2O	.16655-03	CN2	.00000	C2O	.00000	CLF5	.00000	BEM	.00000
FO2	.00000	C2N	.00000	C2N	.00000	C2CL4	.00000	C2CL6	.00000
C2HF	.00000	C2CL2	.00000	C2HCL	.25803-36	CHCL	.00000	CHF	.00000
C2F3N	.00000	F3NO	.00000	F2	.00000	CL2	.10476-20	N2	.10525+00
O2	.00000	CNO	.00000	N3	.00000				

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        GRAPHITE SURFACE KINETICS (GASKET) PROB. 1          0002000001

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNV/DLNP      GAMMA
  .45925-00    .15656+01    -.31404-00    .23647-01    .10684+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,DEG-R,AND DEG-R
    TEMP          VISC          COND          UBAR          PR            SC
  .18000+04     .24455-04     .21791-04     .55747-04     .51634-00     .72386-00
    MU1           MU2          MOL.WT         HTIL          CPTIL         HTIL*
  .90664-00     .22947+02     .24744+02    -.26439+04     .83557-00    -.28858+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA =  .667)
      1             4             6             7             8             9            17            106           44
   .60998-01     .82547-01     .12040-00     .13886-00     .21821-00     .20456-00     .10287-00     .10594-10     .55519-02
   .91602-01     .64916-01     .13756-00     .14577-00     .23323-00     .17659-00     .14517-00     .10000-10     .51141-02

SOLUTION TIMES
        ITERATIONS =     4                          TIME =     2.342 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUGH =     .74900-00
 RHO V WALL/RHOE UE CH =     .10000-10    APRIME =     .10000-10

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  1800.0000 DEG R =  1000.0000 DEG K      PRESS =      31.47833 ATM

                                  GAS              CONDENSED        COMPOSITE
  ENTHALPY = BTU/LBM           -.32690+04          .00000          -.32690+04
  ENTROPY = BTU/LBM DEG R       .21654+01          .00000           .00000
  DENSITY = LBM/FT3             .59382-00                           .59382-00
  MOLECULAR WEIGHT             24.7994             .0000           24.7993


 PUNCHED CARD OUTPUT (80 COLUMNS) . . . .
( 31.4783   .00000  .000001000.0000 .667-1003.237-1010.106 0  CHAR        .000      )

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = APRIME CONDENSED ). . . .

   SPECIES   MOLE FR.    SPECIES   MOLE FR.    SPECIES   MOLE FR.    SPECIES   MOLE FR.    SPECIES   MOLE FR.
   CO2       .31284-02   H2        .26236-00   H2O       .16441-00   CO        .92119-01   C* F      .00000
   CLH       .76699-01   FH        .40702-02   BE        .83947-22   CCLN      .59291-12   C2H2      .54928-09
   C         .27978-33   C2        .14302-34   C3        .34824-32   C4        .00000      C F       .77108-26
   C2 F      .10863-25   C3 F      .72397-19   C4 F      .11171-22   C2HE      .29235-30   BECL      .75103-15
   BECLF     .27936-01   BECL2     .40456-02   BEF       .16947-11   BEF2      .10774+00   BEHO      .14855-13
   BEH2      .10977-15   BEH2O2    .40165-02   BEO       .65663-24   BE2CL4    .16544-07   BE2O2     .22552-19
   BE3O3     .81032-11   BE4O4     .23494-07   BESOS     .37897-05   BE6O6     .10449-01   CCL       .65381-27
   CCLFO     .21459-12   CCLF3     .52771-24   CCL2O     .99471-13   CCL3F     .20929-24   CCL4      .23104-24
   CF        .11223-24   CFN       .28484-17   CF2       .12975-21   CF2O      .22738-12   CF3       .18929-26
   CF4       .13197-23   CH        .78037-26   CHCLF2    .38233-18   CHCL2F    .87041-18   CHCL3     .56170-17
   CHFO      .98119-09   CH2       .38136-16   CHN       .11256-05   CHNO      .55521-07   CHO       .16233-10
   CH2       .30535-14   CH2CLF    .13434-12   CH2CL2    .68993-11   CH2F2     .89994-14   CH2O      .78096-06
   CH3       .31620-08   CH3CL     .23570-05   CH3F      .25304-08   CH4       .16886-00   CN        .34299-18
   C2F2      .53070-32   C2H       .03328-36   C2H4      .14926-05   C2H4O     .19715-14   C2N2      .27690-14
   C3O2      .34476-13   C4N2      .14270-23   CL        .66593-10   CLF       .19379-19   CLFO3     .00000
   CLF3      .00000      CLNO      .75391-14   CLNO      .14504-21   CLO       .28625-21   CLO2      .21626-35

   CL2O      .16734-29   F         .47376-18   FHO       .16112-22   FN        .83582-29   FNO       .32858-26
   FO        .32869-32   F2O       .00000      F3N       .00000      H         .18121-09   HN        .34620-17
   HO        .31243-12   H2N       .38191-11   H2O2      .32786-19   H3N       .57390-03   H4N2      .93498-16
   N         .18488-22   NO        .39554-15   NO2       .31674-26   N2O       .58758-19   N2O3      .00000
   N2O4      .00000      N2O5      .00000      O         .35283-21   O3        .00000      CCL2F2    .22585-24
   CCLO      .49036-11   CFO       .40744-19   C2F6      .00000      FNO2      .00000      CLNO2     .17114-34
   F2N       .21733-37   FNO3      .00000      HNO       .27158-16   HFN       .53168-28   HNO2      .58259-23
   HNO3      .98303-35   BF2O      .23573-23   F4N2      .00000      HO2       .12736-24   NO3       .00000
   CF4O      .00000      CCL2      .38045-22   CCL3      .31827-23   F2N2      .00000      H2N2      .91974-17
   BE2F2O    .47502-02   CN2       .11134-23   C2O       .10976-19   CLF5      .00000      BFH       .00000
   FO2       .00000      C2H       .11404-18   C2H       .54441-23   C2CL4     .43817-27   C2CL6     .00000
   C2HF      .43445-28   C2CL2     .30542-20   C2HCL     .42104-14   CHCL      .78566-21   CHF       .13926-20
   C2F3O     .49419-28   F3NO      .00000      F2        .67271-33   CL2       .86570-12   N2        .12264+00
   O2        .14158-21   C4O       .98361-19   N3        .41858-25
```

GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 5002000061

REACTANT
COEFFICIENTS

REACTION	1	2	3	4
CO2		1		
H2			1	
H2O	1			1
CO				1
C* F	1	1	2	
CLH				
FM				
BE				
CCLN				

PRODUCT
COEFFICIENTS

REACTION	1	2	3	4
CO2				1
H2	1		3	1
H2O			-2	
CO	1	2	2	
C* F				
CLH				
FM				
BE				
CCLN				

KINETIC REACTION---	1	2	3	4
PRE-EXPONENT FACTOR	1.317+01	1.317+01	8.114-01	1.054+00
ACTIVATION ENERGY	4.600+04	4.600+04	5.350+04	0.000
TEMPERATURE EXPONENT	0.000	0.000	0.000	0.000

SPECIES
INHIBITING
FACTORS
PSI/FRR

CO2	1.00/	.00	1.00/	.00	1.00/	.00	.00/	.00
H2	1.00/	.00	1.00/	.00	.00/	.00	.00/	.00
H2O	1.00/	.00	1.00/	.00	1.00/	.00	.00/	.00
CO	1.00/	.00	1.00/	.00	1.00/	.00	.00/	.00
C* F	.00/	.00	.00/	.00	.00/	.00	.00/	.00
CLH	.00/	3.00	.00/	3.00	.00/	.00	.00/	.00
FM	.00/	.00	.00/	.00	.00/	.00	.00/	.00
BE	.00/	.00	.00/	.00	.00/	.00	.00/	.00
CCLN	.00/	.00	.00/	.00	.00/	.00	.00/	.00

Sample Problem 1
Sample Output, Continued

```
DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNM/DLNP      GAMMA
  .42837-00    .12392+01   -.50270-00   -.34647-00    .33396+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DBAR           PR            SC
  .21600+04     .28445-04     .28696-04     .75436-04     .42461-00     .72393-00
     MU1           MU2          MOL.WT         MTIL         CPTIL         MTIL*
  .83886-00     .21896+02     .23804+02    -.17654+04     .71918-00    -.21926+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA =  .667)
      1             4             6             7             8             9            17           106           44
   .45610-01     .80889-01     .11931+00     .13771-00     .20225-00     .20499-00     .16772-00     .19984-24     .41525-01
   .91602-01     .64916-01     .12842-00     .14577-00     .20890-00     .17659-00     .14517-00     .25207-24     .38573-01

SOLUTION TIMES
        ITERATIONS =   10                        TIME =    2.724 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUGH =    .94900-00
 RHO V WALL/RHOE UE CM =    .15066-08   APRIME =    .15066-08

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2160.0000 DEG R =  1200.0000 DEG K      PRESS =     31.47833 ATM

                                  GAS            CONDENSED       COMPOSITE
  ENTHALPY - BTU/LBM           -.27867+04         .00000          -.27867+04
  ENTROPY - BTU/LBM DEG R       .22215+04         .00000           .00000
  DENSITY - LBM/FT3             .47500-00                          .47500-00
  MOLECULAR WEIGHT             23.8042             .0000          23.8042


 PUNCHED CARD OUTPUT (40 COLUMNS) . . . .
( 31.4783  .00000  .00000 1200.0000 .667-1218.115-1548.149 ) C* F       .000     )

 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .72208-10  2=   .28438-10  3=   .12345-10  4=   .75985-03

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = APRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   CO2       .22460-01    H2        .34462-00    H2O       .56987-01    CO        .18384-00    C* F      .00000
   CLH       .52691-01    FH        .38247-02    HE        .13621-16    CCLN      .21612-10    C2H2      .34595-07
   C         .32019-24    C2        .12143-27    C3        .10901-25    C4        .93992-33    C F       .35108-24
   C2 F      .14599-27    C3 F      .34370-25    C4 F      .13585-32    C2BE      .21316-23    BECL      .19141-11
   BECLF     .40732-01    BECL2     .95950-02    BEF       .39543-09    BEF2      .90350-01    BEMO      .13797-10
   BEH2      .43406-12    BEH2O2    .28641-02    BEO       .55942-19    BE2CL4    .47580-07    BE2O2     .25203-15
   BE3O3     .13660-08    BE4O4     .64441-06    BESO5     .20087-04    BE6O6     .64090-02    CCL       .34577-22
   CCLFO     .48326-12    CCLF3     .47859-23    CCL2O     .28644-12    CCL3F     .35121-23    CCL4      .37447-23
   CF        .21053-20    CFN       .86603-15    CF2       .65686-19    CF2O      .35805-12    CF3       .53856-24
   CF4       .64006-23    CH        .98114-21    CHCLF2    .21656-17    CHCL2F    .52602-17    CHCL3     .25380-16
   CHFO      .19832-08    CHF3      .13887-17    CHN       .13412-04    CHNO      .16498-06    CHO       .77268-09
   CH2       .69764-15    CH2CLF    .40957-12    CH2CL2    .11979-10    CH2F2     .30632-13    CH2O      .20703-05
   CH3       .71563-07    CH3CL     .10630-05    CH3F      .45374-08    CH4       .52586-01    CN        .12970-14
   C2F2      .11129-27    C2F4      .51329-33    C2H4      .39120-05    C2H4O     .18467-13    C2N2      .57706-12
   C3O2      .12919-11    C4N2      .11919-19    CL        .28103-08    CLF       .43337-17    CLFO3     .00000
   CLF3      .00000       CLNO      .14465-12    CLNO      .42253-19    CLO       .22652-18    CLO2      .53965-31
   CL2O      .35969-26    F         .43946-15    FHO       .74323-20    FN        .21763-24    FNO       .45118-23
   FO        .15429-27    F2O       .00000       F3N       .00000       H         .20555-07    HN        .39301-14
   HO        .26200-10    H2N       .38226-09    H2O2      .28732-17    H3N       .41364-03    H4N2      .15266-14
   N         .25536-18    NO        .67862-13    NO2       .51033-23    N2O       .88455-17    N2O3      .00000
   N2O4      .00000       N2O5      .00000       O         .16558-17    O3        .45754-37    CCL2F2    .31883-23
   CCLO      .16544-09    CFO       .41540-14    C2F6      .00000       FNO2      .12777-34    CLNO2     .67340-31
   F2N       .15749-32    FNO3      .00000       HNO       .70763-16    HEN       .59609-22    HNO2      .19014-20
   HNO3      .21494-31    BE2O      .99792-18    F4N2      .00000       HO2       .20431-21    NO3       .57818-38
   CF4O      .00000       CCL2      .38991-19    CCL3      .45779-21    F2N2      .31589-38    H2N2      .94386-15
   HE2F2O    .15761-01    CN2       .13030-19    C2O       .41112-16    CLF5      .00000       BEN       .00000
   FO2       .37113-35    C2N       .99891-15    C2N       .16780-18    C2CL4     .24700-25    C2CL6     .72459-38
   C2H       .52342-17    C2CL2     .11280-17    C2HCL     .38579-12    CHCL      .18674-17    CHF       .23211-17
   C2F3N     .52334-26    F3NO      .00000       F4        .21348-28    CL2       .10572-10    N2        .11880+00
   O2        .14007-14    CNO       .45004-15    N3        .15992-21
```

GRAPHITE SURFACE KINETICS (GASKET) PROB. 1 5002000041

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.46349+00	.10410+01	-.72163+00	.47678+01	.11590+01

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

TEMP	VISC	COND	DBAR	PR	SC
.72000+04	.62663-04	.78502-04	.55595-03	.36997+00	.72440+00
MU1	MU2	MOL.WT	MTIL	CPTIL	RTIL*
.75181+00	.19541+02	.19410+02	.76090+04	.89359+03	.48070+04

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

1	4	6	7	8	9	17	106	44
.39015-01	.67724-01	.14835-00	.13877-00	.21986-00	.18440-00	.16237-00	.36207-01	.32169-02
.89557-01	.61282-01	.14882-00	.13828-00	.22291-00	.16664-00	.13641-00	.33311-01	.28135-02

SOLUTION TIMES

ITERATIONS = 8 TIME = [illegible] SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
MASS TRANSFER COEFFICIENT ROUCM = .04900-00
RHO V WALL/RHOE UE CM = .53955-01 B'PRIME = .53955-01

STATE ADJACENT TO THE SURFACE . . . .
TEMP = 7195.9999 DEG R = 4000.0000 DEG K PRESS = 31.47833 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY = BTU/LBM	.19527+04	.00000	.19527+04
ENTROPY = BTU/LBM DEG R	.70271+01	.00000	.00000
DENSITY = LBM/FT3	.11613-02		.11613-02
MOLECULAR WEIGHT	.19419+02	.0000	19.4097

PUNCHED CARD OUTPUT (80 COLUMNS) . . .
(3,1.4783 .00000 .05388+000.0000 .667 2673.355 1025.200) C* F .000)

NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
(MOLES OF REACTION / UNIT SURFACE AREA / TIME - RHOE UE CM). . . .
1= -.23437-03 2= .27058-04 3= .36305-03 4= -.25312-04

CHEMICAL STATE ADJACENT TO THE SURFACE
(MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES)
(MOLE FR FOR CONDENSED = MOLES/TOTAL CONDENSED) . . . .

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.14[illegible]-02	H2	.[illegible]+00	H2O	.12710-01	CO	.23764-00	C* F	.00000
CLH	.30[illegible]-01	[illegible]	[illegible]	BE	.91361-02	CCLN	.16879-05	CBE2	.72038-03
C	.78[illegible]-06	C2	.[illegible]-03	C3	.[illegible]-12	C4	.[illegible]-17	C F	.[illegible]-22
C2 F	.28[illegible]-02	C3 F	.[illegible]-03	C4 F	.10414-03	C2OE	.15[illegible]-03	BECN	.[illegible]-06
BECLF	.[illegible]-01	BECL2	.[illegible]-02	BEF	.61[illegible]-01	BEF2	.[illegible]-01	BENO	.[illegible]-02
BEH2	.11[illegible]-03	BEH2O2	.[illegible]-03	OBE	.[illegible]-03	BE2CL4	.43[illegible]-07	BE2O2	.[illegible]-11
BE3O3	.82[illegible]-15	BE4O4	.[illegible]-05	BE5O5	.[illegible]-08	BE606	.[illegible]-10	CF	.[illegible]-07
CCLF3	.[illegible]-09	CCLF3	.[illegible]-6	CF2O	.[illegible]-09	CCL3F	.48[illegible]-1	[illegible]	.[illegible]-17
CF	.92[illegible]-07	CFN	.[illegible]-04	CF2	.[illegible]-09	CF2O	.44[illegible]-08	CFO	.[illegible]-13
CF4	.[illegible]-07	CH	.[illegible]-05	CHCLF2	.93[illegible]-10	CHCL2F	.[illegible]-14	CHCL3	.[illegible]-10
CHFO	.[illegible]-07	CH2	.92[illegible]-10	CHN	.[illegible]-04	CHNO	.43[illegible]-05	CHO	.[illegible]-04
CH2	.72[illegible]-07	CH2CL	.[illegible]-11	CH2CL2	.[illegible]-11	CH2F2	.71[illegible]-12	CH3	.[illegible]-05
CH3	.21263-06	CH3CL	.[illegible]	CH3F	.[illegible]-10	CH4	.18833-07	CN	.[illegible]-05
C2F2	.[illegible]-13	C2F4	.[illegible]-22	C2H4	.[illegible]-11	C2H4O	.[illegible]-15	C2N2	.[illegible]-09
C3O2	.21[illegible]-10	C4N2	.[illegible]-17	CL	.1[illegible]-01	CLF	.[illegible]-05	CLFO2	.[illegible]-23
CLF3	.[illegible]-28	CLO	.[illegible]-04	CLNO	.[illegible]-07	CLO	.[illegible]-06	CLN2	.[illegible]-10
CL2O	.[illegible]-10	F	.[illegible]-03	FNO	.17306-07	FN	.[illegible]-07	FO2	.[illegible]-07
FO	.[illegible]-07	FO2	.[illegible]-10	H2N	.[illegible]-19	H	.[illegible]	HF	.[illegible]-04
HO	.[illegible]-04	HCN	.[illegible]-06	HCO2	.[illegible]-07	HCN	.[illegible]-05	HCNO	.[illegible]-12
N	.[illegible]-04	NO	.[illegible]-04	NO2	.[illegible]-05	N2O	.[illegible]-07	N2O3	.[illegible]-15
N2O4	.[illegible]-21	N2O5	.[illegible]-25	O	.13684-02	O2	.[illegible]-12	OCLCF2	.[illegible]-15
OCLO	.[illegible]-09	OFO	.[illegible]-08	O2F2	.14575-29	FN2	.[illegible]-14	CLNO2	.[illegible]-13
F2N	.[illegible]-12	FNO2	.[illegible]-13	FNO	.67359-06	HCN	.[illegible]-04	HNO2	.[illegible]-09
HNO3	.[illegible]-14	CF2O	.[illegible]-13	FNO2	.[illegible]-31	NO2	.[illegible]-06	N2	.[illegible]-14
CH4O	.[illegible]-22	CF2	.[illegible]-03	CCL3	.[illegible]-13	F2NO	.[illegible]-16	HCN2	.[illegible]-05
BEF2O	.[illegible]-02	CN2	.[illegible]-07	C2O	.41978-07	CLF3	.[illegible]-35	SEN	.[illegible]-16
FO2	.[illegible]-11	C2H	.[illegible]-07	C2N	.[illegible]-04	C2CL4	.[illegible]-21	C2CL6	.[illegible]-30
C2HF	.[illegible]-10	C2CL4	.[illegible]-13	C2HCL	.[illegible]-03	CHCL	.[illegible]-38	CHF	.[illegible]-05
C2F3N	.26117-19	[illegible]	.[illegible]-24	N2	.[illegible]-03	CL2	.51940-05	N2	.[illegible]-01
O2	.26989-04	CNO	.[illegible]-06	N3	.[illegible]-03				

Sample Problem 2

The shockwave option of GASKET is utilized in this problem. The boundary layer edge state is specified as the stagnation condition behind a normal shock wave with an upstream Mach number of two. The shock is assumed to exist in the divergent section of a nozzle and, thus, conditions upstream of the shock are calculated via an isentropic expansion from input ideal chamber conditions. Since the edge gases contain both hydrogen and oxygen, all three kinetically-controlled surface reactions are possible, requiring that the edge state be recalculated in terms of an elemental set which contains the fictitious element "HOT DRY ICE". Two temperatures are input for both the frozen-edge and surface temperature arrays. Finally, the diffusion factors are updated for sixteen selected species.

```
5091220400 3901.     40.81     -2.0      68.02     0.463     0.0       PROB. 2
 1000.
 1500.

 1200.
 1400.

  6
  1 HYDROGEN   1.008     3.2219
  6 CARBON     12.011     .56490                    1.0
  7 NITROGEN   14.008     0.5366
  8 OXYGEN     16.0       2.2486
 13 ALUMINUM   26.98      1.013
 17 CHLORINE   35.453     0.5396
1              0.0      -9999.          0.0
016
C              0.69180CH          0.74920CH4          0.93570CN          1.02670
CO             1.01700CO2         1.29140C2H2         1.17460H           0.30180
H2             0.38930H2O         0.7749ON            0.74930NO          0.99810
N2             1.026200           0.7397002           1.00000C2          1.02530
```

Sample Problem 2
Listing of Input

```
                GRAPHITE SURFACE KINETICS (GASKET) PROB. 2          0110000*00

RELATIVE ELEMENTAL COMPOSITIONS. ATOMIC WTS/UNIT MASS
   AT.NO.   ELEMENT      ATOMIC WT      ENVE GAS       SURFACE
      1     HYDROGEN       1.00800      .0322228      .0000000
      6     CARBON        12.01100      .0056497      .0000000
      7     NITROGEN      14.00800      .0053666      .0000000
      8     OXYGEN        16.00000      .0224887      .0000000
     13     ALUMINUM      26.98000      .0101312      .0000000
     17     CHLORINE      35.45300      .0053966      .0000000
    106     GRAPHITE      12.01100      .0000000      .0032570

 ELEMENTS          HYDROGEN    CARBON    NITROGEN    OXYGEN    ALUMINUM
                   CHLORINE    GRAPHITE

 BASE SPECIES      H2          CO2         ALN         H2O         AL
                   CLH         C( P

UPDATE OF DIFFUSION FACTORS
      SPECIES     DIFFUSION FACTOR
        CO2          1.24950
        H2            .28302
        H2O           .77040
        CO           1.01720
        C             .68950
        CHN          1.14730
        CH4           .95030
        CN           1.03330
        H             .19396
        HO            .74210
        N             .75530
        O             .70630
        N2           1.02750
        O2            .95530
```

Sample Problem 2
Sample Output

GRAPHITE SURFACE KINETICS (GASKET) SOLUTION PROB. 2

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.42292-00	.12704+01	-.81277-00	.49322-01	.11173+01

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

TEMP	VISC	COND	DBAR	PR	SC
.70218+04	.63390-04	.85944-04	.24081-03	.20630-00	.72419-00
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.72973-00	.19512+02	.33302+02	.65918+04	.96722-00	.43581+04

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

1	6	7	8	13	17	106
.32481-01	.67858-01	.75176-01	.35982-00	.27334-00	.19133-00	.00000
.11385+00	.11708+00	.12939-00	.29554-00	.66241-01	.27791-00	.00000

Sample Problem 2
Sample Output, Continued

SOLUTION TIMES
ITERATIONS = 26 TIME = 3.246 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .72936-00
TEMP = 7021.8000 DEG R. = 3901.0000 DEG K. PRESS = 68.02000 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.19525+04	-.45284+04	-.78083+03
ENTROPY - BTU/LBM DEG R	.29116+01	.98046-00	.20972+01
DENSITY - LBM/FT3	.25542-00		.44171-00
MOLECULAR WEIGHT	19.2566	101.9600	33.3017

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	.66737-02	H2	.32617-00	H2O	.10141+00	C* F	.00000	CLH	.10313+00
AL	.34058-02	ALN	.82812-06	CO	.18139-00	C2H2	.21056+08	C	.61831-07
C2	.82812-11	C3	.55589-14	C4	.61063-20	C F	.00000	C2 F	.00000
C3 F	.00000	C4 F	.00000	CAL	.15831-08	ALCL	.30936-01	ALCLO	.57869-02
ALCL2	.10086-01	ALCL3	.16870-03	ALH	.48001-03	ALHO2	.26118-02	ALO	.22287-02
AL2CL6	.23471-10	AL2O	.14065-02	AL2O2	.13165-04	CCL	.40178-08	CCLN	.59873-07
CCL2O	.13633-08	CCL4	.10457-16	CH	.46306-07	CHCL3	.21823-13	CHN	.12381-04
CHNO	.71154-06	CHO	.43116-04	CH2	.20572-07	CH2CL2	.62541-11	CH2O	.22213-05
CH3	.12184-06	CH3CL	.65646-09	CH4	.21308-07	CN	.81829-06	C2H4	.13289-11
C2H4O	.40597-15	C2N2	.14721-10	C3O2	.67098-11	C4N2	.28976-19	CL	.19085-01
CLHO	.18073-04	CLNO	.20132-06	CLO	.19456-04	CLO2	.46403-09	CL2O	.30312-09
H	.92099-01	HN	.54938-04	HO	.16300-01	H2N	.33594-04	H2O2	.78275-06
H3N	.16738-04	H4N2	.48775-11	N	.43875-04	NO	.14886-02	NO2	.14500-06
N2O	.22029-06	N2O3	.65204-14	N2O4	.67023-19	N2O5	.16930-22	O	.26375-02
O3	.17661-09	CCLO	.12986-04	CLNO2	.17837-11	HNO	.34734-05	HNO2	.28569-07
HNO3	.10025-11	ALHO	.30332-02	HO2	.20304-05	NO3	.31523-12	CCL2	.19414-09
CCL3	.89553-13	H2N2	.31548-08	CN2	.28302-09	C2O	.67846-08	C2H	.10787-08
C2N	.80645-10	C2CL4	.41519-20	C2CL6	.66049-29	ALO2	.30842-03	C2CL2	.88878-13
C2HCL	.27663-10	CHCL	.38207-08	CL2	.24543-04	N2	.88531-01	O2	.32087-03
CNO	.14688-06	N3	.10383-08	ALCLO*	.00000	CLH4N*	.00000	CLH4NO4*	.00000
ALCL3*	.00000	AL4*	.00000	C3AL4*	.00000	AL*	.00000	AL2O3*	.13775-00

GRAPHITE SURFACE KINETICS (GASKET) PROB. 2 2000200*00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.42239-00	.13866+01	-.90232-00	.51733-01	.11154+01

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

TEMP	VISC	COND	DBAR	PR	SC
.68863+04	.62553-04	.84896-04	.39809-03	.20604-00	.72416-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.72632-00	.19417+02	.32991+02	.67808+04	.96810-00	.44581+04

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

1	6	7	8	13	17	106
.32481-01	.67858-01	.75176-01	.35982-00	.27334-00	.19133-00	.00000
.11401+00	.11665+00	.12891-00	.29553-00	.67230-01	.27768-00	.00000

SOLUTION TIMES

ITERATIONS = 4 TIME = .728 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .72535-00

TEMP = 6884.3426 DEG R. = 3824.6348 DEG K. PRESS = 40.81000 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.19713+04	-.45750+04	-.78083+03
ENTROPY - BTU/LBM DEG R	.29649+01	.97375-00	.21278+01
DENSITY - LBM/FT3	.15520-00		.26178-00
MOLECULAR WEIGHT	19.1214	101.9600	32.9911

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	.66537-02	H2	.31918-00	H2O	.53949-01	C* F	.00000	CLN	.10115+00
AL	.38022-02	ALN	.50657-06	CO	.17969-00	C2H2	.74241-09	C	.42786-07
C2	.34514-11	C3	.15460-14	C4	.97634-21	C F	.00000	C2 F	.00000
C3 F	.00000	C4 F	.00000	CAL	.91975-09	ALCL	.31652-01	ALCLO	.60022-02
ALCL2	.87658-02	ALCL3	.12383-03	ALH	.42869-03	ALHO2	.26299-02	ALO	.24448-02
AL2CL6	.79110-11	AL2O	.14643-02	AL2O2	.13718-04	CCL	.23068-08	CCLN	.32715-07
CCL2O	.74638-09	CCL4	.50500-17	CH	.26486-07	CHCL3	.71758-14	CHN	.72295-05
CHNO	.41051-06	CHO	.29750-04	CH2	.10257-07	CH2CL2	.21814-11	CH2O	.12919-05
CH3	.54212-07	CH3CL	.24238-09	CH4	.83042-08	CN	.51453-06	C2H4	.30769-12
C2H4O	.84817-16	C2N2	.49752-11	C3O2	.22958-11	C4N2	.35187-20	CL	.21246-01
CLHO	.15146-04	CLNO	.15334-06	CLO	.18796-04	CLO2	.38034-09	CL2O	.21339-09
H	.10201+00	HN	.43884-04	HO	.17377-01	H2N	.22969-04	H2O2	.60492-06
H3N	.99528-05	H4N2	.14795-11	N	.41831-04	NO	.15439-02	NO2	.13280-06
N2O	.17527-06	N2O3	.37498-14	N2O4	.33785-19	N2O5	.72538-23	O	.31984-02
O3	.16678-09	CCLO	.83870-05	CLNO2	.11840-11	HNO	.27484-05	HNO2	.21329-07
HNO3	.65483-12	ALHO	.30323-02	HO2	.18712-05	NO3	.23762-12	CCL2	.93650-10
CCL3	.34507-13	H2N2	.10033-08	CN2	.13424-09	C2O	.33600-08	C2H	.42864-09
C2N	.30570-10	C2CL4	.77d00-21	C2CL6	.68000-30	ALO2	.34066-03	C2CL2	.28156-13
C2HCL	.92955-11	CHCL	.18479-08	CL2	.21402-04	N2	.87688-01	O2	.38865-03
CNO	.93854-07	N3	.60622-09	ALCLO*	.00000	CLH4N*	.00000	CLH4NO4*	.00000
ALCL3*	.00000	ALN*	.00000	C3AL4*	.00000	AL*	.00000	AL2O3*	.13603-00

Sample Problem 2
Sample Output, Continued

GRAPHITE SURFACE KINETICS (GASKET) PROB. 2 3090100.00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.42269+00	.11586+01	-.62808+00	.13428+01	.11111+01

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

TEMP	VISC	COND	UBAR	PR	SC
.50395+04	.55682-04	.77734-04	.22498-02	.18879+00	.72459+00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.71350+00	.18915+02	.34302+02	.55014+04	.99567+00	.35830+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA = .6667)

1	6	7	8	13	17	106
.32481-01	.07858-01	.75176-01	.33982+00	.27334+00	.19133+00	.00000
.12300+00	.12546+00	.13856+00	.27217+00	.35335-01	.30547+00	.00000

SOLUTION TIMES

ITERATIONS = 8 TIME = 1.345 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .88180+00
TEMP = 5839.4894 DEG R. = 3244.1609 DEG K. PRESS = 5.49552 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.14632+04	-.49298+04	-.15325+04
ENTROPY - BTU/LBM DEG R	.31947+01	.91785+00	.21278+01
DENSITY - LBM/FT3	.23489-01		.44201-01
MOLECULAR WEIGHT	18.2284	101.9600	34.3022

ABOVE ARE STATIC PROPERTIES H-KINETIC = .75171+03 BTU/LBM
VEL. = .6134+04 FT/SEC FLUX = .27115+03 LBM/FT2SEC MACH = 2.00004

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	.57209-02	H2	.35901-00	H2O	.83425-01	C* F	.00000	CLH	.13072-00
AL	.10242-02	ALN	.28258-07	CO	.18807-00	C2H2	.34420-10	C	.22052-08
C2	.38865-13	C3	.86160-17	C4	.75291-24	C F	.00000	C2 F	.00000
C3 F	.00000	C4 F	.00000	CAL	.13461-10	ALCL	.19180-01	ALCLO	.31976-02
ALCL2	.59715-02	ALCL3	.91060-04	ALH	.66581-04	ALHO2	.73140-03	ALO	.43778-03
AL2CL6	.87125-12	AL2O	.22594-03	AL2O2	.16613-05	CCL	.10736-09	CCLN	.39858-08
CCL2O	.87546-19	CCL4	.97773-19	CH	.10628-08	CHCL3	.23143-15	CHN	.14241-05
CHNO	.55785-07	CHO	.50794-05	CH2	.52174-09	CH2CL2	.10684-12	CH2O	.20665-06
CH3	.43098-08	CH3CL	.17695-10	CH4	.87998-09	CN	.49285-07	C2H4	.60162-14
C2H4O	.50490-14	C2N2	.12998-12	C3O2	.52202-13	C4N2	.36829-23	CL	.19774-01
CLHO	.35784-05	CLNO	.14000-07	CLO	.36808-05	CLO2	.12836-10	CL2O	.11578-10
H	.80464-01	HN	.70500-05	HO	.74123-02	H2N	.39382-05	H2O2	.47674-07
H3N	.21445-05	H4N2	.18136-13	N	.76695-05	NO	.46799-03	NO2	.99719-08
N2O	.19280-07	N2O3	.12673-16	N2O4	.26873-22	N2O5	.10826-26	O	.10038-02
O3	.31625-11	OCLO	.16992-05	CLNO2	.23685-13	HNO	.31138-06	HNO2	.11866-08
HNO3	.77978-14	ALHO	.10204-02	HO2	.16204-06	NO3	.23443-14	CCL2	.44773-11
CCL3	.10596-14	H2N2	.74820-19	CN2	.36115-11	C2O	.13471-09	C2N	.13267-10
C2N	.55724-12	C2CL4	.35730-23	C2CL6	.33362-33	ALO2	.49740-04	C2CL2	.61964-15
C2HCL	.31049-12	CHCL	.79977-10	CL2	.10683-04	N2	.91798-01	O2	.93085-04
CNO	.73107-08	N3	.20736-10	ALCLO*	.00000	CLH4N*	.00000	CLH4NO4*	.00000
ALCL3*	.00000	ALN*	.00000	C3AL4*	.00000	AL*	.00000	AL2O3*	.15765-00

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        GRAPHITE SURFACE KINETICS (GASKET) PROB. 2          4000300*00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNM/DLNT    DLNM/DLNP      GAMMA
  .42211-00    .14694*01   -.95477-00    .55541-01    .11133*01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,ANU DEG-R
    TEMP          VISC          COND          DBAR          PR            SC
  .66873*04     .61318-04     .83637-04     .67562-03     .28389-00     .72416-00
     MU1           MU2         MOL.WT          MTIL          CPTIL         MTIL*
  .72173-00     .19279*02     .32841*02     .68743*04     .97282-00     .64948*04

ELEMENTAL R AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .667)
       1             6             7             8            13            17           106
   .32681-01     .67858-01     .75176-01     .35982-00     .27334-00     .19133-00     .00000
   .11506-00     .11712-00     .12962-00     .29348-00     .65858-01     .27987-00     .00000

SOLUTION TIMES
        ITERATIONS =    6                    TIME =    1.030 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

  MASS CONDENSED/MASS GAS =     .73629-00
  TEMP =  6687.2656 DEG R.  =  3715.1476 DEG K.     PRESS =     22.91480 ATM

                                GAS           CONDENSED       COMPOSITE
  ENTHALPY - BTU/LBM           .19547*04      -.40619*04       -.84269*03
  ENTROPY - BTU/LBM DEG R      .30294*01       .96388-00        .21535*01
  DENSITY - LBM/FT3            .88743-01                        .15408-00
  MOLECULAR WEIGHT            18.9142        181.9600          32.8407

  VEL2 =      .1760*04 FT/SEC     MACH2 =     .52408    THETA 2 =    .000000 DEG
 ABOVE ARE STATIC CONDITIONS DOWNSTREAM OF THE SHOCK FOR ....
  VEL1 =   .613*04 FT/SEC   H1-STATIC = -.133*04 BTU/LBM   H-TOT = -.781*03 BTU/LBM
  P1 =      5.49552 ATM    RHO1 =     .44201-01 LBM/FT3 THETA 1 =    .000000 DEG

 STATIC 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       .65564-02    H2        .31647-00    H2O       .95760-01    C* F      .00000     CLH       .10142*00
   AL        .38077-02    ALN       .34484-06    CO        .17895-00    C2H2      .24784-09    C         .25334-07
   C2        .11894-11    C3        .36160-15    C4        .12402-21    C F       .00000     C2 F      .00000
   C3 F      .00000       C4 F      .00000       CAL       .43016-04    ALCL      .31211-01    ALCL0     .59247-02
   ALCL2     .75907-02    ALCL3     .93415-04    ALH       .34178-03    ALHO2     .24153-02    ALO       .23392-02
   AL2CL6    .26957-11    AL2O      .13303-02    AL2O2     .12240-04    CCL       .11576-08    CCLN      .16873-07
   CCL2O     .38401-09    CCL4      .13481-17    CH        .13116-07    CHCL3     .21872-14    CHN       .48872-05
   CHNO      .22344-06    CHO       .19152-04    CH2       .46026-08    CH2CL2    .72890-12    CH2O      .71657-06
   CH3       .22828-07    CH3CL     .86581-10    CH4       .31923-08    CN        .29628-06    C2H4      .67664-13
   C2H4O     .15627-16    C2N2      .19319-11    C3O2      .70615-12    C4N2      .36202-21    CL        .23141-01
   CLHO      .11749-04    CLNO      .11238-06    CLO       .16213-04    CLO2      .25128-09    CL2O      .12834-09
   H         .10941*00    HN        .31837-04    HO        .17248-01    H2N       .14686-04    H2O2      .40443-06
   H3N       .57495-05    H4N2      .48757-12    N         .35504-04    NO        .14003-32    NO2       .10214-06
   N2O       .12314-05    N2O3      .13538-14    N2O4      .11265-19    N2O5      .10562-23    O         .34605-02
   O3        .11904-09    OCLO      .54886-05    OLNO2     .63000-12    OHO       .19268-05    OHO2      .13448-07
   OHO3      .33097-12    ALHO      .28892-02    HO2       .14418-05    NO3       .13371-12    OCL2      .48612-10
   OCL3      .11982-13    H2N2      .72689-09    CN2       .55121-10    C2O       .14722-08    C2H       .15323-09
   C2N       .10107-10    C2CL4     .12804-21    C2CL6     .57316-31    ALO2      .32281-03    C2CL2     .68981-14
   C2HCL     .28984-11    CHCL      .79415-09    CL2       .18123-04    N2        .87344-01    O2        .41154-03
   CNO       .53479-07    N3        .38166-09    ALCLO*    .00000       CLH4N*    .00000       CLH4NO4*  .00000
   ALCL3*    .00000       ALN*      .00000       C3AL4*    .00000       AL*       .00000       AL2O3*    .13659-00
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GRAPHITE SURFACE KINETICS (GASKET) SOLUTION PROB. 2

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.42201-00	.14002+01	-.9798E-00	.57413-01	.11137+01

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

TEMP	VISC	COND	DBAR	PR	SC
.67695+04	.61849-04	.84085-04	.59241-03	.28559-00	.72413-00
MU1	MU2	MOL.WT	MTIL	CPTIL	KTIL*
.72313-00	.19328+02	.3273++02	.69537+04	.96967-00	.45517+04

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

1	6	7	8	13	17	106
.32481-01	.67858-01	.75176-01	.35982-00	.27334-00	.19133-00	.00000
.11425+00	.11636+00	.12059-00	.29538-00	.67808-01	.27761-00	.00000

SOLUTION TIMES

ITERATIONS = 3 TIME = .591 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .72313-00

TEMP = 6769.4887 DEG R. = 3760.8271 DEG K. PRESS = 20.66891 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.19911+04	-.48140+04	-.78083+03
ENTROPY - BTU/LBM DEG R	.38108+01	.96803-00	.21535+01
DENSITY - LBM/FT3	.10247+00		.17658-00
MOLECULAR WEIGHT	18.4969	101.4000	32.7342

ABOVE ARE ISENTROPIC STAGNATION CONDITIONS DOWNSTREAM OF THE SHOCK FOR . . .

VEL1 = .613+04 FT/SEC H1-STATIC = -.133+04 BTU/LBM H-TOT = -.781+03 BTU/LBM

P1 = 5.49552 ATM RHO1 = .44201-01 LBM/FT3 THETA 1 = .000000 DEG

ISEN. STAG. 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	.66236-02	H2	.31348-00	H2O	.96753-01	C* F	.00000	CLM	.99456-01
AL	.41188-02	ALN	.41766-06	CO	.17828-00	C2H2	.31317-09	C	.31169-07
C2	.16523-11	C3	.53144-15	C4	.21191-21	C F	.00000	C2 F	.00000
C3 F	.00000	C4 F	.00000	CAL	.57684-09	ALCL	.32853-01	AL2CL0	.61399-02
ALCL2	.77695-02	ALCL3	.95614-04	ALH	.38619-03	ALHO2	.26195-02	ALO	.26043-02
AL2CL6	.31976-11	AL2O	.14931-02	AL2O2	.13975-04	CCL	.14410-08	CCLN	.19759-07
CCL2O	.45038-09	CCL4	.18794-17	CH	.16507-07	CHCL3	.28378-14	CHN	.46282-05
CHNO	.25959-06	CHO	.21772-04	CH2	.57276-08	CH2CL2	.90860-12	CH2O	.82280-06
CH3	.27674-07	CH3CL	.10615-09	CH4	.38141-08	CN	.35106-06	C2H4	.91792-13
C2H4O	.23109-16	C2N2	.60220-11	C3O2	.94152-12	C4N2	.61269-21	CL	.23104-01
CLHO	.12970-04	CLNO	.12088-06	CLO	.18042-04	CLO2	.31606-09	CL2O	.15699-09
H	.11054+00	HN	.38140-04	HO	.18182-01	H2N	.16678-04	H2O2	.48257-06
H3N	.84636-05	H4N2	.56614-12	N	.39802-04	NO	.15770-02	NO2	.12157-06
N2O	.14358-06	N2O3	.63101-14	N2O4	.18539-19	N2O5	.34507-23	O	.37086-02
O3	.15513-09	CCLO	.81631-05	CLNO2	.82685-12	HNO	.22404-05	HNO2	.16506-07
HNO3	.45050-12	ALHO	.30067-02	HO2	.17220-05	NO3	.18344-12	CCL2	.50729-10
CCL3	.15513-13	H2N2	.90646-09	CN2	.71754-10	C2O	.18646-08	C2H	.19873-09
C2N	.13601-10	C2CL4	.19259-21	C2CL6	.10187-30	ALO2	.36433-03	C2CL2	.10805-13
C2HCL	.37572-11	CHCL	.10041-06	CL2	.18990-04	N2	.86994-01	O2	.44935-03
CNO	.64259-07	N3	.38385-09	ALCLO*	.00000	CLH4N*	.00000	CLH4NO4*	.00000
ALCL3*	.00000	ALN*	.00000	C3AL4*	.00000	AL*	.00000	AL2O3*	.13473-00

Sample Problem 2
Sample Output, Continued

GRAPHITE SURFACE KINETICS (GASKET) PROB. 2 0110090*00

RELATIVE ELEMENTAL COMPOSITIONS. ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	EDGE GAS	SURFACE
1	HYDROGEN	1.00800	.0322228	.0000000
6	CARBON	12.01100	.0054473	.0000000
7	NITROGEN	14.00800	.0053666	.0000000
8	OXYGEN	16.00000	.0220840	.0000000
13	ALUMINUM	26.98000	.0101312	.0000000
17	CHLORINE	35.45300	.0053966	.0000000
106	GRAPHITE	12.01100	.0000000	.0832570
44	HOT DRY ICE	44.01100	.0002023	.0000000

ELEMENTS HYDROGEN CARBON NITROGEN OXYGEN ALUMINUM
CHLORINE GRAPHITE HOT DRY ICE

BASE SPECIES H2 CO ALN H2O AL
CLH C. F CO2

UPDATE OF DIFFUSION FACTORS

SPECIES	DIFFUSION FACTOR
CO2	1.24950
H2	.28302
H2O	.77040
CO	1.01720
C	.68950
CHN	1.14730
CH4	.95030
CN	1.03330
H	.19396
HO	.74210
N	.75530
O	.70630
N2	1.02750
O2	.95530

GRAPHITE SURFACE KINETICS (GASKET) SOLUTION PROB. 2

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.42201+00	.14879+01	-.97745+00	.57344+01	.11138+01

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

TEMP	VISC	COND	DBAR	PR	SC
.67695+04	.61849-04	.84085-04	.59241-03	.26559-00	.72413-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.72313-00	.19328+02	.32734+02	.69537+04	.46967-00	.45517+04

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

1	6	7	8	13	17	106	44
.32481-01	.65428-01	.75176-01	.35334-00	.27334-00	.14133-00	.00000	.89053-02
.11425+00	.11271+00	.12859-00	.20565-00	.67808-01	.27761-00	.00000	.13376-01

SOLUTION TIMES
ITERATIONS = 25 TIME = 3.478 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .72313-00
TEMP = 6769.4887 DEG R. = 3760.8271 DEG K. PRESS = 26.66891 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.19911+04	-.46140+04	-.78083+03
ENTROPY - BTU/LBM DEG R	.30108+01	.96803-00	.21535+01
DENSITY - LBM/FT3	.10247+00		.17658-00
MOLECULAR WEIGHT	18.9969	101.9600	32.7342

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	.66236-02	H2	.31348-00	H2O	.96753-01	CO	.17828-00	C* F	.00000
CLH	.99656-01	AL	.41188-02	ALN	.41766-06	C2H2	.31317-09	C	.31169-07
C2	.16523-11	C3	.53144-15	C4	.21191-21	C F	.00000	C2 F	.00000
C3 F	.00000	C4 F	.00000	CAL	.57684-09	ALCL	.32053-01	ALCLO	.61399-02
ALCL2	.77695-02	ALCL3	.95614-04	ALH	.38619-03	ALHO2	.26195-02	ALO	.26043-02
AL2CL6	.31976-11	AL2O	.14931-02	AL2O2	.13975-06	CCL	.14610-08	CCLN	.19759-07
CCL2O	.45038-09	CCL4	.18794-17	CH	.16507-07	CHCL3	.28376-14	CHN	.46282-05
CHNO	.25959-06	CH2	.21772-04	CH2	.57276-08	CH2CL2	.90860-12	CH2O	.82280-06
CH3	.27674-07	CH3CL	.10615-09	CH4	.38141-08	CN	.35106-06	C2H4	.91792-13
C2H4O	.23109-16	C2N2	.20220-11	C3O2	.94152-12	C4N2	.61269-21	CL	.27104-01
CLHO	.12970-04	CLNO	.12088-06	CLO	.18042-04	CLO2	.31606-09	CL2O	.15699-09
H	.11054+00	HN	.30140-04	HO	.18182-01	H2N	.16678-04	H2O2	.48257-06
H3N	.64637-05	H4N2	.30614-12	N	.39802-04	NO	.15770-02	NO2	.12157-06
N2O	.14358-06	N2O3	.23101-14	N2O4	.18539-19	N2O5	.34507-23	O	.37086-02
O3	.15513-09	CCLO	.61631-05	CLNO2	.82685-12	HNO	.22404-05	HNO2	.16506-07
HNO3	.45060-12	ALHO	.30067-02	HO2	.17220-05	NO3	.18344-12	CCL2	.50729-10
CCL3	.15513-13	H2N2	.70846-09	CH2	.71754-10	C2O	.18646-08	C2H	.19873-09
C2N	.13601-10	C2CL4	.14259-21	C2CL6	.10187-30	ALO2	.36433-03	C2CL2	.10805-13
C2HCL	.37572-11	CHCL	.10041-08	CL2	.18998-04	N2	.86994-01	O2	.44935-03
CNO	.64259-07	NJ	.30385-09	ALCLO*	.00000	CLH4NO*	.00000	CLH4NO4*	.00000
ALCL3*	.00000	ALN*	.00000	C3AL4*	.00000	AL*	.00000	AL2O3*	.13473-00

GRAPHITE SURFACE KINETICS (GASKET) PROB. 2 0090000.00

UPDATE OF DIFFUSION FACTORS

SPECIES	DIFFUSION FACTOR
CO2	1.29140
H2	.38930
H2O	.77490
CO	1.01700
C2H2	1.17460
C	.69180
C2	1.02530
CH	.74920
CH4	.93570
CN	1.02670
H	.30180
N	.74930
NO	.99810
O	.73970
N2	1.02620
O2	1.00000

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.35738-00	.18503+02	-.39451+01	.90394-01	.98993-00

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

TEMP	VISC	COND	DBAR	PR	SC
.18000+04	.23252-04	.21904-04	.65800-04	.24829-00	.72410-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.76890-00	.18497+02	.32734+02	.13642+04	.67112-00	.58801+03

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

1	6	7	8	13	17	106	44
.32481-01	.05428-01	.75176-01	.35334-00	.27334-00	.19133-00	.00000	.89053-02
.96675-01	.11503+00	.13141-00	.29106-00	.69193-01	.28328-00	.00000	.13352-01

SOLUTION TIMES

ITERATIONS = 25 TIME = .317 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

Sample Problem 2
Sample Output, Continued

MASS CONDENSED/MASS GAS = .00000

TEMP = 1800.0000 DEG R. = 1000.0000 DEG K. PRESS = 26.66891 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.25713+03	.00000	-.29777+04
ENTROPY - BTU/LBM DEG R	.24233+01	.00000	.15836+01
DENSITY - LBM/FT3	.38538-00		.66407-00
MOLECULAR WEIGHT	18.9969	.0000	32.7342

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	.66236-02	H2	.31348-00	H2O	.96753-01	CO	.17828-00	C* F	.00000
CLH	.99456-01	AL	.41188-02	ALN	.41766-06	C2H2	.31317-09	C	.31169-07
C2	.16523-11	C3	.53144-15	C4	.21191-21	C F	.00000	C2 F	.00000
C3 F	.00000	C4 F	.00000	CAL	.57684-09	ALCL	.32053-01	ALCLO	.61399-02
ALCL2	.77695-02	ALCL3	.95614-04	ALH	.38619-03	ALHO2	.26195-02	ALO	.26043-02
AL2CL6	.31976-11	AL2O	.14931-02	AL2O2	.13975-04	CCL	.14410-08	CCLN	.19759-07
CCL2O	.45038-09	CCL4	.18794-17	CH	.16507-07	CHCL3	.28376-14	CHN	.46282-05
CHNO	.25959-06	CHO	.21772-04	CH2	.57276-08	CH2CL2	.90860-12	CH2O	.82280-06
CH3	.27674-07	CH3CL	.10615-09	CH4	.38141-08	CN	.35106-06	C2H4	.91792-13
C2H4O	.23109-16	C2N2	.20220-11	C3O2	.94152-12	C4N2	.61269-21	CL	.23104-01
CLHO	.12970-04	CLNO	.12088-06	CLO	.18042-04	CLO2	.31606-09	CL2O	.15699-09
H	.11054+00	HN	.36140-04	HO	.18182-01	H2N	.16678-04	H2O2	.48257-06
H3N	.64637-05	H4N2	.56614-12	N	.39802-04	NO	.15770-02	NO2	.12157-06
N2O	.14358-06	N2O3	.23101-14	N2O4	.18539-19	N2O5	.34507-23	O	.37086-02
O3	.15513-09	CCLO	.61631-05	CLNO2	.82685-12	HNO	.22404-05	HNO2	.14506-0
HNO3	.45060-12	ALHO	.30067-02	HO2	.17220-05	NO3	.18344-12	CCL2	.50729-10
CCL3	.15513-13	H2N2	.90846-09	CN2	.71754-10	C2O	.18646-08	C2H	.19973-09
C2N	.13601-10	C2CL4	.19259-21	C2CL6	.10187-30	ALO2	.36433-03	C2CL2	.10805-13
C2HCL	.37572-11	CHCL	.10041-08	CL2	.18990-04	N2	.86994-01	O2	.44935-03
CNO	.64259-07	N3	.38385-09	ALCLO*	.00000	CLH4N*	.00000	CLH4NO4*	.00000
ALCL3*	.00000	ALN*	.00000	C3AL4*	.00000	AL*	.00000	AL2O3*	.13473-00

GRAPHITE SURFACE KINETICS (GASKET) PROM. 2 0000000*00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.37709-00	.83579*01	-.26263*01	.90394-01	.10051*01

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

TEMP	VISC	COND	DBAR	PR	SC
.27000*04	.3037*-04	.30140-04	.12093-03	.24889-00	.72410-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.76890-00	.18497*02	.3273*-02	.19439*04	.70565-00	.11023*04

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

1	6	7	8	13	17	106	44
.32481-01	.65428-01	.75176-01	.35334-00	.27334-00	.19133-00	.00000	.89053-02
.96675-01	.11503*00	.13141-00	.29106-00	.69193-01	.28328-00	.00000	.13352-01

SOLUTION TIMES

ITERATIONS = 25 TIME = .226 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 2700.0000 DEG R. = 1500.0000 DEG K. PRESS = 26.66891 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.11652*03	.00000	-.26468*04
ENTROPY - BTU/LBM DEG R	.25914*01	.00000	.17324*01
DENSITY - LBM/FT3	.25692-00		.44271-00
MOLECULAR WEIGHT	18.9969	.0000	32.7342

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	.66236-02	H2	.31348-00	H2O	.96753-01	CO	.17828-00	C* F	.00000
CLH	.99456-01	AL	.41188-02	ALN	.41766-06	C2H2	.31317-09	C	.31169-07
C2	.16523-11	C3	.53144-15	C4	.21191-21	C F	.00000	C2 F	.00000
C3 F	.00000	C4 F	.00000	CAL	.57684-09	ALCL	.32053-01	ALCLO	.61399-02
ALCL2	.77695-02	ALCL3	.95814-04	ALH	.38619-03	ALHO2	.26195-02	ALO	.26043-02
AL2CL6	.31976-11	AL2O	.14431-02	AL2O2	.13975-04	CCL	.14410-08	CCLN	.19759-07
CCL2O	.45038-09	CCL4	.18734-17	CH	.16507-07	CHCL3	.28376-14	CHN	.46282-05
CHNO	.25959-06	CHO	.21772-04	CH2	.57276-08	CH2CL2	.90860-12	CH2O	.82280-06
CH3	.27674-07	CH3CL	.10615-09	CH4	.38141-08	CN	.35106-06	C2H4	.91792-13
C2H4O	.23109-16	C2N2	.20220-11	C3O2	.94152-12	C4N2	.61269-21	CL	.23104-01
CLHO	.12970-04	CLNO	.12088-06	CLO	.18042-04	CLO2	.31606-09	CL2O	.15699-09
H	.11054*00	HN	.36140-04	HO	.18182-01	H2N	.16678-04	H2O2	.48257-06
H3N	.64437-05	H4N2	.50014-12	N	.39802-04	NO	.15770-02	NO2	.12157-06
N2O	.14358-06	N2O3	.23101-14	N2O4	.18539-19	N2O5	.34507-23	O	.37086-02
O3	.15513-09	CCLO	.61631-05	CLNO2	.82685-12	HNO	.22404-05	HNO2	.16506-07
HNO3	.45860-12	ALHO	.50067-02	NO2	.17220-05	NO3	.18344-12	CCL2	.50729-10
CCL3	.15513-13	H2N2	.90446-09	CN2	.71754-10	C2O	.18646-08	C2H	.19873-09
C2N	.13601-10	C2CL4	.14259-21	C2CL6	.10187-30	ALO2	.36433-03	C2CL2	.10805-13
C2HCL	.37572-11	CHCL	.10041-08	CL2	.18990-04	N2	.86994-01	O2	.44935-03
CNO	.64259-07	N3	.58385-09	ALCLO*	.00000	CLH4NO*	.00000	CLH4NO4*	.00000
ALCL3*	.00000	ALN*	.00000	C3AL4*	.00000	AL*	.00000	AL2O3*	.13473-00

GRAPHITE SURFACE KINETICS (GASKET) PROB. 2 0003000*00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.31282-00	.50558-00	-.16150-00	.13340-01	.11408+01

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

TEMP	VISC	COND	DBAR	PR	SC
.90000+03	.16097-04	.10002-04	.20836-04	.50343-00	.72558-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.96269-00	.25263+02	.34644+02	-.30373+04	.44230-00	-.28877+04

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

1	6	7	8	13	17	106	44
.66360-01	.85730-01	.10103+00	.19130-00	.10844+00	.43660-00	.95689-19	.12335-01
.96675-01	.11503+00	.13141-00	.29106-00	.69193-01	.28328-00	.10000-18	.13352-01

SOLUTION TIMES

ITERATIONS = 47 TIME = 5.916 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
MASS TRANSFER COEFFICIENT ROUGH = .66300-00
RHO V WALL/RHOE UE CM = .10000-18 RPRIME = .10000-18

STATE ADJACENT TO THE SURFACE . . . .
TEMP = 900.0000 DEG R = 500.0000 DEG K PRESS = 26.66891 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.25766+04	.00000	-.25766+04
ENTROPY - BTU/LBM DEG R	.14642+01	.00000	.00000
DENSITY - LBM/FT3	.14056+01		.14056+01
MOLECULAR WEIGHT	34.6436	.0000	34.6436

CHEMICAL STATE ADJACENT TO THE SURFACE
(MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES)
(MOLE FR FOR CONDENSED = MPRIME CONDENSED). . . .

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.97099-02	H2	.91319-01	H2O	.41422-00	CO	.17763-10	C* F	.00000
CLH	.90894-02	AL	.00000	ALN	.00000	C2H2	.43502-28	C	.00000
C2	.00000	C3	.00000	C4	.00000	C F	.00000	C2 F	.00000
C3 F	.11891-20	C4 F	.00107-19	CAL	.00000	ALCL	.23915-30	ALCLO	.80177-26
ALCL2	.14041-16	ALCL3	.11271-03	ALH	.00000	ALHO2	.65984-28	ALO	.00000
AL2CL6	.69567-01	AL2O	.00000	AL2O2	.00000	CCL	.00000	CCLN	.20130-28
CCL2O	.42873-28	CCL4	.00000	CH	.00000	CHCL3	.35796-32	CHN	.20341-16
CHNO	.22504-17	CHO	.17656-28	CH2	.00000	CH2CL2	.81396-21	CH2O	.21658-15
CH3	.12464-19	CH3CL	.38620-10	CH4	.24727-00	CN	.00000	C2H4	.15129-15
C2H4O	.00081-31	C2N2	.11357-37	C3O2	.00000	C4N2	.00000	CL	.64279-22
CLHO	.84478-27	CLNO	.00000	CLO	.00000	CLO2	.00000	CL2O	.00000
H	.40554-21	HN	.39706-35	HO	.16664-26	H2N	.80112-28	H2O2	.20461-36
H3N	.67568-01	H4N2	.24147-21	N	.00000	NO	.57877-32	NO2	.00000
N2O	.18829-35	N2O3	.00000	N2O4	.00000	N2O5	.00000	O	.00000
O3	.00000	CCLO	.11180-28	CLNO2	.00000	HNO	.10915-35	HNO2	.00000
HNO3	.00000	ALHO	.12276-31	NO2	.00000	NO3	.00000	CCL2	.00000
CCL3	.00000	H2N2	.35806-28	CN2	.00000	C2O	.00000	C2H	.00000
C2N	.00000	C2CL4	.00000	C2CL6	.00000	ALO2	.00000	C2CL2	.00000
C2HCL	.41782-38	CHCL	.00000	CL2	.46021-23	N2	.91143-01	O2	.00000
CNO	.00000	N3	.00000						

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        GRAPHITE SURFACE KINETICS (GASAFT) PROB. #          0002000+00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNW/DLNT    DLNW/DLNP      GAMMA
  .39313-00    .16701+01   -.86553-00    .63549-01    .11141+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          UBAR           PR            SC
  .18000+04     .26778-04     .21303-04     .85000-04     .65720-00     .72457-00
    MU1           MU2         MOL.WT         MTIL          CPTIL         MTIL*
  .88436-00     .22655+02     .28346+02    -.28059+04     .81341-00    -.28130+04

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA =  .667)
      1             6             7             8            13            17           106           44
   .59651-01     .93947-01     .11177+00     .21321-00     .10081+00     .48738-00     .94673-19     .13241-01
   .96675-01     .11503+00     .13141-00     .24106-00     .69193-01     .28328-00     .16000-18     .13352-01

SOLUTION TIMES
          ITERATIONS =   11                        TIME =     1.776 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT POUCH =     .46300-00
 RHO V WALL/RHOE UE CM =     .10000-18   BPRIME =     .10000-18

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  1800.0000 DEG R =  1000.0000 DEG K      PRESS =      20.66861 ATM

                                GAS              CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM          -.19599+04          .00000          -.19599+04
  ENTROPY - BTU/LBM DEG R      .18964+01          .00000           .00000
  DENSITY - LBM/FT3            .57506-00                           .57506-00
  MOLECULAR WEIGHT            28.3465              .0000          28.3465


 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = BPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   CO2        .85284-02     H2         .60435-00     H2O        .29379-00     CO         .83036-01     C* F       .00000
   CLH        .80029-02     AL         .87336-20     ALN        .78338-28     C2H2       .22850-09     C          .18637-30
   C2         .53765-35     C3         .73881-33     C4         .00000        C F        .86732-26     C2 F       .11644-25
   C3 F       .74663-19     C4 F       .10876-22     CAL        .43841-36     ALCL       .54286-09     ALCLO      .11450-07
   ALCL2      .26102-04     ALCL3      .70418-01     ALH        .34634-18     ALHO2      .83201-08     ALO        .93481-20
   AL2CL6     .15735-01     AL2O       .11818-16     AL2O2      .22778-17     CCL        .36595-28     CCLN       .29288-13
   CCL2O      .63995-15     CCL4       .76721-29     CH         .54687-26     CHCL3      .23353-28     CHN        .69612-06
   CHNO       .66969-07     CHO        .13644-18     CH2        .22512-18     CH2CL2     .35913-13     CH2O       .78757-06
   CH3        .24524-08     CH3CL      .15361-06     CH4        .13778-08     CN         .20103-18     C2H4       .68733-06
   C2H4O      .12418-14     C2N2       .81878-15     C3O2       .13686-13     C4H2       .13387-24     CL         .66048-11
   CLHO       .18768-14     CLNO       .17366-22     CLO        .38835-22     CLO2       .48133-36     CL2O       .19878-31
   H          .22582-09     HN         .37938-17     HO         .53137-12     H2N        .18157-18     H2O2       .88139-19
   H3N        .69808-03     H4N2       .18528-15     N          .19259-22     NO         .54868-15     NO2        .61745-26
   N2O        .73886-19     N2O3       .00000        N2O4       .00000        N2O5       .00000        O          .56967-21
   O3         .00000        OCLO       .68178-12     CLNO2      .28028-35     HNO        .48718-18     HNO2       .11946-22
   HNO3       .27572-34     ALHO       .66791-09     HO2        .29592-24     NO3        .00000        CCL2       .17913-24
   CCL3       .12578-26     H2N2       .93576-17     CN2        .78536-24     C2O        .58442-28     C2H        .51033-19
   C2N        .18881-23     C2CL4      .82117-32     C2CL6      .00000        ALO2       .14655-19     C2CL2      .81281-23
   C2HCL      .13992-15     CHCL       .68284-22     CL2        .72146-14     N2         .11274+00     O2         .35708-21
   CNO        .79095-18     N3         .33458-25
```

GRAPHITE SURFACE KINETICS (WASAT) PROB. 2 5002000+00

REACTANT COEFFICIENTS

REACTION	1	2	3	4
CO2		1		
H2			1	
H2O	1			1
CO				1
C* F	1	1	2	
CLH				
AL				
ALN				

PRODUCT COEFFICIENTS

REACTION	1	2	3	4
CO2				1
H2	1		3	1
H2O			-2	
CO	1	2	2	
C* F				
CLH				
AL				
ALN				

KINETIC REACTION---	1	2	3	4
PRE-EXPONENT FACTOR	2.700+01	2.700+01	1.663+00	2.160+00
ACTIVATION ENERGY	4.600+04	4.600+04	5.550+04	0.000
TEMPERATURE EXPONENT	0.000	0.000	0.000	0.000

SPECIES INHIBITING FACTOR PSI/FRR

CO2	1.00/	.00	1.00/	.00	1.00/	.00	.00/	.00
H2	1.00/	.00	1.00/	.00	.00/	.00	.00/	.00
H2O	1.00/	.00	1.00/	.00	1.00/	.00	.00/	.00
CO	1.00/	.00	1.00/	.00	1.00/	.00	.00/	.00
C* F	.00/	.00	.00/	.00	.00/	.00	.00/	.00
CLH	.00/	3.00	.00/	3.00	.00/	.00	.00/	.00
AL	.00/	.00	.00/	.00	.00/	.00	.00/	.00
ALN	.00/	.00	.00/	.00	.00/	.00	.00/	.00

Sample Problem 2
Sample Output, Continued

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.38955-00	.92399-00	-.42571-00	.46219+01	.18340-00

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

TEMP	VISC	COND	DBAR	PR	SC
.21600+04	.27269-04	.26124-04	.8904+1-04	.39715-00	.72456-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.82402-00	.20002+02	.25530+02	-.11400+04	.00145-00	-.13382+04

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

1	6	7	8	13	17	18	44
.49702-01	.84886-01	.11277+00	.17344+00	.96952-01	.29186-00	.21906-24	.71139-01
.96675-01	.99267-01	.13141-00	.20407-00	.69193-01	.28328-00	.30515-24	.71104-01

SOLUTION TIMES

ITERATIONS = 12 TIME = 2.062 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
MASS TRANSFER COEFFICIENT BOUCM = .46300-00
RHO V BAR/RHOE UE CM = .13928-06 BPRIME = .13928-06

STATE ADJACENT TO THE SURFACE . . . .
TEMP = 2160.0000 DEG R = 1200.0000 DEG K PRESS = 20.66891 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.15556+04	.00000	-.15556+04
ENTROPY - BTU/LBM DEG R	.20235+01	.00000	.00000
DENSITY - LBM/FT3	.43160-00		.43160-00
MOLECULAR WEIGHT	25.5298	.0000	25.5298

NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
(MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
1= .89251-08 2= .24120-08 3= .12929-09 4= .13121-02

CHEMICAL STATE ADJACENT TO THE SURFACE
(MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES)
(MOLE FR FOR CONDENSED = BPRIME CONDENSED). . . .

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.41266-01	H2	.42659-00	H2O	.15269-00	CO	.15604-00	C* F	.0A000
CLH	.81607-02	AL	.33739-14	ALN	.39828-21	C2H2	.47262-08	C	.12555-24
C2	.15818-28	C3	.47174-27	C4	.13513-34	C F	.41634-24	C2 F	.17232-27
C3 F	.16961-25	C4 F	.16335-32	CAL	.14305-27	ALCL	.87870-06	ALCLO	.24403-05
ALCL2	.11914-02	ALCL3	.86224-01	ALH	.67500-13	ALHO2	.14474-05	ALO	.20000-14
AL2CL6	.21603-02	AL2O	.28739-10	AL2O2	.10084-11	CCL	.17372-23	CCLN	.93641-12
CCL2O	.39916-14	CCL4	.39579-27	CH	.38596-21	CHCL3	.21639-19	CHN	.46446-05
CHNO	.12367-06	CHO	.87163-09	CH2	.28697-15	CH2CL2	.88878-13	CH2O	.18429-05
CH3	.30137-07	CH3CL	.89735-07	CH4	.22679-01	CN	.43861-15	C2H4	.56048-06
C2H4O	.57270-14	C2N2	.55900-13	C3O2	.26195-12	C4N2	.12744-21	CL	.42502-09
CLNO	.49834-13	CLNO	.11929-19	CLO	.74156-19	CLO2	.38241-31	CL2O	.15088-27
H	.24845-07	HN	.80968-14	HO	.68552-10	H2N	.40807-09	H2O2	.16664-16
H3N	.45220-03	H4N2	.14739-14	N	.25993-18	NO	.14952-12	NO2	.26339-22
N2O	.16808-16	N2O3	.00000	N2O4	.00000	N2O5	.00000	O	.42306-17
O3	.54773-36	CCLO	.17992-1[illegible]	CLNO2	.41152-31	HNO	.15967-15	HNO2	.63561-20
HNO3	.22724-30	ALHO	.31005-06	HO2	.11571-20	NO3	.59690-37	CCL2	.23743-21
CCL3	.37751-24	H2N2	.00892-15	CN2	.37999-20	C2O	.12156-16	C2H	.12628-15
C2N	.18851-19	C2CL4	.00727-30	C2CL6	.00000	ALO2	.74253-15	C2LL2	.24124-20
C2HCL	.10013-13	CHCL	.95054-19	CL2	.20467-12	N2	.10253+00	O2	.77466-18
CNO	.33381-14	N3	.12463-21						

```
        GRAPHITE SURFACE KINETICS (GASKET) PROB. #        5002000+00

                                                                    10  7

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNM/DLNT   DLNM/DLNP      GAMMA
  .38642-00    .55470-00   -.19056-00   .16214+01   .41406-00

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          UBAR          PR            SC
  .25200+04     .30149-04     .29725-04     .11499-03     .38992-00     .72469-00
    MU1           MU2          MOL.WT         HTIL          CPTIL         HTIL0
  .80981-00     .20220+02     .24010+02    -.75954+03     .70870-00    -.10093+04

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEA =  .647)
      1             6             7             8            13            17           106           44
   .48654-01     .91180-01     .11422-00     .21165-00     .96781-01     .38884-00     .84519-20     .48672-01
   .96675-01     .18556-00     .13141-00     .26564-00     .69192-01     .28328-00     .10981-19     .48036-01

SOLUTION TIMES
        ITERATIONS =    8                       TIME =     1.308 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUCM =     .4A300-00
 RHO V WALL/RHOE UE CM =     .20447-05   APRIME =     .20447-05

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2520.0000 DEG R =  1400.0000 DEG K      PRESS =      20.66091 ATM

                                  GAS             CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM           -.13130+04          .00000          -.13130+04
  ENTROPY - BTU/LBM DEG R       .21174+01          .00000           .00000
  DENSITY - LBM/FT3             .35661-00                           .35661-00
  MOLECULAR WEIGHT             24.6097             .0000           24.6097


 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .13568-06  2=   .26393-07  3=   .40819-08  4=   .78786-03

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = APRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   CO2       .27210-01    H2        .94469-00    H2O       .13991-00    CO        .18551-00    C* F      .00000
   C2H       .13313-01    AL        .70432-11    ALN       .30928-17    C2H2      .45205-08    C         .70514-21
   C2        .96773-25    C3        .36244-24    C4        .20113-31    C F       .11958-19    C2 F      .27832-22
   C3 F      .17678-20    C4 F      .10637-26    CAL       .81827-23    ALCL      .39684-04    ALCLO     .52773-04
   ALCL2     .79286-02    ALCL3     .79462-01    ALH       .42997-10    ALHO2     .30898-04    ALO       .31784-11
   AL2CL6    .37751-03    AL2O      .31676-07    AL2O2     .73835-09    CCL       .27374-20    CCLN      .83168-11
   CCL2O     .40587-13    CCL4      .32709-25    CH        .37886-10    CHCL3     .23369-18    CHN       .61037-05
   CHNO      .16774-06    CHO       .71436-08    CH2       .13402-13    CH2CL2    .14616-12    CH2O      .19164-05
   CH3       .43863-07    CH3CL     .68853-07    CH4       .13034-02    CN        .41492-13    C2H4      .39187-07
   C2H4O     .28822-14    C2N2      .18872-12    C3O2      .50177-12    C4N2      .40514-21    CL        .15788-07
   CLHO      .20854-11    CL4O      .99311-17    CLO       .61731-16    CLO2      .10475-26    CL2O      .69350-20
   H         .62685-06    HN        .52910-12    HO        .37878-08    H2N       .42857-08    H2O2      .22351-14
   H3N       .21471-03    HCN2      .96735-14    N         .23974-15    NO        .18842-10    NO2       .37178-19
   N2O       .17260-14    N2O3      .33251-34    N2O4      .00000       N2O5      .00000       O         .49862-14
   O3        .13888-38    CCLO      .20894-29    CLNO2     .30882-27    HNO       .28845-13    HNO2      .20138-17
   HNO3      .10344-26    ALHO      .19988-04    NO2       .14857-17    NO3       .52659-32    CCL2      .55458-19
   CCL3      .57462-22    H2N2      .17175-13    CN2       .66503-10    C2O       .87879-15    C2N       .42394-14
   C2N       .21383-17    C2CL4     .48278-28    C2CL6     .00000       ALO2      .85498-12    C2CL2     .76854-19
   C2HCL     .50967-13    CHCL      .13988-15    CL2       .78962-11    N2        .10022+00    O2        .75253-15
   CNO       .19922-13    NO        .33588-14
```

Sample Problem 3

In this problem, ablation rates at the throat of a rocket nozzle are again calculated. The actual chamber state is input, from which an isentropic expansion to the nozzle throat is performed in order to obtain the boundary layer edge state. Since the propellant gases do not contain oxygen, only one of the three possible kinetically-controlled surface reactions can occur (reaction 3., Section 2.2.2.2) and, therefore, the fictitious element need not be introduced in the edge state definition. No frozen edge solutions are calculated, and an array of three surface temperatures is input.

```
3201020300  4110.      10.0      -1.0       0.0       0.173      0.0      PROB. 3
 1500.
 2000.
 2040.

  4
  1 HYDROGEN     1.008      .2275416
  2 HELIUM       4.003      .0175340
  6 CARBON      12.011                    1.0
 18 ARGON       39.948      .0175340
```

Sample Problem 3
Listing of Input

```
GRAPHITE SURFACE KINETICS (GASKET) PROB. 3          2110200*00

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

 AT.NO.   ELEMENT      ATOMIC WT      EDGE GAS      SURFACE
    1     HYDROGEN      1.00800       .2275419      .0000000
    2     HELIUM        4.00300       .0175340      .0000000
    6     CARBON       12.01100       .0000000      .0000000
   18     ARGON        39.94800       .0175340      .0000000
  106     GRAPHITE     12.01100       .0000000      .0832570

ELEMENTS          HYDROGEN    HELIUM      CARBON      ARGON       GRAPHITE

BASE SPECIES      H2          HE          C2H2        A           C* F

UPDATE OF DIFFUSION FACTORS
      SPECIES     DIFFUSION FACTOR
       H2              .28302
       C               .68950
       CH4             .95030
       H               .19396
```

Sample Problem 3
Sample Output

GRAPHITE SURFACE KINETICS (GASKET) SOLUTION PROB. 3

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.12018+01	.32478+01	-.39428-00	.23593-01	.11938+01

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

TEMP	VISC	COND	DBAR	PR	SC
.59716+04	.52171-04	.19299-03	.11881-02	.32483-00	.72774-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.40470-00	.98612+01	.63981+01	.17508+05	.26118+01	.13730+05

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEA = .667)

1	2	6	18	106
.22936-00	.70189-01	.00000	.70045-00	.00000
.43045-00	.92570-01	.00000	.67698-00	.00000

SOLUTION TIMES

ITERATIONS = 9 TIME = .349 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 5971.5609 DEG R. = 3317.5339 DEG K. PRESS = 10.00000 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.73980+04	.00000	.73980+04
ENTROPY - BTU/LBM DEG R	.69963+01	.00000	.69963+01
DENSITY - LBM/FT3	.15844-01		.15844-01
MOLECULAR WEIGHT	6.3981	.0000	6.3981

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

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2	.68020-00	C* F	.00000	C2H2	.00000
A	.11218+00	HE	.11218+00	C	.00000
C2	.00000	C3	.00000	C4	.00000
C F	.00000	C2 F	.00000	C3 F	.00000
C4 F	.00000	CH	.00000	CH2	.00000
CH3	.00000	CH4	.00000	C2H4	.00000
H	.95432-01	C2H	.00000		

GRAPHITE SURFACE KINETICS (GASKET) PROB. 3 3000100*30

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.11874+01	.28088+01	-.29488-00	.16389-01	.11991+01

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

TEMP	VISC	COND	DBAR	PR	SC
.55228+04	.49589-04	.18886-03	.18487-02	.32650-00	.72793-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.40938-00	.99642+01	.64980+01	.14727+05	.25856+01	.11639+05

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEA = .667)

1	2	6	18	106
.22936-00	.70189-01	.00000	.70045-00	.00000
.42899-00	.92857-01	.00000	.67828-00	.00000

SOLUTION TIMES

ITERATIONS = 4 TIME = .132 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 5522.5600 DEG R. = 3066.0890 DEG K. PRESS = 6.09649 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.63856+04	.00000	.63856+04
ENTROPY - BTU/LBM DEG R	.69963+01	.00000	.69963+01
DENSITY - LBM/FT3	.98220-02		.98220-02
MOLECULAR WEIGHT	6.4980	.0000	6.4980

ABOVE ARE STATIC PROPERTIES H-KINETIC = .10125+04 BTU/LBM

VEL. = .7119+04 FT/SEC FLUX = .69925+02 LBM/FT2SEC MACH = 1.00003

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

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2	.70645-00	C* F	.00000	C2H2	.00000
A	.11394+00	HE	.11394+00	C	.00000
C2	.00000	C3	.00000	C4	.00000
C F	.00000	C2 F	.00000	C3 F	.00000
C4 F	.00000	CH	.00000	CH2	.00000
CH3	.00000	CH4	.00000	C2H4	.00000
H	.65679-01	C2H	.00000		

Sample Problem 3, Sample Output, Continued

```
 GRAPHITE SURFACE KINETICS (GASKET) PROB. 3          0003000-00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNM/DLNP      GAMMA
  .12209+01    .12209+01   -.45175-07   -.14401-07    .13225+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DBAR          PR            SC
  .90000+03    .14956-04     .46023-04     .91147-04     .39675-00     .72842-00
    MU1           MU2          MOL.WT         RTIL          CPTIL         RTIL*
  .41840-00    .10162+02     .66734+01     .69721+03     .21549+01     .54820+03

ELEMENTAL R AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .667)
      1             2             6            18           106
   .23100-00     .69984-01     .00000        .67841-00     .15367-18
   .42999-00     .92807-01     .00000        .47820-00     .10000-18

SOLUTION TIMES
        ITERATIONS =   24                        TIME =      .436 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT BOUCH =    .17300-00
 RHO V WALL/RHOE UE CM =    .10000-18    RPRIME =    .10000-18

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =   900.0000 DEG R =   500.0000 DEG K      PRESS =      0.09649 ATM

                                GAS          CONDENSED        COMPOSITE
 ENTHALPY - BTU/LBM          .27016+03        .00000          .27016+03
 ENTROPY - BTU/LBM DEG R     .48319+01        .00000          .00000
 DENSITY - LBM/FT3           .61896-01                        .61896-01
 MOLECULAR WEIGHT             6.6734           .0000           6.6734

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = RPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   M2         .76666-00    C* F      .00000      C2H2       .00000
   A          .11667-00    ME        .11667-00   C          .00000
   C2         .00000       C3        .00000      C4         .00000
   C F        .30000       C2 F      .00000      C3 F       .70685-21
   C4 F       .20915-19    CH        .00000      CH2        .00000
   CH3        .00000       CH4       .00000      C2H4       .00000
   H          .24576-20    C2H       .00000
```

```
 GRAPHITE SURFACE KINETICS (GASKET) PROB. 3          0002000-00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNM/DLNP      GAMMA
  .10549+01    .10549+01    .00000       -.00000       .13411+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DBAR          PR            SC
  .18000+04    .23615-04     .71835-04     .28784-03     .34812-00     .72842-00
    MU1           MU2          MOL.WT         RTIL          CPTIL         RTIL*
  .41840-00    .10162+02     .66734+01     .26026+04     .21690+01     .21340+04

ELEMENTAL R AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .667)
      1             2             6            18           106
   .23100-00     .69984-01     .00000        .67841-00     .14178-18
   .42999-00     .92807-01     .00000        .47820-00     .10000-18

SOLUTION TIMES
        ITERATIONS =    6                        TIME =      .149 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT BOUCH =    .17300-00
 RHO V WALL/RHOE UE CM =    .10000-18    RPRIME =    .10000-18

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  1800.0000 DEG R =  1000.0000 DEG K      PRESS =      0.09649 ATM

                                GAS          CONDENSED        COMPOSITE
 ENTHALPY - BTU/LBM          .12637+04        .00000          .12637+04
 ENTROPY - BTU/LBM DEG R     .56031+01        .00000          .00000
 DENSITY - LBM/FT3           .30968-01                        .30968-01
 MOLECULAR WEIGHT             6.6734           .0000           6.6734

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = RPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   M2         .76666-00    C* F      .00000      C2H2       .00000
   A          .11667-00    ME        .11667-00   C          .00000
   C2         .00000       C3        .00000      C4         .00000
   C F        .16389-25    C2 F      .95.49-26   C3 F       .20257-19
   C4 F       .16563-23    CH        .00000      CH2        .00000
   CH3        .00000       CH4       .00000      C2H4       .00000
   H          .80149-09    C2H       .00000
```

```
        GRAPHITE SURFACE KINETICS (GASKET) PROB. 3          S002000*60

  REACTANT
    COEFFICIENTS

*REACTION*  1
            --

H2           1
C* F         2
C2H2
A
ME

  PRODUCT
    COEFFICIENTS

*REACTION*  1
            --

H2
C* F
C2H2         1
A
ME


  KINETIC
  REACTION---       1

  PRE-EXPONENT
    FACTOR          4.451*00

  ACTIVATION
    ENERGY          5.550*04

  TEMPERATURE
    EXPONENT        0.000

  SPECIES
   INHIBITING
    FACTORS
    PSI/FKR

    H2              .00/  .00
    C* F            .00/  .00
    C2H2            .00/  .00
    A               .00/  .00
    ME              .00/  .00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNM/DLNP      GAMMA
  .10728*01    .10734*01   -.15815-03    .28014-04    .13839*01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DBAR          PR            SC
  .27650*04    .30849-04     .97937-04     .56401-03    .33791-00    .72842-00
     MU1           MU2          MOL.WT         MTAL          CPTIL         MTIL*
  .41941-00    .10162*02     .46734*01     .45578*04    .22258*01    .37406*04
```

```
ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .667)
      1             2             6            16           106
   .23160-00    .69984-01    .49465-05    .69841-08    .94322-17
   .42899-00    .92807-01    .40861-05    .47820-00    .85060-17

SOLUTION TIMES
        ITERATIONS =   42                        TIME =     1.428 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT POUCH =     .17300-00
 RHO V WALL/RHOE UE CM =     .40861-05   BPRIME =     .40861-05

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2700.0000 DEG R =  1500.0000 DEG K      PRESS =       0.09649 ATM

                              GAS            CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM          .22195*04        .00000           .22195*04
  ENTROPY - BTU/LBM DEG R     .60335*01        .00000           .00000
  DENSITY - LBM/FT3           .20632-01                         .20632-01
  MOLECULAR WEIGHT             0.6734           .0000            0.6734


 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=    .17010-06

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = BPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   H2        .76665-00    C* F      .00000       C2H2      .76275-12
   A         .11667*00    ME        .11667*00    C         .98849-21
   C2        .13944-26    C3        .22700-28    C4        .16684-37
   C F       .31756-17    C2 F      .14627-19    C3 F      .77119-18
   C4 F      .18357-23    CH        .15784-18    CH2       .10727-14
   CH3       .54038-09    CH4       .27477-05    C2H4      .98845-12
   H         .02110-05    C2H       .47505-17
```

```
        GRAPHITE SURFACE KINETICS (GASKET) PHOB. 3          5002000*40

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNM/DLNT    DLNM/DLNP      GAMMA
  .11128+01    .11523+01   -.12504-01    .34352-02    .13539+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DBAR          PR            SC
  .36000+04     .37283-04     .12423-03     .48899-03     .33395-00     .72841-00
    MU1           MU2          MOL.WT          RTIL          CPTIL         RTIL*
  .41846-00     .10162+02     .66741+01     .64404+04     .23406+01     .54375+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .667)
      1             2             6             18            106
   .23160-00     .69958-01     .50815-03     .69794-00     .47169-10
   .42889-00     .92778-01     .41665-03     .47791-00     .35919-10

SOLUTION TIMES
        ITERATIONS =   12                          TIME =      .383 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUCM =     .17300-00
 RHO V WALL/RHOE UE CM =     .41686-03   RPRIME =     .41686-03

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  3600.0000 DEG R =  2000.0000 DEG K      PRESS =       0.09649 ATM

                                GAS             CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM          .32094+04          .00000          .32094+04
  ENTROPY - BTU/LBM DEG R     .63491+01          .00000          .00000
  DENSITY - LBM/FT3           .15476-01                          .15476-01
  MOLECULAR WEIGHT             6.6741             .0000           6.6741


 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .17353-04

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = RPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   M2         .76592-00    C* F       .00000      C2M2       .14492-04
   A          .11660+00    ME         .11664+00   C          .92692-12
   C2         .76148-14    C3         .33232-13   C4         .38485-18
   C F        .54473-11    C2 F       .26299-12   C3 F       .67650-11
   C4 F       .43519-15    CM         .12114-10   CM2        .11027-08
   CM3        .43808-05    CM4        .23784-03   C2M4       .15831-06
   M          .57373-03    C2M        .17555-07
```

```
        GRAPHITE SURFACE KINETICS (GASKET) PHOB. 3          5002000*40

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNM/DLNT    DLNM/DLNP      GAMMA
  .11164+01    .11593+01   -.44180-02   -.29361-03    .13581+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DBAR          PR            SC
  .36720+04     .37772-04     .12635-03     .93935-03     .33374-00     .72841-00
    MU1           MU2          MOL.WT          RTIL          CPTIL         RTIL*
  .41846-00     .10182+02     .66742+01     .68178+04     .23581+01     .55813+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .667)
      1             2             6             18            106
   .23159-00     .69950-01     .65862-03     .69788-00     .11783-09
   .42887-00     .92769-01     .53704-03     .47783-00     .89297-10

SOLUTION TIMES
        ITERATIONS =    5                          TIME =      .201 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUCM =     .17300-00
 RHO V WALL/RHOE UE CM =     .53739-03   RPRIME =     .53739-03

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  3671.9999 DEG R =  2040.0000 DEG K      PRESS =       0.09649 ATM

                                GAS             CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM          .32923+04          .00000          .32923+04
  ENTROPY - BTU/LBM DEG R     .63716+01          .00000          .00000
  DENSITY - LBM/FT3           .15172-01                          .15172-01
  MOLECULAR WEIGHT             6.6742             .0000           6.6742


 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .22371-04

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = RPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   M2         .76572-00    C* F       .00000      C2M2       .41728-04
   A          .11658+00    ME         .11663+00   C          .27682-11
   C2         .33474-13    C3         .17916-12   C4         .39786-17
   C F        .12660-10    C2 F       .70010-12   C3 F       .17137-10
   C4 F       .13467-14    CM         .31209-10   CM2        .23747-08
   CM3        .65836-05    CM4        .27391-03   C2M4       .96068-06
   M          .74971-03    C2M        .50278-07
```


Sample Problem 3, Sample Output, Concluded

Sample Problem 4

Again ablation rates at the throat of a rocket nozzle are calculated. The edge state is computed via an isentropic expansion from input actual chamber conditions. Since the propellant gases do not contain hydrogen, only one of the three possible kinetically-controlled surface reactions can occur (reaction 2., Section 2.2.2.2) and, therefore, the fictitious element need not be introduced in the edge state definition. Unlike the four other sample problems presented in this section, the equal-diffusion coefficient mode is utilized here. No frozen edge solutions are computed, and an array of five surface temperatures is input.

```
3201020200  450.     11.9      -1.0      0.0       0.302     0.00001  PROB. 4
 1200.
 1400.
 1600.
 1800.
 1900.

  4
  2 HELIUM      4.003     .01355
  6 CARBON      12.011    .0127              1.0
  8 OXYGEN      16.0      .0157
 18 ARGON       39.948     .01355
```

Sample Problem 4
Listing of Input

```
 GRAPHITE SURFACE KINETICS (GASAET) PROB. 4          2110200*00

 RELATIVE ELEMENTAL COMPOSITIONS. ATOMIC WTS/UNIT MASS
    AT.NO.   ELEMENT     ATOMIC WT      EDGE GAS       SURFACE
       2     HELIUM        4.00300      .0135590       .0000000
       6     CARBON       12.01100      .0127042       .0000000
       8     OXYGEN       16.00000      .0157114       .0000000
      18     ARGON        39.94600      .0135590       .0000000
     106     GRAPHITE     12.01100      .0000000       .0832570

 ELEMENTS          HELIUM      CARBON      OXYGEN      ARGON       GRAPHITE

 BASE SPECIES      HE          CO2         CO          A           C* F

 UPDATE OF DIFFUSION FACTORS
       SPECIES     DIFFUSION FACTOR
       CO2              1.24950
       CO               1.01720
       C                 .60950
       O                 .70630
       O2                .95530
```

Sample Problem 4
Sample Output

GRAPHITE SURFACE KINETICS (GASKET) SOLUTION PROB. 4

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.25932-00	.56259-00	-.21115-00	.11414-01	.12491+01

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

TEMP	VISC	COND	DBAR	PR	SC
.64659+04	.58211-04	.27142-04	.12303-02	.53705-00	.72707-06
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.91909-00	.22919+02	.24512+02	.11305+04	.34041-00	.81004+03

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA = .000)

2	6	8	18	106
.54280-01	.15265-00	.25138-00	.54169-00	.00000
.54285-01	.15265-00	.25138-00	.54168-00	.00000

SOLUTION TIMES

ITERATIONS = 21 TIME = .645 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 6465.8554 DEG R. = 3592.1419 DEG K. PRESS = 11.90000 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.81000+03	.00000	.81000+03
ENTROPY - BTU/LBM DEG R	.20843+01	.00000	.20843+01
DENSITY - LBM/FT3	.61771-01		.61771-01
MOLECULAR WEIGHT	24.5125	.0000	24.5125

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

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.42006-01	CO	.26953-00	C* F	.00000
A	.33238-00	HE	.33238-00	C	.47610-08
C2	.42608-13	C3	.29650-17	C4	.17872-24
C F	.00000	C2 F	.00000	C3 F	.00000
C4 F	.00000	C3O2	.14924-12	O	.15808-01
O3	.61276-08	C2O	.30273-09	O2	.78883-02

GRAPHITE SURFACE KINETICS (GASKET) PROB. 4 3000100+00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.26035-00	.44441-00	-.14740-00	.74305-02	.12587+01

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

TEMP	VISC	COND	DBAR	PR	SC
.58211+04	.52328-04	.25336-04	.18095-02	.53771-00	.72702-00
MU1	MU2	MOL.WT	MTIL	CPTIL	MTIL*
.92510-00	.23016+02	.24847+02	.97589+03	.34144-00	.51705+03

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA = .000)

2	6	8	18	106
.54280-01	.15265-00	.25138-00	.54169-00	.00000
.54285-01	.15265-00	.25138-00	.54168-00	.00000

SOLUTION TIMES

ITERATIONS = 0 TIME = .292 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 5821.0785 DEG R. = 3233.9326 DEG K. PRESS = 6.57897 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	.51702+03	.00000	.51702+03
ENTROPY - BTU/LBM DEG R	.20843+01	.00000	.20843+01
DENSITY - LBM/FT3	.38451-01		.38451-01
MOLECULAR WEIGHT	24.8467	.0000	24.8467

ABOVE ARE STATIC PROPERTIES H-KINETIC = .29298+03 BTU/LBM

VEL. = .3830+04 FT/SEC FLUX = .14725+03 LBM/FT2SEC MACH = 1.00005

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

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.59892-01	CO	.25589-00	C* F	.00000
A	.33692-00	HE	.33692-00	C	.36467-09
C2	.12967-14	C3	.05665-19	C4	.12101-26
C F	.00000	C2 F	.00000	C3 F	.00000
C4 F	.00000	C3O2	.24457-13	O	.60639-02
O3	.10751-08	C2O	.37628-10	O2	.43192-02

```
        GRAPHITE SURFACE KINETICS (GASKET) PROB. #         0003000*00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNM/DLNP      GAMMA
  .42444-00    .42444-00   -.12753-06    .14981-07    .12292+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP         VISC         COND         DBAR          PR           SC
  .90000+03    .15261-04    .10283-04    .84463-04    .62988-00    .72700-00
    MU1          MU2         MOL.WT        MTIL         CPTIL        MTIL*
  .92970-00    .23086+02    .25107+02   -.87769+03    .47937-00   -.95238+03

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .000)
      2            6            8           18          106
   .54200-01    .15265-00    .25138-00    .54169-00    .10000-18
   .54205-01    .15265-00    .25138-00    .54168-00    .10000-18

SOLUTION TIMES
        ITERATIONS =   27                          TIME =      .576 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUCH =     .30200-00
 RHO V WALL/RHOE UE CM =     .10000-18   HPRIME =     .10000-18

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =   900.0000 DEG R =   500.0000 DEG K      PRESS =       6.57897 ATM

                                GAS          CONDENSED       COMPOSITE
  ENTHALPY - BTU/LBM          -.95238+03      .00000          -.95238+03
  ENTROPY - BTU/LBM DEG R      .15140+01      .00000           .00000
  DENSITY - LBM/FT3            .25130-00                       .25130-00
  MOLECULAR WEIGHT           25.1074           .0000         25.1074

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = HPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   CO2       .75377-01     CO        .24372-00     C* F      .00000
   A         .34045-00     ME        .34045-00     C         .00000
   C2        .00000        C3        .00000        C4        .00000
   C F       .00000        C2 F      .00000        C3 F      .13029-20
   C4 F      .51238-19     C3O2      .18991-10     O         .00000
   O3        .00000        C2O       .95608-31     O2        .00000
```

```
        GRAPHITE SURFACE KINETICS (GASKET) PROB. #         0002000*00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNM/DLNP      GAMMA
  .29119-00    .29119-00   -.21873-07    .29802-07    .13732+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP         VISC         COND         DBAR          PR           SC
  .18000+04    .24097-04    .12491-04    .24073-03    .56174-00    .72700-00
    MU1          MU2         MOL.WT        MTIL         CPTIL        MTIL*
  .92970-00    .23086+02    .25107+02   -.51677+03    .36034-00   -.65003+03

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .000)
      2            6            8           18          106
   .54200-01    .15265-00    .25138-00    .54169-00    .10000-18
   .54205-01    .15265-00    .25138-00    .54168-00    .10000-18

SOLUTION TIMES
        ITERATIONS =   11                          TIME =      .317 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUCH =     .30200-00
 RHO V WALL/RHOE UE CM =     .10000-18   HPRIME =     .10000-18

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  1800.0000 DEG R =  1000.0000 DEG K      PRESS =       6.57897 ATM

                                GAS          CONDENSED       COMPOSITE
  ENTHALPY - BTU/LBM          -.65004+03      .00000          -.65004+03
  ENTROPY - BTU/LBM DEG R      .17513+01      .00000           .00000
  DENSITY - LBM/FT3            .12565-00                       .12565-00
  MOLECULAR WEIGHT           25.1074           .0000         25.1074

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = HPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   CO2       .75377-01     CO        .24372-00     C* F      .00000
   A         .34045-00     ME        .34045-00     C         .28449-29
   C2        .30907-33     C3        .15943-30     C4        .18899-30
   C F       .21567-25     C2 F      .17761-25     C3 F      .69671-19
   C4 F      .62411-23     C3O2      .10719-12     O         .43924-21
   O3        .00000        C2O       .01714-19     O2        .52369-22
```


Sample Problem 4, Sample Output, Continued

```
        GRAPHITE SURFACE KINETICS (GASKET) PROB. 4          5002000.00

  REACTANT
    COEFFICIENTS

*REACTION*  1
           --

CO2          1
CO
C* F         1
A
ME

  PRODUCT
    COEFFICIENTS

*REACTION*  1
           --

CO2
CO           2
C* F
A
ME


  KINETIC
  REACTION---       1

  PRE-EXPONENT
    FACTOR        4.139+01

  ACTIVATION
    ENERGY        4.600+04

  TEMPERATURE
    EXPONENT      0.000

  SPECIES
   INHIBITING
    FACTORS
    PSI/ERR

    CO2          1.00/  .00
    CO           1.00/  .00
    C* F          .00/  .00
    A             .00/  .00
    ME            .00/  .00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN    CP-EQUIL   DLNM/DLNT   DLNM/DLNP     GAMMA
  .27861-00   .27861-00   .00000      .2015-.-01   .13585+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
   TEMP         VISC          COND          UBAR          PR            SC
 .21600+04   .27173-04    .13692-04     .34096-03    .35291-00    .72700-00
   MU1          MU2         MOL.WT        CPTIL         CPTIL*
 .92970-00   .23096+02    .25107+02    -.38097+03    .35582-00   -.54884+03

ELEMENTAL A AND / MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA =  .0001
      2             6             7            18           196
   .54280-01    .15265-00    .25130-00    .54169-00    .98292-24
   .54285-01    .15265-00    .25130-00    .54150-00    .98296-24

SOLUTION TIMES
      ITERATIONS =    6                    TIME =     .278 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUGH =    .30200-00
 RHO V WALL/RHOE UE CM =    .29928-06   RPRIME =    .29928-06

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2160.0000 DEG R =  1200.0000 DEG K     PRESS =      6.57897 ATM

                                GAS            CONDENSED       COMPOSITE
  ENTHALPY - BTU/LBM         -.54050+03        .00000          -.54050+03
  ENTROPY - BTU/LBM DEG R     .19031+01        .00000           .00000
  DENSITY - LBM/FT3           .10471+00                         .10471+00
  MOLECULAR WEIGHT           25.1074             .0000         25.1074

 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .24917-07

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = RPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   CO2       .75377-01    CO        .24372-00    C* F      .00000
   A         .34045-00    ME        .34045-00    C         .16769-24
   C2        .69609-29    C3        .68397-28    C4        .64552-36
   C F       .16798-23    C2 F      .69851-27    C3 F      .68754-25
   C4 F      .65002-32    C3U2      .21941-13    O         .20055-16
   O3        .35504-35    C2O       .82559-17    O2        .42945-17
```

```
      GRAPHITE SURFACE KINETICS (GASAFT) PROB. 4          5002000*40

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN    CP-EQUIL    DLNM/DLNT    DLNM/DLNP     GAMMA
  .27156-00    .27156-00    .00000      .53020-00    .00336-00

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
   TEMP          VISC          COND          DBAR          PR            SC
  .25200*04     .30078-04     .14916-04     .*6812-03     .54760-00     .72700-00
    MU1           MU2          MOL.WT          MTIL          CPTIL         MTIL*
  .92976-00     .23086*02     .25107*02     -.26000*03     .35001-00     -.44954*03

ELEMENTAL X AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .000)
      2             6             8            16            106
   .54280-01     .15265-00     .25138-00     .54168-00     .33582E19
   .54284-01     .15266-00     .25138-00     .54168-00     .3358?E-19

SOLUTION TIMES
        ITERATIONS =    3                    TIME =     .143 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT BOUCM =    .30000-00
 RHO V WALL/RHOE UE CM =    .51845-05    RPRIME =    .51845-05

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2520.0000 DEG R =  1400.0000 DEG K      PRESS =      6.57897 ATM

                                GAS          CONDENSED       COMPOSITE
  ENTHALPY = BTU/LBM          -.44955+03      .00000         -.44955+03
  ENTROPY = BTU/LBM DEG R      .18455+01      .00000          .00000
  DENSITY = LBM/FT3            .89750-01                      .89750-01
  MOLECULAR WEIGHT            25.1073          .0000         25.1073

 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .43164-08

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = RPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   CO2       .75366-01     CO        .24374-03     C* F      .00000
   A         .34045-00     HE        .34045-00     C         .43959-21
   C2        .42774-26     C3        .53438-26     C4        .45606-34
   C F       .48475-19     C2 F      .11282-21     C3 F      .71060-20
   C4 F      .67441-24     C3O2      .32602-13     O         .42548-13
   O3        .49837-20     C2O       .17595-15     O2        .13550-13
```

```
      GRAPHITE SURFACE KINETICS (GASAFT) PROB. 4          5002000*40

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN    CP-EQUIL    DLNM/DLNT    DLNM/DLNP     GAMMA
  .26744-00    .26744-00    .00000     -.19971*01   -.77336-00

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
   TEMP          VISC          COND          DBAR          PR            SC
  .28800*04     .32845-04     .16136-04     .58171-03     .54431-00     .72700-00
    MU1           MU2          MOL.WT          MTIL          CPTIL         MTIL*
  .92975-00     .23086*02     .25106*02     -.13446*03     .34669-00     -.35232*03

ELEMENTAL X AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEX =  .000)
      2             6             8            16            106
   .54276-01     .15269-00     .25137-00     .54167-00     .10884-15
   .54282-01     .15269-00     .25137-00     .54166-00     .10884-15

SOLUTION TIMES
        ITERATIONS =    3                    TIME =     .146 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT BOUCM =    .30000-00
 RHO V WALL/RHOE UE CM =    .41230-04    RPRIME =    .41230-04

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2880.0000 DEG R =  1600.0000 DEG K      PRESS =      6.57897 ATM

                                GAS          CONDENSED       COMPOSITE
  ENTHALPY = BTU/LBM          -.35233*03      .00000         -.35233*03
  ENTROPY = BTU/LBM DEG R      .18815*01      .00000          .00000
  DENSITY = LBM/FT3            .78529-01                      .78529-01
  MOLECULAR WEIGHT            25.1063          .0000         25.1063

 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .34327-05

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = RPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   CO2       .75285-01     CO        .24387-00     C* F      .00000
   A         .34042-00     HE        .34042-00     C         .16448-18
   C2        .21131-23     C3        .14491-24     C4        .12025-32
   C F       .10678-15     C2 F      .89055-18     C3 F      .39646-16
   C4 F      .21357-21     C3O2      .24489-13     O         .13229-10
   O3        .19667-24     C2O       .22183-14     O2        .55761-11
```

GRAPHITE SURFACE KINETICS (GASKET) PROB. # 5002000+00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNR/DLNT	DLNR/DLNP	GAMMA
.26504-00	.26504-00	.00000	-.12951+01	-.10041+01

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

TEMP	VISC	CONU	UBAR	PR	SC
.32400+04	.35497-04	.17350-04	.70725-03	.56229-00	.72700-00
RHO1	RHO2	MOL.WT	MTIL	CPTIL	MTIL*
.92970-00	.23085+02	.25102+02	-.91753+01	.36482-00	-.25534+03

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA = .000)

2	6	8	18	18O
.56209-01	.15282-00	.25133-00	.56159-00	.65828-13
.56276-01	.15282-00	.25133-00	.56157-00	.65829-13

SOLUTION TIMES

ITERATIONS = 3 TIME = .139 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
MASS TRANSFER COEFFICIENT ROUGH = .36200-00
RHO V GALL/RHOE UE CM = .20493-03 RPRIME = .20493-03

STATE ADJACENT TO THE SURFACE . . . .
TEMP = 3240.0000 DEG R = 1800.0000 DEG K PRESS = 0.57897 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.25530+03	.00000	-.25530+03
ENTROPY - BTU/LBM DEG R	.19132+01	.00000	.00000
DENSITY - LBM/FT3	.89791-01		.89791-01
MOLECULAR WEIGHT	25.1010	.0000	25.1010

NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
(MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
1= .17062-04

CHEMICAL STATE ADJACENT TO THE SURFACE
(MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES)
(MOLE FR FOR CONDENSED = RPRIME CONDENSED). . . .

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.74917-01	CO	.24447-06	C* F	.00000
A	.34031-00	N2	.34031-00	C	.16082-16
C2	.16978-21	C3	.19763-23	C4	.16760-31
C F	.42318-13	C2 F	.99186-15	C3 F	.31124-13
C4 F	.66164-18	C3O2	.28465-13	O	.11373-08
O3	.70981-21	C2O	.16473-13	O2	.50535-09

GRAPHITE SURFACE KINETICS (GASKET) PROB. # 5002000+00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNR/DLNT	DLNR/DLNP	GAMMA
.26379-00	.26379-00	.18061-05	-.12813+01	-.19176+01

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

TEMP	VISC	CONU	UBAR	PR	SC
.35640+04	.37790-04	.18420-04	.82660-03	.54111-00	.72701-00
RHO1	RHO2	MOL.WT	MTIL	CPTIL	MTIL*
.92950-00	.23082+02	.25090+02	.18466+03	.34300-00	-.16652+03

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA = .000)

2	6	8	18	13A
.56295-01	.15320-00	.25122-00	.56134-00	.72566-11
.56294-01	.15320-00	.25122-00	.56133-00	.72566-11

SOLUTION TIMES

ITERATIONS = 3 TIME = .139 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

SURFACE IS LAYER-ORIENTED PYROLYTIC GRAPHITE
MASS TRANSFER COEFFICIENT ROUGH = .38200-00
RHO V GALL/RHOE UE CM = .65029-03 RPRIME = .65029-03

STATE ADJACENT TO THE SURFACE . . . .
TEMP = 3564.0000 DEG R = 1980.0000 DEG K PRESS = 0.57897 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.16053+03	.00000	-.16053+03
ENTROPY - BTU/LBM DEG R	.19393+01	.00000	.00000
DENSITY - LBM/FT3	.63415-01		.63415-01
MOLECULAR WEIGHT	25.0897	.0000	25.0897

NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
(MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
1= .54161-04

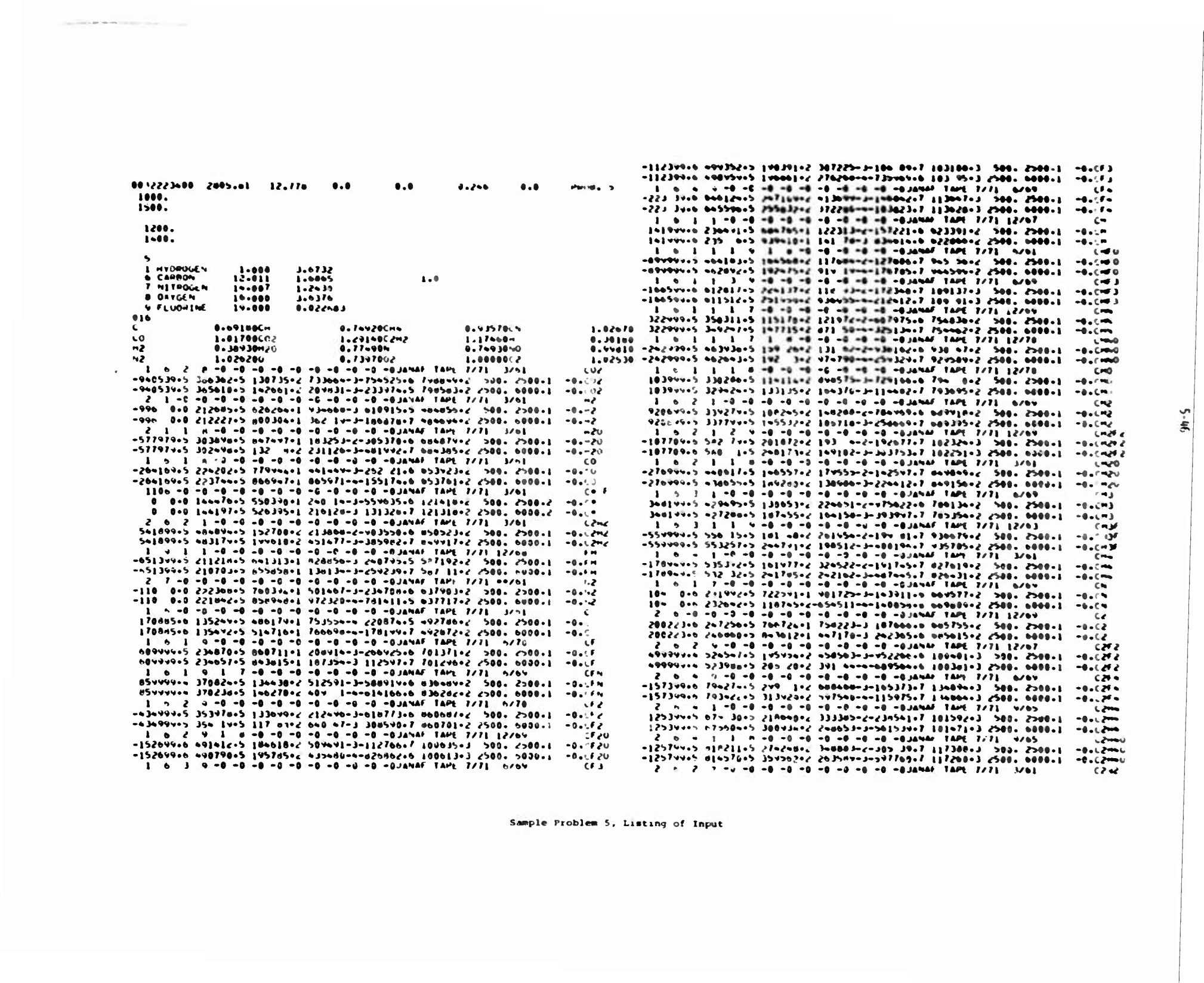
CHEMICAL STATE ADJACENT TO THE SURFACE
(MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES)
(MOLE FR FOR CONDENSED = RPRIME CONDENSED). . . .

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.73918-01	CO	.24918-00	C* F	.00000
A	.33999-00	N2	.33999-00	C	.50493-15
C2	.35105-20	C3	.16262-22	C4	.12825-30
C F	.32689-11	C2 F	.16714-12	C3 F	.30047-11
C4 F	.22533-15	C3O2	.16485-13	O	.28503-07
O3	.25864-18	C2O	.73792-13	O2	.16576-07

Sample Problem 4, Sample Output, Concluded

Sample Problem 5

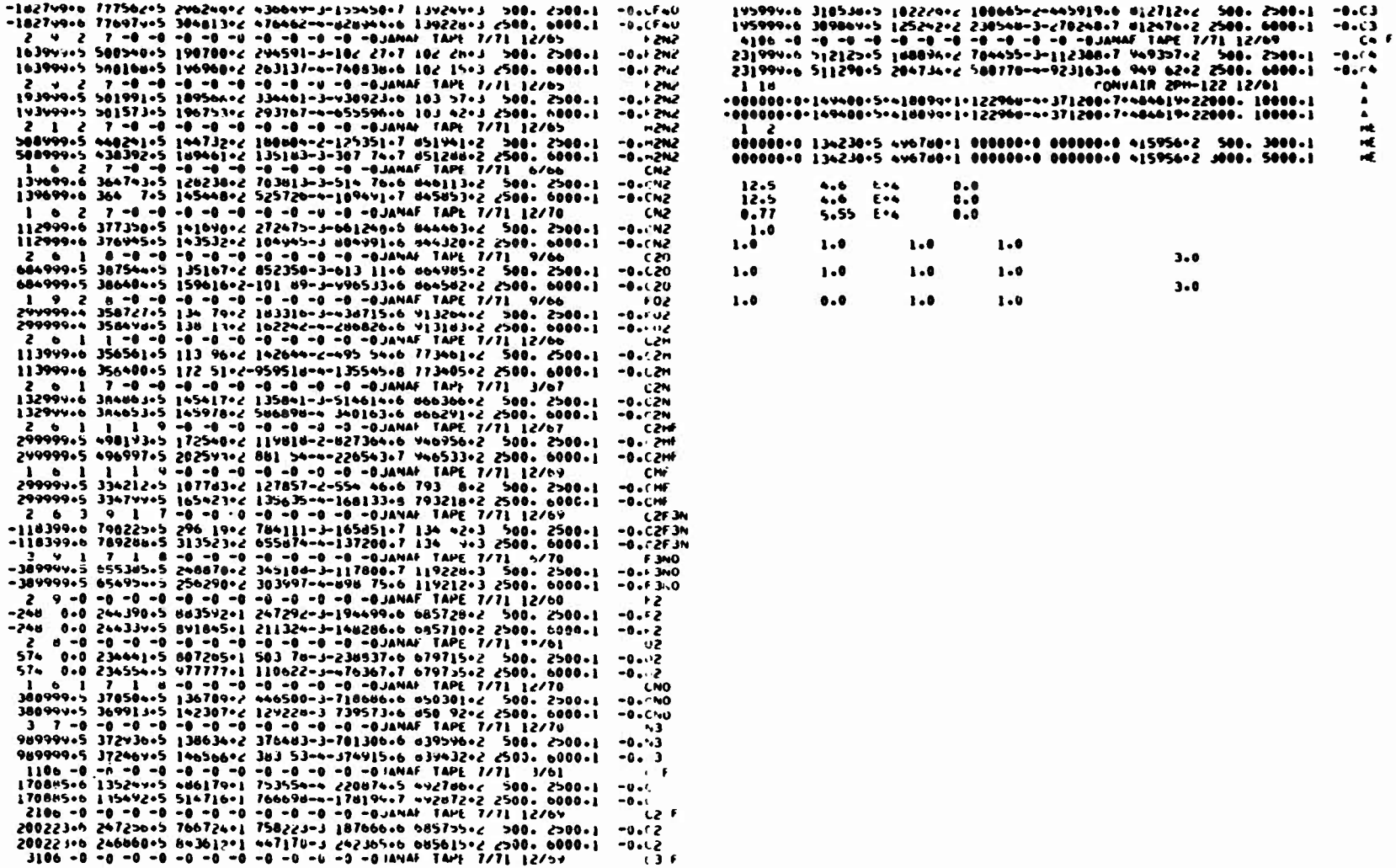
In this problem, all options which require the input of thermophysical properties are utilized. The edge thermodynamic state (2805.81°K and 12.778 atm) is input directly. Diffusion factors for sixteen selected species are input, along with a complete JANAF-type thermochemical data deck. Pre-exponential factors; activation energies, temperature exponents, and inhibiting species partial pressure coefficients are input for each of the four possible kinetically-controlled reactions (the three reactions in Section 2.2.2.2 and the water gas-shift reaction mentioned in Section 3.1.3). Finally, two frozen-edge temperatures and two surface temperatures are input to be used in lieu of the corresponding built-in temperature arrays.



Sample Problem 5, Listing of Input

```
 738699+5 512470+5 183275+2 889 50-3-071640+6 985977+2  500. 2500.1  -0.C2N2
 738699+5 511460+5 203898+2 704552-4-970377+6 985620+2 2500. 6000.1  -0.C2N2
  3  6 -0  -0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0 -0 -0 -0JANAF TAPE 7/71 12/69          C3
 195999+6 31053d+5 102229+2 100665-2-445914+6 812712+2  500. 2500.1  -0.C3
 195999+6 30986d+5 1252+2+2 230548-3-270248+7 812476+2 2500. 6000.1  -0.C3
  3  6  2   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/68          C3O2
-223799+5 654763+5 237207+2 109673-2-134954+7 117669+3  500. 2500.1  -0.C3O2
-223799+5 653493+5 2622d5+2 885573-4-127 91+7 117624+3 2500. 6000.1  -0.C3O2
  4  6 -0  -0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/69          C4
 231999+6 512125+5 186896+2 704455-3-112386+7 9 9357+2  500. 2500.1  -0.C4
 231999+6 511290+5 2047J4+2 580770-4-923163+6 949 62+2 2500. 6000.1  -0.C4
  4  6  2   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  3/61          C4N2
 127499+6 803415+5 289 30+2 136592-2-148718+7 133142+3  500. 2500.1  -0.C4N2
 127499+6 801830+5 3205 0+2 108998-3-153471+7 133 86+3 2500. 6000.1  -0.C4N2
  1  9 -0  -0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  9/65          F
 188599+5 136784+5 503772+1-250 79-4 875998+5 497896+2  500. 2500.1  -0.F
 188599+6 136820+5 498358-1-229881-5 511 68+5 497907+2 2500. 6000.1  -0.F
  1  9  1   1  1  8  -0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  9/65          FHO
-309999+5 324127+5 109339+2 955994+3-550539+6 794 60+2  500. 2500.1  -0.FHO
-309999+5 323249+5 134265+2 696725-4-227199+7 793746+2 2500. 6000.1  -0.FHO
  1  9  1   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/65          FN
 594999+5 237720+5 874469+1 178 15-3-241277+6 709764+2  500. 2500.1  -0.FN
 594999+5 237626+5 889689+1 111780-3-157572+6 709731+2 2500. 6000.1  -0.FN
  1  9  1   7  1  8  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/61          FNO
-156999+5 35232d+5 130324+2 315542-3-527139+6 878299+2  500. 2500.1  -0.FNO
-156999+5 351949+5 137315+2 266130-4-382215+6 878165+2 2500. 6000.1  -0.FNO
  1  9  1   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/66          FO
 259999+5 240268+5 876918+1 213141-3-226  5+6 715186+2  500. 2500.1  -0.FO
 259999+5 240140+5 867377+1 200A90-3 558627+6 715144+2 2500. 6000.1  -0.FO
  2  9  1   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/69          F2O
 585999+4 361673+5 137175+2 718  7-4-434922+6 988332+2  500. 2500.1  -0.F2O
 585999+4 361581+5 138658+2 659989-5-342524+6 888299+2 2500. 6000.1  -0.F2O
  3  9  1   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/69          F3N
-314299+5 508316+5 194630+2 152192-3-872260+6 103348+3  500. 2500.1  -0.F3N
-314299+5 508117+5 197771+2 140580-4-876939+6 103341+3 2500. 6000.1  -0.F3N
  1  1 -0  -0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  9/65          F
 520999+5 134230+5 496799+1 396467-4 118965+1 388627+2  500. 2500.1  -0.F
 520999+5 134229+5 496794+1 921 55-4 232451+3 388627+2 2500. 6000.1  -0.F
  1  1  1   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/65          FN
 869999+5 218531+5 683593+1 797250-3-960831+5 609577+2  500. 2500.1  -0.FN
 869999+5 217912+5 681 13+1 168 34-3-134730+7 609358+2 2500. 6000.1  -0.FN
  1  1  1   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/70          FO
 944199+4 214896+5 6579Z0+1 822769-3-4J0 21+4 613838+2  500. 2500.1  -0.FO
 944199+4 214299+5 6519A0+1 156668-3-175457+7 613627+2 2500. 6000.1  -0.FO
  2  1  1   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/65          F2N
 400699+5 307767+5 931217+1 150567-2-475 47+6 702290+2  500. 2500.1  -0.F2N
 400699+5 306320+5 1310+0+2 107546-3-273450+7 701769+2 2500. 6000.1  -0.F2N
  2  1  2   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/68          F2O2
-325299+5 447647+5 130105+2 242 20-2-417391+6 901302+2  500. 1000.1  -0.F2O2
-325299+5 439112+5 140670+2 174477-2-790461+6 897654+2 1000. 1500.1  -0.F2O2
  3  1  1   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  9/65          F3N
-109699+5 418803+5 120819+2 260909-2-958558+6 769952+2  500. 2500.1  -0.F3N
-109699+5 416923+5 104832+2 939209-3-250 24+7 769297+2 2500. 6000.1  -0.F3N
  4  1  2   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/65          F4N2
 227899+5 684959+5 320594+2 317316-2-187274+7 108246+3  500. 2500.1  -0.F4N2
 227899+5 686442+5 3021e7+2 228174-3-685272+7 108140+3 2500. 6000.1  -0.F4N2
  1  7 -0  -0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  3/61          H
 11296+6 134412+5 492401+1 271304-4 956 3+4 480916+2  500. 2500.1  -0.H
 11296+6 134277+5 277722+1 523356-3 567729+7 480868+2 2500. 6000.1  -0.H
  1  7  1   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/63          HO
 215799+5 227506+5 808175+1 354495-3-276336+6 688669+2  500. 2500.1  -0.HO
 215799+5 227145+5 877301+1 726516-4-192889+6 688541+2 2500. 6000.1  -0.HO
  1  7  2   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  9/64          HO2
 790999+4 34547d+5 128604+2 382 47-3-731 84+6 848188+2  500. 2500.1  -0.HO2
 790999+4 345  4+5 136887+2 329899-4-453910+6 848 21+2 2500. 6000.1  -0.HO2
  2  7  1   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/64          HO2O
 196 99+5 366422+5 133569+2 547758-3-726358+6 816233+2  500. 2500.1  -0.HO2O
 196 99+5 365783+5 146 28+2 446710-4-652692+6 816  7+2 2500. 6000.1  -0.HO2O
  2  7  3   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/64          HO3
 197999+5 618923+5 230372+2 652593-3-123951+7 123258+3  500. 2500.1  -0.HO3
 197999+5 618123+5 244627+2 562183-4-829998+6 123229+3 2500. 6000.1  -0.HO3
  2  7  4   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  9/64          HO4
 216999+4 787376+5 295602+2 812393-3-176876+7 134959+3  500. 2500.1  -0.HO4
 216999+4 786374+5 313221+2 701107-4-126885+7 134924+3 2500. 6000.1  -0.HO4
  2  7  5   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/64          HO2O
 269999+4 916178+5 352907+2 191 87-3-165360+7 156735+3  500. 2500.1  -0.HO2O
 269999+4 915902+5 356432+2 200514-4-118397+7 156725+3 2500. 6000.1  -0.HO2O
  1  8 -0  -0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/62          O
 595549+5 135106+5 496176+1 567346-5 296080+5 500932+2  500. 2500.1  -0.O
 595586+5 135210+5 450112+1 133922-3 964980+6 500947+2 2500. 6000.1  -0.O
  3  8 -0   0 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/61          O3
 340999+5 360506+5 134949+2 279823-3-668694+6 861 14+2  500. 2500.1  -0.O3
 340999+5 360306+5 138156+2 140117-3-430343+6 860944+2 2500. 6000.1  -0.O3
  1  6  1   9  1  8  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/65          CFO
-409999+5 348580+5 129144+2 358914-3-624512+6 873417+2  500. 2500.1  -0.CFO
-409999+5 348145+5 137 55+2 304924-4-437467+6 873263+2 2500. 6000.1  -0.CFO
  2  6  6   9 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/65          C2F6
-321199+6 108190+6 416434+2 405 36-3-222  8+7 165846+3  500. 2500.1  -0.C2F6
-321199+6 108140+6 426449+2 338745-5-220426+7 165826+3 2500. 6000.1  -0.C2F6
  1  9  1   7  2  6  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/65          FNO2
-259999+5 495524+5 186360+2 448868-3-104727+7 101561+3  500. 2500.1  -0.FNO2
-259999+5 494976+5 196111+2 388625-4-734965+6 101541+3 2500. 6000.1  -0.FNO2
  2  9  1   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  3/64          F2N
 100999+5 358 73+5 136 35+2 114 92-3-529 83+6 888773+2  500. 2500.1  -0.F2N
 100999+5 357926+5 138345+2 106264-4-387321+6 888720+2 2500. 6000.1  -0.F2N
  1  9  1   7  3  8  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  3/63          FNO3
 249999+4 6478 4+5 255565+2 413666-4-947439+6 121621+3  500. 2500.1  -0.FNO3
 249999+4 647454+5 255565+2 413666-4-947439+6 121621+3 2500. 6000.1  -0.FNO3
  1  1  1   7  1  8  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  3/63          HNO
 237999+5 328804+5 113718+2 869620-3-887633+6 784313+2  500. 2500.1  -0.HNO
 237999+5 327904+5 134577+2 665408-4-1175d5+7 783981+2 2500. 6000.1  -0.HNO
  1  1  1   7  2  8  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/63          HNO2
-183399+5 470292+5 165708+2 109287-2-100298+7 962851+2  500. 2500.1  -0.HNO2
-183399+5 469203+5 193 75+2 820449-4-231266+7 962466+2 2500. 6000.1  -0.HNO2
  1  1  1   7  2  8  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/63          HNO2
-188399+5 470293+5 165119+2 110 24-2-952 79+6 963403+2  500. 2500.1  -0.HNO2
-188399+5 469226+5 193 31+2 824 45-4-249346+7 963 26+2 2500. 6000.1  -0.HNO2
  1  1  1   7  3  6  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  6/63          HNO3
-320999+5 810921+5 219820 2 128411-2-152322+7 1109J5+3  500. 2500.1  -0.HNO3
-320999+5 809614+5 251557+2 987509-4-283753+7 1108B9+3 2500. 6000.1  -0.HNO3
  4  9  2   7 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  3/64          F4N2
-199999+4 807234+5 310466+2 278142-3-158 39+7 136617+3  500. 2500.1  -0.F4N2
-199999+4 806671+5 316228+2 258462-4-122683+7 136604+3 2500. 6000.1  -0.F4N2
  1  1  2   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71  3/64          HO2
 499999+4 326521+5 111320+2 908314-3-582260+6 800215+2  500. 2500.1  -0.HO2
 499999+4 325647+5 134514+2 664851-4-192589+7 799900+2 2500. 6000.1  -0.HO2
  1  7  3   8 -0 -0  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/64          HO3
 169999+5 498701+5 191696+2 260574-3-112525+7 799138+2  500. 2500.1  -0.HO3
 169999+5 498363+5 197111+2 240749-4-814340+6 799 18+2 2500. 6000.1  -0.HO3
  1  6  4   9  1  8  -0 -0 -0  -0 -0 -0  -0 -0JANAF TAPE 7/71 12/64          CF4O
```

Sample Problem 5, Listing of Input, Continued



Sample Problem 5, Listing of Input, Concluded

GRAPHITE SURFACE KINETICS (GASKET) PROB. 5 0130000+00

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	EDGE GAS	SURFACE
1	HYDROGEN	1.00800	.0367311	.0000000
6	CARBON	12.01100	.0164646	.0000000
7	NITROGEN	14.00700	.0126297	.0000000
8	OXYGEN	16.00000	.0463751	.0000000
9	FLUORINE	19.00000	.0002268	.0000000
106	GRAPHITE	12.01100	.0000000	.0832570

ELEMENTS	HYDROGEN GRAPHITE	CARBON	NITROGEN	OXYGEN	FLUORINE
BASE SPECIES	H2	CO2	N2	H2O	FH
	C* F				

UPDATE OF DIFFUSION FACTORS

SPECIES	DIFFUSION FACTOR
CO2	1.29140
H2	.38430
H2O	.77490
N2	1.02620
CO	1.01700
C2H2	1.17460
C	.69180
CH	.74920
CH4	.93570
CN	1.02670
C2	1.02530
H	.30180
N	.74930
NO	.99810
O	.73970
O2	1.00000

GRAPHITE SURFACE KINETICS (GASKET) SOLUTION PROB. 5

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.46249+00	.65564+00	-.99470-01	.44135-02	.11752+01

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

TEMP	VISC	COND	UBAR	PR	SC
.50505+04	.51634-04	.39295-04	.76050-03	.60771-00	.72573-00
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.90430-00	.24423+02	.23866+02	-.78924+03	.54371-00	-.90231+03

ELEMENTAL R AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMCX = .667)

1	6	7	8	9	106
.37025-01	.20256-00	.17410-00	.58200-00	.43047-02	.00000
.49534-01	.18884-00	.16938-00	.58779-00	.44617-02	.00000

SOLUTION TIMES

ITERATIONS = 35 TIME = 5.063 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 5050.4579 DEG R. = 2805.8100 DEG K. PRESS = 12.77800 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY = BTU/LBM	-.10389+04	.00000	-.10389+04
ENTROPY = BTU/LBM DEG R	.26582+01	.00000	.26582+01
DENSITY = LBM/FT3	.82678-01		.82678-01
MOLECULAR WEIGHT	23.8660	.0000	23.8660

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	.12957-00	H2	.10109+00	H2O	.32744-00	C* F	.00000	FH	.54117-02
N2	.14795-00	CO	.27292-00	C2H2	.69146-12	C	.77736-11	CF	.16781-11
CFN	.17162-11	CF2	.81495-14	CF2O	.75542-11	CF3	.72826-19	CF4	.42956-22
CH	.61978-11	CH2O	.28847-08	CH3	.12704-18	CHN	.22775-06	CHNO	.11418-06
CHO	.24462-05	CH2	.83245-11	CH2F2	.72542-14	CH2O	.20108-06	CH3	.23200-09
CH3F	.54603-13	CH4	.13789-09	CN	.17571-08	C2	.34836-16	C2F2	.33838-22
C2F4	.39976-30	C2H4	.22785-15	C2H4O	.10718-18	C2N2	.88703-14	C3	.55451-20
C3O2	.53113-13	C4	.88885-28	C4N2	.17314-25	F	.17094-05	FHO	.11542-08
FN	.87972-11	FNO	.87085-10	FO	.92544-10	F2O	.23175-18	F3N	.95160-25
H	.73962-02	HN	.86630-06	HO	.67376-02	H2N	.84656-06	H2O2	.30976-06
H3N	.12701-05	H4N2	.85335-14	N	.39018-06	NO	.74492-03	NO2	.78996-07
N2O	.58228-07	N2O3	.37731-15	N2O4	.34929-20	N2O5	.40202-24	O	.31381-03
O3	.19406-10	CF3	.24458-08	C2F6	.00000	FNO2	.94423-15	F2N	.57401-17
FNO3	.20093-21	HNO	.38493-06	HNO2	.10369-07	HNO2	.11668-07	HNO3	.34432-12
F4N2	.00000	HO2	.53589-06	NO3	.39440-13	CF4O	.26116-28	F2N2	.11650-21
F2N2	.11121-21	H2N2	.22739-10	CN2	.20952-14	CN2	.18493-12	C2O	.94486-11
FO2	.32441-12	C2H	.91323-13	C2N	.48729-14	C2HF	.13616-16	CHF	.28473-12
C2F3N	.28234-25	F3NO	.17392-23	F2	.91303-14	O2	.41419-03	CNO	.39465-08
N3	.53328-11	C F	.00000	C2 F	.00000	C3 F	.00000	C4 F	.00000

GRAPHITE SURFACE KINETICS (GASRET) PROB. 5 0150000*00

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	EDGE GAS	SURFACE
1	HYDROGEN	1.00800	.0367311	.0000000
6	CARBON	12.01100	.0114355	.0000000
7	NITROGEN	14.00700	.0124297	.0000000
8	OXYGEN	16.00000	.0655170	.0000000
9	FLUORINE	19.00000	.0002268	.0000000
106	GRAPHITE	12.01100	.0000000	.0832570
44	HOT DRY ICE	44.01100	.0935291	.0000000

ELEMENTS	HYDROGEN	CARBON	NITROGEN	OXYGEN	FLUORINE
	GRAPHITE	HOT DRY ICE			
BASE SPECIES	H2	CO	N2	H2O	FH
	C(s)	CO2			

UPDATE OF DIFFUSION FACTORS

SPECIES	DIFFUSION FACTOR
CO2	1.29140
H2	.38930
H2O	.77430
CO	1.01700
N2	1.02620
C2H2	1.17460
C	.69180
CH	.74920
CH4	.93570
CN	1.02670
C2	1.02530
H	.30140
N	.74930
NO	.99610
O	.73970
O2	1.00000

GRAPHITE SURFACE KINETICS (ASPETI SOLUTION PROB. 5

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.46269+00	.66666+00	-.97669+01	.99961-02	.11776+01

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

TEMP	VISC	COND	UBAR	PR	SC
.50503+04	.51634-04	.39293-04	.74430-03	.68771-00	.72573-09
MU1	MU2	MOL.WT	MTIL	CPTIL	KTIL*
.90436-00	.24423+02	.23806+02	-.78926+03	.56371-00	-.90231+03

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA = .6671)

1	6	7	8	9	10&	66
.37825-01	.13735-00	.17610-00	.49827-03	.43847-07	.00000	.23894-00
.49534-01	.13442-00	.16936-00	.44279-00	.44617-02	.00000	.19942-00

SOLUTION TIMES

ITERATIONS = 31 TIME = 4.442 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 5050.4579 DEG R. = 2805.8100 DEG K. PRESS = 12.77800 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.10389+04	.00000	-.10389+04
ENTROPY - BTU/LBM DEG R	.26582+01	.00000	.26582+01
DENSITY - LBM/FT3	.82078-01		.82078-01
MOLECULAR WEIGHT	23.0660	.0000	23.0660

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	.12957-00	H2	.10109+00	H2O	.32744-00	CO	.47292-00	C* F	.00000
FH	.54117-02	H2	.19745-06	C2H2	.69146-12	C	.77738-11	CF	.16781-11
CFN	.17162-11	CF2	.91495-14	CF2O	.75542-11	CF3	.72826-19	CF4	.42956-22
CH	.81978-11	CHO	.28867-08	CHF3	.12706-18	CHN	.22775-06	CHNO	.11418-08
CHO	.24462-05	CH2	.83265-11	CH2F2	.72542-16	CH2O	.20108-06	CH3	.23208-09
CH3F	.54603-13	CHN	.13769-07	CN	.17571-08	C2	.34036-16	C2F2	.33838-22
C2F4	.39978-30	C2H4	.22795-15	C2H4O	.10718-18	C2H2	.68703-14	C3	.59458-20
C3O2	.53113-17	C4	.88885-25	C4H2	.17316-25	F	.17895-05	FHO	.11542-08
FN	.87972-11	FNO	.87865-10	FO	.92566-10	F2O	.23175-18	F3N	.95168-25
H	.73952-02	HN	.66530-06	HO	.67377-02	H2N	.84656-06	H2O2	.38976-06
H3N	.12701-05	H4N2	.85335-14	N	.39810-06	NO	.74492-03	NO2	.70996-07
N2O	.58228-07	N2O3	.37731-13	N2O4	.34929-20	N2O5	.48282-24	O	.31381-03
O3	.19486-10	C2O	.24858-08	C2F6	.00000	FNO2	.94423-15	F2N	.57481-17
FNO3	.20893-21	HNO	.38493-06	HNO2	.10384-07	HNO2	.11668-07	HNO3	.34432-12
F4N2	.00000	HO2	.53589-06	NO3	.39448-13	CF4O	.26116-28	F2N2	.11658-21
F2N2	.11121-21	H2N2	.22719-13	CN2	.20952-14	CN2	.18493-12	C2O	.94466-11
FO2	.32491-12	C2H	.81323-13	C2N	.68729-14	C2NF	.13616-16	CNF	.28473-12
C2F3N	.28234-24	F3NO	.17392-24	F2	.31303-14	O2	.41419-03	CNO	.39465-08
N3	.53328-11	C F	.00000	C2 F	.00000	C3 F	.00000	C4 F	.00000

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        GRAPHITE SURFACE KINETICS (GASP II) PROB. 5          0000000*00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNM/DLNT    DLNM/DLNP      GAMMA
  .38462-00    .17810*01   -.26874-00    .48304-02    .10763*01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DRAR          PR            SC
  .18000*04     .20162-04     .16443-04     .13733-03     .61196-00     .72573-00
    MU1           MU2          MOL.WT         MTIL          CPTIL         MTIL*
  .90430-00     .20423*02     .23800*02    -.24217*04     .44752-00    -.24398*04

ELEMENTAL X AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEA =  .667)
      1             6             7             8             9            106           44
   .37025-01     .13735-00     .17410-00     .40827-00     .43047-02     .00000        .23894-00
   .49534-01     .13442-00     .16938-00     .44279-00     .44617-02     .00000        .19942-00

SOLUTION TIMES
        ITERATIONS =   31                        TIME =      .187 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

  MASS CONDENSED/MASS GAS =     .00000
  TEMP =  1800.0000 DEG R.  =  1000.0000 DEG K.      PRESS =      12.77800 ATM

                                  GAS              CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM           -.24353*04            .00000          -.24353*04
  ENTROPY - BTU/LBM DEG R       .22222*01            .00000           .22222*01
  DENSITY - LBM/FT3             .23198-00                             .23198-00
  MOLECULAR WEIGHT             23.8660                .0000          23.8660

 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       .12957-00     H2        .10109*00     H2O       .32744-00     CO        .27292-00     C* F      .00000
    FH        .54117-02     N2        .14795-00     C2H2      .69146-12     C         .77738-11     CF        .16781-11
    CFN       .17162-11     CF2       .81495-14     CF2O      .75542-11     CF3       .72826-19     CF4       .42956-22
    CH        .61978-11     CHFO      .20847-08     CHF3      .12704-18     CHN       .22775-06     CHNO      .11418-06
    CHO       .24462-05     CH2       .83245-11     CH2F2     .72542-16     CH2O      .20188-06     CH3       .23200-09
    CH3F      .54603-13     CH4       .13789-09     CN        .17571-08     C2        .34836-16     C2F2      .33838-22
    C2F4      .39976-30     C2H4      .22785-15     C2H4O     .10714-18     C2N2      .88793-14     C3        .55450-20
    C3O2      .53113-13     C4        .98885-28     C4N2      .17314-25     F         .17595-05     FNO       .11542-08
    FN        .87972-11     FNO       .87085-10     FO        .92544-10     F2O       .23175-18     F3N       .95168-25
    H         .73962-02     HN        .86530-06     HO        .67376-02     H2N       .84658-06     H2O2      .30976-06
    H3N       .12701-05     H4N2      .95335-14     N         .39010-06     NO        .74492-03     NO2       .78996-07
    N2O       .58228-07     N2O3      .37731-15     N2O4      .34929-20     N2O5      .40202-24     O         .31381-03
    O3        .19406-10     CFO       .24858-08     C2F6      .00000        FNO2      .94423-15     F2N       .57401-17
    FNO3      .20093-21     HNO       .38493-06     HNO2      .10369-07     HNO2      .11660-07     HNO3      .34432-12
    F4N2      .00000        HO2       .93589-06     NO3       .39440-13     CF4O      .26116-28     F2N2      .11650-21
    F2N2      .11121-21     H2O2      .22739-10     CN2       .20952-14     CN2       .18493-12     C2O       .94466-11
    FO2       .32441-12     C2H       .81323-13     C2N       .48729-14     C2HF      .13616-16     CHF       .28473-12
    C2F3N     .28234-26     F3NO      .17392-29     F2        .91303-14     O2        .41419-03     CNO       .39465-08
    N3        .53328-11     C F       .00000        C2 F      .00000        C3 F      .00000        C4 F      .00000
```

Sample Problem 5, Sample Output, Continued

GRAPHITE SURFACE KINETICS (GASEQ) PROB. 5 0000000.00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.41239+00	.10432+01	-.18072+00	.43042-02	.11197+01

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

TEMP	VISC	COND	DBAR	PR	SC
.27000+04	.36175-04	.23040-04	.24909-03	.81171+00	.72573+00
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.90436+00	.24423+02	.23860+02	-.20034+04	.48067+00	-.20448+04

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

1	6	7	8	9	106	44
.37025-01	.13735+00	.17410+00	.40827+00	.43097-02	.00000	.23894+00
.49534-01	.13442+00	.16938+00	.44279+00	.44617-02	.00000	.19942+00

SOLUTION TIMES

ITERATIONS = 31 TIME = .186 SEC.

CLOSED SYSTEM EQUILIBRIUM SOLUTION OUTPUT

MASS CONDENSED/MASS GAS = .00000

TEMP = 2700.0000 DEG R. = 1500.0000 DEG K. PRESS = 12.77800 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.20760+04	.00000	-.20760+04
ENTROPY - BTU/LBM DEG R	.23837+01	.00000	.23837+01
DENSITY - LBM/FT3	.15465-00		.15465-00
MOLECULAR WEIGHT	23.8660	.0000	23.8660

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	.12957-00	H2	.10109+00	H2O	.32744-00	CO	.27292-00	C* F	.0n000
FH	.54117-02	N2	.14795-00	C2H2	.69146-12	C	.77738-11	CF	.16781-11
CF2	.17162-11	CF2	.81495-14	CF2O	.75542-11	CF3	.72826-19	CF4	.42956-22
CH	.81978-11	CHFO	.20847-06	CHF3	.12704-18	CHN	.22775-06	CHNO	.11418-06
CHO	.24462-05	CH2	.83245-11	CH2F2	.72542-16	CH2O	.20108-06	CH3	.23200-09
CH3F	.54603-13	CH4	.13789-09	C4	.17571-08	C2	.34836-16	C2F2	.33838-22
C2F4	.39976-30	C2H4	.22785-15	C2H2O	.10718-18	C2N2	.88703-14	C3	.55450-20
C3O2	.53113-13	C4	.88885-28	C4N2	.17314-25	F	.17095-05	FHO	.11542-08
FN	.47972-11	FNO	.87095-10	FO	.92544-10	F2O	.23175-18	F3N	.95160-25
H	.73962-02	HN	.86530-06	HO	.67376-02	H2N	.84656-06	H2O2	.30976-06
H3N	.12701-05	H4N2	.85335-14	N	.39010-06	NO	.74492-03	NO2	.70996-07
N2O	.58228-07	N2O3	.37731-15	N2O4	.34929-20	N2O5	.40202-24	O	.31381-03
O3	.19406-10	CF0	.24658-08	C2F6	.00000	FNO2	.94623-15	F2N	.57401-17
FNO	.20093-21	HNO	.38493-06	HNO2	.10369-07	HNO2	.11660-07	HNO3	.34432-12
F4N2	.00000	HO2	.53589-06	NO3	.39440-13	CF4O	.26116-28	F2N2	.11650-21
F2N2	.11121-21	H2N2	.22739-10	CN2	.20952-14	CN2	.18493-12	C2O	.94466-11
FO2	.32441-12	C2H	.81323-13	C2N	.48729-14	C2NF	.13616-16	CNF	.28473-12
C2F3N	.28234-26	F3NO	.17342-29	F2	.91303-14	O2	.41619-03	CNO	.39465-08
N3	.53328-11	C*	.00000	C2 F	.00000	C3 F	.00000	C4 F	.00000

Sample Problem 5, Sample Output, Continued

```
        GRAPHITE SURFACE KINETICS (GASKET) PROB. 5          0003000-00

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL     DLNM/DLNT     DLNM/DLNP      GAMMA
  .32220-00    .32371-00   -.34102-03     .13262-04    .10213+01

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
    TEMP          VISC          COND          DBAR          PR            SC
  .90000+03     .10732-04     .80063-05     .43487-04     .67347-00     .72575-00
    MU1           MU2          MOL.WT         HTIL          CPTIL         HTIL0
  .95035-00     .25917+02     .25256+02    -.32246+04     .33922-00    -.31547+04

ELEMENTAL A AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMEA =  .667)
      1             6             7             8             9            106           44
   .43602-01     .13600-00     .17404-00     .40178-00     .43227-02     .12444-18     .23966-00
   .49534-01     .13442-00     .16938-00     .44279-00     .44617-02     .10000-18     .19942-00

SOLUTION TIMES
        ITERATIONS =    37                        TIME =     3.969 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS EDGE-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUCM =     .24000-00
 RHO V WALL/RHOE UE CM =     .10000-18   BPRIME =     .10000-18

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =   900.0000 DEG R =   500.0000 DEG K      PRESS =     12.77800 ATM

                                GAS              CONDENSED        COMPOSITE
  ENTHALPY - BTU/LBM          -.30318+04          .00000          -.30318+04
  ENTROPY - BTU/LBM DEG R      .19174+01          .00000           .00000
  DENSITY - LBM/FT3            .49098-00                           .49094-00
  MOLECULAR WEIGHT           25.2561               .0000          25.2561

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = BPRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   CO2       .13753-00    H2        .41230-04    H2O       .41327-00    CO        .21095-00    C* F      .00000
   FH        .57460-07    N2        .15744-00    C2H2      .14273-18    C         .06000       CF        .00000
   CFN       .17458-28    CF2       .10694-33    CF2O      .28020-09    CF3       .59360-36    CF4       .20480-21
   CH        .00000       CHO       .83351-09    CHF3      .11239-17    CHN       .15326-11    CHNO      .37421-09
   CHO       .35999-20    CH2       .00000       CH2F2     .13930-15    CH2O      .58256-09    CH3       .22336-18
   CH3F      .67769-11    CH4       .65825-01    CN        .95462-38    C2        .00006       C2F2      .00000
   C2F4      .00000       C2H4      .10750-09    C2H4O     .94111-22    C2N2      .14271-24    C3        .00000
   C3O2      .11612-16    C4        .00000       C4N2      .00000       F         .22665-34    FHO       .18762-38
   FN        .00000       FNO       .00000       FO        .00000       F2O       .00000       F3N       .00000
   H         .12446-22    HF        .11083-36    HO        .11311-24    H2N       .32896-23    H2O2      .45169-33
   H3N       .40903-06    H4O2      .19472-28    N         .00000       NO        .24294-28    NO2       .00000
   N2O       .71859-32    N2O3      .00000       N2O4      .00000       N2O5      .00000       O         .00000
   O3        .00000       OF2       .53485-25    C2F6      .00000       FNO2      .00000       F2N       .00000
   FNO3      .00000       HNO       .57361-34    HNO2      .32182-38    HNO2      .52776-18    HNO3      .00000
   F4N2      .00000       HO2       .00000       NO3       .00000       CF4O      .00000       F2N2      .00000
   F2N2      .00000       H2N2      .13376-31    CN2       .00000       CN2       .00000       C2O       .33223-37
   FO2       .00000       C2H       .00000       C2N       .00000       C2HF      .63510-35    CHF       .33429-38
   C2F3N     .13211-33    F3O       .00000       F2        .00000       O2        .00000       CNO       .12309-31
   N3        .00000       C F       .00000       C2 F      .00000       C3 F      .13713-20    C4 F      .64390-19
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Sample Problem 5, Sample Output, Continued

GRAPHITE SURFACE KINETICS (ASPEII PROB. 5) 00U2000*00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DL T	DLNM/DLNP	GAMMA
.30550-00	.54344-00	-.74174-01	.55106-02	.12043+01

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

TEMP	VISC	COND	DHAR	PR	SC
.18000+04	.26250-04	.16347-04	.13733-03	.61917-00	.72579-00
MU1	MU2	MOL.WT	HTIL	CPTIL	HTIL*
.91015-00	.24660+02	.24085+02	-.25919+04	.44340-00	-.25712+04

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

1	6	7	8	9	106	44
.37661-01	.13730-00	.17419-00	.40748-00	.43118-02	.11444-18	.23906-00
.49534-01	.13442-00	.16938-00	.44279-00	.44617-02	.10000-18	.19942-00

SOLUTION TIMES
ITERATIONS = 13 TIME = 1.342 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

SURFACE IS EDGE-ORIENTED PYROLYTIC GRAPHITE
MASS TRANSFER COEFFICIENT ROUGH = .2.600-00
RHO V WALL/RHOE UE CH = .10000-10 MPRIME = .10000-10

STATE ADJACENT TO THE SURFACE . . . .
TEMP = 1800.0000 DEG R = 1000.0000 DEG K PRESS = 12.77800 ATM

	GAS	CONDENSED	COMPOSITE
ENTHALPY - BTU/LBM	-.25207+04	.00000	-.25207+04
ENTROPY - BTU/LBM DEG R	.22090-01	.00000	.00000
DENSITY - LBM/FT3	.23410-00		.23410-00
MOLECULAR WEIGHT	24.0847	.0000	24.0847

CHEMICAL STATE ADJACENT TO THE SURFACE
(MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES)
(MOLE FR FOR CONDENSED = MPRIME CONDENSED). . . .

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.13882-00	H2	.45297-01	H2O	.34230-00	CO	.27105-00	C* F	.00000
FH	.54657-02	N2	.14972-00	C2H2	.19478-10	C	.10862-30	CF	.93610-25
CFN	.16716-17	CF2	.13418-21	CF2O	.10308-11	CF3	.24240-20	CF4	.20942-23
CH	.23080-24	CHFO	.15409-05	CHF3	.21455-18	CHN	.23417-06	CHNO	.50520-07
CHO	.18415-19	CH2	.34659-19	CH2F2	.18309-14	CH2O	.44389-06	CH3	.18066-09
CH3F	.17912-09	CH4	.42360-02	CN	.16233-18	C2	.26234-35	C2F2	.14990-32
C2F4	.27536-36	C2H4	.10237-07	C2H4O	.54025-16	C2N2	.25192-15	C3	.17470-33
C3O2	.33054-13	C4	.00000	C4N2	.96930-26	F	.14531-17	FHO	.94651-22
FN	.17977-29	FNO	.30716-25	FO	.43952-31	F2O	.00000	F3N	.00000
H	.19418-04	HN	.26379-17	HO	.14821-11	H2N	.29513-11	H2O2	.29066-18
H3N	.84502-04	H4N2	.42502-17	N	.31984-22	NO	.29218-14	NO2	.10517-24
N2O	.31378-19	N2O3	.00000	N2O4	.00000	N2O5	.00000	O	.38042-20
O3	.00000	CFO	.14687-15	C2F6	.00000	FNO2	.30107-37	F2N	.57966-37
FNO3	.00000	HNO	.40572-18	HNO2	.65152-22	HNO2	.84900-22	HNO3	.67898-33
F4N2	.00000	HO2	.26403-23	NO3	.00000	CF4O	.00000	F2N2	.00000
F2N2	.00000	H2N2	.21687-17	CN2	.12862-29	CH2	.50474-24	C2O	.08176-20
FO2	.00000	C2H	.10417-19	C2N	.70362-24	C2HF	.43964-21	CHF	.51045-21
C2F3N	.10909-28	F3NO	.00000	F2	.25462-32	O2	.70263-28	CHO	.20370-17
N3	.35967-25	C F	.14322-25	C2 F	.15175-25	C3 F	.70480-19	C4 F	.08133-23

Sample Problem 5, Sample Output, Continued

GRAPHITE SURFACE KINETICS (BASED) PROB. 5 5002000*60

REACTANT
COEFFICIENTS

REACTION	1	2	3	4
CO2		1		
H2			1	
H2O	1			1
CO				1
C* F	1	1	2	
FM				
N2				

PRODUCT
COEFFICIENTS

REACTION	1	2	3	4
CO2				1
H2			3	1
H2O		2		
CO	1	2	2	
C* F				
FM				
N2				

KINETIC REACTION---	1	2	3	4
PRE-EXPONENT FACTOR	5.081+01	5.081+01	3.130+00	4.065+00
ACTIVATION ENERGY	4.600+04	4.600+04	5.250+04	-0.060
TEMPERATURE EXPONENT	0.000	0.000	0.000	-0.000

SPECIES
INHIBITING
FACTORS
PSI/FKR

CO2	1.00/ -.00	1.00/ -.00	1.00/ -.00	-.00/ -.00
H2	1.00/ -.00	1.00/ -.00	.00/ -.00	-.00/ -.00
H2O	1.00/ -.00	1.00/ -.00	1.00/ -.00	-.00/ -.00
CO	1.00/ -.00	1.00/ -.00	1.00/ -.00	-.00/ -.00
C* F	-.00/ -.00	-.00/ -.00	-.00/ -.00	-.00/ -.00
FM	-.00/ 3.00	-.00/ 3.00	-.00/ -.00	-.00/ -.00
N2	-.00/ -.00	-.00/ -.00	-.00/ -.00	-.00/ -.00

DERIVATIVE PROPERTY OUTPUT

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
.39305-00	.39740-00	.10000+01	-.10000+01	-.00000

Sample Problem 5, Sample Output, Continued

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PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
  TEMP         VISC         COND         GRAN         PR           SC
 .21600+04    .28958-04    .19391-04    .18584-03    .58636-00    .72568-00
  MU1          MU2          MOL.WT       HTIL         CPTIL        HTIL*
 .92377-00    .24489+02    .25184+02   -.24103+04    .47780-00   -.24529+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA =  .667)
     1            6            7            8            9            106          44
 .33683-01    .88870-01    .16806-00    .20680-00    .41600-02    .44420-24    .41843-00
 .49534-01    .90108-31    .16938-00    .32473-00    .44617-02    .55940-24    .36179-00

SOLUTION TIMES
      ITERATIONS =   11                          TIME =    1.652 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS EDGE-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT RHOUCM =     .26600-00
 RHO V WALL/RHOE UE CM =     .11134-05    MPRIME =     .11134-05

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2150.0000 DEG R =  1200.0000 DEG K     PRESS =      12.77800 ATM

                                    GAS           CONDENSED       COMPOSITE
 ENTHALPY - BTU/LBM             -.25041+04        .00000         -.25041+04
 ENTROPY - BTU/LBM DEG R         .21981+01        .00000          .00000
 DENSITY - LBM/FT3               .20399-00                        .20399-00
 MOLECULAR WEIGHT                25.1841           .0000          25.1841

 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / MMOE UE CM). . . .
 1=   .48669-07  2=   .43934-07  3=   .60151-10  4=   .36877-02

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = MPRIME CONDENSED ). . . .
```

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
CO2	.23944-00	H2	.15236-00	H2O	.20524-00	CO	.18610-00	C* F	.00000
FH	.55139-02	N2	.15105-00	C2H2	.23317-10	C	.30857-25	CF	.27943-21
CFN	.64020-14	CF2	.12027-19	CF2O	.09104-12	CF3	.13580-24	CF4	.22287-23
CH	.39142-22	CHFO	.11734-08	CH3	.14836-10	CHN	.39580-06	CHNO	.51261-07
CHO	.33158-09	CH2	.12044-16	CH2F2	.10084-14	CH2O	.37624-06	CH3	.52360-09
CH3F	.45766-19	CH4	.16286-03	CN	.90361-16	C2	.45567-30	C2F2	.79631-30
C2F4	.79243-35	C2H4	.47368-09	C2H4O	.23489-16	C2H2	.11375-14	C3	.15994-29
C3O2	.20982-13	C4	.53834-38	C4N2	.35875-25	F	.14936-14	FNO	.11268-18
FN	.53633-24	FNO	.11698-21	FO	.55204-26	F2O	.93000	F3N	.00000
H	.21448-07	HN	.24709-14	HO	.28788-09	H2N	.12245-09	H2O2	.14080-15
H3N	.56136-24	HNO2	.03453-16	N	.45484-18	NO	.12752-11	NO2	.10094-20
N2O	.12942-15	N2O3	.53680-37	N2O4	.00000	N2O5	.00000	O	.42958-16
O3	.13158-31	CFO	.50343-14	C2F6	.00000	FNO2	.34885-32	F2N	.53521-32
FNO3	.00000	HNO	.30417-15	HNO2	.86789-19	HNO2	.10985-18	HNO3	.19013-28
F4N2	.00000	HO2	.21838-19	NO3	.12039-34	CF4O	.00000	F2N2	.17308-37
F2N2	.77629-38	H2O2	.21843-15	CN2	.15147-25	CN2	.05810-21	C2O	.17867-17
FO2	.13987-32	C2H	.15997-17	C2N	.45655-21	C2HF	.11487-19	CHF	.13049-18
C2F3N	.37449-28	F3N	.00000	F2	.10011-27	O2	.30250-16	CNO	.33453-15
N3	.15416-21	C F	.00540-24	C2 F	.35924-27	C3 F	.35413-25	C4 F	.33470-32

Sample Problem 5, Sample Output, Continued

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        GRAPHITE SURFACE KINETICS (GASKET) PROB. 5          5002000*40

                                                                    9  7

DERIVATIVE PROPERTY OUTPUT
 CP-FROZEN     CP-EQUIL    DLNM/DLNT   DLNM/DLNP      GAMMA
  .40440-00    .40457-00    .10000+01  -.10000+31   -.00000

PROPERTY ROUTINE OUTPUT IN  LB-MASS,FT,SEC,BTU,AND DEG-R
   TEMP          VISC          COND          UBAR          PR            SC
  .25200+04    .32256-04     .21931-04     .23999-03     .59480-00     .72560-00
    MU1           MU2         MOL.WT         CPTIL         CPTIL*        HTIL*
  .91873-00    .24511+02     .24826+02    -.22365+04     .48515-00    -.22759+04

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . . (GAMMA =  .667)
      1             6             7             8             9            10            44
   .34699-01     .10301+00     .16983-00     .32205-00     .42038-02     .17508-14     .36620-00
   .49533-01     .10335+00     .16937-00     .35996-00     .44616-02     .19721-14     .31332-00

SOLUTION TIMES
        ITERATIONS =    7                       TIME =     1.046 SEC.

OPEN SYSTEM CHEMICAL KINETICS SOLUTION OUTPUT

 SURFACE IS EDGE-ORIENTED PYROLYTIC GRAPHITE
 MASS TRANSFER COEFFICIENT ROUCM =     .24600-00
 RHO V WALL/RHOE UE CM =     .17684-04   APRIME =     .17684-04

 STATE ADJACENT TO THE SURFACE . . . .
  TEMP =  2520.0000 DEG R =  1400.0000 DEG K      PRESS =      12.77800 ATM

                                  GAS            CONDENSED       COMPOSITE
  ENTHALPY - BTU/LBM           -.23199+04         .00000          -.23199+04
  ENTROPY - BTU/LBM DEG R       .22779+01         .00000           .00000
  DENSITY - LBM/FT3             .17236-00                          .17236-00
  MOLECULAR WEIGHT             24.8257            .0000           24.8257


 NET FORWARD RATE OF KINETICALLY CONTROLLED REACTIONS
  (MOLES OF REACTION / UNIT SURFACE AREA / TIME / RHOE UE CM). . . .
  1=   .85446-06  2=   .61545-06  3=   .11881-08  4=   .25847-02

 CHEMICAL STATE ADJACENT TO THE SURFACE
  (MOLE FR FOR GASES = MOLECULES / TOTAL GAS MOLECULES )
  (MOLE FR FOR CONDENSED = APRIME CONDENSED ). . . .

   SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.     SPECIES   MOLE FR.
   CO2       .20657-00    H2        .13772-00    H2O       .28679-00    CO        .21291-00    C* F      .00000
   FH        .54928-02    N2        .15049-00    C2H2      .96829-11    C         .12255-21    CF        .77959-19
   CFN       .60062-15    CF2       .33975-16    CF2O      .12092-11    CF3       .34391-23    CF4       .41600-23
   CH        .24753-19    CHFO      .19343-08    CHF3      .13162-18    CHN       .34608-06    CHNO      .62903-07
   CHO       .31547-08    CH2       .34730-15    CH2F2     .44733-15    CH2O      .32658-06    CH3       .43568-09
   CH3F      .83471-11    CH4       .44853-05    CN        .61045-14    C2        .13950-26    C2F2      .61044-28
   C2F4      .95678-34    C2H4      .12677-13    C2H4O     .58883-17    C2N2      .18751-14    C3        .43487-27
   C3N2      .26306-13    C4        .20059-35    C4N2      .29099-25    F         .26386-12    FHO       .35489-16
   FN        .10406-20    FNO       .10506-18    FO        .60696-22    F2O       .32110-34    F3N       .36417-30
   H         .50247-06    HN        .36094-12    HO        .20146-07    H2N       .11266-08    H2O2      .30306-13
   H3N       .21751-04    H4N2      .18744-13    N         .42364-15    NO        .19720-09    NO2       .28705-17
   N2O       .17140-13    N2O3      .14429-31    N2O4      .00000       N2O5      .00000       O         .68768-13
   O3        .79019-28    OF2       .14926-12    C2F6      .00000       FNO2      .73969-28    F2N       .2A874-28
   FNO3      .00000       HNO       .90453-13    HNO2      .44107-16    HNO2      .60067-16    HNO3      .20467-24
   F4N2      .00000       NO2       .51580-16    NO3       .26967-29    CF4O      .19132-37    F2N2      .14186-33
   F2N2      .76860-34    H2N2      .38240-14    CN2       .91234-23    CN2       .83043-19    C2O       .87888-16
   FO2       .14594-27    C2H       .23577-16    C2N       .26160-19    C2HF      .66303-19    CHF       .50494-17
   C2F3N     .98829-28    F3NO      .00000       F2        .29354-24    O2        .68726-13    CNO       .19389-13
   N3        .64348-19    C* F      .24494-19    C2 F      .5A044-22    C3 F      .36910-20    C4 F      .34726-26
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Sample Problem 5, Sample Output, Concluded

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