THE CONTROL OF OXIDES OF NITROGEN EMISSIONS FROM AIRCRAFT GAS TURBINE ENGINES

Volume 2: The NOx Formation Process

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The contents of this report reflect the views of the Northern Research and Engineering Corporation which is responsible for the facts and the accuracy of the data presented herein. The contents do not necessarily reflect the official views or policy of the Department of Transportation or the Environmental Protection Agency. This report does not constitute a standard, specification or regulation.
The objective of this study was to develop criteria for use in the design of aircraft gas turbine combustion chambers to minimize nitrogen oxide emissions. The approach adopted involved the development of a mathematical model of NOx emission from aircraft engine combustors; a parametric analysis, using the model, to determine the sensitivity of NOx emissions to variations of model parameters and engine design variables; evaluation of critical model parameters by means of experimental measurements; and the incorporation of the model into combustor design methods to provide guidelines for minimizing NOx emission while maintaining other performance and emission characteristics. The results of the study and the NOx emission control criteria are described in Volume 1 (FAA-RD-71-111-1). Volume 2 (FAA-RD-71-111-2) describes the nitric oxide formation process and a computer program (NOXRAT) for calculating thermodynamic data. The program is based upon a six-reaction model of NO formation. Volume 3 (FAA-RD-71-111-3) describes combustion and flow processes in gas turbine combustors and a computer program (GASNOX) for calculating gas properties and NO concentrations throughout a combustor. This program is based upon a three-zone, heterogeneous model of gas turbine combustor operation. Program GASNOX is used with input data from Program NOXRAT to calculate NO emission rates.
The study reported here was carried out under the technical direction of Dr. D. M. Dix with Dr. Ronald S. Fletcher assuming project responsibilities. Other participants in the program were Dr. R. D. Siegel, Dr. E. K. Bastress, and Mr. R. J. Murad; Professors J. B. Heywood, A. H. Lefebvre, and Mr. E. R. Norster served in a consulting capacity during the course of the study.

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1. INTRODUCTION

Volume 1 of this report carries a full description of the complete program but omits mathematical details of the model developed to predict the nitric oxide (NOx) emissions from aircraft gas turbine combustors and also the details of two computer programs developed as part of the study for obtaining predictions from the model. It is the purpose of Volumes 2 and 3 of the report to present full descriptions of both the model and the computer programs.

It is convenient to consider the model in two parts, one part being concerned with the NOx formation process and the other with modeling the flow behavior within gas turbine combustors. The convenience arises not only due to the basic difference in the studies of these two parts, but also due to the fact that a separate computer program has been developed for each part. This approach has been adopted in the interests of economy of computation as calculation of the necessary data for the determination of the NOx formation process requires appreciable computer time, but, of course, the data once collected can be applied to any combustor calculation with the same reference conditions (in this case, combustor inlet conditions) of pressure and temperature. The computer program developed for this task has the name NOXRAT, and its function is to compute the rate terms of the NOx formation process and all relevant thermodynamic data for a series of fuel-to-air ratios with a common reference state.

Volume 2 of this report is solely concerned with the nitric oxide formation process. It presents a mathematical description of the process, a full description of the program NOXRAT, and also includes a section which is essentially a user's manual for the program. Volume 3 produces the same details for the flow model developed to describe the flow conditions in a gas turbine combustor. The corresponding computer program is named GASNOX and it is so arranged that the rate terms and all relevant thermodynamic data computed in NOXRAT are punched onto a deck of computer cards which serves as input data to the main program GASNOX.
The objective of this volume of the report, therefore, is to present the theory behind the NOx formation process and details of the computer program developed for its application.
2. THE NOx FORMATION PROCESS

While engine exhaust emissions are often expressed as nitrogen oxides (NOx), or as nitrogen dioxide (NO₂), the pollutant present in the exhaust gas as it leaves the engine is almost completely nitric oxide, NO, with only a few per cent of NO₂ (Ref 1). The conversion to NOx or NO₂ is made because many of the techniques used to measure nitric oxide require first that it be oxidized to nitrogen dioxide. Thus, inside the engine, the important oxide of nitrogen to consider is nitric oxide, NO.

Several authors have proposed reaction schemes for nitric oxide formation, e.g., Caretto, Sawyer, and Starkman (Ref 1), Bartok, et al (Ref 2), Newhall (Ref 3), Lavoie, Heywood, and Keck (Ref 4). The set of reactions proposed by Lavoie, et al (Ref 4) is the most complete for predicting nitric oxide formation, and it has been evaluated experimentally for a range of equivalence ratios (0.9-1.2), pressures (10-30 atm), and temperatures (2200-2800 deg K) in a spark-ignition engine (Refs 4 and 5). These conditions are directly comparable to those occurring in the gas turbine combustor primary zone as shown by Heywood et al (Ref 5), and the reaction scheme does predict NO emission levels which are in good agreement with measurements made on such combustion systems.

The set of reactions included in the analyses of References 4, 5, and 6 are incorporated in the model and are shown below.

\[
\begin{align*}
N + NO & \rightleftharpoons N_2 + O \quad (1) \\
N + O_2 & \rightleftharpoons NO + O \quad (2) \\
N + OH & \rightleftharpoons NO + H \quad (3) \\
H + N_2O & \rightleftharpoons N_2 + OH \quad (4) \\
O + N_2O & \rightleftharpoons N_2 + O_2 \quad (5) \\
O + N_2O_2 & \rightleftharpoons NO + NO \quad (6)
\end{align*}
\]

Note that the reaction 2NO \rightleftharpoons N_2 + O_2 has been omitted from this scheme as it is very slow and does not proceed directly. In References 4 through 6 the rate constants selected for these reactions were taken from Schofield (Ref 7) except for reaction 3 which was taken from
Campbell and Thrush (Ref 8). These constants are,

\[ \begin{align*}
  k_1 &= 2 \times 10^{-11} \\
  k_2 &= 2 \times 10^{-11} \exp(-7.1/RT) \\
  k_3 &= 7 \times 10^{-11} \\
  k_4 &= 5 \times 10^{-11} \exp(-10.8/RT) \\
  k_5 &= 6 \times 10^{-11} \exp(-24.0/RT) \\
  k_6 &= 8 \times 10^{-11} \exp(-24.0/RT)
\end{align*} \]

and are in \( \text{cm}^3/\text{sec}\)-molecule. \( R \) is in kcal/gm-mole-deg K. Since the equilibrium constants for these reactions are known, the kinetic scheme is thus completely defined.

Recently completed analyses of data and correlations available in the latest literature have raised some question as to the reliability of the above constants. A group at Leeds University (Ref 9) reports \( k_1 \) better correlated in the form \( A \exp(-E/RT) \) while both Leeds and Newhall (Ref 3) show reaction 2 to be correlated more satisfactorily in the form \( AT \exp(-E/RT) \). Newhall also correlated reaction 6 with a pre-exponential factor 3.6 times greater, and an activation energy 1.16 times greater, than the corresponding values determined by Schofield.

With this lack of agreement of the rate constants, it was decided to represent all six reactions in the reaction scheme in the general form,

\[ k_i = A_i T_i^n \exp(-E_i/RT) \]  \hspace{1cm} (7)

This format allows maximum flexibility in comparing the different fits of the kinetic rate data for each of the expressions. Further, as new data and correlations become available, it will be a simple matter to adjust the three constants to correspond accordingly to those correlations and data.

Not all of the above reactions are equally important over the equivalence ratio and temperature range of interest. The first two reactions, the Zeldovich chain mechanism, are the two most important reactions at high temperatures (greater than 2200 deg K) in fuel-lean mixtures. The importance of this pair of reactions is well established. The third reaction becomes important in fuel-rich mixtures. Reactions
4, 5, and 6 involving \( N_2O \) as an intermediary become important at temperatures about 2000 deg K. It can be shown that the small amount of \( NO_2 \) present is in equilibrium with the NO and other reactions with \( NO_2 \) need not be included (Ref 5).

Conditions in gas turbine combustors fall into all of these regimes, but calculations indicate that the reactions 4, 5, and 6 do not contribute greatly to the nitric oxide formation rate. In fact, if one accepts the probable limits of accuracy for any such kinetic scheme, a case may be made for their exclusion. However, these reactions are included in the reaction scheme for the sake of completeness.

In order to apply this reaction scheme to gas turbine combustors, it is necessary to be able to predict the concentration levels of all species active in the set of six reactions specified above at all thermodynamic states typical of the combustor. At the pressure and temperature levels that exist in such combustors during high thrust, low altitude operation, the hydrocarbon oxidation reactions go rapidly to completion compared with the nitric oxide formation processes. In order to predict these species concentrations therefore, the following assumptions are made:

a. Combustion is mixing controlled and not rate-limited, and therefore, in the combustor, \( N_2, O_2, O, OH, H, \) and \( H_2 \) concentrations are the equilibrium concentrations corresponding to the combustor inlet temperature and pressure, and to the equivalence ratio. This assumption limits the usefulness of the model to high pressure, high temperature operating conditions, but it is precisely these conditions at which most nitric oxide is produced and are therefore of most interest to this study.

b. \( N \) and \( N_2O \) concentrations are given by the steady-state assumption; that these concentrations are not in equilibrium but are in steady-state with NO can be shown by deriving rate equations for \( N \) and \( N_2O \) which have relaxation times short compared with the NO rate equation.

If these assumptions are applied to Equations 1 through 7, then the change, \( \dot{n} \), in total nitric oxide per unit time per unit volume,
that results from chemical reaction over a fixed element can be written as

\[ \dot{\alpha} = 2M_{NO} (1 - \alpha^2) \left[ \frac{R_1}{1 + \alpha K_1} + \frac{R_6}{1 + K_2} \right] \]  

where \( M_{NO} \) is the molecular weight of NO, \( \alpha = [NO]/[NO]_e \) is the local nitric oxide concentration divided by the equilibrium nitric oxide concentration, \( R_1 \) is the "one-way" equilibrium rate of reaction 1, i.e., \( R_1 = k_1 [N]_e [NO]_e \); \( K_1 = R_1/(R_2 + R_3) \) with \( R_2 \) and \( R_3 \) defined analogously to \( R_1 \) but for reactions 2 and 3; and \( R_6 = k_6 [O]_e [N_2O]_e \) and \( K_2 = R_6/(R_4 + R_5) \).

It is interesting to consider the form of the equation above when applied to the gas turbine combustor. In this case the thermodynamic base state is represented by the combustor inlet pressure and temperature, both of which are nonvariable with time for a fixed operating condition. If the fuel-to-air ratio is specified, therefore, the terms \( R_1, R_6, K_1 \) and \( K_2 \) all become constants as a consequence of assumptions a and b above. The molecular weight \( M_{NO} \) is a constant, hence the only variable is \( \alpha \) and the equation reduces to the simple form,

\[ \frac{dNO}{dt} = f(NO) \]

which may readily be integrated to follow the nitric oxide concentration levels through the combustor.

Maximum utility has been made of this simplicity, chiefly in the interests of reducing the computer operating costs for each sample case tested in the flow model. The computational procedure, as previously explained in the introduction, was separated into two tasks; the first task primarily determines the rate terms \( R_1, R_6, K_1 \), and \( K_2 \) for a specified combustor inlet temperature and pressure over the complete range of fuel-to-air ratios that cause sufficiently high temperatures to form nitric oxide, and the second task computes the flow conditions throughout the combustor and uses the data collected from task one to predict nitric oxide emission levels.

A computer program has been developed for each task and the program for Task 1 will be described in the next section.
3. PROGRAM NOXRAT

3.1 INTRODUCTION

3.1.1 Program Function and Capabilities

Program NOXRAT is a modified version of CEC, a NASA developed digital computer program written in Fortran IV (Refs 10, 11 and 12). NOXRAT is designed to evaluate the chemical equilibrium products, the adiabatic flame temperature, and the kinetic properties used in the nitric oxide formation model (previously described) for the combustion of a reactive fuel, or a fuel mixture with an oxidant or mixture of oxidants. NOXRAT iteratively calculates the equilibrium properties of the combustion products based on a minimized Gibbs free energy. In a typical equilibrium computation NOXRAT prints the following properties for each assigned fuel-to-air ratio:

a. The equilibrium temperature and pressure; the sonic velocity, the enthalpy, entropy, mean molecular weight, \( \frac{\partial V}{\partial P} \), the heat capacity, and the heat capacity ratio \( \frac{C_p}{C_v} \), of the combustion stream.

b. The mole fraction of each of the combustion products present at equilibrium at concentrations greater than \( 5 \times 10^{-6} \).

c. The chemical formula, weight fraction in the total fuel or oxidant, and the base enthalpy, temperature, density, and physical state of each of the specified reactants.

d. The total oxidant to total fuel weight ratio, the per cent fuel, the equivalence ratio, and the average density of the reaction mixture.

e. The equilibrium mole fraction of each of the species of interest in the nitric oxide kinetic scheme (Ref 18) and the equilibrium mole fractions of \( C(S) \), \( CO \), and \( CO_2 \).

f. The molecular weight and the adiabatic flame temperature of the combustion products; the assigned inlet pressure; the

* Normal output of CEC.
fuel-to-air ratio; and the atomic composition, inlet temperature, and enthalpy of both the fuel(s) and the oxidant(s).

For each assigned pressure the program also prints and punches:

a. The atomic composition of the fuel (C_{x}H_{y}); the inlet air temperature; a code number identifying the set of kinetic constants used in the NO rate formation calculations; the assigned pressure; and the stoichiometric equivalence ratio.

b. For each specified fuel-to-air ratio: the mixture ratio (mass of fuel to mass of fuel and air); the equivalence ratio; the density and adiabatic flame temperature of the combustion products; the equilibrium concentration of NO, CO, C_{(s)}, and CH_{2} (unburned fuel); and the kinetic parameters* R_1, R_6, K_1, and K_2 where R_1 and R_6 are forward reaction rates for reactions 1 and 6 and K_1 and K_2 are ratios of forward reaction rates used in the kinetic scheme (see Appendix V).

NOXRAT also permits calculation of:

a. Chemical equilibrium for assigned temperatures and pressures.

b. Theoretical rocket performances for both frozen and equilibrium compositions during expansion.

c. Chapman-Jouguet detonation properties.

The latter two options were not exercised in this study.

3.1.2 Analysis Procedures

The analytical procedures on which NOXRAT is based are described in Section 2. A detailed description of the changes that have been incorporated into these procedures to permit calculation of the reaction rate constants and the thermal properties used in the chemical reactions is provided.

* These parameters are used to compute the rate of change of the NO mass fraction due to chemical reaction by:

\[
\frac{d\chi_{NO}}{dt} = \frac{2M_{NO}}{\rho} (1-\phi^2) \left[ \frac{R_1}{K_{1}} + \frac{R_6}{K_{2}} \right]
\]

where \(M_{NO}\) is the molecular weight of NO, \(\rho\) is the gas density, \(\chi_{NO}\) is the mass fraction concentration of NO and \(\phi\) is the ratio of NO concentration to the NO concentration at equilibrium.
reaction scheme for the formation of nitric oxide are presented in the appendices of this report. Reference to any of these procedures is unnecessary for operation of the computer program.

3.1.3 Report Arrangement

The main body of the report begins with a section in which the input data necessary for the solution of any case are described in detail; this includes instructions for preparing and supplying these data to the program and a sample case in the appropriate format. The next section contains a discussion of the various types of output data which are obtained from the program and also the output data from the sample case. Following that is a section containing miscellaneous information regarding the operation of the program with the CDC 6600 computing system. The next section is a description of the error messages printed by the program.

The first appendix consists of a general discussion of the overall logic structure of the program. The next appendix gives the Fortran nomenclature for the major new variables incorporated into the original CEC program. The remaining appendices, except the last two, provide detailed description of the changes made to existing routines and of the subroutines which have been developed and incorporated into the program, one appendix for each routine. The appendix for each new subroutine contains a presentation of the input and output variables, an internal Fortran nomenclature, a description of the step-by-step calculation procedure, and a Fortran listing of the subroutine. The last two appendices are respectively a listing of the program in its entirety and a listing of the THERMO data.

3.2 INPUT DATA

3.2.1 General Description

The input data to Program NOXRAT is nearly identical with that of NASA's Program CEC. Although the input format for CEC has been described in a preliminary guide (Ref 13) and detailed in a NASA report (Ref 14), NREC has elected to present here
a description of NOXAT input (and output) data. This description is suitable to allow the reader to understand the mechanics of how to operate the program. Much of this information is taken directly from Reference 13.

Program input data will be discussed under four categories. Three of the categories are required and one is optional. The three required categories and the code names by which they will be referred are as follows:

a. Library of thermodynamic data for reaction products (THERMO data).

b. Data pertaining to reactants (REACTANTS cards).

c. Namelist data which includes the type of problem, required schedules, and options (NAMELISTS Input).

d. The optional category of data are chemical formulas of species which are singled out for special purposes (OMIT and INSERT cards).

**THERMO Data**

The thermodynamic data are in the form of 7 least squares coefficients (a_i) for the following equations:

\[
\frac{C_p^0}{RT} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4
\]

(1)

\[
\frac{H^0}{RT} = a_1 + \frac{a_2}{2} T + a_3 T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{6}
\]

(2)

\[
\frac{S^0}{RT} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7
\]

(3)

\[
\frac{G^0}{RT} = \frac{H^0}{RT} - \frac{S^0}{T}
\]

(4)

For each species, two sets of coefficients are included for two adjacent temperature intervals. The data provided cover the temperature intervals 300 deg K to 1000 deg K and 1000 deg K to 5000 deg K.
The supplied data for each species were made by the PAC program described in NASA TN D-4097 (Ref 15). For the gases, the PAC program calculated the thermodynamic functions from the molecular data given in JANAF (Ref 16). For the condensed species, the thermodynamic functions were taken directly from JANAF. However, NASA added the functions at the transition points since they were not included in the JANAF data. The PAC program does a least squares fit of the functions for the two specified temperature intervals. The fits are constrained to give consistent data at transition points and at the common interval temperature (1000 deg K).

Heats of formation and transition were also taken from JANAF. They were combined with sensible heats to give assigned enthalpies $H^\circ_T$. By definition,

$$H^\circ_T = H^\circ_{298.15} + \left[ H^\circ_T - H^\circ_{298.15} \right]$$  \hspace{1cm} (5)

It has been arbitrarily assumed that $H^\circ_{298.15} = (\Delta H^E_f)_{298.15}$. Equation 5 then becomes

$$H^\circ_T = (\Delta H^E_f)_{298.15} + \left[ H^\circ_T - H^\circ_{298.15} \right]$$  \hspace{1cm} (6)

For the JANAF reference elements, $H^\circ_{298.15} = 0$. In general, $H^\circ_T \neq (\Delta H^E_f)_T$ for $T \neq 298.15^\circ K$.

**REACTANTS Data**

Reactants data consists of the following physical data for each of the reaction species in the combustion stream.

a. Atomic symbols and formula numbers.

b. Relative weights or number of moles (for fuel in total fuels or oxidant in total oxidants).

c. Enthalpy.

d. Physical state (solid, liquid, gas).

e. Temperature associated with enthalpy in item c above.

f. Density.
NAMELISTS Data

NAMELISTS data is specified on two input NAMELISTS; only the first is necessary for generation of the chemical equilibrium and kinetic rate data of interest. The second NAMELIST is associated with the rocket performance option of NOXRAT described in the introduction to this report. This latter option was not exercised in this study but will be described in the following subsection. The information required in the first NAMELIST is:

a. The type of problem.
b. One or more pressures.
c. One or more temperatures for assigned temperature problems (e.g., rocket problems with an assigned chamber temperature).
d. The relative amount of fuel(s) and oxidant(s).

The information required in the second NAMELIST is:

a. The pressure ratio schedule.
b. The subsonic area ratio values (optional).
c. The supersonic area ratio values (optional).
d. Whether only frozen or equilibrium performance is to be calculated (optional).

OMIT and INSERT Data

OMIT and INSERT cards are optional. They contain the names of particular species in the library of thermodynamic data for the specific purposes stated below.

OMIT Cards. These cards list species to be omitted from the THERMO data.

INSERT Cards. These cards contain the names of condensed species only.

3.2.2 Detailed Description of Input Data

The information required to prepare the input data for a case is furnished in the table given below. This information contains a description of each input item as well as a description of the form in
which these items are written on input data sheets. The descriptions of the input items refer frequently to several points, relevant to the selection of input values, which are discussed in the subsequent subsection. The discussions of these points provide additional detailed information useful in preparing the input data for any case.

The first input item read by Program NOXRAT is the code word THERMO. The second input line contains the three temperature values 300, 1000, 5000. This input is followed by the thermodynamic data for any number of species. The last line of the THERMO input contains the code word END and follows the last set of species data (see point a).

<table>
<thead>
<tr>
<th>Line</th>
<th>Location</th>
<th>Input Item</th>
<th>Type of Number</th>
<th>Fortran Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-6</td>
<td>A</td>
<td></td>
<td></td>
<td>This is the code word &quot;THERMO&quot; that identifies the beginning of the thermodynamic data</td>
</tr>
<tr>
<td>2</td>
<td>1-10</td>
<td>FP</td>
<td>TLOW</td>
<td></td>
<td>Low temperature for lowest temperature interval of thermodynamic data</td>
</tr>
<tr>
<td>2</td>
<td>11-20</td>
<td>FP</td>
<td>TMID</td>
<td></td>
<td>Common temperature for the two temperature intervals of the thermodynamic data</td>
</tr>
<tr>
<td>2</td>
<td>21-30</td>
<td>FP</td>
<td>THIGH</td>
<td></td>
<td>High temperature for highest temperature interval of thermodynamic data</td>
</tr>
<tr>
<td>3</td>
<td>1-12</td>
<td>A</td>
<td>DATA</td>
<td></td>
<td>Species name</td>
</tr>
<tr>
<td>3</td>
<td>19-24</td>
<td>A</td>
<td>DATA</td>
<td></td>
<td>Date</td>
</tr>
<tr>
<td>3</td>
<td>25-26</td>
<td>A</td>
<td>DATA</td>
<td></td>
<td>Atomic symbol</td>
</tr>
<tr>
<td>3</td>
<td>27-29</td>
<td>FP</td>
<td>DATA</td>
<td></td>
<td>Atomic formula number</td>
</tr>
<tr>
<td>3</td>
<td>30-31</td>
<td>A</td>
<td>DATA</td>
<td></td>
<td>Atomic symbol</td>
</tr>
<tr>
<td>3</td>
<td>32-34</td>
<td>FP</td>
<td>DATA</td>
<td></td>
<td>Atomic formula number</td>
</tr>
<tr>
<td>Line</td>
<td>Location</td>
<td>Input Item</td>
<td>Type of Number</td>
<td>Fortran Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>------------</td>
<td>----------------</td>
<td>----------------</td>
<td>-------------</td>
</tr>
<tr>
<td>3</td>
<td>35-36</td>
<td>A</td>
<td>DATA</td>
<td>Atomic symbol</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>37-39</td>
<td>FP</td>
<td>DATA</td>
<td>Atomic formula number</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>40-41</td>
<td>A</td>
<td>DATA</td>
<td>Atomic symbol</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>42-44</td>
<td>FP</td>
<td>DATA</td>
<td>Atomic formula number</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>45</td>
<td>A</td>
<td>DATA</td>
<td>Species phase (S = solid; L = liquid; G = gas)</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>46-55</td>
<td>FP</td>
<td>DATA</td>
<td>Low temperature of temperature interval</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>56-65</td>
<td>FP</td>
<td>DATA</td>
<td>High temperature of temperature interval</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>80</td>
<td>Int</td>
<td>NCD</td>
<td>Integer 1 to identify card</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1-15</td>
<td>a&lt;sub&gt;1&lt;/sub&gt;</td>
<td>FP</td>
<td>Coefficient in equations 1-4 for upper temperature interval</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>16-30</td>
<td>a&lt;sub&gt;2&lt;/sub&gt;</td>
<td>FP</td>
<td>Coefficient in equations 1-4 for upper temperature interval</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>31-45</td>
<td>a&lt;sub&gt;3&lt;/sub&gt;</td>
<td>FP</td>
<td>Coefficient in equations 1-4 for upper temperature interval</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>46-60</td>
<td>a&lt;sub&gt;4&lt;/sub&gt;</td>
<td>FP</td>
<td>Coefficient in equations 1-4 for upper temperature interval</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>61-75</td>
<td>a&lt;sub&gt;5&lt;/sub&gt;</td>
<td>PP</td>
<td>Coefficient in equations 1-4 for upper temperature interval</td>
<td></td>
</tr>
<tr>
<td>Line</td>
<td>Location</td>
<td>Item</td>
<td>Type of</td>
<td>Fortran Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>------</td>
<td>---------</td>
<td>----------------</td>
<td>-------------</td>
</tr>
<tr>
<td>4</td>
<td>80</td>
<td></td>
<td>Int</td>
<td>NCD</td>
<td>Integer 2 to identify card</td>
</tr>
<tr>
<td>5</td>
<td>1-15</td>
<td>a₆</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for upper temperature interval</td>
</tr>
<tr>
<td>5</td>
<td>16-30</td>
<td>a₇</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for upper temperature interval</td>
</tr>
<tr>
<td>5</td>
<td>31-45</td>
<td>a₁</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for lower temperature interval</td>
</tr>
<tr>
<td>5</td>
<td>46-60</td>
<td>a₂</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for lower temperature interval</td>
</tr>
<tr>
<td>5</td>
<td>61-75</td>
<td>a₃</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for lower temperature interval</td>
</tr>
<tr>
<td>6</td>
<td>83</td>
<td></td>
<td>int</td>
<td>NCD</td>
<td>Integer 3 to identify card</td>
</tr>
<tr>
<td>6</td>
<td>1-15</td>
<td>a₄</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for lower temperature interval</td>
</tr>
<tr>
<td>6</td>
<td>16-30</td>
<td>a₅</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for lower temperature interval</td>
</tr>
<tr>
<td>6</td>
<td>31-45</td>
<td>a₆</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for lower temperature interval</td>
</tr>
</tbody>
</table>
### Input Type of Fortran Line Location Item Number Symbol Description

<table>
<thead>
<tr>
<th>Line</th>
<th>Location</th>
<th>Item</th>
<th>Type of Number</th>
<th>Fortran Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>46-60</td>
<td>a,</td>
<td>FP</td>
<td>DATA</td>
<td>Coefficient in equations 1-4 for lower temperature interval</td>
</tr>
<tr>
<td>6</td>
<td>80</td>
<td>int</td>
<td>NCD</td>
<td></td>
<td>Integer 4 to identify card</td>
</tr>
</tbody>
</table>

Lines 3-6 are repeated for each species in the thermodynamic data. The last line of the thermodynamic data, designated as line N below, contains the word END. This word is a signal to the computer that it has reached the end of the thermodynamic data.

N 1-3 A This is the code word "END" that identifies the end of the thermodynamic data.

The next set of input data read by Program NOXRAT are reactant cards (see point b). These cards are required for all problems; they contain specific data on the reactants to be combusted. The first item in the set contains the code word REACTANTS; the last card in the set is blank. In between the first and last cards may be any number of cards up to a maximum of 15, one for each reactant species being considered. There is no limit to the number of sets of reactants to be considered by the program; each must, however, be followed by appropriate data from input categories (3) and (4). The input for each series or set of reactants begins with a new data line N+1 and concludes with data line M.

<table>
<thead>
<tr>
<th>Line</th>
<th>Location</th>
<th>Item</th>
<th>Type of Number</th>
<th>Fortran Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>N+1</td>
<td>1-9</td>
<td>A</td>
<td>A</td>
<td>NAME</td>
<td>This is the code word &quot;REACTANTS&quot; that identifies the beginning of reactants data</td>
</tr>
<tr>
<td>N+2</td>
<td>1-2</td>
<td>A</td>
<td>NAME</td>
<td></td>
<td>Atomic symbol</td>
</tr>
<tr>
<td>N+2</td>
<td>3-9</td>
<td>FP</td>
<td>ANUM</td>
<td></td>
<td>Atomic formula number</td>
</tr>
<tr>
<td>N+2</td>
<td>10-11</td>
<td>A</td>
<td>NAME</td>
<td></td>
<td>Atomic symbol</td>
</tr>
<tr>
<td>Line</td>
<td>Location</td>
<td>Item</td>
<td>Type of Number</td>
<td>Fortran Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>-------</td>
<td>----------</td>
<td>--------</td>
<td>----------------</td>
<td>----------------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>N+2</td>
<td>13-18</td>
<td></td>
<td>FP</td>
<td>ANUM</td>
<td>Atomic formula number</td>
</tr>
<tr>
<td>N+2</td>
<td>19-20</td>
<td></td>
<td>A</td>
<td>NAME</td>
<td>Atomic symbol</td>
</tr>
<tr>
<td>N+2</td>
<td>21-27</td>
<td></td>
<td>FP</td>
<td>ANUM</td>
<td>Atomic formula number</td>
</tr>
<tr>
<td>N+2</td>
<td>28-29</td>
<td></td>
<td>A</td>
<td>NAME</td>
<td>Atomic symbol</td>
</tr>
<tr>
<td>N+2</td>
<td>30-36</td>
<td></td>
<td>FP</td>
<td>ANUM</td>
<td>Atomic formula number</td>
</tr>
<tr>
<td>N+2</td>
<td>37-38</td>
<td></td>
<td>A</td>
<td>NAME</td>
<td>Atomic symbol</td>
</tr>
<tr>
<td>N+2</td>
<td>39-45</td>
<td></td>
<td>FP</td>
<td>ANUM</td>
<td>Atomic formula number</td>
</tr>
<tr>
<td>N+2</td>
<td>46-52</td>
<td></td>
<td>FP</td>
<td>PECWT</td>
<td>Relative weight (or number of moles) of fuel in total fuel or oxidant in total oxidant*</td>
</tr>
<tr>
<td>N+2</td>
<td>53</td>
<td></td>
<td>A</td>
<td>MOLE</td>
<td>Symbol to identify if PECWT is relative weight or number of moles = blank if relative weights = M if number of moles</td>
</tr>
<tr>
<td>N+2</td>
<td>54-62</td>
<td></td>
<td>FP</td>
<td>ENTH</td>
<td>Enthalpy in calories/gm mole (see point c.)</td>
</tr>
<tr>
<td>N+2</td>
<td>63</td>
<td></td>
<td>A</td>
<td>FAZ</td>
<td>State</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>= S for solid</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>= L for liquid</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>= G for gas</td>
</tr>
<tr>
<td>N+2</td>
<td>64-71</td>
<td></td>
<td>FP</td>
<td>RTEMP</td>
<td>Temperature in deg K associated with enthalpy in columns 54-62</td>
</tr>
<tr>
<td>N+2</td>
<td>72</td>
<td></td>
<td>A</td>
<td>FOX</td>
<td>Symbol to identify if reactant is an oxidant or a fuel = F if fuel = 0 if oxidant</td>
</tr>
<tr>
<td>N+2</td>
<td>73-80</td>
<td></td>
<td>FP</td>
<td>DENS</td>
<td>Density in gm/cc (optional)</td>
</tr>
</tbody>
</table>

* A fuel (or oxidant) may be composed of more than one fuel (or oxidant).
Line N+2 is repeated for each reactant in the set up to a maximum of 15 reactant species. The last line in this sequence (M) is blank.

```
M  1-80
```

The next input items are read into Program NOXRAT using a NAMELIST statement. Input data referring to a NAMELIST statement begins with a $ in the second location on a new line, immediately followed by the NAMELIST name, immediately followed by one or more blank characters. Any combination of three types of data items may then follow. The data items must be separated by commas. If more than one line is needed for the input data, the last item on each line, except the last line, must be a number followed by a comma. The first location on each line should always be left blank since it is ignored. The end of a group of data is signaled by a $ immediately after the last item of data. The form that data items may take is:

a. Variable name = constant, where the variable name may be an array element or a simple variable name. Subscripts must be integer constants.

b. Array name = set of constants separated by commas where \( k^* \) constant may be used to represent \( k \) consecutive values of a constant. The number of constants must be equal to the number of elements in the array.

c. Subscripted variable = set of constants separated by commas where, again, \( k^* \) constant may be used to represent \( k \) consecutive values of a constant. This results in the set of constants being placed in consecutive array elements, starting with the element designated by the subscripted variable.

The first input NAMELIST is necessary for all of the options associated with Program NOXRAT. The items in this NAMELIST, INPT2 are:

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Input Item</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>KASE</td>
<td></td>
<td>Optional assigned number associated with the case</td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Input Item</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>------------</td>
<td>-------------</td>
</tr>
<tr>
<td>P</td>
<td>P</td>
<td>Assigned pressures (maximum of 26) Chamber pressure (one value) for rocket problems. Values in atm unless PSIA or MMHG are set TRUE (see below)</td>
</tr>
<tr>
<td>T</td>
<td>T</td>
<td>Assigned temperature in deg K (maximum of 26) (see point d)</td>
</tr>
<tr>
<td>MIX</td>
<td></td>
<td>Value of fuel-to-oxidant air weight ratios if FA is set TRUE (maximum of 40). For rocket problems (RKT is set TRUE) there must be as many sets of RKTINP NAMELIST inputs as there are MIX values (see point e)</td>
</tr>
<tr>
<td>FA</td>
<td></td>
<td>If variable is set TRUE, fuel-to-air weight ratios given in MIX. Value before read: FALSE</td>
</tr>
<tr>
<td>TP</td>
<td></td>
<td>If variable is set TRUE, problem type is assigned temperature and pressure. Value before read: FALSE (see point f)</td>
</tr>
<tr>
<td>HP</td>
<td></td>
<td>If variable is set TRUE, problem type is assigned enthalpy and pressure. Value before read: FALSE (see point g)</td>
</tr>
<tr>
<td>RKT</td>
<td></td>
<td>If variable is set TRUE, problem type is rocket. Value before read: FALSE (see point h)</td>
</tr>
<tr>
<td>DETN</td>
<td></td>
<td>If variable is set TRUE, problem type is detonation. Value before read: FALSE (see point i)</td>
</tr>
<tr>
<td>PSIA</td>
<td>P</td>
<td>If set TRUE, pressure is in psia units. Values are converted to atm internally. Value before read: FALSE</td>
</tr>
<tr>
<td>MMHG</td>
<td>P</td>
<td>If set TRUE, pressure is in mmHg. Values are converted to atm internally. Value before read: FALSE</td>
</tr>
<tr>
<td>IONS</td>
<td></td>
<td>If set TRUE, ionic species are considered in the combustion products. Value before read: FALSE</td>
</tr>
</tbody>
</table>
Fortran Symbol | Input Item | Description
--- | --- | ---
IDEBUG | If set TRUE, intermediate output is printed. Value before read: FALSE.

The second NAMELIST, RKTINP, is required only for rocket (RKT) problems. It follows the INPT2 namelist. The items in this NAMELIST are

- **PCP**
  Ratio of chamber pressure to exit pressure (maximum of 22 values). See point j.
- **EQL**
  If set FALSE, program will not calculate rocket performance assuming equilibrium composition during expansion. Value before read: TRUE. This is an optional input. See point k.
- **FROZ**
  If set FALSE, program will not calculate rocket performance assuming frozen composition during expansion. Value before read: TRUE. This is an optional input. See point k.
- **SUBAR**
  Subsonic area ratio. This is an optional input. See point l.
- **SUPAR**
  Supersonic area ratio. This is an optional input. See point l.

The remaining input items to Program NOXRAT are optional. These are OMIT and INSERT cards. Each card contains the word OMIT (in card columns 1 through 4) or INSERT (in card columns 1 through 6) and the names of from 1 to 4 species starting in columns 16, 31, 46, and 61. The names must be exactly the same as they appear in the THERMO data. See point m for further discussion of these input items.

### 3.2.3 Discussion of Input Data

Some important aspects to be considered in appropriately specifying the input data are discussed below. Reference to these discussions has been made in the preceding subsection in which the input format was described. The points referred to are as follows:
a. The library of thermodynamic data for reaction products may be read either from cards or from tape. If the data are read in from cards, the program will write these data on tape 4. During a computer run, the appropriate reaction product data for each new set of REACTANTS cards will be selected from tape 4 and stored.

THERMO data may be read in from cards for each run. However, a permanent tape or disc containing the data may be made during any run by using the required type of control cards preceding the operating deck. Two advantages of using a permanent tape or disc are that the scratch tape will not be made for each run and handling the cards is eliminated.

b. The fuel specification card(s) must precede the oxidant card(s) in the input deck. Further, the oxygen must be the second specie specified in the oxidant air atomic formula; the atomic formula of the fuel must be specified in the order: carbon, hydrogen.

For gaseous mixtures (such as air) specify equivalent formula numbers on an atomic basis—e.g., air is 78.03 per cent $N_2$, 20.99 per cent $O_2$, 0.98 per cent $Ar$. Air's equivalent formula is then $0.7803N_2, 0.2099O_2, 0.0049Ar$ where the sum of the relative weights is as close to 1.0 as possible.

c. This enthalpy is not required for assigned temperature problems, i.e., $TP$.

d. If no $T$ value is given the program uses the temperature and enthalpies on the reactant cards. When $T$ values are assigned in the INPT2 NAMELiST, the program calculates the enthalpy from the library of THERMO data if the following two conditions are satisfied:
   i. The reactant card has zeros punched in card columns 37 and 38.
   ii. The reactant is a species in the library of THERMO data.

e. Relative amounts of fuel(s) and oxidizer(s). These quantities
may be specified by assigning 1 and 40 values or FA if no value is assigned for any of these, the program assumes the relative amounts of fuel(s) and oxidizer(s) to be those specified on the reactants cards.

t. TP Problem. Thermodynamic properties will be calculated for all combinations of assigned values for pressure P and temperature T in the NAMELIST. Thus, if 26T values and 26P values are included in the INPT2 lists, properties will be calculated for 676 P and T combinations.

g. HP Problem. Combustion temperature and corresponding properties will be calculated for each pressure specified.

h. RKT Problem. One pressure value P is required for the chamber pressure. The T schedule is used only if expansion from an assigned chamber temperature is desired (such as for a nuclear rocket). Otherwise it should be omitted.

The RKT problem requires a second namelist for input (RKTINP) discussed in the previous subsection.

i. DETN Problem. The temperature and pressures in the T and P input refer to the unburned gas.

j. The list of pressure ratios should not include values for the chamber and the throat. Values should be in increasing order.

k. The program will calculate both equilibrium and frozen performance unless RKTINP contains FROZ = F or EQL = F.
If FROZ = F, only equilibrium performance will be calculated.
If EQL = F, only frozen performance will be calculated.*

l. The subsonic area ratio values (SUBAR) and/or the supersonic area ratio values (SUPAR) are optional. When assigned area ratios are included, the PCP input should contain values of pressure ratios whose corresponding area ratios will be in the range of the assigned area ratios.

m. If OMIT cards are not used, the program will consider as possible species all those species in the THERMO data which are consistent with the chemical system being considered.

* F is the symbol for FALSE.
Occasionally, it may be desired to specifically omit one or more species from consideration as possible species. This may be accomplished by means of OMIT cards.

INSERT cards have been included as options for two reasons. The first and less important reason is that if one knows that one or several particular condensed species will be present among the final equilibrium compositions for the first assigned point, then a small amount of computer time can be saved by using an INSERT card. Those condensed species whose chemical formulas are included on an INSERT card will be considered by the program during the initial iterations for the first assigned point. If the INSERT card were not used, only gaseous species would be considered during the initial iterations. However, after convergence, the program would automatically insert the appropriate condensed species and reconverge. Therefore, it usually is immaterial whether or not INSERT cards are used. For all other assigned points the inclusion of condensed species is handled automatically by the program.

The second and more important reason for including the INSERT card option is that, in rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low (say several degrees K). In these rare cases, the use of an INSERT card containing the name of the required condensed species will eliminate this kind of convergence difficulty. When this difficulty occurs, an error message is generated. This message is described in the subsection Description of Error Messages.

3.2.4 Description of Sample Case Input

A completed input data sheet is shown on page 29 for an assigned enthalpy pressure problem (HP). In this table, lines 1 through 6 identify
the start of the thermodynamic data and include, as examples, data for solid phase aluminum. Lines 10 through 13 identify that the reactant components for this problem are kerosene \((C_{1}H_{1923})\) and air \((N_{0.7803O_{0.2099Ar_{0.0049}}})\). The kerosene (fuel) is supplied as liquid at 298.15 deg K with an enthalpy of \(-5430\) cal/gm-mole. The air (oxidant) is gaseous at 350 deg K with an enthalpy of 195.0 cal/gm-mole. The density of the kerosene is specified as 0.773 gm/cc while that of the air is omitted. Lines 15 through 18 are the NAMELISTS $INPT2$ input. Here the case is given the code number 1, HP is identified as the problem type, the combustor pressure is set at 1.80 atm, and the MIX matrix is assigned 35 fuel-to-air ratios for test.

2.3 OUTPUT DATA

The output of Program NOXRAT consists of both printed and punched data. The data falls into two main categories: normal output and error messages. The normal output consists of the printed and punched results usually obtained with each run of the program. If any difficulties are encountered in the solution of a case, one or more error messages are printed. These messages are diagnostic statements which describe the nature of the difficulty. They are described in greater detail in subsection 3.3.2.

3.3.1 Normal Output

The normal output from NOXRAT falls into two main categories: printed output for each fuel-to-air ratio for each assigned condition (e.g., pressure); and printed and punched output for each assigned pressure. The normal output from the first category is:

- \(\ast\) a. The chemical formula of each reactant specie.
- \(\ast\) b. The weight fraction of each reactant specie in the total fuel or oxidant.
- \(\ast\) c. The base enthalpy of each reactant in cal/gm-mole.
- \(\ast\) d. The input temperature of each reactant in deg-K.

\(\ast\) Also normal output of CEC.
e. The density of each reactant (if specified in the input) in gm/cc.
f. The physical state of each of the specified reactants.
g. The total oxidant to fuel weights ratio.
h. The per cent fuel in the reactant mixture.
i. The equivalence ratio of the reactants.
j. The weight average density of the reaction mixture in gm/cc (printed as zero if the density of any species is omitted from the input).
k. The equilibrium pressure in atm.
l. The equilibrium temperature in deg K.
m. The sonic velocity of the combustion production mixture in meters/sec.
n. The mean enthalpy of the combustion products in cal/gram.
o. The mean entropy of the combustion products in cal/gram-deg K.
p. The mean molecular weight of the combustion products in grams.
q. The differential \( \frac{\partial V}{\partial P} \) in cc/atm.
r. The differential \( \frac{\partial V}{\partial T} \) in cc/deg K.
s. The mean heat capacity of the combustion products in cal/gram-deg K.
t. The mean heat capacity ratio \( (C_p/C_v) \) of the combustion products.
u. The mole fraction and chemical formula of each of the combustion products present at equilibrium at a concentration greater than \( 5 \times 10^{-6} \).
v. The mole fraction of each of the species of interest in the nitric oxide kinetic scheme (Refs 4 through 6) and the mole fractions of \( C_3 \), \( CO \), \( CO_2 \).
w. The mean molecular weight of the combustion products in grams.
x. The adiabatic flame temperature of the combustion products in deg K.
y. The assigned inlet pressure in atm.
z. The fuel-to-air weight ratio of the reactants.
zl. The atomic composition, inlet temperature (in deg K) and enthalpy (cal/gm-mole) of both the fuel(s) and the oxidant(s).

* Also normal output of CEC.
With the exception of the descriptive characteristics of the fuel(s) and oxidant(s) (output #21), the output from this category is clearly labeled and requires no further discussion.

The fuel and oxidant are described by seven characteristic numbers, the first five of which give the atomic composition while the sixth and seventh are the enthalpy in cal/gm-mole at the inlet temperature in deg K. These two lines of output appear directly below the fuel-to-air ratio with the first line always referring to the fuel and the second to the oxidant. Since the fuel used in this analysis has been assumed to be of the form \( C_x H_y \), the first two figures printed describing the fuel are "x" and "y" while the third, fourth, and fifth figures are printed as zero. In this analysis, the oxidant has been taken to be air comprised of nitrogen, oxygen, and argon with the equivalent chemical formula \( N_A O_B A_r C \). Hence, the first three numerals printed describing the oxidant are "A", "B", and "C" respectively. The fourth and fifth figures are printed as zero; inclusion of other trace components in the air will change these latter digits accordingly. Further description of this output is included in Appendix IV. The output for the sample data case corresponding to this category of the output is shown on pages 30 and 31.

The normal output for the second category is:

a. The atomic composition of the fuel \( (C_x H_y) \).

b. The inlet air temperature in deg ...

c. A code number identifying the set of kinetic constants used in the NO rate formation calculations (see Appendix V).

d. The assigned pressure in atm.

e. The stoichiometric fuel-to-air ratio.

f. For each fuel-to-air ratio specified, the program prints and punches two lines of output containing twelve items of data. This data is (consecutively): the mixture ratio (mass fuel to mass fuel and air); the equivalence ratio; the density of the combustion products in gm/cm\(^3\); the adiabatic flame temperature of the combustion products in deg K; the equilibrium mole fraction of NO, CO,
C(s), and CH₂ (unburned hydrocarbons). and the kinetic parameters $R_1$, $R_6$ (in gm-moles/cm³·sec), $K_1$, and $K_2$ (dimensionless). The output for the sample data case corresponding to this category of the output is shown on page 32.

Program NOXRAT prints intermediate output for each input set of REACTANT cards and for each fuel-to-air ratio. The former consists of a listing of the input data for the case and a listing of the species being considered as products of the combustion process. The latter data is the result of intermediate calculations within NOXRAT and is not described here. It is generally not of any interest to the user; however, the output for one fuel-to-air ratio for the sample data case is shown on page 33.

3.3.2 Description of Error Messages

The known error messages in Program NOXRAT* are:

a. In rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low (say several deg K). In these rare cases, the use of an INSERT card containing the name of the required condensed species will eliminate this kind of convergence difficulty. When this difficulty occurs, the following message is printed by the program: "LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD".

b. If the user mixes the order of the cards for a particular species in the thermodynamic data file, the program will print: "ERROR IN ORDER OF DATA CARDS FOR --------(specie name)". This is a nonfatal error and the program will continue to execute, however, the specie in error will be deleted from the thermodynamic inventory.

c. If there are cards in the input data deck that do not belong, the program will write the card and: "ERROR IN ABOVE CARD: IGNORE CONTENTS". This is a nonfatal error to the program, but causes it to skip to the next data set.

* These are as those for CEC.
d. If there are errors in the REACTANTS data cards the program will write: "ERROR IN REACTANT CARDS". This is a nonfatal error to the program but causes it to skip to the next data set.

e. If the convergence tests are not satisfied for the equilibrium products the program will print: "ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS FOR THE POINT _____".

f. If the temperature calculated for the combustion is out of the range of the thermodynamic data the program will print: "THE TEMPERATURE = ______ IS OUT OF RANGE FOR POINT _____".

g. If the phases of a condensed specie are out of order, the program will print: "PHASES OF A CONDENSED SPECIE ARE OUT OF ORDER".

3.4 MISCELLANEOUS OPERATIONAL INFORMATION

Program NOXRAT occupies approximately 71,000 core locations during loading and approximately 63,000 core locations during execution on the CDC 6600 computer. Actual program length is approximately 38,000 core locations. Hence, the total storage requirement for this program is comfortably within the CDC 6600 core capacity of 131,000 locations.

The execution time of Program NOXRAT depends primarily upon the number of assigned pressure levels and upon the number of fuel-to-air ratios at each of the pressure levels to be tested. A typical operating condition of one assigned pressure and 35 fuel-to-air ratios requires approximately 66 systems seconds (central processor time is approximately 52 secs) for execution. Each succeeding point at any given pressure and any selected fuel-to-air ratio will require approximately one second of over-all machine time.

A "scratch" tape is required by the program. This scratch tape number is not assigned a Fortran name but is given the value of 4 by the program. The instructions necessary for mounting this tape must be supplied to the computer/computer operator upon submission of a run.
NORTHERN RESEARCH AND ENGINEERING CORPORATION

3.5 DATA INPUT SHEET

ENGINEER: RDS  PROJECT: Turbine Combustors  PROJECT NO: 1152

TITLE: Sample to Illustrate the Use of Program NOXRAT  SHEET: 1 OF 1

<table>
<thead>
<tr>
<th>LOCATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Line 1</td>
</tr>
<tr>
<td>Line 2</td>
</tr>
<tr>
<td>Line 3</td>
</tr>
<tr>
<td>Line 4</td>
</tr>
<tr>
<td>Line 5</td>
</tr>
<tr>
<td>Line 6</td>
</tr>
<tr>
<td>Line 7</td>
</tr>
<tr>
<td>Line 8</td>
</tr>
<tr>
<td>Line 9</td>
</tr>
<tr>
<td>Line 10</td>
</tr>
<tr>
<td>Line 11</td>
</tr>
<tr>
<td>Line 12</td>
</tr>
<tr>
<td>Line 13</td>
</tr>
<tr>
<td>Line 14</td>
</tr>
<tr>
<td>Line 15</td>
</tr>
<tr>
<td>Line 16</td>
</tr>
<tr>
<td>Line 17</td>
</tr>
<tr>
<td>Line 18</td>
</tr>
</tbody>
</table>

Note: The table contains data related to thermal analysis, including location specifications, reaction rates, and input parameters for a turbine combustor project.
### 3.6 Sample Case Output

#### Theoretical ThermoDynamic Combustion Properties

<table>
<thead>
<tr>
<th>CASE NO.</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Chemical Formula</strong></td>
<td><strong>WT Fraction</strong></td>
</tr>
<tr>
<td><strong>Fuel</strong></td>
<td>C</td>
</tr>
<tr>
<td><strong>Oxidant</strong></td>
<td>N</td>
</tr>
<tr>
<td><strong>(see note)</strong></td>
<td><strong>Cal/ Mol</strong></td>
</tr>
<tr>
<td></td>
<td>1.90000</td>
</tr>
<tr>
<td></td>
<td>1.90000</td>
</tr>
<tr>
<td><strong>O/F</strong></td>
<td>5.2549</td>
</tr>
</tbody>
</table>

#### ThermoDynamic Properties

<table>
<thead>
<tr>
<th>P</th>
<th>Atmosphere</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>1608.4</td>
</tr>
<tr>
<td>H</td>
<td>25.088</td>
</tr>
<tr>
<td>M</td>
<td>2.4465</td>
</tr>
<tr>
<td>M mol wt</td>
<td>22.018</td>
</tr>
<tr>
<td>(DLV/DLP)T</td>
<td>-1.00326</td>
</tr>
<tr>
<td>(DLV/DLP)IP</td>
<td>1.2988</td>
</tr>
<tr>
<td>Cp</td>
<td>1.3974</td>
</tr>
<tr>
<td>Gamma</td>
<td>1.3123</td>
</tr>
<tr>
<td>Non vel/w sec</td>
<td>766.1</td>
</tr>
</tbody>
</table>

#### Mole Fractions

| AR | 0.0026 |
| CH4 | 0.00061 |
| CO | 0.24395 |
| CO2 | 0.0742 |
| HCN | 0.0001 |
| H2 | 0.2916 |
| NO | 0.00429 |
| NH3 | 0.0003 |
| NZ | 0.49887 |

#### Additional Products Which Were Considered But Whose Mole Fractions Were Less Than 0.00005 For All Assumed Conditions:

| C2H(L) | N | NH | NH2 | NO | NO2 | N2E | N2H | N2H2 | N2O | N2O2 | N2O3 | N2O4 | N2O5 | N2O6 | N2O7 | N2O8 | N2O9 | N2O10 | N2O11 | N2O12 | N2O13 | N2O14 | N2O15 | N2O16 | N2O17 | N2O18 | N2O19 | N2O20 | N2O21 | N2O22 | N2O23 | N2O24 | N2O25 | N2O26 | N2O27 | N2O28 | N2O29 | N2O30 | N2O31 | N2O32 | N2O33 | N2O34 | N2O35 | N2O36 | N2O37 | N2O38 | N2O39 | N2O40 | N2O41 | N2O42 | N2O43 | N2O44 | N2O45 | N2O46 | N2O47 | N2O48 | N2O49 | N2O50 | N2O51 | N2O52 | N2O53 | N2O54 | N2O55 | N2O56 | N2O57 | N2O58 | N2O59 | N2O60 | N2O61 | N2O62 | N2O63 | N2O64 | N2O65 | N2O66 | N2O67 | N2O68 | N2O69 | N2O70 | N2O71 | N2O72 | N2O73 | N2O74 | N2O75 | N2O76 | N2O77 | N2O78 | N2O79 | N2O80 | N2O81 | N2O82 | N2O83 | N2O84 | N2O85 | N2O86 | N2O87 | N2O88 | N2O89 | N2O90 | N2O91 | N2O92 | N2O93 | N2O94 | N2O95 | N2O96 | N2O97 | N2O98 | N2O99 | N2O100 |

**Note:** Weight Fraction of Fuel in total fuels and of oxidant in total oxidants.
<table>
<thead>
<tr>
<th></th>
<th>FUEL</th>
<th>OXIDANT</th>
<th>MIXTURE</th>
</tr>
</thead>
<tbody>
<tr>
<td>H/CAL/O</td>
<td>-3.88719620E+02</td>
<td>1.35636455E+01</td>
<td>-5.08381779E+01</td>
</tr>
<tr>
<td>V*</td>
<td>4.25394067E-01</td>
<td>0</td>
<td>6.80101579E-02</td>
</tr>
<tr>
<td>V&lt;</td>
<td>0</td>
<td></td>
<td>-2.43508462E-02</td>
</tr>
<tr>
<td>ATOMS/O</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>7.15074437E-02</td>
<td>0</td>
<td>1.14450899E-02</td>
</tr>
<tr>
<td>H</td>
<td>1.3904292E+01</td>
<td>0</td>
<td>2.22297982E-02</td>
</tr>
<tr>
<td>N</td>
<td>0</td>
<td></td>
<td>4.52619469E-02</td>
</tr>
<tr>
<td>O</td>
<td>0</td>
<td></td>
<td>1.21754231E-02</td>
</tr>
<tr>
<td>AR</td>
<td>0</td>
<td></td>
<td>2.84228553E-04</td>
</tr>
<tr>
<td>PT</td>
<td>-2.632</td>
<td>-0.000</td>
<td>-2.326</td>
</tr>
<tr>
<td>C</td>
<td>-0.000</td>
<td>-9.396</td>
<td>-12.706</td>
</tr>
<tr>
<td>H</td>
<td>-0.000</td>
<td>-0.000</td>
<td>-35.262</td>
</tr>
<tr>
<td>N</td>
<td>-0.000</td>
<td>-24.674</td>
<td>-15.000</td>
</tr>
<tr>
<td>O</td>
<td>-0.000</td>
<td>-24.674</td>
<td>-15.000</td>
</tr>
<tr>
<td>AR</td>
<td>-0.000</td>
<td>-24.674</td>
<td>-15.000</td>
</tr>
</tbody>
</table>
4. REFERENCES


5. TABLES
TABLE 1

KINETIC DATA FOR THE NITRIC OXIDE REACTION SCHEME

<table>
<thead>
<tr>
<th>Reaction No.</th>
<th>$A_i (\text{cm}^3/\text{sec gm-mole deg K})$</th>
<th>$n_i$</th>
<th>$E_i (\text{kcal/gm-mole})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICODE = 1 (from Refs 4, 5)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$1.2046 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>$1.2946 \times 10^{13}$</td>
<td>0.0</td>
<td>7.1</td>
</tr>
<tr>
<td>3</td>
<td>$4.2161 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>$3.0115 \times 10^{13}$</td>
<td>0.0</td>
<td>10.8</td>
</tr>
<tr>
<td>5</td>
<td>$3.6138 \times 10^{13}$</td>
<td>0.0</td>
<td>24.0</td>
</tr>
<tr>
<td>6</td>
<td>$4.8184 \times 10^{13}$</td>
<td>0.0</td>
<td>24.0</td>
</tr>
<tr>
<td>ICODE = 2 (from Refs 9, 17)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$3.1 \times 10^{13}$</td>
<td>0.0</td>
<td>0.334</td>
</tr>
<tr>
<td>2</td>
<td>$6.4 \times 10^{9}$</td>
<td>1.0</td>
<td>6.25</td>
</tr>
<tr>
<td>3</td>
<td>$4.1 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>$2.9513 \times 10^{13}$</td>
<td>0.0</td>
<td>10.77</td>
</tr>
<tr>
<td>5</td>
<td>$3.8146 \times 10^{13}$</td>
<td>0.0</td>
<td>24.1</td>
</tr>
<tr>
<td>6</td>
<td>$4.5775 \times 10^{13}$</td>
<td>0.0</td>
<td>24.1</td>
</tr>
<tr>
<td>ICODE = 3 (from Ref 18)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>$3.0717 \times 10^{13}$</td>
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<td>0.33</td>
</tr>
<tr>
<td>2</td>
<td>$1.3251 \times 10^{10}$</td>
<td>1.0</td>
<td>7.1</td>
</tr>
<tr>
<td>3</td>
<td>$4.2161 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>$2.9513 \times 10^{13}$</td>
<td>0.0</td>
<td>10.77</td>
</tr>
<tr>
<td>5</td>
<td>$3.8146 \times 10^{13}$</td>
<td>0.0</td>
<td>24.1</td>
</tr>
<tr>
<td>6</td>
<td>$4.5775 \times 10^{13}$</td>
<td>0.0</td>
<td>24.1</td>
</tr>
<tr>
<td>ICODE = 4 (from Ref 18)</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>1</td>
<td>$1.0239 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>$3.7945 \times 10^{12}$</td>
<td>0.0</td>
<td>7.0</td>
</tr>
<tr>
<td>3</td>
<td>$4.1559 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>$2.5513 \times 10^{13}$</td>
<td>0.0</td>
<td>10.77</td>
</tr>
<tr>
<td>5</td>
<td>$3.8146 \times 10^{13}$</td>
<td>0.0</td>
<td>24.1</td>
</tr>
<tr>
<td>6</td>
<td>$4.5775 \times 10^{13}$</td>
<td>0.0</td>
<td>24.1</td>
</tr>
</tbody>
</table>

where

$k = A_i T^{n_i} \exp(-E_i/RT)$

$T =$ Temperature in deg K

$R = 1.987 \times 10^{-3}$ kcal/gm-mole deg K
<table>
<thead>
<tr>
<th>Program or Subprogram</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOXRAT</td>
<td>Main program to calculate chemical equilibrium compositions with applications; the main program controls the calculation and directs the input and output</td>
</tr>
<tr>
<td>REACT</td>
<td>Subroutine to read and convert reaction input data</td>
</tr>
<tr>
<td>SEARCH</td>
<td>Subroutine to search tape for thermodynamic data for species to be considered</td>
</tr>
<tr>
<td>EQUILBRM</td>
<td>Subroutine to calculate equilibrium composition and properties</td>
</tr>
<tr>
<td>CPHS</td>
<td>Subroutine to calculate thermodynamic properties for individual species</td>
</tr>
<tr>
<td>MATRIX</td>
<td>Subroutine to perform matrix inversion</td>
</tr>
<tr>
<td>MGAUSD</td>
<td>Subroutine to solve any linear set of up to 20 equations</td>
</tr>
<tr>
<td>VARFMT</td>
<td>Subroutine to set variable formats</td>
</tr>
<tr>
<td>OUT1</td>
<td>Subroutine to write output</td>
</tr>
<tr>
<td>OUT2</td>
<td>Subroutine to write output</td>
</tr>
<tr>
<td>OUT3</td>
<td>Subroutine to write output</td>
</tr>
<tr>
<td>HCALC</td>
<td>Subroutine to calculate enthalpy for propellant using coefficients</td>
</tr>
<tr>
<td>MOLIER</td>
<td>Subroutine to calculate thermodynamic equilibrium properties at assigned temperatures and pressures</td>
</tr>
<tr>
<td>CMBSTN</td>
<td>Subroutine to calculate theoretical thermodynamic combustion properties</td>
</tr>
<tr>
<td>DETON</td>
<td>Subroutine to calculate Chapman-Jouguet detonations</td>
</tr>
<tr>
<td>SHCK</td>
<td>Subroutine to terminate program if a shock occurs</td>
</tr>
<tr>
<td>ROCKET</td>
<td>Subroutine to calculate rocket performance</td>
</tr>
<tr>
<td>Program or Subprogram</td>
<td>Description</td>
</tr>
<tr>
<td>-----------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>RKTOUT</td>
<td>Subroutine to write output for rocket performance</td>
</tr>
<tr>
<td>RATIO</td>
<td>Subroutine to interpolate area ratio</td>
</tr>
<tr>
<td>SET</td>
<td>Subroutine to interpolate area ratio</td>
</tr>
<tr>
<td>FROZEN</td>
<td>Subroutine to calculate frozen composition expansion only</td>
</tr>
<tr>
<td>RATES</td>
<td>Subroutine to calculate rate constants for the NO reaction scheme</td>
</tr>
</tbody>
</table>
6. FIGURES
FIGURE 1 - MODULAR TREE DIAGRAM
### 7. NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_p$</td>
<td>Specific heat at constant pressure</td>
<td>cal/gm-deg K</td>
</tr>
<tr>
<td>$C_v$</td>
<td>Specific heat at constant volume</td>
<td>cal/gm-deg K</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
<td>atm</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>deg K</td>
</tr>
<tr>
<td>$V$</td>
<td>$V_{cc}$</td>
<td>cc</td>
</tr>
</tbody>
</table>
8. APPENDICES
The over-all computer flow of NOXRAT is identical to that of CEC excepting the additional CALL to Subroutine RATES by Subroutine OUT3. The other modifications to OUT3 and to the main program (NOXRAT) do not affect the over-all program logic. A complete description of the program logic is available in References 11, 13, 14, and 15. A modular diagram of NOXRAT is provided as Figure 1 (Ref 13). Table 2 contains a brief statement as to the role of each routine in the program.
APPENDIX II - COMMON FORTRAN NOMENCLATURE

The following tables contain the COMMON Fortran nomenclature for Program NOXRAT that was added to that of Program CEC. COMMON consists of labeled blocks; the nomenclature is arranged in alphabetical order for each block. The metric system of units is included in the nomenclature.

### Nomenclature for COMMON/SNEW

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>INDFA</td>
<td></td>
<td>Index of equivalence ratios</td>
<td></td>
</tr>
<tr>
<td>RON</td>
<td>F/A</td>
<td>Fuel-to-air mass ratio</td>
<td></td>
</tr>
</tbody>
</table>

### Nomenclature for COMMON/DICK

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATT(j,1)</td>
<td>T_j</td>
<td>jth value of the adiabatic flame temperature (in the combustor) at a particular fuel-to-air mass ratio</td>
<td>deg K</td>
</tr>
<tr>
<td>BCON1(j,1)</td>
<td>Y_C(s)_j</td>
<td>Equilibrium mole fraction of carbon at the jth pressure level at a particular fuel-to-air mass ratio</td>
<td></td>
</tr>
<tr>
<td>BCON2(j,1)</td>
<td>Y_CO_j</td>
<td>Equilibrium mole fraction of carbon monoxide at the jth pressure level at a particular fuel-to-air mass ratio</td>
<td></td>
</tr>
<tr>
<td>BCON6(j,1)</td>
<td>Y_NO_j</td>
<td>Equilibrium mole fraction of nitric oxide at the jth pressure level at a particular fuel-to-air mass ratio</td>
<td></td>
</tr>
<tr>
<td>CH2(j,1)</td>
<td>Y_CH2_j</td>
<td>Equilibrium mole fraction of unburned hydrocarbons in the combustion products (excluding C(s) and CO) expressed as CH2 at the jth pressure level at a particular fuel-to-air mass ratio</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>----------------</td>
<td>--------</td>
<td>------------------------------------------------------------------------------</td>
<td>---------------</td>
</tr>
<tr>
<td>EKI(I,J)</td>
<td>(K1)j</td>
<td>Ratio of forward reaction rate at the i-th pressure level for a particular fuel-to-air mass ratio i</td>
<td></td>
</tr>
<tr>
<td>EK2(J,I)</td>
<td>(K2)j</td>
<td>Ratio of forward reaction rate at the j-th pressure level for a particular fuel-to-air mass ratio i</td>
<td></td>
</tr>
<tr>
<td>F(I)</td>
<td>F</td>
<td>Mixture ratio</td>
<td></td>
</tr>
<tr>
<td>MIX(I)</td>
<td></td>
<td>Matrix of specified fuel-to-air mass ratios</td>
<td></td>
</tr>
<tr>
<td>PHI(I)</td>
<td>φ</td>
<td>Equivalence ratio</td>
<td></td>
</tr>
<tr>
<td>ROH(J,I)</td>
<td>ρj</td>
<td>Equilibrium density at the j-th pressure level at a particular fuel-to-air mass ratio i</td>
<td>gm/cm³</td>
</tr>
<tr>
<td>R1(J,I)</td>
<td>(R1)j</td>
<td>Forward reaction rate for the first reaction at the j-th pressure level at a particular fuel-to-air mass ratio i</td>
<td>gm-mole/cm³-sec</td>
</tr>
<tr>
<td>R6(J,I)</td>
<td>(R6)j</td>
<td>Forward reaction rate for the sixth reaction at the j-th pressure level at a particular fuel-to-air mass ratio i</td>
<td>gm-mole/cm³-sec</td>
</tr>
</tbody>
</table>
APPENDIX III - MAIN ROUTINE - NOXRAT

The changes to the main routine of CEC are as follows:

a. The main program was renamed NOXRAT, thus replacing the CEC name "MAIN".

b. The subscripted variable MIX was expanded from 15 to 50. MIX is the matrix of specified fuel-to-air ratios.

c. Labeled COMMON blocks SNEW, DICK, and EQNEW were added. Definitions of the variables contained in these blocks are provided in Appendix II.

d. The statement DO 303 $1 = 1, 15$ was modified to DO 303 $1 = 1, 50$. This is consistent with the expansion of the MIX matrix from 15 to 50.

e. Statement number 322:DO 625 IST = 1, 5 was modified to read DO 625 IST = 1, 40. This is consistent with the decision to limit each set of specified fuel-to-air ratios to between 35 and 40 entries.

f. The statement INDFA = IST was inserted directly after the statement numbered 322. The statement RON = MIX(IST) was inserted directly after the statement numbered 323. Both of these new variables are part of the new labeled COMMON blocks and are used only in Subroutine RATES.
APPENDIX IV - SUBROUTINE OUT3

Subroutine OUT3 is an entry point to Subroutine OUT1. The main purpose of this subroutine had been to provide the written output for the CEC program. The modifications incorporated into OUT3 permit identification of the species of interest in the kinetic scheme (previously described). Once identified, these variables are transmitted to Subroutine RATES by means of COMMON and a call statement from OUT3. The specific changes to OUT3 are as follows:

a. The subscripted variable MIX was expanded from 15 to 50. MIX is the matrix of specified fuel-to-air ratios.

b. A dimension statement was added for the variables "SIEGEL" and "CONCKI". "SIEGEL" is a singly-subscripted variable containing the alphanumeric characters used in the identification of the chemical species of interest in the kinetic scheme. The variable "CONCKI" is a doubly-subscripted array representing the equilibrium mole fraction of a given species for a particular pressure level at a specified fuel-to-air ratio.

c. Labeled COMMON blocks SNEW, DICK, and EQNEW were added. Definitions of the variables contained in these blocks are provided in Appendix II.

d. The elements of the "SIEGEL" array were entered into the program via a DATA statement.

e. Statement number 1000 was changed from a RETURN statement to a CONTINUE statement.

f. 34 statements were added to the program after statement number 106', in order to identify which elements of the CLC array EN (containing the moles of a given species present in a particular reaction mixture) were the ones of interest in the kinetic analysis. This problem was created by the storage of the alphanumeric characters identifying reaction species in the CEC generated array.
"SUB". This array was created in such a manner that
determination of the specific elements of interest to
NREC had to be accomplished by a direct comparison of the
alphanumeric data in the "SUB" array with the specific
names in the input "SIEGEL" array. This comparison and the
calculation of the equilibrium mole fractions was accom-
plished in the DO 3000 loop of OUT3. The remaining state-
ments added to OUT3 allow the equilibrium mole fractions
and names of the species of interest, the molecular weight
and adiabatic flame temperature of the combustion products,
the assigned pressure, the fuel-to-air ratio, and the
atomic and thermal characteristics of the fuel and oxidant
to be printed for each specified fuel-to-air ratio. This
output appears directly beneath the "normal" output (i.e.,
regular CEC type) generated by OUT3. The final cards
added to OUT3 are the CALL statement to Subroutine RATES
and the Subroutine RETURN statement.
APPENDIX V - SUBROUTINE RATES

The primary function Subroutine RATES is to produce data, in the form of a deck of cards, which specify all of the kinetic properties required by Program GASNOX at the equilibrium combustor conditions.

Subroutine RATES is called by Subroutine OUT3 of Program NOXRAT; it does not call any other subroutines. Subroutine RATES does not require external input but does provide external output in the form of punch cards and paper. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

- **A** ANUM
- **ENTH** ICODE
- **NREAC** PPP

The internal output consists of:

- **ATT** BCON1
- **EK1** EK2
- **R1** R6

The external output consists of:

- **ANUM** ATT
- **CH2** EKS
- **ICODE** PHI
- **AI** R6

Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine RATES which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(I)</td>
<td>A_i</td>
<td>Pre-exponential factors in the kinetic equations</td>
<td>cm^3/sec-gm mole deg K</td>
</tr>
<tr>
<td>ANUM(I,J)</td>
<td>a_i,j</td>
<td>Atomic number</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>a_1,1 = carbon</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>a_1,2 = hydrogen</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>a_2,2 = oxygen</td>
<td></td>
</tr>
</tbody>
</table>

* See Volume 3.
<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONC(J,I)</td>
<td>$y_{i,j}$</td>
<td>Equilibrium mole fraction of the $i^{th}$ species for the $j^{th}$ pressure at a particular fuel-to-air mass ratio $i$.</td>
<td></td>
</tr>
<tr>
<td>CONMCM(K,J,I)</td>
<td>$y_{i,j}$</td>
<td>Equilibrium concentration of the $k^{th}$ species for the $j^{th}$ pressure at a particular fuel-to-air mass ratio $i$.</td>
<td>gm moles/cm$^3$</td>
</tr>
<tr>
<td>E(I)</td>
<td>$E_i$</td>
<td>Activation energies for the kinetic equations</td>
<td>kcal/gm-mole</td>
</tr>
<tr>
<td>EKS</td>
<td>$k_s$</td>
<td>Fuel-to-air mass ratio at stoichiometric conditions</td>
<td></td>
</tr>
<tr>
<td>EN(J)</td>
<td>$n_i$</td>
<td>Temperature exponent for the kinetic equations</td>
<td></td>
</tr>
<tr>
<td>ENTH(N)</td>
<td>$H_n$</td>
<td>Enthalpy of reactant $n$</td>
<td>cal/gm-mole</td>
</tr>
<tr>
<td>ICODE</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\text{ICODE} = 1$ if kinetic rate constants of Lavoie are employed (Refs 4, 5)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\text{ICODE} = 2$ if &quot;best&quot; kinetic data are employed (Refs 9, 17)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\text{ICODE} = 3$ if &quot;high&quot; kinetic data are employed</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\text{ICODE} = 4$ if &quot;low&quot; kinetic data are employed</td>
<td></td>
</tr>
<tr>
<td>IPRINT</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\text{IPRINT} = 0$ if data is not to be printed and punched</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\text{IPRINT} = 1$ if data is to be printed and punched</td>
<td></td>
</tr>
<tr>
<td>IST</td>
<td></td>
<td>Index of equivalence ratios</td>
<td></td>
</tr>
<tr>
<td>NPT</td>
<td></td>
<td>Index of pressures</td>
<td></td>
</tr>
<tr>
<td>NREAC</td>
<td>$n_{\text{react}}$</td>
<td>Number of the $n^{th}$ reactant species</td>
<td></td>
</tr>
<tr>
<td>PPP(J)</td>
<td>$P_j$</td>
<td>$j^{th}$ value of the pressure in the combustor</td>
<td>atm</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
<td></td>
</tr>
<tr>
<td>-----------------</td>
<td>-----------------------------------------------------------------------------</td>
<td>----------------------------</td>
<td></td>
</tr>
<tr>
<td>RATEK(K,J,I)</td>
<td>jth value of the reaction rate for the kth kinetic equation at a particular fuel-to-air mass ratio i</td>
<td>cm³/sec·gm mole</td>
<td></td>
</tr>
<tr>
<td>RATWTS</td>
<td>Ratio of atomic numbers</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RTEMP(N)</td>
<td>Inlet temperature of reactant n</td>
<td>deg K</td>
<td></td>
</tr>
<tr>
<td>R2(J,I)</td>
<td>Forward Reaction rate for the second reaction at the jth pressure level at a particular fuel-to-air mass ratio i</td>
<td>gm-mole/cm³·sec</td>
<td></td>
</tr>
<tr>
<td>R3(J,I)</td>
<td>Forward reaction rate for the third reaction at the jth pressure level at a particular fuel-to-air mass ratio i</td>
<td>gm-mole/cm³·sec</td>
<td></td>
</tr>
<tr>
<td>R4(J,I)</td>
<td>Forward reaction rate for the fourth reaction at the jth pressure level at a particular fuel-to-air mass ratio i</td>
<td>gm-mole/cm³·sec</td>
<td></td>
</tr>
<tr>
<td>R5(J,I)</td>
<td>Forward reaction rate for the fifth reaction at the jth pressure level at a particular fuel-to-air mass ratio i</td>
<td>gm-mole/cm³·sec</td>
<td></td>
</tr>
<tr>
<td>TTT(J)</td>
<td>jth value of the temperature (in the combustor) at a particular fuel-to-air mass ratio</td>
<td>deg K</td>
<td></td>
</tr>
<tr>
<td>WM(J,I)</td>
<td>jth value of the molecular weight of the reaction products at a particular fuel-to-air mass ratio</td>
<td>gm/gm-mole</td>
<td></td>
</tr>
</tbody>
</table>

**Analysis Procedure**

The step-by-step procedure of Subroutine RATES is given below.

At the conclusion of the step-by-step procedure, the Fortran listing of the subroutine appears:

a. Establish the printing and punching control.

b. Convert equilibrium mole fractions of $C(s), CO, CO_2, H_2, N, NO, N_2O, O, O_2$ to moles/cm³ by the relationship

$$ \left( y_{ij} \right)_j = \left[ y_{ij} \right] \left[ P_j / 82.07 T_j \right]$$
c. Compute the forward reaction rate constants as
\[
(R_k)_j = A_k T_j^0 \exp \left[ -\frac{E_k}{RT_j} \right]
\]

d. Calculate \((R_1)_j, (R_2)_j, (R_3)_j, (R_4)_j, (R_5)_j\), and \((R_6)_j\)
\[
\begin{align*}
(R_1)_j &= (R_1)_j (N_2)_j (NO_2)_j \\
(R_2)_j &= (R_2)_j (N_2)_j (O_3)_j \\
(R_3)_j &= (R_3)_j (N_2)_j (O_3)_j \\
(R_4)_j &= (R_4)_j (He)_j (N_2O_2)_j \\
(R_5)_j &= (R_5)_j (O_3)_j (N_2O_2)_j \\
(R_6)_j &= (R_6)_j (O_3)_j (N_2O_2)_j
\end{align*}
\]

e. Compute \((K_1)_j\) and \((K_2)_j\)
\[
\begin{align*}
(K_1)_j &= (R_1)_j / [(R_2)_j + (R_3)_j] \\
(K_2)_j &= (R_4)_j / [(R_5)_j + (R_6)_j]
\end{align*}
\]
If \((R_2)_j\) and \((R_3)_j\) equal zero, \((K_1)_j = 10^{35}\)
If \((R_4)_j\) and \((R_5)_j\) equal zero, \((K_2)_j = 10^{35}\)

f. Compute \(\phi_j\) as
\[
\phi_j = \frac{P_j MW_j}{82.057 T_j}
\]

g. Compute \(k_s\) as
\[
k_s = \frac{(2 a_{1,1} + 1 a_{1,2}) a_{2,2}}{28.99 (a_{1,1} + a_{1,2})}
\]

h. Compute \(\phi\) as
\[
\phi = \frac{F/A}{k_5}
\]

i. Compute \(F\) as
\[
F = \phi k_s / (1 + \phi k_5)
\]

j. Compute \(Y_{CH_2,j}\)
\[
Y_{CH_2,j} = 1 \left\{ \frac{a_{1,1}}{1 + \frac{12a_{1,2}}{a_{1,1}}} \right\} \left[ \frac{MW_j (F/A)}{F/A + 1} \right] y_{C_1} - y_{C_2} - y_{C_3}
\]

k. Repeat steps a through j for each of the specified pressure levels.
1. If all of the input fuel-to-air mass ratios have been examined, proceed to step m. If not, return to subroutine OUT of Program NOXRAT and repeat the set of calculations in NOXRAT leading up to the calling of subroutine RATES.

m. If this is the first fuel-to-air mass ratio at the particular pressure in question, write and punch a heading card. If not, go to step n.

n. Write and punch the required output data at the jth pressure level (for each fuel-to-air mass ratio at that pressure level). This data is: $F; \phi; Y_j; T_j; Y_{NO,j}; Y_{CO,j}; Y_{C(s),j}; Y_{CH_2,j}; (R_1)_j; (R_6)_j; (K_1)_j; \text{ and } (K_2)_j$.

o. If this is the last fuel-to-air mass ratio at the jth pressure level, proceed to step p. If not, return to step m at the next ratio.

p. If this is the last pressure specified, proceed to step q. If not, return to step m.

q. Return.
SUBROUTINE RATES(CONCKI, WM, TTT, PPP, ANUM, ENTH, RTEMP, NPT, NREAC)
REAL MIX(50)
DIMENSION CONCKI(10,30), TTT(13), PPP(13), WM(13), ANUM(15,5), ENTH(15), RTEMP(15),
MIX(50)
DIMENSION R2(30,40), R3(30,40), R4(30,40), R5(30,40), RATEK(6,30,40), CRAT(6,30,40)
DIMENSION (I, J, IST) = (CONCKI(I, J) * PPP(J) / (82.057 * TTT(J)))
DO 1000 J = 1, NPT
1000 CONTINUE
C课程
C置
C压
C置
C计算浓度

CON1(J, IST) = CONCKI(1, J)
CON2(J, IST) = CONCKI(2, J)
CON6(J, IST) = CONCKI(6, J)
GO TO 1000
CONM1(J, IST) = (CONCKI(I, J) * PPP(J)) / (82.057 * TTT(J))
1000 CONTINUE
C课程
C计算速率常数
C置
C压
C置
C计算指向反应常数

R1(J, IST) = (RATK(1, J, IST) * CONWCM(5, J, IST) * CONM(6, J, IST))
R2(J, IST) = (RATK(2, J, IST) * CONWCM(5, J, IST) * CONM(9, J, IST))
R3(J, IST) = (RATK(3, J, IST) * CONWCM(5, J, IST) * CONM(10, J, IST))
R4(J, IST) = (RATK(4, J, IST) * CONWCM(4, J, IST) * CONM(7, J, IST))
R5(J, IST) = (RATK(5, J, IST) * CONWCM(4, J, IST) * CONM(7, J, IST))
R6(J, IST) = (RATK(6, J, IST) * CONWCM(8, J, IST) * CONM(7, J, IST))
C课程
C计算K1, K2, RNO, KS, AND PHI
C置
C压
C置
C计算指向反应常数

IF(R2(J, IST) = 0.0, AND(R3(J, IST) = 0.0)) EK1(J, IST) = 1.0E+35
IF(R2(J, IST) = 0.0, AND(R3(J, IST) = 0.0) GO TO 2500
EK1(J, IST) = (R2(J, IST) / R3(J, IST))
2500 CONTINUE
IF(R4(J, IST) = 0.0, AND(R5(J, IST) = 0.0) EXP(J, IST) = 1.0E+35
IF(R4(J, IST) = 0.0, AND(R5(J, IST) = 0.0) GO TO 2750
EK2(J, IST) = (R4(J, IST) / R5(J, IST))
2750 CONTINUE
R(1, IST) = (PPP(J) * WM(J)) / (82.057 * TTT(J))
NOTE... FUEL CARD IS PHYSICALLY BEFORE OXIDANT CARD IN INPUT, OXYGEN RATIO
IS SECOND SPECIE SPECIFIED IN OXIDANT AIR, FUEL IS SPECIFIED C-A.

C** EKS = ((12*ANUM(1,1)+1*ANUM(1,2))*ANUM(2,2))/(28.99*(ANUM(1,1)+(RATIO(660)))
1*ANUM(1,2))

PHI(IST) = RON/EKS

F(IST) = PHI(IST)*EKS/(1+(PHI(IST)*EKS))

C** CALCULATE CONCENTRATION OF CH2

C** RATWTS = ANUM(1,1)/ANUM(1,2)

CH2(J,IST) = ((RATWTS/(1+12*RATWTS))*(WM/J)*RON/(RON+1.0)) - CONCRAT(720)

C** CALCULATE CONCENTRATION OF CH

C** STORE VALUES OF T

C** PRINT AND PUNCH OUTPUT

C** IF(IPRINTZ.EQ.0) GO TO 9999

DO 9500 J = 1,NPT

IF(I,NE.1) GO TO 8500

WRITE(6,1800) ANUM(1,1), ANUM(1,2), RTEMP(2), PEXP(J), ICODE, EKS

WRITE(7,1800) ANUM(1,1), ANUM(1,2), RTEMP(2), PEXP(J), ICODE, EKS

8000 FORMAT(1X,7HFUEL= CN15.8*1HM=CN15.8,18H INLET AIR T(K)= CN15.8/1XRAT=9840

WRITE(6,1820) F(I), PHI(I), RON(J,1), ATT(J,1), RC0N6(J,1), BCON2(J,1)

WRITE(7,1820) F(I), PHI(I), RON(J,1), ATT(J,1), RC0N6(J,1), BCON2(J,1)

8200 FORMAT(1X,6E12.5/1X,6E12.5)

WRITE(6,1850) F(I), PHI(I), RON(J,1), ATT(J,1), RC0N6(J,1), BCON2(J,1)

WRITE(7,1850) F(I), PHI(I), RON(J,1), ATT(J,1), RC0N6(J,1), BCON2(J,1)

8500 FORMAT(1X,6E12.5/6E12.5)

CONTINUE

9999 RETURN
APPENDIX VI - LISTING OF PROGRAM NOXRAT
PROGRAM NOXHAT (INPUT, OUTPUT, PUNCH, TAPE 5 = INPJT, TAPE 6 = OUTPUT, NOX=0000)
TAPE 7 = PUNCH, TAPE 4)

C MAIN PROGRAM

C DOUBLE PRECISION G*X
REAL MIX (50)
INTEGER DATA, OMIT, INSERT, REAC, ALANK, THR, END, SUB
LOGICAL HP, SP, TP, INERUG, NEW, IONS, HOLES, FROZ, E2L, PSA, RKT
LOGICAL SHOCK, MMH, PASCAL, EVIC, OETN, CPCVF, CPCVEQ, SIUNIT, EUNITS
LOGICAL FA, OF, ERAT, FPCT

C DIMENSION OMIT (3, 3), NCO (4), INSERT (3, 3), LH (2), LV (2), LM (2)
COMMON/POINTS/NSUM (13), SSUM (13), CPR (13), DLVT (13), DLVPT (13)
1*ANMAS (13), P (26), T (26), V (13), PPP (13), WH (13), SONVEL (13), TTT (13)
2*TON (13)
COMMON/SPECIES/COEF (2*7*150), S (150), EN (150), ENL (150), H (150)
1*DELN (150), a (15*150), SUR (150), T (150), IUE (150), TEMP (150)
COMMON/MISC/ENN, SUM, TT, S, A, OH (3*101), LLM (15), BO (15), BP (15)
1*TH, LOM, TM, THIG, PP, CPSUM, OF, EDRATE, FPCT, R, R, HSUR, AC (2), AM (2)
2*PP (2), RHO (2), VMN (2), VMPL (2), VPL (2), DATA (22), NAME (15, 5)
3*ANUM (15, 5), PFCNT (15), ENTH (15), FAZ (15), RTEMP (15), FCK (15), DENS (15)
4*ÄNOMP, ANW (15), TLN
COMMON/DUAL/ G (20*21), X (20)
COMMON/INDX/ THEBUG, CONV, TP, HP, SF, HPS, TPSP, HOLES, NP, NT, NPT, NNL
1*NS, X4T, IMAT, T101, T102, NOMIT, TP, NEW, nsSUB, NSUP, TN, CPCVF, CPCVEQ
2*INS, NC, INSERT, JSOL, LTO, KASE, NREA, IC, JS1, VOL, SHOCK
COMMON/PERF/PCP (26), VMOC (13), SPNT (13), VAC (13), SUBAR (13), SUF, R (13)
1*CORF (13), ARE (13), CSTR, EQL, FROZ, SSO
COMMON/GNEW/RON, IINDA
COMMON/DICK/MIX
COMMON/GNEW/ R (30*40), R (6*30*40), EK1 (30*40), EK2 (30*40), ROH (30*40)
1CH2 (30*40), ATT (13*40), F (40), PHI (40), BCON (30*40), BCON2 (30*40), BCONEQ (13)
26*15)
COMMON/GNEW/R (30*40), R (6*30*40), EK1 (30*40), EK2 (30*40), ROH (30*40), BCON2 (30*40), BCONEQ (13)
COMMON/GNEW/R (30*40), R (6*30*40), EK1 (30*40), EK2 (30*40), ROH (30*40), BCON2 (30*40), BCONEQ (13)

C EQUIVALENCE (OMIT, ENLN), (INSERT, EN (1, 3)), (NL, M, L), (OF, OXFL)
C DATA MIX/4HOMIT/BLANK/1H/PSIA/4HPSIA/REAC/4HREAC/I2/2H0/2
1*INPUT/4HINPUT/IF/1HE/INSERT/HSH/SHIN/SHM/4TH/THRE/END/END/END/
DATA LH/4HCA, 4HML, G/, LV, 2HV, 1H/, LVM, 2HV, 1H/, NMLT/4HNAME/
C VMELIST/INP, KASE, P, TERA, IO, OF, FPCT, FA, TP, HP, SP, RKT
1*PSIA, MMH, SHOCK, IONS, EV, V, OETN, CPCVF, CPCVEQ, IDEBUG
2*SIUNIT, EUNITS, MIX
C
T LOW = 0,
VAR = "FALSE"
C
1 WRITE (6, 400)
400 FORMAT (1H1)
293 READ (5, 204) (DATA (I), I = 1, 15)
204 FORMAT (5, 3-14, 13)
WRITE (6, 245) (DATA (I), I = 1, 15)
2045 FORMAT (4X, 2-14, 3, X)
IF (DATA (1), EQ, THR) GO TO 90
IF (DATA (1), EQ, REAC) GO To 11
IF (DATA (1), EQ, MIT) Go To 205
IF (DATA (1), EQ, INSERT) Go To 180
IF (DATA (1), EQ, INPUT, OR, DATA (1), EQ, NMLT) Go To 210
IF (DATA (1), EQ, BLANK) Go To 203

C
1023 WRITE(6,1024)
1024 FORMAT(4H0ERROR IN ABOVE CARD. IGNORE CONTENTS.)
   GO TO 203
10 CALL REACT
   IF(.EQ.0) WRITE(4,52)
52 FORMAT(4H0ERROR IN REACTANT CARDS)
   GO TO 203
C
C       READ THERMO DATA FROM CARDS AND STORE ON TAPE 4
C
90 VERW = .TRUE.
   REWIND 4.
   READ(5,5) TLOw, THID, THIGH
5 FORMAT(3F10.3)
   WRITE (4,5) TLOw, THID, THIGH
   READ (5,10) (DATA(I),I=1,16),NCD(1)
10 FORMAT(9A4*5X,2A3*,4(A2+F2.0),1A1,2F10.3,1I5)
   IF((DATA(1),EQ.BLANK) OR (DATA(1) = END))
   WRITE (4,10) (DATA(I),I=1,16)!
   IF((DATA(1),EQ.END) GO TO 203
   READ(5,10) (DATA(I),I=1,15),NCD(2),(DATA(J),J=6,10),NCD(3),(DATA(K),K=1,15)
10 IF(1.EQ.14)*NCD(4)
20 FORMAT(5E15.8,5/E15.8,5/E15.8,4/E15.8,12)
   WRITE (4,20) (DATA(I),I=1,14)
21 FORMAT(5E15.8,5/E15.8,4/E15.8)
   DO 25, I=1,4
25 IF(NCD(I),EQ.1) GO TO 25
   WRITE(6,22) (DATA(J),J=1,3)
22 FORMAT(25H0ERROR IN ORDER OF CARDS FOR +SA4)
   CONTINUE
   GO TO 97
C
C       CHECK INSERT CARDS
C
180 DO 185, I=4,15,3
185 IF((DATA(1),EQ.BLANK) GO TO 185
   NSERT = NSERT+1
   NSERT(I+1) = DATA(I)
   NSERT(2*NSERT) = DATA(I+1)
   NSERT(3*NSERT) = DATA(I+2)
   CONTINUE
   GO TO 203
C
C       CHECK OMIT CARDS
C
205 DO 208, I=4,15,3
208 IF((DATA(I),EQ.BLANK) GO TO 208
   NOMIT = NOMIT+1
   OMIT(I+NOMIT) = DATA(I)
   OMIT(2+NOMIT) = DATA(I+1)
   OMIT(3+NOMIT) = DATA(I+2)
   CONTINUE
   VERW = .TRUE.
   GO TO 203
C
C       BEGIN NAMELIST INPT2
C
210 DO 300 I=1,26
   300 CONTINUE
   V1 = 0.
   V2 = 0.
   R40P = 0.
   KASE = 0
   TP = *FALSE*
   HP = *FALSE*
   SP = *FALSE*
   RXT = *FALSE*
   CPCVR = *FALSE*
   CPCVEQ = *FALSE*
   SHOCK = *FALSE*
   DETN = *FALSE*
   EV = *FALSE*
   PASCAL = *FALSE*
   MMHG = *FALSE*
   PSIA = *FALSE*
   R = 1.0*67165
   RR = 4134.5R
   SIUNIT = *FALSE*
   EUUNITS = *FALSE*
   IONS = *FALSE*
   TDERUG = *FALSE*
   FA = *FALSE*
   DF = *FALSE*
   ERATIO = *FALSE*
   FPCT = *FALSE*
   DO 303 I = 1,50
      MIX(I) = 0.
   303 CONTINUE
   EQL = *TRUE*
   READ(5*INPT2)
   DO 305 I=1,26
      IF (P(I).EQ.0.) GO TO 322
      IF (MMHG) P(NP) = P(NP)/760.
      IF (PASCAL) P(NP) = P(NP)/101325.
      IF (PSIA) P(NP) = P(NP)/14.696006
   305 CONTINUE
   DO 625 IST = 1,44
      INOFA = IST
      IF (IST.NE.1) WRITE(6*1400)
      IF (MIX(IST).NE.0.) GO TO 323
      IF (IST.NE.1) GO TO 1
      WRITE(6*724)
   322 FORMAT(4*NOINO INPT? VALUE GIVEN FOR OF* EQRAT* FA* OR FPCT)
   IF (WP(2).NE.0.) OXFL = WP(1)/WP(2)
   GO TO 333
   323 OXFL = MIX(IST)
   GON = MIX(IST)
   IF (FA) GON = 1./ MIX(IST)
   IF (FPCT) OXFL = (100.* MIX(IST))/ MIX(IST)
   IF (NOT.ERATIO) GO TO 333
   IF (EQRAT.EQ.1.) EQRAT = 1.0*000005
S(2)/(VS(1)*EQRATOVM!N(I)) X*80

3XFL = (-EORAT*VT2)VPLN{2))/vpi

333 SUM = OXFL *1* 
V2 = (OXFL*VMIN(1)+VMIN(2))/SUM 
V1 = (OXFL+VPLS(1)+VPLS(2))/SUM 
IF(V2+NE,0) EORAT=ABS(V1/V2) 
IF (RHO(1)*NF. 0. *AND. RHO(2) *NE. 0.) GO TO 744 
RHO = RHO(2) 
IF (RHOP *EQ. 0.) RHOP = RHO(1) 
GO TO 745

744 RHOP =(OXFL+1)*RHO(1)*RHO(2)/(RHO(1)+OXFL*RHO(2)) 

745 LL = L 
IF (*NOT.IONS) GO TO 746 
LL = L+1 
IF (LLMT(L)+EQ.IE) GO TO 746 
LL = L+1 
LLMT(L) = IE 
3D(L) = 0.

746 DD 747 IF1+LL 
B0(I1) = (OXFL +B0P(I+1) + B0P(I+2))/SUM

747 CONTINUE 
NPT = 1 
MSUA=10OXFL*HPP(1) + HPP(2))/SUM 
IF (*NOT.NEW) GO TO 786 
CALL SEARCH 
IF(SHOCK.OR.DETN) GO TO 760 
DO 755 N=I,NREA 
TT = RT(N) 
CALL HCALC 
GO TO 760

755 CONTINUE 
760 WRITE(*,INPT2) 
766 EVN = +1 
SUM = ENN 
XI = NS - NC 
X = ENN/XI 
XLN = ALOG(XI) 
DO 432 J=1,NS 
IF(IUSE(J)+EQ.+10000) IUSE(J)=0 
IF (IUSE(J)+NE,0) GO TO 432 
EV(J+1) = XI 
EVLN(J) = XLN 

432 CONTINUE 
WRITE (6,770)

770 FORMAT (1H0+17X*4FUEL +13X*7OXIDANT +12X*7H4MIXTURE //)

780 FORMAT (1H2 2A4,3E19.8/) 
L:7200 H=HPP(1)+HPP(2)+SUSB0+LVP*VPLS(2)+VPLS(1)*V1* 

785 LOAD (SH ATOMS/G) 
WRITE (4,780)(LLMT(I)+BLANK*B0P(I+1)+B0P(I+2)+B0P(I+1)+B0P(I+1)+B0P(I)*1*I:;L) }

CONTINUE 
WRITE (6,780)

780 FORMAT (1H2 2A4,3E19.8/) 
L:7200 H=HPP(1)+HPP(2)+SUSB0+LVP*VPLS(2)+VPLS(1)*V1* 

785 LOAD (SH ATOMS/G) 
WRITE (4,780)(LLMT(I)+BLANK*B0P(I+1)+B0P(I+2)+B0P(I+1)+B0P(I)+1*I:;L) }

CONTINUE 
WRITE (6,780)
IF(NSERT=0) GO TO 302
DO 301 I=1,NSERT
IF(SUB(J+1) .NE. ENSERT(1+I)) GO TO 301
IF(SUB(J+2) .NE. ENSERT(2+I)) GO TO 301
IF(SUB(J+3) .NE. ENSERT(3+I)) GO TO 301
ENSERT(1+I) = 0.
I01= I01+1
IUSE(J)= -IUSE(J)
301 CONTINUE
302 CONTINUE
790 ITN= 35
IC = .FALSE.
JSQL = 0
JLIQ = 0
IF(OM) CALL DETON
IF(RKT) CALL ROCKET
IF(TP) CALL MOLIER
IF(HP) CALL CMBSIN
IF(SHOCK) CALL SHCK
625 CONTINUE
NSERT = 0
GO TO 1
END
SUBROUTINE REACT

DOUBLE PRECISION Gx
LOGICAL HP,SP,TP,INEJ,UG,CONVG,NEWR,IONS,MOLES,eqL,FRoZ

C

DIMENSION ANAME(15,5),V(15)

C

COMMON/PIX/ANN,SUM+TT+SN+AToM(3,101),LLMT(15),G0(15),GOP(15,2)
1+T,THMIN,THIGH,PP,CPSUM,OF,EDRAT,FPCT,R,RH,HSUAN,AC(2),AM(2)
2+HP(2),RNC(2),VMIN(2),VPL(2),WP(2),DATA(22),NAME(15,5)
3+ANUM(15,5),PECW(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
4+RHP,AM(15),TLY

COMMON/INDX/NS,,new,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NL,LM
1+NS,KMAT,THAY,101,102,NODIT,IP,NEWR,NSUB,NSUP,ITN,CPCVF,CPCEQ
2+IONS,NC,INSERT,JSEL,JNIQ,KASE,NREC+IC,J31+VOL,SHC

C

EQUIVALENCE (NAME,ANAME),(NL,LM)

C

DATA MOL/1HH/*0X/1H0/*LANK/1H/*ZERO/2H00/

C

DO 10 K=1,2
WP(K)=0.
HP(K)=0.
RHO(K)=0.
VPLS(K)=0.
VMIN(K)=0.
AC(K)=0.
AM(K)=0.
DO 8 J=1,15
LLMT(J)=0.
DATA(J,K)=0.
8 CONTINUE
10 CONTINUE

=1
L=1

20 READ(5,21): (NAME(N),ANUM(V+1),I=1,5),PECW(T),MOLE,ENTH(N),FAZ(N)
1+RTEMP(T),FOX(N),DENS(N)

21 FORK=N(40+F4,1)+F7,S+A1,F9,5,A1+F8,5,A1+F8,5
IF .EQ.0 GO TO 20
WRITE(6,0) (NAME(N),ANUM(N),I=1,5),PECW(T),MOLE,ENTH(N),FAZ(N)
3+RTEMP(N),R0(1-DENS(N)

3+NAME(1X,5)(A2,1X,F7,4,2X,F8,4,2X,A1,F11,2X,A2,F8,3,2X)
1,W,F8,5)
35 IF (MOLE.EQ.MOL) MOLES=TRUE.

=2
IF (FOX(N),EQ,OK) K=1
DO 38 J=1,15
DATA(J)=0.
38 CONTINUE
R4=0.
DO 40 J=1,5
IF (ANUM(N,J),EQ,0.) GO TO 101
DO 41 J=1,15
NJ=J
IF (LLMT(J).EQ.N) GO TO 45
IF (NAME(N,J),EQ,LLMT(J)) GO TO 46
41 CONTINUE
45 L=NJ
LLMT(J)=NAME(N,J)
46 DO 48 KK=1,101
  IF(ATOM(1,KK).EQ.ANAME(N,JJ))GO TO 50
48 CONTINUE
  L=0
  GO TO 20
50 R(N)=R(N)+NUM(N,JJ)*ATOM(Z,KK)
  V(J)=ATOM(3,KK)
  DATA(J)=NUM(N,JJ)
100 CONTINUE
101 PCWT=PCWT(N)
  IF(NOLES) PCWT=PCWT/RM
  WP(K)=WP(K)*PCWT
  IF(NAME(N,N),NE,0) HPP(K)=HPP(K)+ENTH(N)*PCWT/RM
  AM(K) = AM(K)+PCWT/RM
  DO 110 J=1,L
  WP(J,K)=DATA(J)*PCWT/RM + WP(J,K)
110 CONTINUE
  IF(DENS(N),NE,0) GO TO 115
  GO TO 117
115 RHO(K)=RHO(K)*PCWT/DENS(N)
117 RW(N)=RM
  N = N+1
  IF(N*NE,16) GO TO 20
200 NREAC=N-1
  IF(L,EQ,0) GO TO 1000
  DO 220 K=1,L
  IF(WP(K),EQ,0) GO TO 220
  HPP(K)=HPP(K)/WP(K)
  AM(K)=AM(K)/AM(K)
  IF(RHO(K),NE,0) RHO(K)=WP(K)/RHO(K)
  DO 215 J=1,L
  WP(J,K)=WP(J,K)/WP(K)
  IF(V(J),LT,0) VMIN(K)=VMIN(K)+WP(J,K)*V(J)
  IF(V(J),GT,10) VPLS(K)=VPLS(K)+WP(J,K)*V(J)
215 CONTINUE
  IF(NOLES) GO TO 220
  DO 218 N=1,NREAC
  IF(FIXX(N),EQ,0X,AND,K,EQ,2) GO TO 218
  IF(FIXX(N),NE,0X,AND,K,EQ,1) GO TO 218
  PECWT(N) = PECWT(N)/WP(K)
218 CONTINUE
220 CONTINUE
  NREAC='TRUE'
  DO 230 N=1,NREAC
  IF(DENS(N),NE,0) GO TO 230
  RHO(1)=0
  RHO(2)=0
  SG TO 1000
230 CONTINUE
1000 RETURN
END
SUBROUTINE SEARCH

C SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED

INTEGER SU*MIT,END

C LOGICAL NFWR

C DIMENSION DATE(2,3),MT(4),3(4),OMIT(3,3)

COMMON/SPCES$LOE$FN(2,7,150),S(150),EN(150,13),ENL(150),H(150)
1,DELN(150),A(15,150),SUB(150,3),USE(150),TEMP(50,2)
COMMON/MISC/ENN,TT$0,ATOM(3,101),LLMT(15),B0(15),BO(15)
1,TMP(3,101),THOM,THG,PP*,CPSUM*OF,EGRT,TFC,PR,FR,HSUB0,AC(2),AM(2)
2,PP(2),RGT(2),VMTN(2),VPS(2),HPS(2),DATA(22),NAME(15,5)
3,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
4,RP,ROMN(15),TLN

COMMON/INII/DEB,CONVG,IP,HP,SP,HPSP,IPSP,MOLES,NS,NT,NPT,NLM
1,NS,PHA*,IMAT,IP,IO*,NOMIT,IP,NEW,NSUB,NSUP,IN,PCVFR,CPCVEQ
2,ION,NS,NE,NSET,JS0,LJL,J,AS*,VOL,SHOCK

C EQUIVALENCE (DATE,EN),(OMIT,ENL),(END,END),(L,NLM)

C DATA GAS/1HG,END/3END/

C

QC=0

I=0

COEF(1,1,1)=END

I=1

DO 3 I=1,150

IF(A(1,1),EQ,END) GO TO 4

DO 3 J=1,L

A(1,1)=0

3 CONTINUE

4 A=M5=1

AIND=4

R=0(4,5) TLW,TMD,THIG

5 FORMAT (3F10.3)

NS=1

6 READ (4,10) (SUR(NS,J),J=1,3),DATE(1,NS),DATE(2,NS),(HT(J),J=1,L)

1 J=1,NS,PHA,IMAT,1

10 FORMAT (3F10.4,6X,2A3,4,A2,F3.0,A12,F10.3)

IF(SUR(NS,J),END) GO TO 71

READ (4,29) (COEF(I,J+NS),J=1,7)*I=+2

20 FORMAT (5I15.8)

IF(NOMIT,F3.0) GO TO 810

DO 805 I=1,NOMIT

DO 804 J=1,3

IF(OMIT(J,1),NE,SUR(NS,J)) GO TO 805

804 CONTINUE

3 CONTINUE

805 CONTINUE

810 R=0*K=1,4

IF(R(K),EQ,0) GO TO 825

810 CONTINUE

810 CONTINUE

810 DO 925 K=1,4

IF(R(K),EQ,0) GO TO 925

DO 925 I=1,L

925 CONTINUE

925 CONTINUE

R=0.5,NS=0

GO TO 7

920 K(*)=R(K)
825 IF(NS.EQ.MAXNS) GO TO 870
     IUSF(NS) = 0
     IF(PHAZ.EQ.GAS) GO TO 170
     NC = NC+1
     TE = T(NC+1) = T1
     TE = T(NC+2) = T2
     IX = IX+1
     IF(IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145
     DO 830 I = 1,L
     IF(A(I+NS).NE.A(I+NS-1)) GO TO 145
     830 CONTINUE
     IX = IX-1
   145 IUSE(NS) = -IX
   170 NS = NS+1
     GO TO 7
   870 WRITE(6,871) (SUB(NS,J),J=1,3)
   871 FORMAT (45H001IMENSIONS IN SPECIES TOO SMALL TO CONSIDER *3A4)
     GO TO 7
   171 NS = NS-1
     NWR = *FALSE*
     WRITE(6,172)
   172 FORMAT (42H0SPECIES BEING CONSIDERED IN THIS SYSTEM)
     DO 174 I = 1,NS+5
      IS = I+4
      IF(NS.LT.IS) IS = NS
     174 WRITE (6,176) (DATE(I+J),DATE(I+J),SUB(J,1),SUB(J,2),SUB(J,3),J=1,IS)
   176 FORMAT (5(5X,2A3,2X,3A4))
     RETURN
   END
SUBROUTINE EQLARM
C ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES
C
C DOUBLE PRECISION X, G
LOGICAL HP, SP, TP, INEBUG, CONVG, IONS, MOLES, FROZ, EQL, LOGV, HPSP, TPSP
LOGICAL ISING, IC SHOCK
C
C DIMENSION PROW(18)
C
C COMMON/POINTS/HSUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13)
1,GAMMA(13), P(26), T(26), V(13), PPP(13), WM(13), SDVNL(13), TT1(12)
2,TOTN(13)
C COMMON/SPTES/Coeff(2, 7, 150), S(150), EN(150, 13), ENLN(150), H0(150)
C COMMON/HINC/ENLN(150), EN(150), SUB(150), IUSE(150), TEMP(50, 2)
C COMMON/HSC/EN(150), HINC(150), LHM(150), ATOM(3, 101), LLMT(15), B0(15), AOP(15)
C COMMON/HSO/FPSU, FPO, FPSO, FPSO, FPSO, FPSO, FPSO, FPSO, FPSO, FPSO
C COMMON/HS4/H4O, H4O, H4O, H4O, H4O, H4O, H4O, H4O, H4O
C COMMON/DOUBLE/ G(20, 21), X(20)
C COMMON/INX/ INEBUG, CONVG, TP, HP, SP, HPSP, TPSP, MOLES, NP, NT, NPT, NLM
C COMMON/INX/ INEBUG, CONVG, TP, HP, SP, HPSP, TPSP, MOLES, NP, NT, NPT, NLM
1, NSKMAT, THAT, 101, 102, NOMIT, TP, NEWNS, SUBNS, TN, CPCVFR, CPCVEQ
2, IONS, N, N, N, N, N, N, N, N, N
C COMMON/PERF/PCP(26), VMC(13), SM(13), VACI(13), SUBAR(13), SUPAR(13)
C COMMON/PERF/PCP(26), VMC(13), SM(13), VACI(13), SUBAR(13), SUPAR(13)
1, CPRF(13), AEAT(13), CSTR, EQL, FROZ, SS0
C
C EQUIVALENCES (NLM, L)
C
C DATA
C
C SIZE= 1A5
SIZEF = 0
INGS = .FALSE.
ENLN = ALOG(ENN)
LOGV = .FALSE.
PPLN = ALOG(PP)
TLN = ALOG(TT)
CONVG = .FALSE.
ITNUMB = ITN
JS1 = 1
CALL CPSH
TM = PPLN - FNVL
C
C IF (IC) PREVIOUS POINT HAD SINGULAR MATRIX
C
C IF (IC) GO TO 966
IF (NOT IONS, OR IE EQ LLM(L)) GO TO 33
L = L + 1
IS1 = IC + 1
DO 499 J = 1, NS
IF (A(L, J) EQ 0.) GO TO 499
EN(J, NPT) = SMNALO
ENVL(J) = SMNOD
IUSE(J) = 0
499 CONTINUE
33 IF (NP, EQ, 3) AND (NOT SHOCK) WRITE(6, *344) (LLMT(I)) I = 1, L
C 244 FORMAT (4AMPT, 16(5X, A4))
C
C BEGIN ITERATION
C
C
43 CONTINUE
IF (IC) GO TO 171
IF (.NOT. CONVG OR JSOL .EQ. 0) GO TO 62
ENSOL = EN(JSOL, NPT)
ENSOL = EN(JSOL, NPT) * EN(JLIQ, NPT)
IUSE(JLIQ) = -IUSE(JLIQ)
IQ = IQ - 1
DLVT(NPT) = 0
CPR(NPT) = 0
GAMMAS(NPT) = 0
LOGV = .TRUE.
62 CALL MATRIX
NUMR = ITN - ITNUMB - 1
IF (.NOT. CONVG) GO TO 67
IF (LOGV .AND. JSOL .EQ. 0) GO TO 63
DO 182 I = 1, L
PROW(I) = G(IQ1, I)
182 CONTINUE
IF (.NOT. LOGV) GO TO 67
C LOGV = .TRUE. -- SET UP MATRIX TO SOLVE FOR DLVT(NPT)
63 G(IQ1, IQ2) = ENN
IQ = IQ1 - 1
DO 777 I = 1, IQ
G(I, IQ2) = G(I, IQ1)
777 CONTINUE
67 IF (.NOT. IFERLIG) GO TO 72
WRITE(6, 772) NUMR
772 FORMAT (1H0, 'NUMR = ', J3, 6X, 7HMATRIX //)
DO 911 I = 1, IMAT
IF (.NOT. CONVG) IMAT = IMAT - 1
ITST = IMAT
CALL MGAUSD
IF (ITST .NE. IMAT) GO TO 774
WRITE (4, 773) (LLMT(I), I = 1, L)
WRITE (4, 373) (LLMT(I), I = 1, IMAT)
373 FORMAT (7H0, 5, 9(A4, 1X))
WRITE (4, 911) (G(I, K), K = 1, IMAT)
911 CONTINUE
73 IF (.NOT. CONVG) GO TO 85
773 CONTINUE
IF (.NOT. LOGV) GO TO 174
IF (JLIQ .NE. 0) EN(JSOL, NPT) = ENSOL
GO TO 171
174 SUM = 0
DO 175 J = 1, L
SUM = SUM + PROW(J) * X(J)
175 CONTINUE
DLVT(NPT) = 1. * G(IQ2, IQ1) / (ENN * SUM / ENSOL - X(IQ1)
CPR(NPT) = G(IQ2, IQ2)
DO 176 J = 1, IQ
CPR(NPT) = CPR(NPT) - G(IQ2, J) * X(J)
176 CONTINUE
LOGV = .TRUE.
GO TO 82
C SINGULAR MATRIX
C IF(ISING) SINGULAR ONCE
C IF (IC) SINGULAR TWICE

774 IF (*NOT*CONVG) GO TO 775
WRITE(6,172)
172 FORMAT(20H?DERIVATIVE MATRIX SINGULAR )
IC = *IC*
GO TO 1171
775 IF (*NOT*HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.) GO TO 871
WRITE(6,874)
874 FORMAT(6X"LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE"
1"BEEN INCLUDED ON AN INSERT CARD; RESTART")
GO TO 873
871 WRITE (6,74)
74 FORMAT(16H0SINGULAR MATRIX)
IF (IC) GO TO 773
IF (ISING) GO TO 997
VTZERO = 0
966 DO 970 JJ = 1, NS
IF (IUSE(JJ)) 970, 968, 967
967 IF (EN(JJ,NPT).NE.0.) GO TO 873
GO TO 969
968 IF (EN(JJ,NPT).NE.0.) GO TO 969
EN(JJ,NPT) = SMALNO
ENLN(JJ) = SMNOL
GO TO 970
969 VTZERO = VTZERO+1
970 CONTINUE
IF (*NOT*IC) GO TO 971
IC = *FALSE*
GO TO 43
971 ISING = *TRUE*
WRITE(6,776)
776 FORMAT (AH0RESTART)
GO TO 43
997 IF (VTZERO.NE.(L-1)) GO TO 873
IF (ERAT.GT.1.00001.OR.ERAT.LT.0.99999) GO TO 873
ENN=0
NEN = 0
DO 98 I=1,L
98 LEN=0
DO 99 J=1,NS
IF (EN(J,NPT).EQ.0.) GO TO 80
IF (I*I+J*J).EQ.0.) GO TO 80
IF (EN(J,NPT).NE.0.) GO TO 83
99 JEN = J
R0 CONTINUE
NEN = NEN+1
EN(J,NPT) = R0(I)/A(I*JEN)
93 CONTINUE
IF (NEN.LT.VTZERO) GO TO 873
CONVG = *TRUE*
IC = *TRUE*
HSMN(NPT) = 0
DO 94 J=1,NS
IF (EN(J,NPT).EQ.0.) GO TO 84
ENN = EN(J,NPT)*ENN
TEM = EN(J,NPT)
ENLN(J) = ALOG(TEM)
HSMN(NPT) = HSMN(NPT) + EN(J,NPT)*H0(J)
94 CONTINUE

C
T4 = ALOG(PP/ENN)
GO TO 40
70

A5 ITNUMY= ITNUMA-1

OBTAIN CORRECTIONS TO THE ESTIMATES

KK = L + 1
DLNT = X(I01)
IF (TP) DLNT=0
DO 10 J=1*NS
IF (IUSE(J)) 101,99,100
99 DELN(J) = HO(J)*DLNT-HO(J)*S(J) - ENLN(J) - TM*X(I01)
DO 99 K=1*L
DELN(J) = DELN(J) + A(K,J)*X(K)
99 CONTINUE
GO TO 101
100 DELN(J) = X(KK)
KK = KK + 1
101 CONTINUE
AMBDAA = 1.
AMBDAV = 1.
SUM = X(I01)
IF(SUM.LT.0.) SUM=SUM
IF(DLNT.GT.SUM) SUM=DLNT
IF(DLNT.GT.SUM) SUM=SUM
DO 917 J=1*NS
IF (IUSE(J).NE.0) GO TO 917
IF((EN(J,NPT).GT.0.).AND.(A*ENLN(J).GT.SUM)) SUM = DELN(J)
917 CONTINUE
IF (SUM.LT.0.) SUM=-SUM
IF (SUM.LT.25) SUM=-SUM
AMBDAA = AMBDAA
AMBDAV = AMBDAV
IF (.NOT.IDERUG) GO TO 111
WRITE(6,923) T+ENN+ENN+PP+PPLN+AMRDA
923 FORMAT(3HI0=15,R,6HN=15,8,7HM ENNL=E15.8,5H PP=E15.8
1 7H PPLN=E15.8,8H AMRDA=E15.8)
WRITE(6,924)
924 FORMAT(1HN,1R,2HN,12X,5HN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HS0)
1R=12X=6HM=6/RT=9X=M=6/RT
DO 921 J=1*NS
FVEGI = S(J)-H0(J)
FNEG2 = FNEG2-ENLN(J1)-TM
WRITE(6,925) SUB(J,1),SUB(J,2)
1SUB(J+1)*EN(J,NPT)+ENLN(J)+DELN(J)+H(J)+S(J)+FNEG1+FNEG2
925 FORMAT(1X=3A4,7E15.6)
926 CONTINUE
WRITE(6,110)
110 FORMAT(1HO)

APPLY CORRECTIONS TO ESTIMATES

111 SUM = 0.
ENNL = ENNL+AMRDA*X(I01)
ENN = EX2(ENNL)
TM = PPLN - FNL
DO 113 J=1*NS
IF (IUSE(J)) 113 112 114
112  ENLN(J) = ENLN(J) + AMBDA * DELN(J)
   EN(J,NPT) = 0.
   IF (ENLN(J) = ENLN(J) + SIZE) * LE*O*) GO TO 113
   EN(J,NPT) = EXP(ENLN(J))
   SUM = SUM + EN(J,NPT)
   GO TO 113
114  EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)
113  CONTINUE
   SUMN = SUM
   IF (TP) GO TO 115
   TLN= TLN*AMBDA*DLN
   TT = EXP(TLN)
   JS1 = 1
   CALL CPHS
115  IF (LLMT(L) .NE. IE) GO TO 116
DO 116 J = 1,NS
   IF (A(L,J) .NE. O.) GO TO 116
   IF (EN(J,NPT) .GT. O.) GO TO 116
116  CONTINUE
DO 117 J = 1,NS
   IF (A(L,J) .NE. O.) IUSE(J) = -10000
117  CONTINUE
L = L - 1
   I01 = 101 - 1
   GO TO 43
C
C TEST FOR CONVERGENCE
C
116  IF (ITNUMA .EQ. O.) GO TO 13
   IF (AMBDA .LT. O.) GO TO 43
   SUM = (ENN-SUHN)/ENN
   IF (SUM .LT. O.) SUM = -SUM
   IF (SUM .GT. O.5E-5) GO TO 43
   DO 130 J = 1,NS
      AA = DELN(J)/SUHN
      IF (A(L,J) .LT. O.) AA = -AA
      IF (IUSE(J) .EQ. O.) AA = AA*EN(J,NPT)
   129  IF (AA .GT. O.5E-5) GO TO 43
   CONTINUE
C
C CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS
C
   SSUM(NPT) = 0.
   DO 133 J = 1,NS
      IF (NPT .EQ. O.) SS0 = SS0 + EN(J,1)*S(J)
      SS = SS(J)
      IF (IUSE(J) .EQ. O.) SS = SS = ENLN(J) + TM
      SSUM(NPT) = SSUM(NPT) + SS*EN(J,NPT)
   133  CONTINUE
   IF (NPT .EQ. O.) SS0 = SS0 + SSUM(NPT) * F801
   SS = SSUM(NPT) - SS0
   IF (SS .LT. O.5E05) OR (SS .GT. 0.00005) GO TO 43
   IF (IDERUG) WRITE(6*1183) SS
   130 CONTINUE
C
C CHECK ON REMOVING IONS
C
   DO 116 J = 1,NS
      IF (A(L,J) .EQ. O.) GO TO 116
      IF (EN(J,NPT) .GT. O.) GO TO 116
   116  CONTINUE
   DO 117 J = 1,NS
      IF (A(L,J) .NE. O.) IUSE(J) = -10000
   117  CONTINUE
C
C EXAMINE SHAPE
C
   IF (LLMT(L) .NE. IE) GO TO 116
   IF (SSUM(NPT) .NE. SSUM) GO TO 13
   RETURN
130 CONTINUE
IF (TT .LT. TLOW*OAR*TT .GT. THIGH) WRITE (6,306) TT , NPT EQL '3000
306 FORMAT (17H0 THE TEMPERATURE=E12.4*26H IS OUT OF RANGE FOR POINT=15) EQL '3010
WRITE (6,973) TT, NPT
973 FORMAT (1HL*12*I2*69H IUTS FOR THE POINT =15)
IF (.NOT. HP OR. NPT, NE=.1 OR. NC. E0.0 OR. TT. GT. 100.) GO TO 873
WRITE (6,874) TT = T(1)
RETURN

CONVERGENCE TESTS ARE SATISFIED: TEST CONDENSED SPECIES.
160 IF (INC. E0.0) GO TO 143
143 SIZEF = 0.
INC = 0.
DO 170 J = 1, 85
IF ((IUSE(J)*E0.0 .OR. IUSE(J)*EQ.-10000) GO TO 170
INC = INC + 1
IF (IDUSE(J)) WRITE (6,144) (SUB(J+I)*I13)+TEMP(INC+1)*TEMP(INC+2),
144 FORMAT (1H0,344*,2F10.3,3X,5HUSE=,I4,E15.7)
IF (EN(J*NPT)) 144*148*169
146 IF (J*NE. J SOL *AND* J*NE. JLIQ) GO TO 147
JSOL = J.
JLIQ = 0.
147 IIE = I1D - 1
EV(J*NPT) = 0.
GO TO 166
148 KG = 1.
154 IF (IUSE(J)*EQ.-IUSE(J*1)) GO TO 154
151 IF (J*EQ.1.0 OR. IUSE(J)*NE. IUSE(J*1)) GO TO 153
KG = -1.
154 JKG = J + KG
IF (EN(JKG*NPT)*LT. 0.) GO TO 170
TMELT = TEMP(INC+1)
IMP = INC - KG
IF (TMELT. EQ. TEMP(IMP+2)) GO TO 158
TMELT = TEMP(INC+2)
IF (TMELT. EQ. TEMP(IMP+1)) GO TO 157
WRITE (6,156)
156 FORMAT (150H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER)
C
C JTH SPECIES A SOLID (EN=0), (J*KG)TH SPECIES A LIQUID (EN IS +)
C
157 IF (TT*GT.TMELT) GO TO 169
158 IF (TP*AND.TT*EQ*TMELT) GO TO 169
159 IF (TP) GO TO 1165
160 IF (TT*LE.*TMELT-150.) GO TO 1165
JSOL = J.
JLIQ = JKG
GO TO 159
C
C JTH SPECIES A LIQUID (EN=0), (J*KG)TH SPECIES A SOLID (EN IS +)
C
158 IF (TT*LT.TMELT) GO TO 169
159 IF (TP*AND.TT*EQ*TMELT) GO TO 169
160 IF (TP) GO TO 1165
161 IF (TT*GT.TMELT-150.) GO TO 1165
JSOL = JKG
JLTQ = J
JL9 TLN = ALOG (TMELT)
          TT = TMELT
          EN(JKG, NPT) = EN(JKG, NPT) X 5
          EN(J, NPT) = EN(JKG, NPT)
          GO TO 165
C
C WRONG PHASE INCLUDED FOR T INTERVAL; SWITCH EN
C
1645 EN(J, NPT) = EN(JKG, NPT)
          IUSE(J) = -IUSE(J)
          IUSE(JKG) = -IUSE(JKG)
          EN(JKG, NPT) = 0.
          GO TO 60

153 IF (TT = LT.Temp(INC, 1) .AND. Temp(INC, 1) .NE. TLOW) GO TO 169
       IF (TT, GT, Temp(INC, 2)) GO TO 169
C
C SUM = 0.
       DO 167 I = 1, L
              SUM = SUM + A(I, J) * X(I)
       CONTINUE
       DELF = HO(J) - S(J) - SUM
       IF (DEBUG) WRITE (6, 168) DELF, SIZEF
       IF (DEBUG) FORMAT (17H GO-.SUM(A(I,J)*X(I)) = E15.7)
       GO TO 169

168 FORMAT (17H GO-.SUM(AIJ*PI) =E15.7*10*X*18H(SELECT DELTA G = E15.7)
       GO TO 169
       SIZEF = DELF
       JNEFLF = J
       IF (INC, EQ, NC) GO TO 1160
       CONTINUE

1160 IF (SIZEF.EQ.0.) GO TO 143
       J = JDELF

165 I01 = 101 * 1
166 IUSE(J) = IUSE(J)
       IF (NPT, EQ, 1) SS0 = 0.
       JSI = 1
       CALL CPHS

163 TN = NUMB
       IF (N.EQ., SHOCK) WRITE (6, 771) NPT, (X(IL), IL = 1, L)*TN

771 FORMAT (13, 14F9.3)
       ITNUMB = ITN
       JSI = 1
       IF (TP .AND. CONVG) CALL CPHS
       GO TO 43
C
C CALCULATE EQUILIBRIUM PROPERTIES
C
1171 DLVT(NPT) = -1.
       DLVT(NPT) = 1.
       CP(R(NPT)) = CPSUM
       GO TO 199

171 SUM = 0.
       DO 179 J = 1, L
              SUM = SUM + PROW(J) * X(J)
       CONTINUE

184 IF (JL10.EQ.0) GO TO 199
       IUSE(JL10) = -IUSE(JL10)
       HSUM(NPT) = HSUM(NPT) + EN(JL10,NPT)*(HO(JL10) - HO(JSO))
**74**

```plaintext
TQ1 = TQ1+1
GAMMAS(NPT) = -1/DLVPT(NPT)
GO TO 186
186 GAMMAS(NPT) = -1/(DLVPT(NPT)*DLVTP(NPT)*2)*ENN/CPR(NPT))

200 IF (.NOT.IDER(i)) RETURN
PRATIO = 1.
IF(SP) PRATIO=PP/P(1)
*RITE(6*201) NPT,PRATIO,PP,T,T,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NPT)
1T1 = DLVPT(NPT)*DLVTP(NPT)*GAMMAS(NPT)
201 FORMAT (7HOPOINT=I3,3X;4HPCP=I3*6,3X,2HP=I3,6*3X,3X,2HT=I3,6*3X,4HEQ=I3*5)
SO TO 1000

C.
ERROR SET TT=0

873 TT=0
NPT = NPT-1
1000 RETURN
END
```
SUBROUTINE CPHS
CALLS THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES

COMMON/SPECIES/COEF(2,7,150)*S(150)*EN(150,13)*NLN(150)*H0(150)
1*DELT(150)*A(15,160)*SUR(150,3)*IUSE(150)*TEM(150,2)

COMMON/MISC/SUM,T,T,T,ATM3(3,101)*LMT(151,30,15)*R0P(15,2)
1*TM*TLW*TM*THPP*CPSUM*OF*EDRA*TFCR*R*R*HSURG*AC(2)*AM(2)

COMMON/INDEX/TN/BUG,TN/TP,H,SP,HPSP,TTPS,MOLES,NP,NT,NT,NLH
1*NS*KMAT/KMAT/IQ, IQ2*NOMIT/IP,NEWR,NSUR,NSUP,TIT,CPCVCF,CPCVE
2*IONS,NC,NSERT,JSOL, JLIQ,KASE,NREAIC,IC,JS1,VOL,SHOCK

EQUIVALENCE (J,JS1)

K = 1
IF(TT.LE.TMID) K = 2
KK = 0
CPH SUM = 0.

90 IF(COEF(K+1,J).NE.0) GO TO 97
IF(IUSE(J).LT.0) GO TO 100

100 RETURN

CPH**0000
CPH**0010
CPH**0020
CPH**0030
CPH**0040
CPH**0050
CPH**0060
CPH**0070
CPH**0080
CPH**0090
CPH**0100
CPH**0110
CPH**0120
CPH**0130
CPH**0140
CPH**0150
CPH**0160
CPH**0170
CPH**0180
CPH**0190
CPH**0200
CPH**0210
CPH**0220
CPH**0230
CPH**0240
CPH**0250
CPH**0260
CPH**0270
CPH**0280
CPH**0290
CPH**0300
CPH**0310
CPH**0320
CPH**0330
CPH**0340
CPH**0350
CPH**0360
CPH**0370
CPH**0380
IF (CONV.G) GO TO 175
   DO 145 I=1,L
   X(I)=0(I)=G(I,101)
   G(I,KMAT)=G(I,KMAT)*X(I)
   CONTINUE
   G(I01,KMAT)=G(I01,KMAT)*ENN-SMN

C  COMPLETE ENERGY ROW AND TEMPERATURE COLUMN

175 G(I02,102)=G(I02,102)+CP5UM
185 RETURN
END
SUBROUTINE MGUSD
C SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS
C DOUBLE PRECISION G*X+COEFX(20)*SUM,Z
C COMMON/DODULE/G(20:21)*X(20)
C COMMON/INDX/ID,ERUG,CONVG,TP,HP,SP,HPSP,IPS,IP,NM,NP,NPT,NLM
C COMMON/NMAT,IMA,TQ,IO2,NOIT,IP,NEWR,NSUB,NSUP,ITN,CPUCVF,CPCVEQ
C EQUIVALENCE (IUSE,IMAT)
C DATA BIGNO/1,E,38/
C BEGIN ELIMINATION OF NNTH VARIABLE
C IUSE1=IUSE+1
6 DO 45 NN=IUSE1
83 IF (G(NN,NN).EQ.0.) GO TO 18
45 CONTINUE
B1 IF (G(NN,NN).EQ.0.) GO TO 18
C SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
C 8 DO 18 I=NN+IUSE
C 18 CONTINUE
C INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NNTH
C VARIABLE FROM THE REMAINING EQUATIONS
C INTERCHANGE EQUATIONS I AND NN
28 IF (NN=I) 29,31,29
29 DO 30 J=NN+IUSE1
30 CONTINUE
B2 IF (I) 2R,23,22
C 28 IF (NN=I) 29,31,29
C 29 DO 30 J=NN+IUSE1
C 30 CONTINUE
31 K = NN + 1
DO 36 J = K*, IUSE1
   IF(G(NN+NN),EQ,0.) GO TO 23
   G(NN,J) = G(NN+J) / G(NN,NN)
36 CONTINUE
   IF(K-IUSE1) 88,45,88
88 DO 44 I = K*, IUSE1
   DO 44 J = K*, IUSE1
      G(I,J) = G(I,J) - G(I,NN) * G(NN+J)
44 CONTINUE
45 CONTINUE
C
46 K = IUSE
47 J = K + 1
48 DO 50 I = J*, IUSE1
   SUM = SUM + G(K+I)* X(I)
50 CONTINUE
51 X(K) = G(K, IUSE1) - SUM
C
52 IF(K > 15) GO TO 47
53 IUSE = IUSE + 1
54 RETURN
55 END
SUBROUTINE VARFMT(V,NPT)

C
DIMENSION V(1)

COMMON/OUTP/FMT(30)*FP(4)*FT(4)*FM(4)*FS(4)*FC(4)

1: FC(4)*FG(4)*FB+FMT13+F1+F2*F3*F4*F5*FL(4)*FMT19*FA1*FA2

2: FR1*FC1+FN(4)*FR(4)*FA(4)*FI(4)*FMT9*X*F0

C

DO 45 I=1,NPT

X = 2*I*3

FMT(K) = F4

IF (V(I)*GE.10.) FMT(K) = F3

IF (V(I)*GE.100.) FMT(K) = F2

IF (V(I)*GE.1000.) FMT(K) = F1

IF (V(I)*GE.10000.) FMT(K) = F0

45 CONTINUE

RETURN

END
SUBROUTINE OUTJ
C
DOUBLE PRECISION G,X
REAL HX(40)
LOGICAL EQL,FANZ,TP,HP,SP,HPSP,TPSP,MOLES
C
DIMENSION NV(13),Z(10,3),HEAD(15),XY(5),YN(5)
DIMENSION SIEGEL(30),CONCTK(10,30)
C
COMMON/POINTS/NSUM(13),SSUM(13),CPFR(13),DLVTP(13),DLVPT(13)
C
1 *GAMMAS(13),PI(26),T(26),V(13),PPF(13),WM(13),SONVEL(13),TTT(13)
2 ,TOIN(13)
C
COMMON/SPECIES/COEF(2,150),S(150),POF,EQRAT,PPCT,RR,NSUB0,AC(2),AM(12)
2 ,TPSP,SPS,MOLES
C
1 ,THMP(2),RHO(2),VINN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
2 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
C
5 ,RHP,PRM(15),TLN
C
COMMON /DOUBLE/ G(20,21),X(20)
COMMON/IND/ IDERUG,CNV,G,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
4 ,NP,NT,NLM
C
1 ,NS,KA,IMAT,IQ,192,
2 ,NOMIT,IP,NEWR,NSUB,NSUP,INT,CPCVFR,CPCVEQ
C
1 ,CPCVFR,CPCVEQ
C
COMMON/PERF/PP(26),VMO(113),SP(M13),VACI(13),SUBAR(13),SUPAR(13)
C
1 ,SUPAR(13)
C
1 ,CPRF(13),AEAT(13),CSR,EQL,FROZ,SS0
C
COMMON/OUT/FPMT(203),FP(4),FT(4),FH(4),FS(4),FM(4),V(4),FD(4)
1 ,FC(4),FG(4)
C
2 ,FR,FC1,FR(4),FM(4),SI(4),FI(4),FT9X,F0
C
COMMON/SNEW/R0N/INDFA
C
COMMON/EQNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40)
C
1 ,CH2(30,40)+ATT(13,40)+F(40)+PHI(40)+BCON1(30,40)+BCON2(30,40)+BCONDOUT(30,40)
C
C
EQUIVALENCE A4(VN),(A2,H03),SX,7X.the.F2F,OUT
C
DATA HEAD,'4H(1H94Hv2A492H#S,4H(A2.,4H49F5 94H*3X),214,5 s2HXv
C
DATA FUEL/4HFUEL/,OX10/4HK0ID/,ANT/3iKANT/,,OX/1q(O,,Z/,K0O;
C
2 ,FR,FC1,FR(4),FM(4),SI(4),FI(4),FT9X,F0
C
DATA CHEMICAL FORMULA,(SEE NOTE)
C
1 ,CH2(30,40)+ATT(13,40)+F(40)+PHI(40)+BCON1(30,40)+BCON2(30,40)+BCONDOUT(30,40)
C
C
IF(KASE.NE.0) WRITE (6,3) KASE
C
3 FORMAT (9H CASE No.,15)
IF(AUC,MOLES) WRITE (6,5)
C
5 FORMAT 17X,4H WHT FRACTION ENTHALPY STATE TEMP DENSITY/
1 10X *CHEMICAL FORMULA,51X,21H(SEE NOTE) CAL/MOL,10X,5MD9EG K,OUT
C
2 4X,4HGC
C
2 IF(MOLES) WRITE (6,6)
C
6 FORMAT 17X,4HMOLC,7X,33H ENTHALPY STATE TEMP DENSITY/
1 10X *CHEMICAL FORMULA,66X,7HCAL/MOL:10X,13HDEG K /GC/C
2 30 15 N=1 NREAC
IF(FOX(N).NE.O) GO TO 10
C
MN = 0X10
M02 = ANT
C
OUT*0000
OUT*0010
OUT*0020
OUT*0030
OUT*0040
OUT*0050
OUT*0060
OUT*0070
OUT*0080
OUT*0090
OUT*0100
OUT*0110
OUT*0120
OUT*0130
OUT*0140
OUT*0150
OUT*0160
OUT*0170
OUT*0180
OUT*0190
OUT*0200
OUT*0210
OUT*0220
OUT*0230
OUT*0240
OUT*0250
OUT*0260
OUT*0270
OUT*0280
OUT*0290
OUT*0300
OUT*0310
OUT*0320
OUT*0330
OUT*0340
OUT*0350
OUT*0360
OUT*0370
OUT*0380
OUT*0390
OUT*0400
OUT*0410
OUT*0420
OUT*0430
OUT*0440
OUT*0450
OUT*0460
OUT*0470
OUT*0480
OUT*0490
OUT*0500
OUT*0510
OUT*0520
OUT*0530
OUT*0540
OUT*0550
OUT*0560
OUT*0570
OUT*0580
OUT*0590
GO TO 11
10 HD1 = FUEL
   HD2 = FR
11 DO 13 J=1,5
   IF(NAME(N,J) .EQ. "IZ" .OR. NAME(N,J) .EQ. "IB") GO TO 14
   CONTINUE
   J=6
   14 J=J-1
   HEAD(3) = YN(J)
   HEAD(7) = YX(J)
   HEAD(9) = F75
   IF(PECWT(N) .GE. 10.) HEAD(9) = F73
   WRITE(6,HEAD) HD1*HD2* (NAME(N,J)) * ANUM(N,J) * JJ=1,J ) * PECWT(N) * ENTH (OUT*10)
   1) N, FAZ(N) * RTEP(N) * DENS(N)
   CONTINUE
   15 CONTINUE
   FPC = 100./ (1. + OF)
   WRITE(6,20) OF, FPC, EGRAT, RHP
20 FORMAT (1H0, 1SX9, 4W0/F7.4, 4X/F8, 4X, 2X/DENSITY)
C AGV = 9,80665.
RETURN
C ENTRY OUT2
C PRESSURE
C FMT(4) = FMT(6)
CALL VARFMT (PPP, NPT)
WRITE (6,FMT) (FP(I), I=1,4), (PPP(J), J=1,NPT)
C TEMPERATURE
C DO 65 I=1,NPT
   V(I) = HSUM(I) * R
65 CONTINUE
FMT(4) = FMT13
FMT(5) = FMT19
WRITE (6,FMT) (FT(I), I=1,4) + (NV(J), J=1,NPT)
C ENTHALPY
C DO 75 I=1,NPT
   V(I) = HSUM(I) * R
75 CONTINUE
FMT(5) = FR
FMT(7) = F1
WRITE (6,FMT) (FH(I), I=1,4) + (V(J), J=1,NPT)
C ENTROPY
C FMT(7) = F4
DO 78 I = 1,4
   V(I) = SSUM(I) * R
78 CONTINUE
WRITE (6,FMT) (FS(I), I=1,4) + (V(J), J=1,NPT)
WRITE (6,A0)
90 FORMAT (1H0)
C MOLECULAR WEIGHT
C
C

FMT(7) = F3
WRITE (6,FMT) (FMT(I),I=1,4) *(WM(J)*J=1,NPT)
C

(DLV/OLDP)
C

FMT(7) = F5
IF(EQL) WRITE (6,FMT) (FV(I),I=1,4) *(DLVPT(J)*J=1,NPT)
C

(DLV/OLDP)
C

FMT(7) = F4
IF(EQL) WRITE (6,FMT) (FD(I),I=1,4) *(DLVTP(J)*J=1,NPT)
C

HEAT CAPACITY
C

DO 85 I=1,NPT
V(I) = CPR(I) * R
85 CONTINUE
WRITE (6,FMT) (V(I),I=1,4) *(V(J)*J=1,NPT)
C

GAMMA(S)
C

WRITE (6,FMT) (FG(I),I=1,4) *(GAMMAS(J)*J=1,NPT)
C

SOV: VELOCITY
C

FMT(7) = F1
DO 95 I = 1,NPT
SONVEL(I) = SQRT(2*GAMMAS(I)*TTT(I)/WM(I))
95 CONTINUE
WRITE (6,FMT) (FL(I),I=1,4) *(SONVEL(J)*J=1,NPT)
RETURN
C

ENTRY OUT3
IF(.NOT.EQL) GO TO 331
DO 309 I = 1,NPT
DATA (I) = 0.
DO 308 K = 1,NS
DATA(I) = DATA(I) + EN(K,I)
308 CONTINUE
309 CONTINUE
C

MOLE FRACTIONS = EQUILIBRIUM
C

WRITE (6,AR0)
FMT(7) = F5
WRITE (6,310)
310 FORMAT(15HMOLE FRACTIONS //)
DO 330 K=1,NS
DO 315 I=1,NPT
V(I) = EN(K,I) / DATA (I)
315 CONTINUE
DO 316 I=1,NPT
IF (V(I)*GE*(5.E-6)) GO TO 320
316 CONTINUE
GO TO 330
320 WRITE (6,FMT) SUB(K+1)*SUB(K+2)*SUB(K+3)*FB*(V(I),I=1,NPT)
330 CONTINUE
331 WRITE(6,335)

335 FORMAT(188H
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE M0OUT=1800
14E FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS/) OUT=1 190
LINE= 0
NN = 1
IF(FQL) NN=NPT
DO 350 K=1,NS
DO 340 I=1,NN
IF ((EN(K,I)/DATA(I)) • GE*(5•E-6)) GO TO 343
340 CONTINUE
LINE= LINE+1
Z(LINE+1)= SUR(K+1)
Z(LINE+2)= SUR(K+2)
Z(LINE+3)= SUR(K+3)
343 IF ((LINE. NE.1) AND K. NE .NS) GO TO 350
IF (LINE. EQ.0) GO TO 1000
WRITE(6*345) (Z(LINE+1),Z(LINE+2),Z(LINE+3),LIN•=1 LINE)
345 FORMAT (10(1X,3A4))
LINE= 0
350 CONTINUE
IF (. NOT. MOLES) WRITE (6•360)
360 FORMAT (78H
NOTE: WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANTS IN TOTAL OXIDANTS )
1000 CONTINUE
DO 3000 I =1,10
II = 3•I+ 2
DO 2000 K=1,NS
IF (SIEGEL(II, NE. SUB(K,1)) GO TO 2000
IF (SIEGEL(II-1, NE. SUB(K,2)) GO TO 2000
IF (SIEGEL(II+2, NE. SUB(K,3)) GO TO 2000
DO 1500 J=1, NPT
1500 CONCI(1,J) = EN(K,J)/DATA(J)
GO TO 3000
2000 CONTINUE
3000 CONTINUE
C***
C*** VOTE** FOR MORE THAN NPT=6, THESE PRINT STATEMENTS MUST BE MODIFIED OUT=2150
C***
DO 5000 K=1,10
II = 3•K+ 2
WRITE (6•4000) SIEGEL(II), SIEGEL(II+1), SIEGEL(II+2), (CONCI(K,J),J=1,NPT)
11,NPT)
4000 FORMAT (1X,3A4,2X,6(E15.8,1X))
5000 CONTINUE
WRITE (6*5000) (WM(J),J=1,NPT)
5000 FORMAT (11H MOLEC. WT. X,6(E15.8,1X))
WRITE (6*7000) (TTI(J), J=1,NPT)
7000 FORMAT (9H TEMP. (K) X,6(E15.8,1X)
WRITE (6*8000) (PPP(J), J=1,NPT)
8000 FORMAT (12H PRESS. (ATM)) X,6(E15.8,1X)
WRITE (6*9000) RON
9000 FORMAT (14H FUEL AIR RAT. X,E15.8)
DO 9500 N =1, NREAC
WRITE (6*9500) (ANUM(N,J),J=1,5) * ENTH(N) * RTEMP(N)
9500 FORMAT (1X,E15.8)
9600 CONTINUE
CALL RATES(CONCI,YH,TIT,PPP,ANUM,ENTH,RTEMP,NPT,NREAC)
9999 RETURN
END
SUBROUTINE RATES(CONCKI,WH,TTT,PPP,ANUM,ENTH,TEMP,NPT,NREAC)

REAL MIX(50)
DIMENSION CONCKI(10,30),TTT(13),PPP(13),WH(13),ANUM(15,5),ENTH(15)
RTEMP(15)
DIMENSION R2(30,40),R3(30,40),R4(30,40),R5(30,40),RATEK(6,30,40),CRAT(6,30,40)
10CONMC(10,30,40),A(1),EN(6),E(6)
COMMON/SNEN/RON,INFRA
COMMON/DICK/ MIX
COMMON/EQNEW/RON,INFFA
RATINS(10)
COMMON/EQNEW/RON,INFFA
COMMON/EQNEW/RON,INFFA

DATA(A(I),I=1,6)/3.1E13,6.4E09,4.1E13,2.9513E13,3.8146E13,4.5816E13/1775E13/(E(I),I=1,6)/0.334E00,0.334E00,0,0/1775E13/(E(I),I=1,6)/0.334E00,0.334E00,0,0/1775E13/(E(I),I=1,6)/0.334E00,0.334E00,0,0/

C**** TEST FOR WRITE CONTROL
C****

IST = INDFA
IPRINT = 0
IF(MIX.(IST+1),EQ.0.0) IPRINT = 1
C****
C**** SET PRESSURE LOOP
C****
DO 800 J = 1,NPT
C****
C**** CALCULATE CONCENTRATIONS
C****
BCON1(J,IST) = CONCKI(J+1,J)
BCON2(J,IST) = CONCKI(2,J)
BCON6(J,IST) = CONCKI(6,J)
DO 1000 I = 1,10
CONMC(J,I,IST) = (CONCKI(I,J)*PPP(J))/(82.057*TTT(J))
1000 CONTINUE
C****
C**** COMPUTE RATE CONSTANTS
C****
DO 2000 I = 1,6
RATEK(J,IST) = A(I)*(TTT(J)*EN(I)).EXP(-C(I))/(1.987E03*TTT(J))
2000 CONTINUE
C****
C**** CALCULATE FORWARD REACTION CONSTANTS
C****
R1(J,IST) = (RATEK(J,IST)*CONMC(5,J,IST)*CONMC(6,J,IST))
R2(J,IST) = (RATEK(2,J,IST)*CONMC(5,J,IST)*CONMC(6,J,IST))
R3(J,IST) = (RATEK(3,J,IST)*CONMC(5,J,IST)*CONMC(6,J,IST))
R4(J,IST) = (RATEK(4,J,IST)*CONMC(5,J,IST)*CONMC(6,J,IST))
R5(J,IST) = (RATEK(5,J,IST)*CONMC(5,J,IST)*CONMC(6,J,IST))
R6(J,IST) = (RATEK(6,J,IST)*CONMC(5,J,IST)*CONMC(6,J,IST))
C****
C**** CALCULATE K1,K2,RHO,K5 AND PHI
C****
IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) EK1(J,IST) = 1.0E+35
IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) EK2(J,IST) = 1.0E+35
2500 IF(R2(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) EK2(J,IST) = 1.0E+35
2750 RK1(J,IST) = (PPP(J)*WH(J))/(82.057*TTT(J))
**NOTE**...FUEL CARD IS PHYSICALLY BEFORE OXIDANT CARD IN INPUT.

**NOTE** IS SECOND SPECIE SPECIFIED IN OXIDANT AIR, FUEL IS SPECIFIED C**

C** = 8

EKS = (((12*ANUM(1,1)+1)*ANUM(1,2)*ANUM(2,2))/(28*99*ANUM(1,1))*ANUM(1,2))

PHI(IST) = RON/EKS

F(IST) = PHI(IST)*EKS/(1+(PHI(IST)*EKS))

**CALCULATE CONCENTRATION OF CH2**

RATWTS = ANUM(1,1)/ANUM(1,2)

CH2(J*IST) = ((RATWTS/(1+12+RATWTS)))*(WM(J)*RON/(RON+1)))

1KI(2+J) = CONCNI(3+J) = CONCNI(1+J)

**STOP VALUES OF T**

ATT(J*IST) = T.SET(J)

8000 CONTINUE

**PRINT AND PUNCH OUTPUT**

IF(IPRINT,EQ.0) GO TO 9999

DO 9500 J = 1,NPT

DO 9000 I = 1,IST

IF(I.NE.1) GO TO 8500

WRITE(6,8100) ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2)

WRITE(7,8100) ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2),ANUM(1,1)*ANUM(1,2)*ANUM(2,2)

8100 FORMAT('X,7FUEL = C*E15.8*11H*E15.8*18H INLET AIR T*(K) = *E15.8*1XRAT*880

1,13HPPR, (ATM) = *E15.8,7HICOD = *12,13HPHI STICCH = *E15.8

8500 WRITE(6,8200) F(I),PHI(I),ROH(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I)

13CON1(J,I)*CH2(J,I)*R1(J,I)*R6(J,I)*EKL(J,I)*EKL2(J,I)

8200 FORMAT(1X,6E12.5/1X,6E12.5)

WRITE(7,8250) F(I),PHI(I),ROH(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I)

13CON1(J,I)*CH2(J,I)*R1(J,I)*R6(J,I)*EKL(J,I)*EKL2(J,I)

8250 FORMAT(6E12.5/6E12.5)

9000 CONTINUE

9500 CONTINUE

9999 RETURN

END
SUBROUTINE HCALC

CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS

LOGICAL MOLES
DIMENSION NUM(15,5)

COMMON/SPECIES/COEF(2,7,150),RF(150),EN(150),ENL(150),HO(150)
1+DELN(150),A(15,150),SUB(150,3),USE(150),TEP(150,2)
COMMON/HSC/EN,SMN,ST,SN,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
1+TM(LOW,TMN,THIGH,PP,CPX,OF,ERAT,FPCX,RR,HSUB,AC(2),AM(2))
2+HPP(RH0,?),(VHS(2),VPLS(2),NP(2),DATA(22),NAME(15,5)
3+ANUM(15,5),PECMW(15),ENTH(15),FAZ(15),TPEM(15),FOX(15),DENS(15)
4+RH0,P,RW(15),TLN
COMMON/TENX/DBUG,CONV,X,TP,HP,SP,HP,P,TM,MOLES,MDP,NT,NPT,LM
1+NS,KMAT,IMAT,IQ,1Q,NOMIT,IP,NEWR,NSUB,NSUP,IN,CPCVFR,CPCVEQ
2+IONS,NC,NSERT,JSOL,JLIG,KASE,NREAC,IC,JS1,VOL,SHOCK

DATA AG/1HG/1ZEO/2H00/0X/1HC/10BLK/1H

IS TT IN RANGE

IF(TT LT (TLOW=1000).OR.TT GT (THIGH=1000)) GO TO 75
HPP(1)=0.
HPP(2)=0.
AC(1)=0.
AC(2)=0.
DO 900 N=1,NREAC
K=2
IF(FOX(N),EQ,0,K=1
PCW=PECM(1,0).
IF(.MOLES)PC=PECM(RM(N)
IF(NAME(N),EQ,1ZER0)GO TO 5
AC(1)=0.
AC(2)=0.
GO TO 500
5 J=NUM(N,S)
IF(J=NE.0) GO TO 90
DO 10 J=1,L
DATA(J)=0.
10 CONTINUE
DO 10 I=1,L
IF(ANUM(I),EQ,1,GO TO 50
DO 20 J=1,L
IF(LLMT(J),EQ,NAME(N+1)) GO TO 30
20 CONTINUE
30 DATA(J)=ANUM(N,I)
40 CONTINUE
50 IS=I
DO 70 J=1,NS
IF(USE(J),EQ,0) GO TO 55
IS = IS+1
IF(FAZ(N),EQ,1,GO TO 70
IF(TT GT TEMPS(NP) AND TEMPS(NP) NE. THIGH) GO TO 70
IF(TT LT TEMPS(NP) AND TEMPS(NP) NE. TLOW) GO TO 70
GO TO 56
55 IF(FAZ(N),EQ,AG AND FAZ(N),NE,RLK) GO TO 70
56 DO 60 IS=1,L

HCA*0000
HCA*0010
HCA*0020
HCA*0030
HCA*0040
HCA*0050
HCA*0060
HCA*0070
HCA*0080
HCA*0090
HCA*0100
HCA*0110
HCA*0120
HCA*0130
HCA*0140
HCA*0150
HCA*0160
HCA*0170
HCA*0180
HCA*0190
HCA*0200
HCA*0210
HCA*0220
HCA*0230
HCA*0240
HCA*0250
HCA*0260
HCA*0270
HCA*0280
HCA*0290
HCA*0300
HCA*0310
HCA*0320
HCA*0330
HCA*0340
HCA*0350
HCA*0360
HCA*0370
HCA*0380
HCA*0390
HCA*0400
HCA*0410
HCA*0420
HCA*0430
HCA*0440
HCA*0450
HCA*0460
HCA*0470
HCA*0480
HCA*0490
HCA*0500
HCA*0510
HCA*0520
HCA*0530
HCA*0540
HCA*0550
HCA*0560
HCA*0570
HCA*0580
HCA*0590
IF((I,J),NE,DATA(I)) GO TO 70
60 CONTINUE
   SUM(N+5) = J
   GO TO 90
70 CONTINUE
   GO TO 80
90 NSS = NS
   VS = J
   DELN(J) = EN(J*NPT)
   EN(J*NPT) = 1.
   CALL CPHS
   EN(J*NPT) = DELN(J)
   NS = NSS
   IF (H(J),GT,0.01 .AND. H(J)*LT,0.01) H(J) = 0.
   RTEMP(N) = TT
   ENTH(N) = H(J)*R*TT
   AC(K) = AC(K) + CPSUM*PCWT/RMW(N)
580 HPP(K) = HPP(K) + ENTH(N)*PCWT/RMW(N)
960 CONTINUE
   IF (.NOT.,MOLES) GO TO 951
   DO 950 K=1,2
   IF(WP(K)*EQ,0.) GO TO 950
590 HPP(K) = HPP(K)/WP(K)
   AC(K) = AC(K)/WP(K)
950 CONTINUE
   WRITE(6,75)
   75 WRITE(*,76) 'SOMOREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA '
   WRITE(*,85) 'N'
   85 FORMAT(1H40,12*34H TH REACTANT IS NOT IN THERMO DATA )
1000 RETURN
END
C ROUTINE MOLIER

COMMON/PONTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
1 *GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SOVEL(13),TT(13),
2*TOTN(13)
COMMON/SCPECIES/SCOF(2,7,150),SSUM(150),EN(150,13),ENLN(150),HO(150),
1 *DELN(150),A(15,150),SUR(150),3**,IUSE(150),TEMP(50,2)
COMMON/HSCPY/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2),
1 *T4,TL0W,THTN,THGH,PP,CPSUM,OF,EDRAT,FPCT,R,RR,HSUB0,AC(2),AM(2),
2 *HP2(2),RH0(2),VMIN(2),VPL5(2),NP(2),DATA(22),NAME(15,5)
3 *ANUM(15,5),PECYT(15),ENTH(15),FAL(15),RTEP(15),FOX(15),DENS(15)
4 *RHOP,RH0V(15),TN,
COMMON/INDX/DEBUG,CONVG,TP,HP,SP,HPST,TPSP,N0LES,NP,NT,NPT,NLM,
1 *NS*KMAT,IMAT,101,102,DOMIT,1P,NWNR,NSUB,NSUP,1TN,CPCVFR,CPCVED
2 *IONS,NC,NSES,JSOL,JLIQ,KASE,ENRAC,IC,J1,VS,SH0C

DO 91 IT = 1,26
IF (T(TT),EQ.0.) GO TO 95
VT = IT
91 CONTINUE

C SET ASSIGNED P
95 DO 902 IP = 1,NT
PP = P(IP)
C SET ASSIGNED T
C DO 902 IT=1,NT
IT = T(TT)
CALL EQLBRM
IF(IT*NE.0.) GO TO 800
IF(NP*EQ.0.) GO TO 1000
800 K = 0
IF(IP*EQ.0.,AND.MM,IT.EQ.NT0R,IT.EQ.0.) GO TO 850
K = NPT
IF(NP*NE.13) GO TO 870
860 WRITE (6,865) 5 FORMAT (1H1,'*X,48|HERMODYNAMIC EQUILIBRUM PROPERTIES AT ASSIGNED|P1)
1 */53X,12' THMODYNAMIC EQUILIBRUM PROPERTIES AT ASSIGNED|P1)
C CALL OUT1
WRITE (6,863) 863 FORMAT (25H0:|HERMODYNAMIC PROPERTIES//)
C CALL OUT2
CALL OUT3
865 IF(K*EQ.0.) GO TO 1000
WRITE (6,868) 868 FORMAT (1H1)
NPT = 0
870 NPT = NPT + 1
C SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C DO 866 I = 1,NS
EN(I*NPT) = EN(I*K)
880 CONTINUE
972 CONTINUE
1000 RETURN
END

MO*0000
MOL*0010
MOL*0020
MOL*0030
MOL*0040
MOL*0050
MOL*0060
MOL*0070
MOL*0080
MOL*0090
MOL*0100
MOL*0110
MOL*0120
MOL*0130
MOL*0140
MOL*0150
MOL*0160
MOL*0170
MOL*0180
MOL*0190
MOL*0200
MOL*0210
MOL*0220
MOL*0230
MOL*0240
MOL*0250
MOL*0260
MOL*0270
MOL*0280
MOL*0290
MOL*0300
MOL*0310
MOL*0320
MOL*0330
MOL*0340
MOL*0350
MOL*0360
MOL*0370
MOL*0380
MOL*0390
MOL*0400
MOL*0410
MOL*0420
MOL*0430
MOL*0440
MOL*0450
MOL*0460
MOL*0470
MOL*0480
MOL*0490
MOL*0500
MOL*0510
MOL*0520
MOL*0530
MOL*0540
MOL*0550
MOL*0560
MOL*0570
SUBROUTINE CHASTN
COMMON/POINTS/HSM(10)•SSUM(10)•CPR(10)•DLVTP(10)•DLVPT(10)
1 •GAMMAS(10)•P/26)•T(26)•V(13)•PPP(13)•WM(13)•SONVEL(13)•TTT(13)
2 •TGTN(13) COMMON/SFPCES/COEF(2,7,150)•5(150)•FRN(150)•GHIL(150)•HO(150)
1 •JELN(150)•11(150)•SUB(150)•IU(150)•TEMP(150)
COMMON/NISC/EN+SUN+TT+S1+ATOM(13•101)+LLMT(15)•BO(15)•BLP(15)•2
1 •TON(1)•TM(1)•TH(1)•PP•CPSUH•DFEQRAT•TPCT•R•R•HSR•AC(2)•AM(2)
2 •NAME(15)•150)•NAME(15•150)•NAME(15•150)
3 •ANOM(15)•PECW(15)•ENTH(15)•FAZ(15)•RTEMP(15)•DEN(15)•DEN(15)
4 •RHOP•RMW(15)•TLM COMMON/INDEX/IDBGN/CONVG+TP+HP+SP+HPSP+TPSP+MOLE•NP•NT•NPT•NLM
1 •NS•LAM•IMN•I01•102•NOMIT•IP•NEWR•NSUB•NSUP•INN•CPCVFR•CPCVEQ
2 •IONS•NC•NRT•JSOL•J•AQ•KASE•NRAC•IC•JS1•VOL•SHOCK
SET ASSIGNED P
TT = 38000.
DO 02 IP = 1, NP
PP = P(IP)
CALL EQRBM
T(NPT) = TT
IF(IT(NP)•NE•0) GO TO 800
IF(INPT•EQ•0) GO TO 1000
800 K = 0
IF(IP•EQ•NP OR TT•EQ•0) GO TO 850
K = NPT
IF(INPT•NE•13) GO TO 870
860 WRITE (6,6)
6 FORMAT (1H1,42X,4HTHEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES)
1CMB•0300
1
CALL OUT1
CALL OUT2
CALL OUT3
865 IF(K•EQ•0) GO TO 1000
NPT = 0
870 NPT = NPT + 1
SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
DO 820 I = 1, NS
EN(I•NPT) = EN(I•K)
820 CONTINUE
902 CONTINUE
1000 RETURN
END
SUBROUTINE DETON

CHAPMAN-JOUGUET DETONATIONS

LOGICAL HP, SP, TP, INERUG, NE, R1, R2, IONS, MOLES, FROZ, EQL, PSI, A, RKT
LOGICAL CPCVFR, CPCVF, CALCH

DIMENSION GH(13), CP(13), H(13), PUB(13), TUB(13), GM(13), RRR(13)

COMMON/POINTS/HSUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13)
1 *GAMMAS(13), P(26), T(26), V(13), PPP(13), VM(13), SDNVEL(13), TTT(13)
2 *T(26), H(26), V(26), VOLS(26), WP(26), DATA(22), NAME(13, 5)
3 *SUM(13), SPCT(13), ENTH(13), FAZ(15), RTMP(15), FOX(15), DENS(15)
4 *RHO, RV(15), T/LN

COMMON/INDX/ IEBUG, CNCVG, TP, HP, SP, HSUM, NSUM, NT, NPT, NLM
1 *NS, KMAT, IMAT, IO1, IO2, N, NMAT, IP, NWIR, NSUB, N1T, CPCVF, CPCVFR
2 *IONS, NSC, JRT, JSO, JLIQ, KASE, NREA, IC, JS1, VOL, SHOCK

COMMON/PERF/PCP(26), VHOC(13), SPIN(13), VACI(13), SUBAR(13), SUPAR(13)

COMMON/SUB/CMAT(31), AEAT(13), CURS, EQL, FROZ, SS0

COMMON/OUPF/MT(130), FP(4), FT(4), FH(4), FI(4), V(13), F(13)

COMMON/OUTF/MT(130), FP(4), FT(4), FH(4), FI(4), V(13), F(13)

COMMON/OUPF/MT(130), FP(4), FT(4), FH(4), FI(4), V(13), F(13)

EQUIVALENCE(CP, DATA), (GM, SPIN), (H, VACI), (PUB, SUBAR), (TUB, SUPAR)

EQUIVALENCE(GM, AEAT), (PCP(14), RHH)

DATA FT1/4HT1, D/, FP1/4HP1, A/, FH1/4H11, C/, FM1/4HM1, H/
1 * FC1/4HCPI, FP1/4HA1, / / FPP/4HP/P1, / / FTT/4HT/T1/
2 * FDP/4HDET, / / FM1/4HM1, / / FRA/4HR/00/, / / FDB/4HR/01/
3 * FPA/4HMA1, / / FMB/4H NO, / / IZERO/2H00/

C

D(C) = A11*A22-A21*A12
XX(Y) = (B1*A22-A2*B1)/D(C)
YY(Y) = (B2*A11-A1*B2)/D(C)

C

NT = 1
HSW1 = HSUM1R
CALCH = *FALSE*

TT = 0*

IF(T(T1), EQ, 0.) T(T1) = RTEMP(1)

DO 2 N = 1, NREA

IF(NAME(N), EQ, IZERO) CALCH = *TRUE*

2 CONTINUE

DO 3 IT = 1, 26

IF(T(T1), EQ, 0.) GO TO 7

VI = IT

3 CONTINUE

7 IF(AM(1), NE, 0.), AM(1) + AM(2), NE, 0) GO TO 4

AM(1) = AM(2)

IF(AM(2), EQ, 0.0) AM(1) = AM(1)

GO TO 9

4 AM(1) = 0, 0, AM(2) = AM(1) / AM(1) + 0, 0, AM(2)

9 CONTINUE

FORMAT(33H1) DETONATION VELOCITY CALCULATIONS)

DO 903 IT = 1, NT
T1 = T(T)
T2 = T2
IF (T1 G.T. T1CALC) GO TO 15
CALL MCALC
CALL OUT
15 CP1 = (OF*AC(1) * AC(2))/(OF+1)
DO 50 I=1,NP
P1 = P(I)
H1(NPT) = HSU0
TU3(NPT) = T1
PU3(NPT) = P1
CP(NPT) = CP1*R
ITER = 0
TT = 3800.
PP1 = 15.
PP = PP1*P1
HSU80 = H1(NPT)/R * 75*T1*PP1/AM1
TP = .FALSE.
HP = .TRUE.
CALL EQLBRM
HSU80 = H1(NPT)
HP = .FALSE.
IF (TT EQ. 0.) GO TO 1000
GAM = GAMMAS(NPT)
TT1 = TT/T1
II = 0
TEM = T1 * 75*PP1/(CPR(NPT)*AM1)
AMM = AM(NPT)/AM1
WRITE(16,190) TT
190 FORMAT (AHOT EST.*F8.2/11X*4H/P/1.17X*4HT/T1)
WRITE(6,203) II,PPI,TT1
C 200 DO 202 II=1,4
ALFA = AM/TT1
PPI = (1. + GAM) * (1. - 4.*ALFA*ALFA/(1. + GAM)**2)**.5/(2.*GAM*ALFA)
RK = PPI*ALFA
TT1 = TEM * 5*PPI*GAM*(RK*RK - 1.)/(AH1*CRF(NPT)*RK)
WRITE(6,203) II,PPI,TT1
203 CONTINUE
IF (II EQ. 2.) CONTINUE
C 205 II = II*4
PP = PI*PP1
CALL EQLBRM
IF (NP1 EQ. 0.) GO TO 1000
IF (TT1 Eq. 0.) GO TO 860
GAM = GAMMAS(NPT)
CIF (PCRF(NPT) * CRF(NPT) EQ. 0.*W(NPT))
C 207 IF (PCRF(NPT) * GAMMAS(NPT) * DLTVP(NPT))
A1 = KM(NPT)/AM1
RH1 = PPI*AMM/TT1
A11 = 1./PPI + GAM*RH1*DLTV(NPT)
A12 = GAM*RH1*DLTV(NPT)
A21 = 5.*GAM1(RR1*P2=1. - DLTVP(NPT) C (1. + RR1*21) * DLTVP(NPT) - 1.
A22 = 5.*GAM1*DLTV(NPT) * (RR1*P2=1.) * W(NPT) * CRF(NPT)
B1 = 1./PPI1 + GAM * (RR1 = 1.)
B2 = W(NPT) * (HSUM(NPT) = H1(NPT)/R) / TT * 5*GAM1(RR1*RR1=1.)
X1 = XX(Y)
X2 = YY(Z)
DALM = 1.*
TEN = X1
IF (X1 < 0.9) TEN = -TEN
IF (X2 > GT.TEN) TEN = X2
IF (X2 < -GF.TEN) TEN = -X2
IF (X1 > GT.TEN) DALM = 0.5/TEN
PP1 = P1*EXP(X1*DALM)
PP2 = T1*EXP(X2*DALM)
T1 = T1+T1
US = (RR*GAM*TT/V4(NPT))*5
UP = RR1*JS
WRITE(6,10) ITR
10 FORMAT (2H0, 15D9.3) PP1, PP2, X1, X2, US
30 FORMAT (6X, 4HP/P110X, 1H=E20.8/6X, 4HT/T110X, 1H=E20.8/6X, 4HT/RH0/RHDT*160
1015X11=T20.8/6X, 11HDEL LN P/P13X, 1H=E20.8/6X, 11HDEL LN T/T13XDELT=170
2*1H=E20.8/6X, 2HUS*12X, 1H=E20.8)
C
C CONVERGENCE TEST
C
IF (ITR.LT.10 .AND. TEN>GT.5E-04) GO TO 205
RRH0(NPT)=RR1
IF (CP(NPT)<EQ.0.) GO TO 40
G1(NPT) = CP(NPT) /(CP(NPT)-R/AM1)
V4OC(NPT) = UD/(RR*GAM1(NPT)*T1/AM1)**5
GO TO 41
40 GAM1(NPT) = 0.
V4OC(NPT) = 0.
GO TO 150
C
C DERIVATIVES
C
41 WRITE(6,55)
55 FORMAT (17H0, DERIVATIVE OF 13X*4HLN P16X*4HLN TDELT=150
1*16X*2HUD,
B1 = 1./PP1*GAM*RR1
B2 = GAM*RR1**2
X1 = XX(Y)
X2 = YY(Z)
AA = .5* (1.-DLVPT(NPT))
BB = -.5*DLVPT(NPT)
DUD = UD*(AA*X1+BB*X2+1.)
X1 = X1-1.0
RITE(6,8) X1*X2*DUD
81 FORMAT (6X,13HLNIP1 AT T1+HI, 6X, 1H=E3E17.8)
B1 = GAM*RR1
B2 = B1*RR1+M*P(T)*CP(NPT)/(R*TT1)
X1 = XX(Y)
X2 = YY(Z)
DUD = UD*(AA*X1+B1*X2+1.)*X2 = X2-1.
RITE(6,9) X1*X2*DUD
A4 FORMAT (6X, 16HLNIT1 AT P1+HI, 13X, 1H=E3E17.8)
B1 = 0.
B2 = M(NPT)/(R*TT)
X1 = XX(Y)*1000.
X2 = YY(Z)*1000.
DUD = UD*(AA*X1+B1*X2)
WRITE (6,65) A1, X2, D11D
5 FORMAT (6X*20M4) AT T1*P1*M1 =3E17.8)

C 150 K = 0
IF (IPEQ .AND. JT.EQ.0 OR T1.EQ.0) GO TO 530
K = NPT
IF (NPT = 13) GO TO 870

C OUTPUT

840 WRITE (6,65)
5 FORMAT (1H1*42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS)
CALL OUT1

46 FORMAT (134 UNBURNED GAS//)
FMT(4) = FMT13
FMT(5) = FA
FMT(7) = FA
WRITE (6,FMT) FP1*FP(2)*FB*FB*(PUB(J)*J=1*NPT)
FMT(7) = FA
WRITE (6,FMT) FT1*FT(2)*FB*FB*(TUB(J)*J=1*NPT)
WRITE (6,FMT) FH1*FH(2)*FB*FB*(HL(J)*J=1*NPT)
DO 56 J = 1,NPT
V(I) = AM1
SONVEL(I) = RR*GM1(I)*TUB(I)/AM1*2.5
56 CONTINUE

FMT(7) = FA
WRITE (6,FMT) FM1*FM(2)*FM(3)*FA*(V(J)*J=1*NPT)
FMT(7) = FA
WRITE (6,FMT) FP1*FP(2)*FP(3)*FC(4)*(CP(J)*J=1*NPT)
WRITE (6,FMT) FG1*FG(1)*FG(2)*FG(3)*(GM1(J)*J=1,NPT)
FMT(7) = FA
WRITE (6,FMT) FL1*FL(1)*FL(2)*(SONVEL(J)*J=1,NPT)
WRITE (6,6A)

56 FORMAT (122HDETONATION PARAMETERS//)
FMT(7) = FA
DO 70 J = 1,NPT
V(I) = PUB(I)
PUB(I) = PUB(I)/TUB(I)
SONVEL(I) = SONVEL(I)*RRHO(I)
70 CONTINUE
WRITE (6,FMT) FPP*FB*FB*(V(J)*J=1,NPT)
WRITE (6,FMT) FTT*FB*FB*(PCP(J)*J=1,NPT)
DO 73 J = 1,NPT
V(I) = AM1
73 CONTINUE

FMT(7) = FA
WRITE (6,FMT) FM4*FB*FB*(V(J)*J=1,NPT)
WRITE (6,FMT) FRA*FB*FB*(RRHO(J)*J=1,NPT)
WRITE (6,FMT) FMA*FB*FB*(VOC(J)*J=1,NPT)
FMT(7) = FA
WRITE (6,FMT) FU*FL(2)*FL(3)*FL(4)*(SONVEL(J)*J=1,NPT)
EQL = TRUE.
CALL OUT3
865 IF (K.EQ.0) 0 TO 1000
WRITE (6,68)
SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT

DO 890 I = 1, N
EN(I*NPT) = EN(I*K)
890 CONTINUE
WRITE (6,866)
902 CONTINUE
903 CONTINUE
1000 TP = .FALSE.
RETURN
END
SU-Routine SHCK
RETURN
END
SUBROUTINE ROCKET

ROCKET PERFORMANCE

EITHER HPSP OR TPSP IS TRUE

LOGICAL HP*SP*TP*INEBUG*NEW*IONS*MOLES*FROZ*EQL*LOG*HPSP*TPSP

DIMENSION AA(2),BB(2),CC(2)

COMMON/POTNTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
1*GAHMAS(3)*P(26)*T(26)*V(13)*PPP(13)*WM(13)*SDEV(13)*TTT(13)
2*IGYN(13)
COMMON/SPCE/COEF(2,7,150),S(150),EN(150,13),PLN(150),MO(150),
1*DELN(150)*S(150),SUB(150,3),USE(150),TEMP(50,2)
COMMON/HSCP/NN,SUMN,SP,ATOM(3,101),LLMT(15),BO(15),BP(15,2)
1*TEMP(2),THLT,THIN,PP,CSUM,OF,ERAT,FPCT,RR,HSUB,AC(2),AM(2)
2*HP(2),RHO(2),VKTN(2),VPLS(2),NP(2),DATA(22),NAME(15,5)
3*ANUM(15,5),PECT(15),ENTH(15),FAZ(15),RTMP(15),DES(15)
4*HPSP,PWH(15),TLN
COMMON/INDX/INEBUG,CONVE,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPF,NLM
1*NSXMTI,IMAT(10),INTG,NOINIT,TP,NEWR,NSUB,NSUP,INTN,CPCFVR,CPCVEQ
2*IONS,NSR,ART,JSOL,JSOL,JSOL,JSOL,JSOL,JSOL,JSOL,JSOL,JSOL,JSOL
COMMON/PTRF/PCP(26),VNOC(13),TPMT(13),VACI(13),SUBAR(13),SUPAR(13)
1*PERF(13),AEAT(13),CSTR*EQL,FROZ,SSO

NAMELIST/RKTINP/EQL*FROZ,SUBAR,SUPAR,PCP

ITH = 0

210 DO 300 I=1,NP
PCP(I) = 0
SUBAR(I) = 0
300 CONTINUE

TT = 38000
HPSP = TRUE
HP = TRUE
TPSP = FALSE
EQL = TRUE
FROZ = TRUE
READ (5,RKTINP)
IF (TT(I) .EQ. 0.) GO TO 303
TPSP = TRUE
TT = TT(I)
TP = TRUE
HPSP = FALSE
303 IF (PCP(I) .LT. 0.) GO TO 308
DO 305 I=1,NP
X = NP(I)+2
P(K) = P(K+1)
305 CONTINUE
GO TO 311
310 NP = 2
DO 310 I=1,24
IF (I .GT. 2) GO TO 309
IF ((PCP(I) .EQ. 0.) .OR. PCP(I) .EQ. 1.) GO TO 310
310 CONTINUE
309 IF (PCP(I) .EQ. 0.) GO TO 310
NP = NP + 1
P(NP) = P(1)/PCP(I)
310 CONTINUE

311 VSUP = 0
VSUP = 0
DO 320 1=13
IF(SUPAR(I).NE.0.)NSUB=NSUB+1
IF(SUPAR(I).NE.0.)NSUP=NSUP+1
320 CONTINUE

WRITE (6,AKTP) SS0 = 0.
TT=0T=.3

CONT ASSIGNED P

DO 902 IP = 1*NP
PP = P(IP)
CALL EQL9PM
IF(TT*NE.0.) GO TO 333
IF(NPT.EQ.0.) GO TO 100
GO TO 900
333 P(NPT) = P(1)/PP
IF(IP*GT.1) GO TO 195

COMBUSTION CHAMBER

IF = *FALSE*
HP = *FALSE*
SP = *TUS*
SO = SSUM(1)
PCP(2) = (GAMMAS(1)+1.)/2.*GAMMAS(1)/(GAMMAS(1)-1.)
P(2) = P(1)/PCP(2)
TT = 2.*TT/(GAMMAS(1)+1.)
GO TO 900
195 IF(IP*GT.2) GO TO 900

THROAT

IF (ITH+NE.2) GO TO 191
ITH = 0
GAMMAS(2) = 0.
GO TO 900
191 DH = HSUM(1)-HSUM(2)
DHST = DH=GAMMAS(2)*TT*ENN/2.
IF (ITER.GE.3) WRITE(6,923)DHSTAR,HSUM(1),HSUM(2),PCP(2)
923 FORMAT(4E25.8)
DH = DHSTAR/DH
IF(JH*LE.0.*4E-4.OR.ITROT*EQ.0) GO TO 900
IF(JSOL*NE.0) ITH =1
IF(JSOL*EQ.0. AND ITH*EQ.1) ITH=2
IF(ITH*EQ.0) GO TO 192

SPECIAL THROAT INTERPOLATION IF ITH = 2:

DLN1: = .5*TT*ENN/(HSUM(1)-HSUM(2))
A1(ITH) = .5*DLN1*2.*DLN1/ GAMSAS(2)-1.)/GAMMAS(2)
XX = ALOG(PCP(2))
BB(ITH) = 1. /GAMMAS(2)-DLN1-2.*XX*AA(ITH)
CC(ITH) = ENN*TT/(PP* (HSUM(1)-HSUM(2))*5.)
CC(ITH) = ALOG(CC(ITH)) .XX*BB(ITH)*AA(ITH)*XX
IF(ITH*EQ.1) GO TO 192
SB(1) = BB(1)-RR(2)
AA(1) = AA(1)-AA(2)
PCP(2) = (-BB(1)+BB(1)*SB(1)-4.*AA(1)*(CC(1)-CC(2)))*5.)/(2.*AA(1))
1) \[ PCP(2) = \exp(PCP(2)) \]
GO TO 193

192 \[ PCP(2) = \frac{PCP(2)}{(1 + 2 \times \text{DHSTAR}/(\text{ENN} \times \text{TT} \times (\text{GAMMAS}(2) + 1)))} \]

193 \[ P(2) = \frac{P(1)}{PCP(2)} \]
PP = P(2)
ITR01 = ITR01 - 1
CALL EQLRM
IF(ITT = EQ.0) GO TO 1000
GO TO 190

C

900 \( k = 0 \)
IF (*NOT.EQ. *AND. FROZ) GO TO 990
IF(IP.EQ.NP.OR.TT.EQ.0) GO TO 860
K = NPT
IF(NPT = NE.13) GO TO 870
860 CALL RKTOUT
IF((NSUB + NSUP).NE.0) CALL RATIO
IF(K = EQ.0) GO TO 990
WRITE(6,865)
865 FORMAT(1H1)
NPT = 2
870 NPT = NPT + 1
C
SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C
DO 880 I = 1,NS
EN(I+NPT) = EN(I*K);
880 CONTINUE
END
SUBROUTINE RKTOUT

C ROCKET PERFORMANCE PARAMETERS

C LOGICAL EQL*FROZ *TP*HP*SP*HPSP*TPSP*SHOCK

C DIMENSION NV(13)*Z(10*4)

C COMMON/POINTS/4SUM(13)*SSUM(13)*CPR(13)*DLVTP(13)*DLVPT(13)
1 *GAMMAS(13)*P(26)*T(26)*V(13)*PPP(13)*WM(13)*SONVEL(13)*TTT(13)
2 *T0N(13)
C COMMON/SPECIES/OEF(2*7*150)*S(150)*EN(150*13)*ENLN(150)*H0(150)
1 *JELN(150)*A(15*150)*SUR(150*3)*USE(150)*C70750*2
2 COMMON/MISC/ENN*SUM*TT*50*A(3*101)*LLMK(15*150)*B0(15*2)
1 *T1*TMN*THIG*PP*PSUM*F*FORAT*FPCT*R*RS*HE360*AC(2)*AM(2)
2 *HPF(2)*RHO(2)*VMHN(2)*VPLS(2)*WP(2)*DATA(22)*NAME(15*5)
3 *ANUM(15*5)*PCWTT(15)*ENTH(15)*FAZ(15)*TEMP(15)*FOX(15)*DENS(15)
4 *RP*AW(15)*TLN
C COMMON/IN*V/ IDEBUB٬TP٬HP٬SP٬HP*SP*TPSP*DOES*NP*NT*NPT*NLM
1 *NS*KMAT*MAT(101)*IO*2*HOMIT*TP*NEW*NSUB*NSUP*ITN*CPCVFR*CPCVEQ
2 *INNS*NC*NSERT*JSOL*JL1*IC*T*KAC*IJS*JS*VOL*SHOCK
C COMMON/PERF/PCP(26)*JMO(G13)*SPIM(13)*VACI(13)*SUBAR(13)*SUPAR(13)
1 *CPFR(13)*AFAT(13)*CSTR*EQL*FROZ*SS0
C COMMON/OUP/T/FMT(30)*F(4)*FT(4)*FH(4)*FS(4)*FM(4)*TV(4)*FP(4)
1 *FC(4)*FG(4)*FB*FMT(13)*F1*F2*F3*F4*F5*FL(4)*FTM(4)*TFA1*FA2
2 *F1*FC1*FN(4)*FR(4)*F4*FI(4)*FMT2*FO
C EQUIVALENCE (V*NV)*(Z;H0)

C DATA EXIT/4EXIT/

C IF(EQL) WRITE (6,37)

37 FORMAT(1H1,26X,84THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRKRT=32
1UM COMPOSITION DURING EXPANSION //)
IF(*NOT.EQL) WRITE(6,38)
38 FORMAT(1H1,26X,78THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CRRT=25.
1UM COMPOSITION DURING EXPANSION //)
C IF (TPSP) WRITE (6,737)

737 FORMAT(52X,28AN AN ASSIGNED TEMPERATURE
V(1) = PPP(1)*14.696006
WRITE (6,40) V(1)
40 FORMAT(5H PC = *F8.1*SH PSIA
CALL OUT1
NEX = NPT - 2
DO 862 I = 1*NEX
862 VI = EXIT
WRITE(6,44A) (V(I),T=1*NEX)
48 FORMAT(1H0,16X,16CHAMBER THROAT *11(5X,A4))

C PRESSURE RATIO:

C F41(4) = FMT(6)
CALL VARFMT (PCP*NPT)
WRITE (6,FMT) FR1*FB*FB*FB*FB*FB*FB*PCP(J),J=1*NPT)
CALL OUT2

C AVG = 9.80655
DO 202 K=2,NPT
SPH(K) = (2.*RR*(HSUM(1)*4SUM(K)))*S/AGV
C
C AW (A/W) IN UNITS OF SEC/ATM
C
AW = RR*TTT(K)/(PPP(K)*WH(K)*SPIN(K)*AGV*2)
IF(K*NE.2) GO TO 200
W=AW
CSTR=32.174*P(i)*AWT
200 AEAT(K)=AW/AWT
VACI(K)=SPIN(K)*PPP(K)*AW
IF (SONVEL(K).*NE.0.) VMOC(K)=SPIN(K)*AGV/SONVEL(K)
NV(K)= CSTR * 5
212 CONTINUE
C
MACH NUMBER

VMOC(1)=0.
IF (GAMMAS(2) .EQ. 0.) VMOC(2)=0.
FMT(7) = F3
WRITE(6,FMT) (FN(I)*I=1,4);(VMOC(J)*J=1,NPT)
WRITE (6*208)
208 FORMAT (1H )
C
C FMT(4) = FMT0X
FMT(5) = FMT13
FMT(6) = FMT19
FMT(7) = FB
WRITE (6*FMT) (FR(I)*I=1,4);(NV(J)*J=2,NPT)
C
CF = THRUST COEFFICIENT

FMT(6) = FMT(8)
FMT(7) = F3

DO 212 I=2,NPT
212 V(I)=32.174*SPIN(I)/CSTR
WRITE(6,FMT) (FA1*FB1*FB2*FB3*V(J)*J=2,NPT)
C
AREA RATIO

CALL VARFMT (AEAT,NPT)
FMT(5) = FB
WRITE(6,FMT) FA1*FA2*FB1*FB2*(AEAT(J)*J=2,NPT)
C
VACUUM IMPULSE

FMT(5) = FMT13
FMT(7) = FI
WRITE(6,FMT) (FA(I)*I=1,4);(VACI(J)*J=2,NPT)
C
SPECIFIC IMPULSE

WRITE(6,FMT) (FI(I)*I=1,4);(SPIN(J)*J=2,NPT)
WRITE (6*208)
FMT(4) = FR
FMT(5) = FMT13
FMT(7) = FS
IF(EQL) GO TO 312
WRITE (6*310)
310 FORMAT (15HOMOLE FRACTIONS //)
C MOLE FRACTIONS = FROZEN

C
DO 309 I=1,NPT
DATA(I) = 0.
DO 308 K=1,NS
DATA(I) = DATA(I) + EN(K,I)
308 CONTINUE
309 CONTINUE
LINE = 0
DO 430 K = 1,NS
V(LINE+1) = EN(K+1)/DATA(I)
IF (V(LINE+1) .LT. (5.0E-6)) GO TO 424
LINE = LINE+1
Z(LINE+1) = SUR(K+1)
Z(LINE+2) = SUR(K+2)
Z(LINE+3) = SUR(K+3)
Z(LINE+4) = V(LINE)
424 IF (LINE .NE. 40 .AND. K .NE. NS) GO TO 430
IF (LINE.EQ.0) GO TO 312
WRITE (6,426) (Z(LN+1),Z(LN+2),Z(LN+3),Z(LN+4),LN=1,LINE)
426 FORMAT (1H4(3A4,F9.5,1X))
LINE = 0
430 CONTINUE
312 CALL OUT3
310 RETURN
END
SUBROUTINE RATIO

(USED FOR AREA RATIO INTERPOLATION ONLY)

DOUBLE PRECISION G,X
LOGICAL EQ1, FROZ, TPPS

DIMENSION PER(2,2), AI(13), ACP(13), AT(13), AMT(13), RP(2), NV(13)
1, RP(2)

COMMON POINTS/NSUM(13), SSUM(13), CPR(13), DLVT(13), DVTP(13)
1, GMAPS(13), P(26), T(26), V(13), PPL(13), WMT(13), SVOLVE(13), TTT(13)
2, TOT(13)

COMMON SEPEC/COEF(2,7,150), S(150), EN(150,13), EALN(150), MC(150)
1, DELN(150), A(15,150), SUR(150,3), USE(150), TEM(50,2)

COMMON/NSIC/EN1, SUM, TTT, S(0), ATOC(13), LCTT(15), G0(15), R0P(15,2)
1, TV(1), TMD, TMIH, P(1), CPSUM, ODF, EQRAT, FPCF, RRT, RSPS, A(2), AM(2)
2, H(2), R(1), WTN(2), VPLS(2), N(2), DATA(22), NAME(15,5)

3, ANUM(15,5), PECNT(15), ENTH(15), FAZ(15), RTEMP(15), FOX(15), DENS(15)
4, R(0), RWM(15,15), TLN

COMMON /DOUBLE/ G10, G2, X(20)

COMMON INDX, IDST, TP, HP, SP, THPS, HPS, THP, NPLE, NP, NT, NPT, NLM
1, NLS, KMAT, MAT(10,10), IO2, NOMIT, TP2, NMS, SNS, SUP, TN, CPCVF, CPCVEQ
2, IN, NTS, NTS(13), JSOL, JUIO, KASE, NREA, IC, JSI, VOL, SHOCK

COMMON PER/HPCP(26), VMC(13), SIM(13), VAC(13), SUBAR(13), SUPAR(13)
1, CRF(13), AEAT(13), CRST1, EQL, FROZ, FROZ

COMMON DUW/FTM(30), FP(4), FT(4), FH(4), FS(4), FN(4), NV(4), FG(4)
1, FC(4), FG(4), FB, FMT13, F1, F2, F3, F4, F5, FL(4), FNTI9, FAI, F4
2, FFR, FCI, FN(4), FR(4), FA(4), FI(4), FMT9X, F0

C EQUIVALENCE (V,NV)

NBM0 = NPT-2
DO 22 J3=3,NPT
IF(PCP(J),GT,PCT(2)) GO TO 30
22 CONTINUE

GO TO 31

30 NAL0=F3=J

31 DO 1200 ISOMIC=1,2

L1 = 1
IF (1SONIC, EQ.2) GO TO 34
IF (NSUB, EQ.0) GO TO 1200
VAR = NSUB
GO TO 36

34 IF (NSUB, EQ.0) GO TO 1200
VAR = NSUB

36 DO 1100 I=1,NAR
IF (1SONIC, EQ.2) GO TO 40
IF (NSYLO, LE.1) GO TO 1100
<2>N=0
DO 38 J=4,K
V(LL) = SUBARD
IF (V(LL),GE,AEAT(J)) GO TO 56
38 CONTINUE

GO TO 56

40 IF (NPT=1, NAL0=LE.3) GO TO 1100
V(LL) = SUPARD
K=4+NBL0
DO 42 J=K,NPT
IF (V(LL),LE,AEAT(J)) GO TO 56
42 CONTINUE
IF (V(LL) \* GE. AEAT(J) \* 3.) GO TO 85
56
KJ = J - 1
K = KJ
DO 64 JJ = 1, 2
IF (CPR(K), NE, 0.) GO TO 63
WRITE(66, 62) K
62 FORMAT (I10) ! NO CAN NOT USE POINT I 2 \* 3X \* 4HC P = 0)
GO TO 85
63 PER(JJ + 1) = 1. / (CPR(K) \* WM(K))
IF (EQL) PER(JJJ1) = PER(JJ1) \* DLVT(K)
PER(JJJ = TTT(K/I2) \* WM(K) \* (HSUM(1) - HSUM(K)))
RP(JJ) = J / (1. / GAMMAS(K) - PER(JJ + 1))
IF (EQL) RP(JJ) = 1. \* DLVT(K) \* (1. \* DLVT(K) \* PER(JJ1))
K = KJ + 1
64 CONTINUE
AMWT(LL) = WM(1)
CALL SET (PCP(KJ) \* RP(1) \* AEAT(KJ), V(LL), APCP(LL))
CALL SET (TTT(KJ) \* PER(1), PCP(KJ) \* APCP(LL) \* AT(LL))
IF (EQL) CALL SET (WM(KJ) \* RPP(1) \* PCP(KJ) \* APCP(LL) \* AMWT(LL))
K = KJ
DO 74 JJ = 1, 2
6(G(jj + 7) = 5SPI(K)** 2
6(G(jj + 2, 7) = 2 \* 6(G(JJ, 7) \* PER(JJ, 2))
6(G(jj, 7) = (1. \* GAMMAS(K)) \* G(JJ2, 7)
G(jj, 1) = 1. 0
G(jj, 2, 1) = 0
G(jj, 4, 1) = 0
G(JJJ2) = ALOGP(CP(K))
G(JJ + 2, 1) = 1. 0
G(JJ + 2, 2) = 0
DO 70 M = 3, 6
6(G(jj + M) = G(JJ2, M)**(M - 1)
G(jj + 2,M) = G(JJ2, M) \* (M - 2)** FLAT(M - 1)
G(jj + 4, M) = G(JJ2, M) \* (M - 2)** FLAT(M - 1)
70 CONTINUE
K = KJ + 1
74 CONTINUE
IMAT = 6
CALL MSGAUD
AI(LL) = X (1)
DO 84 JJ = 2, 6
AI(LL) = AI(LL) \* X (JJ) \* ALOGP(APCP(LL)) \* (JJ - 1)
84 CONTINUE
IF (AI(LL) \* LE. 0.) GO TO 85
AI(LL) = AI(LL)**.5
GO TO 86
85 LL = LL - 1
86 IF (LL \* GE. 13. OR. 1 \* GE. NAR) GO TO 90
LL = LL - 1
GO TO 1100
IF (TPSP) WRITE (6,99)
99 FORMAT (52X,2AHAT AN ASSIGNED TEMPERATURE
WRITE (6,91)
91 FORMAT (52X,2AHFOR ASSIGNED AREA RATIOS //)
PC= P(1)*1.4*69606
WRITE(6,101)PC
101 FORMAT(5H PC = *F8.1*SH PSIA)
CALL OUT1
IF(ISONIC.EQ.1) WRITE(6,33)
33 FORMAT(18H0SUBSONIC FLOW //)
IF (ISONIC.EQ.2) WRITE (6,35)
35 FORMAT(18H0SUPERSONIC FLOW //)
C AREA RATIO
C FMT(6)= FMT(8)
FMT(4)= FMT(6)
CALL VARFMT (V*NPT)
WRITE(6,FMT) F1*FA2*FB*FR; (V(M)*M=1,LL)
C VACUUM SPECIFIC IMPULSE AND SPECIFIC IMPULSE
DO 93 M=1,LL
V(M)=AI(M)*CSTR*V(M)/(32*174* APCP(M))
93 CONTINUE
FMT(4)= FMT13
FMT(5)= F8
FMT(7)= F1
WRITE(6,FMT) (FA(N)*N=1,4) * (V(M)*M=1,LL)
WRITE(6,FMT) (FI(N)*N=1,4) * (AI(M)*M=1,LL)
C C
C FMT(5)= FMT19
DO 94 M=1,LL
NV(M)=CSTR * 0.5
94 CONTINUE
WRITE(6,FMT) (FR(N)*N=1,4) * (NV(M)*M=1,LL)
C CF - THRUST COEFFICIENT
C DO 95 M=1,LL
V(M)=AI(M)*32*174/CSTR
95 CONTINUE
FMT(5)= FA
FMT(7)= F3
WRITE(6,FMT) FC1*FR*FB*FB; (V(M)*M=1,LL)
WRITE(6,96)
96 FORMAT(1H 1)
C PRESSURE RATIO
C FMT(4)= FMT(6)
CALL VARFMT (APCP*NPT)
C CALL VARFMT (APCP*NPT)
C PRESSURE
WRITE(6,FMT) FR1*FR2*FR3*(APCP(M)*M=1*LL)
10 DO 98 M=1*LL
98 CONTINUE
CALL VariFMT(V,NPT)
WRITE(6,FMT) (FP(N),N=1,4) , (V(M)*M=1*LL)
WRITE(6,FMT) FR1*FR2*FR3*(APCP(M)*M=1*LL)
20 CALL VariFMT(V,NPT)
WRITE(6,FMT) (FP(N),N=1,4) , (V(M)*M=1*LL)
30 CONTINUE
WRITE(6,FMT) FR1*FR2*FR3*(APCP(M)*M=1*LL)
40 CALL VariFMT(V,NPT)
WRITE(6,FMT) (FP(N),N=1,4) , (V(M)*M=1*LL)
50 CONTINUE
WRITE(6,FMT) FR1*FR2*FR3*(APCP(M)*M=1*LL)
60 CALL VariFMT(V,NPT)
WRITE(6,FMT) (FP(N),N=1,4) , (V(M)*M=1*LL)
70 CONTINUE
WRITE(6,FMT) FR1*FR2*FR3*(APCP(M)*M=1*LL)
80 CALL VariFMT(V,NPT)
WRITE(6,FMT) (FP(N),N=1,4) , (V(M)*M=1*LL)
90 CONTINUE
WRITE(6,FMT) FR1*FR2*FR3*(APCP(M)*M=1*LL)
100 CALL VariFMT(V,NPT)
WRITE(6,FMT) (FP(N),N=1,4) , (V(M)*M=1*LL)
110 CONTINUE
 WRITE(6,FMT) FR1*FR2*FR3*(APCP(M)*M=1*LL)
120 CONTINUE
RETURN
END
SUBROUTINE SET(ONE, TWO, THREE, ARG, HAL)

(USED FOR AREA RATIO INTERPOLATION ONLY)
SETS UP ALL 4 BY 5 MATRICES

DOUBLE PRECISION &*ANS*G*X

DIMENSION ANS(6), ONE(2), TWO(2), THREE(2), A(20, 21)

COMMON /DOUBLE/ G(20, 21), X(20)
COMMON/INJ/ IDEBUG, CONVG, TP, HP, SP, HPSP, TPSP, MOLES, NP, NT, NPT, NLM
1 *NS*XMAT, IMAT, IQ2, NOMIT, TP, NNEW, NSUB, NSUP, IT4, CPCVPR, CPCVEQ
2 *IONS, NC, NSETR, JSOL, JLIQ, KASE, NREAC, IG, JS1, VOL, SHOCK

EQUIVALENCE (&*GA*) (&*XANS*)

DO A J=1, 2
A(J, 5) = ALOG(ONE(J))
A(J, 2, 5) = TWO(J)
A(J, 2, 2) = ALOG(THREE(J))
END CONTINUE

DO 1 I=1, 2
A(I, 1) = 1.0
A(I, 2, 1) = 0.0
A(I, 2, 2) = 1.0
END CONTINUE

A(I, J+1) = A(I, J) = I
A(I, J+1) = A(I, 2) = J
END CONTINUE

CALL MGUSD
HAL = ANS(1)
SUM = ALOG(ARG)
DO 10 J=1, 3
HAL = HAL + SUM(J, ANS(J+1))
END CONTINUE

HAL = EXP(HAL)
RETURN

END
SUBROUTINE FROZEN

LOGICAL EOL,FROZ,CONVG

COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVT(13),DLVTP(13)
1,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2,TOTN(13)

COMMON/SPACING/DO(27),S(150),EN(150),LEN(150),HO(150)
1,DELN(150),A(150),SUB(150),IUSE(150),TEMP(50,2)

COMMON/MISC/SSUM,TT,SO,ATOM(3,101),LLMT(15),S(150),BOP(15,2)
1,TM,TLMT,SK,TS,TH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBC,AC(2),AM(2)
2,MP(2),RHO(2),VNH(2),VPLS(2),NP(2),DATA(22),NAME(15,5)
3,ANUM(15,5),PECKT(15),ENTH(15),FAZ(15),RTHP(15),F0Z(15),SENS(15)
4,RHOP,RMX(15),T,COMMON/INDX/INDEB(2),CONVG,TP,NP,SP,HPSP,TPSP,MLES,NS,NT,NPT,NLM
1,NS,NMAT,IMAT,IDQ,HOMIT,IP,NSW,NSUR,NSUP,TIN,CPVF,CPVEQ
2,IONS,NC,NSERTS,JSL,LIQ,KASE,REAC,IC,JSI,VO,SHOCK

COMMON/PERF/CP(26),VMOC(13),SHVH(13),VACI(13),SUBAR(13),SUPAR(13)
1,CPRF(13),AEAT(13),CSTR,EOL,FROZ,SSG

COMMON/OUTF/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),VO(4)
1,FC(4),FG(4),FB,FM(13),F,FF(4),FV(4),FD(4)
2,FR1,FC1,FM(13),FR(4),FA(4),FI(4),M9T8,F0

45 CONVG = .FALSE.
46 PCPLN= ALG(4,PPC(NPT))
47 SG = SS, CPCLN,WM(1)
48 SUMH = 0.

S1 TT=EXP(TLN)
51 SUMS=0.
52 JSI = 1
53 VPT = 1
54 CALL CPHS
55 VPT = NNN
56 DO 50 J=1,NS
57 IF(EN(J),EQ,0.) GO TO 60
58 SUMS = SUMS + S(J,EN(J))
59 IF(CONV) SUMH=SUMH+H(J)*EN(J)
60 CONTINUE
61 IF (CONVG) GO TO 81
62 DLNT=SUMS=50/CPSUM
63 TNL=TN-DLNT
64 IF((DLNLT.LT.0.) DLNT=DLN)
65 IF((NLNLT.LT.5 E=4) CONVG=.TRUE.
66 GO TO 51
67 A1 TTT(NPT)= TT
THROAT CALCULATIONS

\[ DH = \text{SSUM}(1) - \text{SSUM}(2) \]
\[ DHSTAR = DH - (\text{GAMMAS}(2) \times TT/(2 \times WH(1))) \]
\[ DH = DHSTAR/DH \]
IF \((DH < 0.0)\) \(DH = -DH\)
IF \((DH \geq 0.0)\) \(DH > 0.0\)
GO TO 90

PCP(2) = PCP(2)/(1.0 + 2.0 \times DHSTAR \times WH(1)/(TT \times \text{GAMMAS}(2) - 1.0))

ITROT = ITROT - 1
GO TO 45

90 WM(NPT) = WM(1)
PP(NPT) = P(IP)
CP(NPT) = CPSUM

IF (TT > 0.0) GO TO 903
IF INC > EQ(0) GO TO 700
INC = 0
GO 901 = 1
IF (IUSE(1) < EQ(0) OR IUSE(1) = EQ(1000)) GO TO 90
INC = INC + 1
IF (EN(1) > EQ(0)) GO TO 901
IF (TT > 0.0) GO TO 1000
IF \((\text{TEMP}(\text{INC} + 1) = 50.0) OR (\text{TT} < \text{TEMP}(\text{INC} + 2) = 50.0)\) GO TO 903
901 CONTINUE

700 IF (IP = EQ(0) OR IP = EQ(1) OR IP = EQ(2)) GO TO 863
K = NPT
IF (NPT = NE = 13) GO TO 870
GO TO 863

963 CALL RTOUT
IF (NSUSUP = NE = 0) CALL RATIO
865 IF (K = EQ(0) OR K = EQ(1)) GO TO 1000
K = 2
870 NPT = NPT + 1
962 CONTINUE
1000 RETURN
END
### Table: DIMENSION ATOM(3*50)

<table>
<thead>
<tr>
<th>ATOM</th>
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<th>Y</th>
<th>Z</th>
<th>ELEMENT</th>
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### Table: ATOMIC SYMBOLS, WEIGHTS, AND VALENCES

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### Table: BLOCK DATA

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### Table: EQUIVALENCE (ATOM(1*52) + ATBM)

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### Table: INFORMATION USED IN VARIABLE OUTPUT FORMAT

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</table>
DATA  
1. FT/4HT, D@4HEG K@4H  @2H /FH/4HH, C@4HAL/5@2H  @1H /  
2. FS/4HS, C@4HAL/(@4HG) (K+2H) /FH/4HM, M@4HOL @2HT  @1H /  
3. FV/4H(DLV/4H/DLP/4H)T @2H /FD/4H(DLV/4F/DLT/2H)T @1H /  
4. FC/4MC/4HCAL/4H(G) (@2H) /FG/4HGM/4HA (S+2H) @1H /  
5. FL/4HSON @4HVEL, @4HM/SE+2HC /  

INFORMATION USE IN PERFORMANCE OUTPUT  
DATA  
1. FT/4HC/P/4FC/P/4HPC/P@4HC/P  
2. FR/4HC/4HC/P/4HPC/P/4HC/P/4HPC/P  
3. FL/4HC/P/4HPC/P/4HC/P/4HPC/P  
4. FA/4HPC/P/4HC/P/4HPC/P  
5. FA/4HPC/P/4HC/P/4HPC/P  

END
APPENDIX VII - LISTING OF THERMO DATA