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MODIFIED NASA-LEWIS CHEMICAL EQUILIBRIUM CODE FOR MHD APPLICATIONS

by

R. A. Sacks, H. K. Geyer, S. J. Grammel, and E. D. Doss

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CONTENTS

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ABSTRACT

A substantially modified version of the NASA-Lewis Chemical Equilibrium Code (1) has recently been developed. The modifications were designed to extend the power and convenience of the Code as a tool for performing combustor analysis for MHD systems studies. This report describes the effect of the programming details from a user point of view, but does not describe the Code in detail.

I. INTRODUCTION

The NASA-Lewis Chemical Equilbrium Code [1] had gained wide acceptance as a valuable and accurate tool for computing thermodynamic properties and chemical equilibrium compositions. In a companion publication [2], two of the authors have described a preprocessor program (GPSAP) written to facilitate general systems analysis studies. By adapting the NASA code to the format that GPSAP requires for component models, the very powerful systems analysis capabilities are obtained (e.g., execution time parameter alterations, automated sensitivity studies, and optimization features).

Several additional capabilities were also added to the new code, to implement or simplify combustor studies, especially as related to MHD applications. These new features include:

1) a routine for computing the electrical properties of the equilibrium mixture,

2) a shorthand data input option for treating standard hydrocarbon fuels,

3) a facility for incorporating heat losses (as a fraction of thermal input) into the NASA HP mode computations, and

4) a standard printed summary of equilibrium thermodynamic properties.

Section II describes the modifications that have been made. Section III is a users guide, detailing the input data and giving information necessary for efficient systems studies. Two examples, both demonstrating the power of the modified code and illustrating its use are presented in Section IV. Throughout, it is assumed that the reader is familiar with both the original version of the NASA code and the fundamentals of GPSAP usage.

II. CODE MODIFICATIONS

A. GPSAP Compatibility

As described in Ref. 2, GPSAP requires certain standard features from the component models. Specifically, it is necessary that the data input, calculational, and data output modules be clearly separated entities, each with its own entry point, and that there are appropriate facilities for communicating data between the main program and the calculational block.

Although it is quite generally possible to write PL/1 drivers properly modularized for FORTRAN models, the coupling is most easily accomplished with PL/1 models. The NASA code, as originally written, did not permit alteration of the input data at execution time. The most straightforward approach to remedying this situation was to translate into PL/1 the routines for data input and reduction, output, and the calculational driver, and to rearrange the program logic according to GPSAP requirements. In doing so, the rocket, detonation, and constant volume equilibrium modes were discarded for the sake of execution efficiency. Aside from eliminating these options, the equilibrium calculations (EQLBRM, MATRIX, GAUSS, and CPHS) were left unaltered in FORTRAN.

The three PL/1 entry points to the new version are,

NASAIN,
NASA,
NASAOUT.

NASAIN simply reads the input data from file CARDIN and stores it. NASA performs any desired alterations to the input, reduces the resulting set of data to array form, calls EQLBRM repeatedly to perform the requested tasks, and, if instructed, prints various amounts of intermediate output. NASAOUT prints the summary of thermodynamic and electrical properties and, if instructed, stores the same on disk file FITDAT for post processing.

As in all GPSAP modes, the different entry points are now completely independent. Thus, from a single call to NASAIN, NASA can be (and typically is) called repeatedly, the input data being altered each time from MAIN. The power of the approach derives from the fact that those input data alterations to one NASA call can (and typically do) derive from the results of a previous call. Thus, parameter optimizations may be performed in a single computer job. It has been extensively verified that, for a given set of input data, the answers obtained with the new code are identical to those obtained previously.

B. Electrical Conductivity Procedure

1. Model Description

The plasma electrical conductivity and mobility are computed by use of the algorithm of Demetriades and Argyropoulos [3]. This method calculates the electrical conductivity, using Grad's 13-moment approximation to derive a generalized Ohm's law for a multicomponent plasma. The electrical properties of the plasma are obtained in two successive approximations that are equivalent to the first and second approximations in the expansion of Sonine polynomials in the Chapman-Enskog approach.

In this method, the coefficients of Ohm's law (electrical properties of plasma) are computed if three electron-neutral parameters are known as functions of electron temperature [4]: The effective collision cross section for momentum transfer, Q_{ek}, and the two weighting factors, $A_{ek}^{(2)}$ and $A_{ek}^{(5)}$, that characterize the electron-neutral interaction.

The equations used in the calculation of the electrical properties of plasma that are required in Ohm's law are as follows:

Ohm's law: $E + U \times B = \left(\frac{1}{\sigma}\right) J + \chi J \times B$

where the coefficients, σ and χ, are given by

$$\sigma_o = e^2 n_e/m_e \nu t$$

$$\sigma = \sigma_o/(1-\Delta)$$

$$\chi = (e\, n_e)^{-1}$$

where

$$\nu t \equiv \sum_{k\neq e} \tau_{e,k}^{-1}$$

$$\tau_{e,k}^{-1} \equiv \frac{4}{3} n_k (8k\, T_e/\pi m_e)^{1/2} Q_{ek}$$

$$\Delta \equiv \frac{5}{2} \nu_o^2 \tau_e^*/\nu_t$$

$$\nu_o \equiv \sum_{k\neq e} A_{ek}^{(2)} \tau_{e,k}^{-1}$$

$$(\tau_e^*)^{-1} \equiv \frac{2}{5}\left[1 - (2\ \ell n\ \Lambda_{ee})^{-1}\right]\tau_{ee}^{-1} + \sum_{k\neq e} A_{ek}^{(5)}\ \tau_{e,k}^{-1}$$

$$\Lambda_{ee} \equiv 3\lambda\ (4\pi\varepsilon_o/e^2)\ kT$$

$$\lambda^{-2} = \frac{1}{\varepsilon_o} \Sigma_s \frac{n_s\ e_s^2}{k\ T_s}$$

or $\Lambda_{ee} = 8.7592 \cdot 10^6\ T_e^{3/2}/n_e^{1/2}$

These equations are the ones used in Ref. 3. However, in Ohm's law, the effective electric field term resulting from electron temperature and pressure gradients is neglected. Also, the effect of magnetic field on the Hall field coefficient (χ) is neglected; it will be discussed later.

2. Input Data

In the computation of the electrical properties of the plasma, the following species are considered: OH, Cs, Ar, CO, CO_2, N_2, O_2, H_2O, NO, KOH, SO_2, K, and e (electrons). However, the NASA code considered all the possible species for the particular fuel used. The momentum cross sections, Q's, and the weighting factors, $A^{(2)}$'s and $A^{(5)}$'s, for the specie considered are tabulated as functions of plasma temperature and are given in Table I. The values follow closely the data given by Spencer and Phelps.[5]. However, these data are subject to change should new experimental results become available.

For the calculation of the electrical properties of plasma at other temperatures than those given in the table, linear interpolation is used.

Table 1

Q's, A(2)'s and A(5)'s
(as functions of temperature from 1700 to 3000K)

OH

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
87.00, 82.19, 77.90, 74.05, 70.58, 67.42, 64.54,
61.91, 59.48, 57.25, 55.18, 53.26, 51.48, 49.81,
-.1981,-.1969,-.1958,-.1948,-.1939,-.1930,-.1922,
-.1914,-.1908,-.1901,-.1895,-.1889,-.1883,-.1878,
.921, .920, .920, .920, .919, .919, .918,
.918, .917, .917, .917, .916, .916, .916,

Cs

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
685.48, 645.31, 607.81, 572.99, 540.78, 511.07, 483.71,
458.56, 435.45, 414.24, 394.77, 376.91, 360.50, 345.44,
-.2116, -.2334, -.2520, -.2677, -.2806, -.2909, -.2989,
-.3046, -.308, -.3100, -.3101, -.3085, -.3055, -.3012,
.501, .539, .582, .626, .673, .720, .768,
.815, .862, .907, .951, .994, 1.034, 1.073,

Ar

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
.494, .526, .560, .596, .632, .669, .707,
.745, .783, .821, .860, .899, .937, .976,
.6356, .6574, .6723, .6822, .6882, .6913, .6924,
.6919, .6904, .6880, .6851, .6819, .6784, .6749,
3.085, 3.062, 3.033, 3.000, 2.965, 2.930, 2.896,
2.863, 2.832, 2.803, 2.775, 2.750, 2.727, 2.705,

CO

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
13.050, 13.360, 13.669, 13.979, 14.290, 14.601, 14.911,
15.219, 15.523, 15.823, 16.117, 16.403, 16.680, 16.947,
.3617, .3668, .3722, .3777, .3823, .3872, .3908,
.3933, .3948, .3951, .3943, .3924, .3894, .3855,
1.771, 1.800, 1.230, 1.840, 1.850, 1.851, 1.844,
1.829, 1.807, 1.779, 1.746, 1.708, 1.668, 1.626,

CO2

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
19.15, 18.13, 17.22, 16.39, 15.64, 14.96, 14.34,
13.77, 13.25, 12.77, 12.33, 11.92, 11.55, 11.20,
-.1802, -.1823, -.1836, -.1841, -.1840, -.1831, -.1816,
-.1796, -.1769, -.1738, -.1700, -.1658, -.1610, -.1558,
.857, .870, .883, .897, .911, .926, .942,
.957, .974, .992, 1.010, 1.029, 1.049, 1.070,

Table 1, Cont'd

N2

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.F2, 30.E2,
9.080, 9.178, 9.270, 9.358, 9.445, 9.532, 9.620,
9.710, 9.804, 9.903, 10.007, 10.115, 10.229, 10.349,
.2757, .2741, .2737, .2747, .2769, .2804, .2852,
.2911, .2980, .3058, .3143, .3234, .3330, .3427,
1.428, 1.444, 1.467, 1.495, 1.529, 1.568, 1.611,
1.657, 1.705, 1.753, 1.801, 1.847, 1.891, 1.931,

O2

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
5.624, 5.696, 5.765, 5.832, 5.896, 5.958, 6.018,
6.075, 6.129, 6.181, 6.231, 6.278, 6.322, 6.364,
.2896, .2896, .2897, .2898, .2898, .2895, .2890,
.2881, .2869, .2855, .2837, .2816, .2793, .2768,
1.498, 1.501, 1.502, 1.501, 1.496, 1.490, 1.482,
1.472, 1.460, 1.447, 1.433, 1.419, 1.404, 1.388,

H2O

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
108.532, 102.550, 97.229, 92.443, 88.120, 84.197, 80.620,
77.344, 74.333, 71.555, 68.985, 66.598, 64.377, 62.305,
-.1968, -.1955, -.1942, -.1931, -.1921, -.1911, -.1903,
-.1895, -.1887, -.1881, -.1874, -.1869, -.1863, -.1859,
.923, .923, .922, .922, .921, .920, .919,
.919, .918, .917, .916, .916, .915, .915,

NO

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.F2, 30.E2,
16.592, 17.05, 17.43, 17.735, 17.97, 18.15, 18.28,
18.369, 18.42, 18.44, 18.43, 18.39, 18.34, 18.27,
.4080, .3766, .3478, .3212, .2969, .2745, .2539,
.2351, .2177, .2017, .1869, .1734, .1608, .1493,
1.269, 1.19, 1.124, 1.071, 1.027, .991, .962,
.938, .919, .904, .892, .883, .876, .871,

KOH

17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
620.30, 585.90, 555.12, 527.42, 502.37, 479.59, 458.79,
439.72, 433.17, 405.98, 390.97, 377.03, 364.05, 351.93,
-.1994, -.1993, -.1922, -.1990, -.1990, -.1990, -.1990,
-.1990, -.1991, -.1991, -.1992, -.1993, -.1994, -.1995,
.903, .903, .902, .901, .901, .900, .900,
.899, .898, .898, .898, .897, .897, .897,

SQ2

```
17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
84.93,  80.25,  76.08,  72.33,  68.95,  65.88,  63.08,
60.51,  58.15,  55.98,  53.97,  52.098, 50.359, 48.736,
-.197,  -.1957, -.1945, -.1934, -.1923, -.1914, -.1905,
-.1897, -.1890, -.1884, -.1878, -.1872, -.1867, -.1863,
.923,   .923,   .922,   .922,   .921,   .920,   .919,
.918,   .917,   .916,   .916,   .915,   .915,   .914,
```

K

```
17.E2, 18.E2, 19.E2, 20.E2, 21.E2, 22.E2, 23.E2,
24.E2, 25.E2, 26.E2, 27.E2, 28.E2, 29.E2, 30.E2,
300.143, 284.791, 271.027, 258.609, 247.345, 237.076, 227.674,
219.029, 211.053, 203.669, 196.814, 190.432, 184.477, 1[illegible]06,
-.1679,  -.1669,  -.1661,  -.1654,  -.1648,  -.1644,  -.1[illegible]40,
-.1636,  -.1633,  -.1630,  -.1627,  -.1624,  -.1620,  -.1616,
.921,    .919,    .917,    .915,    .914,    .912,    .911,
.911,    .911,    .911,    .912,    .913,    .915,    .917,
```

For electron-ion interaction, the values for Q_{ei}, $A_{ei}^{(2)}$, and $A_{ei}^{(5)}$ are calculated as follows:

$$Q_{ei} \equiv \frac{\pi}{2} \left(\frac{e^2}{4\pi\varepsilon_o} \frac{1}{kT_e}\right)^2 \ln \Lambda \qquad \text{(Ref.6)}$$

or $$Q_{ei} = \frac{4.387 \cdot 10^{-10}}{Te^2} \ln \Lambda$$

$$\left.\begin{aligned} A_{ei}^{(2)} &= -0.6 \\ A_{ei}^{(5)} &= 1.3 \end{aligned}\right\} \text{(Ref. 4, for coulomb interaction)}$$

3. Calculation of the Hall Parameter, β

According to the algorithm adapted [4] for the calculation of electrical properties of plasma, the Hall parameter, β, is

$$\beta = \chi \cdot \sigma \cdot B,$$

where B is the magnetic field.

However, χ is also a function of the magnetic field, where [4]

$$\chi = (en_e)^{-1} \left(1 + [\Delta\tau_e^* \nu_t/(1 + \omega_e^2\tau_e^{*2})]\right) ,$$

and

$$\omega_e = \frac{eB}{m_e} .$$

The above equation for χ can be simplified, after substituting for the variables Δ, τ_e^*, and ω_e, and the equation becomes:

$$\chi = (e\, n_e)^{-1} \frac{C_1 + B^2}{C_o + B^2},$$

where

$$C_o = (m_e/e)^2 (\tau_e^*)^{-2} \text{ and}$$

$$C_1 = C_o + \frac{5}{2} \left(\frac{m_e}{e}\right)^2 \nu_o^2.$$

The influence of the magnetic field on the Hall coefficient, χ, has been investigated for zero magnetic field, up to 20 T for a typical MHD plasma composition. The results are presented in Fig. II-1. These results indicate that there is a very weak dependence of the coefficient, χ, on the magnetic field. This is a result of C_o and C_1 being very small and, also, almost equal.

Based on these results, the effect of the magnetic field on the Hall coefficient, χ, is neglected, and the equation for the computation of χ is reduced to

$$\chi = (en_e)^{-1}.$$

4. Error Bounds on Electrical Conductivity

For the same method used to compute the electrical conductivity of the

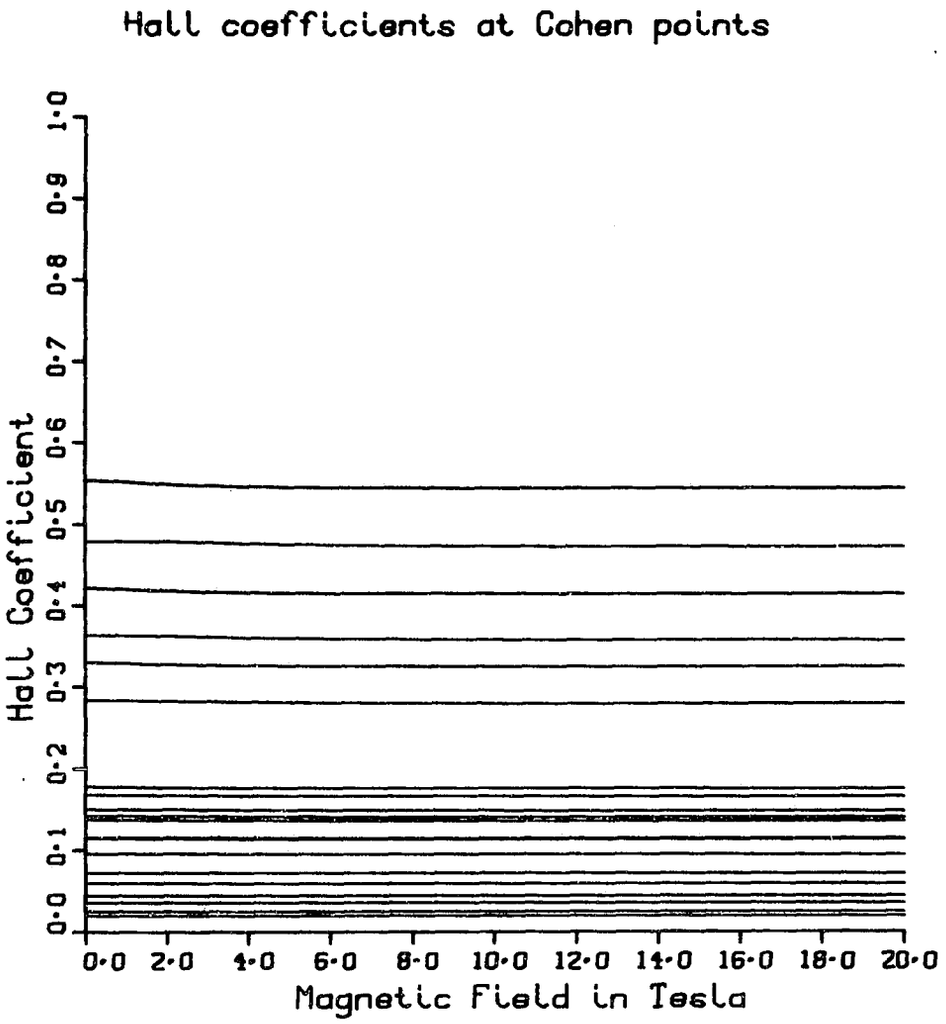

Fig. II-1
Effect of the magnetic field on the Hall Coefficient (as defined in Ref. 4)

plasma, there are two major sources of errors that can contribute to the uncertainty of the computed values for conductivity. The first source of error is the thermochemical data for the heat of formation of some of the species, which can significantly affect the concentration of the electrons in the plasma. The most important species are KOH, AlO_2, and CO_2. The second source of error is the values for the momentum collision cross sections. Reference 7 discussed the error bounds on the electrical conductivity, which result from the uncertainty of the data of the first kind. At ANL, independent calculations were done to investigate such effects.

For CO_2: Using the JANAF data of December, 1975, σ is reduced by 5 % at a reference point (p = 3.5 atm, T = 2600 K, for Montana Rosebud coal with 5 % moisture, 85 % slag rejection, and 34 % oxygen enrichment) as compared to the case where CO_2 is neglected. Based on the investigation of References 7 through 9, it has been shown that, with the new data for the heat of formation for CO_2, there is very little effect of CO_2 on the electron concentration in the plasma and, correspondingly, very little effect on the electrical conductivity of the plasma. On this basis, until the JANAF tables are officially updated, CO_2 is neglected in our analysis.

For AlO_2: Using the old JANAF data of December, 1968, σ is reduced by approximately 13 %. The error bounds on the heat of formation in the new data (12/75) are smaller, which makes the range of uncertainty smaller ($\sim$13 %) than before.

For KOH: Reference 7 showed that s can vary by as much as 50 % because of the uncertainty of + 3 kcal/mol in the heat of formation. Therefore, it is important to reduce experimentally the range of uncertainty. In the meantime, ANL uses the JANAF medium value.

C. Heat Losses

When run in the HP mode, the original NASA code yielded a single calculational point for each pressure input. The heat of formation of each reactant, as input or as computed, was multipled by the mole fraction of that reactant, and the products were summed to give the total enthalpy, HSUBO. Chemical equilibrium was then calculated for that total enthalpy

and each specified pressure. For many purposes, especially combustor studies, it is valuable to be able to find equilibrium properties as a function of combustion chamber heat loss. The new version has been adjusted to allow these studies.

These heat loss studies are performed by computing chamical equilibrium at an enthalpy that is reduced by some amount from HSUBO. Because enthalpy is a relative measure, a reference value, REFH, was added to the inputs. This is typically the enthalpy of the same reactants when brought to equilibrium at some standard set of conditions, and is treated as the enthalpy when heat loss is '100 %.' For a given fractional heat loss, f, the enthalpy at which equilibrum is computed is

H=HSUBO - f (HSUBO - REFH).

To save space, the heat loss fractions are input and stored in the T array, the same array as is used for temperatures in TP mode calculations. Because this array is internally counted by looking for the first zero element, and because no heat loss should be an option, the values actually input to T are from (1-f), rather than f.

Thus, for example, to compute the combustor temperature for a 2.5% combustor heat loss (based on the total thermal input), the HP input mode is used and the value 0.975 is entered in the T array of the NASA input.

D. Shorthand Data Input

The reactants for virtually all MHD combustor studies, and for a large number of other applications, conform to a standard model. A hydrocarbon fuel (coal, oil, natural gas, or some combination of them) of given chemical analysis and heating value is burned in a preheated air/oxygen mixture with some weight fraction of potassium, injected as K_2CO_3. The air, fuel, and K_2CO_3 may be accompanied by some given amount of water.

Although, relatively straightforward, inputting this standard analysis data by REACTANTS cards is rather tedious. For use in coal combustion, the weight fractions must be adjusted from the 'as received' to the 'as determined' basis, in order to correct for various moisture content and ash rejection ratios. The weight fraction of air and pure oxygen must be adjusted to meet the desired O_2-enrichment and stoichiometric ratios. The weight fraction of K_2CO_3 must be adjusted to the proper fraction of potassium seeding. And a fictitious heat of formation for one reactant is required, so that enthalpy of the total mixture will correspond to the given heating value of the fuel as correctly adjusted to the 'as determined' basis.

To simplify treatment of this standard problem, a new input group, FUEL, has been added. As described in detail in Section IV, a FUEL group defines the following:

the chemical composition of the fuel,

fuel heating value,

moisture content,

ash rejection,

stoichiometry of the combustion,

O_2-enrichment,

fuel temperature,

air temperature,

O_2 temperature,

potassium (seed) weight fraction,

water-to-seed weight fraction.

Within the computational entry, NASA, the relative weights and the fictitious enthalpy of the carbon are computed. All the information from

the FUEL group is then stored in the appropriate internal arrays - duplicating the situation that would have occurred if the reduced data had been read from REACTANTS cards.

The computations that are performed in this setup process are as follows:

1) From the ultimate analysis of the fuel, the total fuel weight (TOT_WT) is readjusted to yield the specified value of fuel moisture content (FUEL.H2O_ADJUST).

TOT_WT = TOT_WT*(1.0-H2O_FRAC_FUEL)/(1.0-FUEL.H2O_ADJUST)

The 'as received' heating value for the fuel (FUEL.HHV) is readjusted to account for this moisture change.

HHV = HHV*(1.0-FUEL.H2O_ADJUST)/(1.0-H2O_FRAC_FUEL)

2) From the specified fraction of ash rejection (FUEL.ASH_REJECT), the weights, weight fractions, and HHV are readjusted.

SLAG_WT = total weight of ash content as received,

HHV = HHV*TOT_WT/(TOT_WT-ASH_REJECT*SLAG_WT),

TOT_WT = TOT_WT-ASH_REJECT*SLAG_WT,

X = X*(1.0-ASH_REJECT),

where X is the weight of any ash species (e.g., SiO_2, SO_3).

3) From the input carbon (C), hydrogen (H), sulfur (S), and oxygen (O) content of the fuel and the stoichimetry (STOICH), the total weight of oxygen (OWT) needed in the oxidizer mixture is determined.

OWT = STOICH*(32.0*(C/12.0111) + 0.5*(H/2.016) + (S/32.066))-O,

where the molecular weights of O_2, C, H_2, and S are 32.0, 12.011, 2.016, and 32.066, in that order.

4) From the oxygen enrichment, the total amount of air (AIRWT) is determined.

AIRT = OWT/O2_AIR

5) From the air weight and oxygen weight, the weight of pure oxygen (O2WT) is determined, and, from the humidity (H2OA), the amount of water (H2OWTA) in the oxidizer mixture is determined.

O2WT = OWT-0.2315*AIRWT

H2OWTA = H2OA*AIRWT,

where the mass ratio of oxygen in dry air is 0.2315.

6) From the air temperature (AIRT), its enthalpy (AIRH) is obtained from the polynomial fit.

```
AIRH = -1.174E-10*(AIRT)**4+3.823E-7*(AIRT)**3
       +2.3485E-4*(AIRT)**2+6.713*(AIRT)-2059.76
```

7) From the seed fraction (SF), the fuel weight (FW), and the moisture fraction (H2OS), the amount of K_2CO_3 (SEEDWT) and the amount of water (H2OWTS) accompanying it are determined.

SEEDWT = SF*(FW+O2WT+AIRWT+H2OWTA)/(0.5658-SF*(1+H2OS))

H2OWTS = H2OS*SEEDWT,

where 0.5658 is the mass ratio of K in K_2CO_3.

8) From the heating value (HHV) of the fuel, its total weight, and its carbon, hydrogen, and sulfur content, the appropriate fictitious carbon heat of formation ('Hf') is determined.

Hf = -94052+12.011/C*(HHV*FW-H/2.016*6837.0-S/32.066*70947.0),

where the heat of formation values for CO_2, H_2O, and SO_2 are -94052, 68317, and 70947 cal/g, in that order.

These steps are applied to each FUEL group automatically, loading the internal arrays within the NASA code as if a set of REACTANTS cards had been furnished.

E. Thermodynamic and Electrical Properties Summary Output

When the output routine, NASAOUT, is called, it causes the printing of a summary sheet containing the overall thermodynamic properties of the equilibrium mixture. This summary consists of the following labeled columns of data.

Column	Label	Description
1	P	pressure in atmospheres (input quantity)
2	T	Temperature in kelvins (input quantity in TP mode)
3	MW	Equilibrium molecular weight
4	H	Enthalpy in joules/kg
5	S	Entropy in joules/kg·K (input quantity in SP mode)
6	RHO	Density in kg/m^3
7	CP	Specific heat in joules/kg·K
8	SON VEL	Sonic velocity in m/s
9	SIG	Electrical conductivity in S/m (present only if conductivity calculation required)
11	NE	Electron number density in $10^{20}/m^3$ (present only if conductivity calculation is required)

These numbers are stored internally as the rows of the PL/1-based structure array, NASAP->OUT.A (cf Ref. 2) whenever the calculational entry, NASA, is called. Thus, for example, the values

NASAP->OUT.A(10,J)

for J = 1, 2, . . . , NASAP->IFIN refer, in order, to the conductivities resulting from each equilibrium point calculated. Because the pointer, NASAP, is an external variable, all of these data points are known to (and may be used in) the MAIN Program.

III. USER'S GUIDE

This section will describe in detail the input data to the NASA code and the output that may be obtained with the various options. The variable names into which the input data is stored are also listed and explained, because knowledge of these names is necessary to effect control from GPSAP over parameters in NASA.

A. Input Data

Data input to NASAIN, contained in file CARDIN, is divided into categories, each introduced by a keyword. The keywords and the type of input data following each are:

	Keyword	Type of data
1)	REACTANTS	Description of chemical reactants introduced into the combustor
2)	FUEL	Shorthand description of reactants
3)	NAMELIST	Type of problem, prescription of "givens," selection of options
4)	OMIT	Chemical species to be excluded in computing equilibria
5)	INSERT	Condensed species to be included in first iteration
6)	END	Signifies the completion of problem prescription

These keywords must appear, starting in Column 1. Any additional data on the same line (card) with REACTANTS, FUEL, NAMELIST, or END key cards is ignored; thus, comments may be entered in those lines.

REACTANTS, OMIT, and INSERT all trigger 'GET EDIT' statements, and the data must, therefore, occur in specified columns.

FUEL and NAMELIST trigger 'GET DATA' statements, allowing more free-form input.

END returns program control to the calling (MAIN) program. Inclusion of this key card in the program vocabulary allows the other input categories to occur in any order. The various categories are discussed in detail below.

1. REACTANTS

Except for omitting the division of reactants into "fuels" and "oxidants," the REACTANTS group format has not been changed from that of the original NASA-Lewis code. Thus, the REACTANTS groups from any existing data sets for that code can be used directly in the present one. The names, meanings, and input format for each REACTANTS card (from 1 to NREAC, where NREAC is the total number of reactants read) are as follows:

Variable	Meaning	Format	Columns
NAME(N,I),NUM(N,I)	Atomic symbol and formula numbers for element I (maximum 5) of reactant N (if NAME(N,5) ='00,' the enthalpy is calculated by the code).	5(A(2),F(7,5))	1-45
PECWTS(N)	Relative weight or number of moles of reactant N in total reactants. Arbitrary base.	F(7,5)	46-52
MOLE	If MOLE='M' for any N, then variable MOLES is set to '1'b, signifying that all PECWTS are interpreted as relative numbers of moles. MOLES is alterable at execution time, MOLE is not.	A(1)	53
ENTH(N)	Assigned enthalpy in cal/g·mol [see note regarding NAME(N,5)].	F(9,5)	54-62
FAZ(N)	'S', if solid 'L', if liquid 'G', if gas	A(1)	63

RTEMP(N)	Reactant temperature in K	F(8,5)	64-71
DENS(N)	(optional) reactant density in g/cm^3	F(8,5)	73-80

Note that column 72 is ignored. All of the above, except MOLE (but including MOLES), can be altered with 'AAA' statements at execution time, as shown in the examples in Section IV.

2. FUEL

The FUEL keyword is a local extension, designed to simplify data input for the most common MHD applications. After the keyword, any members of the structure FUEL are input as free-form assignment statements (e.g., FUEL.O = 86.4) separated by commas and/or any number of blanks. The end of a FUEL group is designated by a semicolon. The names, meanings, and default values of the variables input in a FUEL group are

Variable	Meaning	Default
FUEL.C	Relative weight of carbon in fuel	0.0
FUEL.H	Relative weight of hydrogen in fuel	0.0
FUEL.S	Relative weight of sulfur in fuel	0.0
FUEL.N	Relative weight of nitrogen in fuel	0.0
FUEL.O	Relative weight of oxygen in fuel	0.0
FUEL.H2O	Relative weight of H_2O in fuel	0.0
FUEL.SiO2	Relative weight of SiO_2 in fuel	0.0
FUEL.SO3	Relative weight of SO_3 in fuel	0.0
FUEL.AL2O3	Relative weight of Al_2O_3 in fuel	0.0
FUEL.CAO	Relative weight of CaO in fuel	0.0

FUEL.MGO	Relative weight of MgO in fuel	0.0
FUEL.FE2O3	Relative weight of Fe_2O_3 in fuel	0.0
FUEL.K2O	Relative weight of K_2O in fuel	0.0
FUEL.TOT_WT	Total weight to which the above components are normalized	100.0
FUEL.T	Temperature of fuel	300.0
FUEL.HHV	Higher heating value of fuel in cal/g	0.0
FUEL.DENS	density of fuel	0.0
FUEL.STOICH	Ratio of total oxygen supplied in fuel, air, and pure O_2 to total oxygen required for complete combustion of all carbon, hydrogen, and sulfur	1.0
FUEL.O2_AIR	Weight ratio of the total O_2 to the air + O_2 mixture supplied	0.2315
FUEL.H2O_AIR	Weight of water carried by the air, as a fraction of the dry air weight	0.0
FUEL.AIR_TEMP	Temperature of air and its water	300.0
FUEL.O2_TEMP	Temperature of the pure O_2	300.0
FUEL.SEED_FRAC	Weight fraction of potassium in total to be introduced as K_2CO_3	0.01
FUEL.H2O_SEED	Weight of water accompanying the K_2CO_3 as a fraction of the K_2CO_3 weight	0.0
FUEL.H2O_ADJUST	Weight fraction of H_2O required in the fuel. Thus, if FUEL.H2O_ADJUST is not equal to the moisture fraction in the fuel, the weight fractions of water and the HHV of the fuel are readjusted to this new moisture fraction.	0.0
FUEL.ASH_REJECT	Fraction of the total ash content of the fuel to be rejected	0.0

Notes:

(1) If FUEL.C is not entered, the entire FUEL group is ignored.

(2) The seed fraction is calculated as a fraction of the total of the reactants generated by this FUEL group.

(3) As many as three FUEL groups and one REACTANTS group may be entered to describe the reactants for a given problem. At input, each FUEL group is tagged by the keyword, FUEL, and input as

FUEL.xxx=vvv

(4) For modification at execution time, members of the second and third FUEL groups entered are modified by

AAA 'FUEL2.xxx' vvv

and

AAA 'FUEL3.xxx' vvv,

respectively.

3. NAMELIST

The keyword, NAMELIST, triggers a GET DATA statement, which reads a number of parameters and switches that control the calculations to be performed. Although the basic idea is the same as in the original NASA-Lewis code, considerable modification of this input categroy was necessary, both to accomodate the PL/I environment and to serve the locally available options. The variables, types, meanings, and defaults are, at present:

Variable	Dimension	Type	Meaning	Default
TP	1	BIT(1)	If '1'B, equilibria calculated at given temperatures and pressures	'0'B
HP	1	BIT(1)	If '1'B, equilibria calculated at given enthalpies and pressures	'0'B
SP	1	BIT(1)	If '1'B, equilibria calculated at given entropies and pressures	'0'B
OTTO	1	BIT(1)	If '0'B, JANAF chemical table search is skipped whenever the preceding NASA call had the same elements and omissions	'0'B

Variable	Dimension	Type	Meaning	Default
MMHG	1	BIT(1)	If '1'B, pressures are in mm Hg	'0'B
INGH	1	BIT(1)	If '1'B, pressures are in in. Hg	'0'B
PSIA	1	BIT(1)	If '1'B, pressures are in psi	'0'B
NSQM	1	BIT(1)	If '1'B, pressures are in N/m^2. Note that, if none of MMHG, INHG, PSIA, or NSQM, then pressures are in atmospheres	'0'B
FIT	1	BIT(1)	If '1'B, summary output is written onto file FITDAT for subsequent polynomial fit	'0'B
CONDUC	1	BIT(1)	If '1'B, conductivity routine is called after equilibrium calculation	'0'B
IONS	1	BIT(1)	If '1'B, ionized species are included in equilibrium calculation	'1'B
PRINT	1	BIN(15)	Determines the amount of intermediate output	0
IDEBUG	1	BVIN(31)	If > 0, causes equilibrium iterations to be output	0
TRACE	1	DEC(6)	If > 0, signifies that, when mole fractions are printed, all species with fraction > TRACE are shown	0
REFH	1	DEC(6)	Reference enthalpy: enthalpy of the same reactants if brought to equilibrium at standard temp and pres. In TP mode, this is used as a "zero set" for the reported enthalpies. In HP mode, it is used as a reference point to define heat loss	0
SO	1	DEC(6)	Total entropy at which equilibria are calculated in SP mode	0
P	26	DEC(6)	Schedule of pressures at which equilibria are to be calculated. End of the schedule is signified by the first 0	26*0

Variable	Dimension	Type	Meaning	Default
T	26	DEC(6)	If TP mode, schedule of temperatures (in K) at which equilibria are calculated. If HP mode, schedule of heat retention fractions at which equilibria are calculated (see below)	26*0

The use of the T array in HP mode is a locally written extension to the original NASA-Lewis code. In this application, the values 1 - T(I) represent the combustor heat loss as a fraction of the enthalpy difference between the reactants as introduced to the combustor and the enthalpy REFH. Thus, e.g., if REFH is the enthalpy of the same reactants at 300 K, 1 atm, then a value T = .96 represents a heat loss of 4% of the total thermal input.

Note that, in a NAMELIST input from a call to NASAIN, all variables are redefined to their default values before the NAMELIST is read. This can be important when GPSAP is used to do parameter sweeps and optimizations.

4. OMIT and INSERT

OMIT and INSERT cards are identical in both function and format to those in the original NASA-Lewis code. The keyword is followed by the names (chemical symbols) of from one to four species, starting in columns 16, 31, 46, and 61. The names on OMIT cards signify particular species that are to be deleted from consideration in computing the equilibrium composition. INSERT cards contain the names of condensed species that are assumed to be present when the program is begun. The variables, NSERT and NOMIT, contain, respectively, the number of inserted and omitted species; ENSERT (3,30) and OMIT(3,3) [both CHAR(4)] contain the species names. At execution time, the last species in either list may be removed by decreasing NSERT or NOMIT. A species may be changed to a new one by assigning the appropriate new character strings to the array elements. The name of the Nth species is left-justified in the 12-character field,

(XXX(1,N), XXX(2,N), XXX(3,N)),

where XXX stands for either OMIT or ENSERT. If the old species name is longer than the new one, the extra spaces must be explicitly blanked. A new species may be added to the list by increasing NSERT or NOMIT and assigning the new name to the array.

5.0 END

The END card does not signal additional input but, rather, indicates that a problem is now fully specified and that control should be returned to the main program for further processing.

B. Program Output

Primary output from the calculation is the thermodynamic and electrical properties summary printed upon a call to NASAOUT. This output consists of a table for all the points on the P and T schedules of the following:

pressures (atm)

temperatures (K)

molecular weights (kg/kg-mol)

enthalpies(J/kg)

entropies (J/kg·K)

densities (kg/m^3)

specific heats (J/kg·K)

gas constants

sonic velocities (m/s)

conductivities (S/m)

electron number densities ($10^{20}/m^3$)

These same values are also accessible from the driver as NASP->OUT(I,J), where I goes from 1 to 13 and refers to the properties (in the order given)

and J goes from 1 to the number of output points (T varies more rapidly than P).

In addition, various amounts of intermediate output may be obtained, depending on the value of PRINT.

If PRINT=0, all that is obtained is a copy of the input data and any error messages. Error messages will be on file FT06F001 if errors occurred in the equilibrium calculation and on SYSPRINT otherwise. The messages and their meanings are identical to those in the original code and will not be repeated here.

If PRINT=1, the output also includes a list of the species considered each time the JANAF thermodynamic data are scanned, the value (HSUB0) of the total enthalpy of the reactants as introduced, the number of gram atoms of each element present per kg of the mixture (B0's), a listing of any inserted species, and a list of the REACTANTS cards that are equivalent to any FUEL groups used and a list of the reactants, weight fractions (normalized to a total of 1), enthalpies (as input or calculated), phases, reference temperatures, and densities (if input), as well as the net mixture density at input.

PRINT=2 adds a brief summary of the net thermal and electrical properties printed once every 13 points on the calculation schedule.

PRINT=3 yields all of the above plus 1) a listing of the mole fractions for every species of mole fraction greater than or equal to 5×10^{-6} if TRACE=0 (TRACE otherwise), 2) a trace of the LaGrange multiplier values, and 3) the names of added or removed condensed species as the equilibrium calculation proceeds (this last is on file FT06F001).

IV. ILLUSTRATIVE EXAMPLE

Two examples will both demonstrate the method of using the new GPSAP-driven NASA code and illustrate the new capabilities it affords. Any confusion as to variable names and meanings may be resolved by reference to Section III.

A. Example 1

1. Problem

Determine the thermodynamic and electrical propeties of a coal burned in an air/oxygen mixture. The coal has an 'as received' composition analysis of:

Species	Weight
C	52.2
H	3.38
S	0.8
N	0.8
O	11.02
SiO_2	1.732
SO_3	2.055
Al_2O_3	1.214
CaO	1.481
MgO	0.517
Fe_2O_3	0.499
H_2O	24.30

Before being burned, the coal is dryed to 5% moisture content; furthermore, it is assumed that the ash rejection is 75%. (For the analysis, it

is assumed sufficient to remove 75% of the ash species before the combustion, rather than 75% of the condensed species during the combustion process.)

The oxygen/air mixture is to have a preheat temperature of 1000 K and 30 mass % O_2. Sufficient air will be added to obtain a stoichiometric ratio of 0.92. The air is assumed to have moisture content of 1 mass %.

The combustion process is also seeded with 1 mass % potassium. The seed and coal are input at a temperature of 300 K. Also, the higher heating value of the coal is assumed to be 4968 cal/g.

Specifically, the flame temperatures of the combustion are to be determined for pressures is of 4, 5, 6, 7, and 8 atm with no heat loss. In addition, the thermodynamic and electrical properties are to be determined for pressures in the range of 1-8 atm, in 1 atm increments, and for temperatures in the range of 1600-3000 K, in 200 K increments.

2. Input

The total input required for this analysis is shown in Fig. IV-1. This input will now be discussed in detail, on the basis of the line numbers shown at the left in the figure.

Lines 1 to 29 comprise the standard JCL, common to all GPSAP analysis. The in-line procedure, SYSTEM, that is executed (line 29) is composed of three steps: ONE, PLO, and TWO. Step ONE executes GPSAP, which reads the structure in file STRUCIN and expands it into a PL/1 MAIN program on scratch file SYSDRV. Step PLO compiles that program, and step TWO loads it, using library SYSLTB.

Lines 33 to 38 complete the JCL, defining the various data files referenced by NASA. CNDCT contains the table of coefficients used to compute the conductivity. JANAF contains the thermochemical data (JANAF table) used by NASA. FITDAT is a scratch file used to store the NASA

Figure IV-1

```
 1.  JOB
 2.  CUA
 3.  //SYSTEM  PROC
 4.  //ONE EXEC PGM=GPSAP
 5.  //STEPLIB  DD  DSN=C115.B25236.SYSLIB.LOAD,DISP=SHR
 6.  //STRUCT   DD  DDNAME=STRUCIN
 7.  //SYSPRINT DD  SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1511)
 8.  //SYSDRV   DD  DISP=(NEW,PASS),UNIT=SASCR,SPACE=(TRK,(2,1))
 9.  //PLO  EXEC PGM=IEL0AA,PARM='NS,NA,NK,NAG,NOESD,NSTG'
10.  //STEPLIB  DD  DSN=PLI.OPT.LINKLIB,DISP=SHR
11.  //SYSIN    DD  DSN=*.ONE.SYSDRV,DISP=(OLD,DELETE)
12.  //SYSLIN   DD  UNIT=SASCR,SPACE=(CYL,4),
13.  //  DISP=(NEW,PASS),DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)
14.  //SYSPRINT DD  DUMMY
15.  //SYSPUNCH DD  DUMMY
16.  //SYSUT1   DD  SPACE=(CYL,4),UNIT=(SASCR)
17.  //TWO  EXEC PGM=LOADER,REGION=150K,COND=(9,LT,PLO)
18.  //SYSLIB   DD  DSN=SYS1.PLIBASE,DISP=SHR
19.  //         DD  DSN=SYS1.FORTLIB,DISP=SHR
20.  //         DD  DSN=C115.B25236.LOAD,DISP=SHR
21.  //SYSLIN   DD  DSN=*.PLO.SYSLIN,DISP=(OLD,DELETE)
22.  //SYSLOUT  DD  SYSOUT=A,DCB=(RECFM=FB,LRECL=121,BLKSIZE=1573)
23.  //SYSPNCH  DD  DUMMY
24.  //SYSPRINT DD  SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1511)
25.  //SYSPUNCH DD  DUMMY
26.  //PROGREP  DD  SYSOUT=A,DCB=(RECFM=FB,LRECL=133,BLKSIZE=1596)
27.  //FT06F001 DD  SYSOUT=A,DCB=(RECFM=FB,LRECL=133,BLKSIZE=1596)
28.  //  PEND
29.  //  EXEC SYSTEM
30.  //ONE.STRUCIN  DD  *
31.   MMM  NASAIN  NASA  NASAOUT  ;
32.   MMM  NASAIN  NASA  NASAOUT  ;
33.  //TWO.CNDCT  DD  DSN=B25445.TABLE.DATA,DISP=SHR
34.  //JANAF      DD  DSN=B25445.THERMO.DATA,DISP=SHR
35.  //SUMMARY    DD  SYSOUT=A,DCB=(RECFM=FB,LRECL=133,BLKSIZE=1596)
36   //FITDAT     DD  DISP=(NEW,PASS),UNIT=SASCR,SPACE=(TRK,(5,5)),
37   //   DCB=(RECFM=FB,LRECL=80,BLKSIZE=1520)
38   //CARDIN     DD  *
39   FUEL
40     FUEL.C=52.2  FUEL.H=3.38  FUEL.S=0.8  FUEL.N=0.8  FUEL.O=11.02
41     FUEL.SIO2=1.732  FUEL.SO3=2.055  FUEL.AL2O3=1.214  FUEL.K2O=0.0
42     FUEL.CAO=1.481  FUEL.MGO=0.517  FUEL.FE2O3=0.499  FUEL.H2O=24.3
43     FUEL.ASH_REJECT=0.75  FUEL.H2O_ADJUST=0.05
44     FUEL.SEED_FRAC=0.01  FUEL.H2O_SEED=0.00
45     FUEL.HHV=4968.  FUEL.STOICH=0.92
46     FUEL.T=300.  FUEL.AIR_TEMP=1000.  FUEL.O2_TEMP=1000.
47     FUEL.H2O_AIR=0.01  FUEL.O2_AIR=0.3  ;
48
49   NAMELISTS
50     HP='1'B FIT='0'B P(1)=8 P(2)=7 P(3)=6 P(4)=5 P(5)=4  ;
51   END
52   NAMELISTS
53     TP='1'B CONDUC='1'B FIT='1'B PRINT=2
54     P(1)=8 P(2)=7 P(3)=6 P(4)=5 P(5)=4 P(6)=3 P(7)=2 P(8)=1 P(9)=0.5
55     T(1)=3000 T(2)=2800 T(3)=2600 T(4)=2400 T(5)=2200 T(6)=2000
56     T(7)=1800 T(8)=1600 T(9)=1400 T(10)=1200 T(11)=1000 T(12)=800
57     ;
58   END
```

answers for further processing by other procedures. The input data to NASAIN is found in file CARDIN. The names, CNDCT, JANAF, FITDAT, and CARDIN, are built into the NASA code and, hence, cannot be changed.

This problem requires two distinct operations, 1) the determination of the flame temperatures, and 2) the calculations of the thermodynamic and electrical properties. Each of these, in turn, requires three processes: 1) inputting data, 2) calculating the results, and 3) printing the results. Line 31 indicates the simplest GPSAP input for performing these three tasks with the NASA code. The MMM statement will call the NASAIN entry, which will read the input data on file CARDIN down to the first END keyword. It will then call NASA and perform the computations as dictated in the input data. Finally, it will call NASAOUT to print a summary of the results, which will be the flame temperatures in this case.

The second line, 32, in file STRUCIN will perform exactly the same. This time, the first call to NASAIN will read down to the next END keyword, encompassing the inputs necessary to perform the calculations of the thermodynamic properties.

Lines 39 to 58 represent the input data to the NASA code for this problem. As stated, the problem can be input directly without any prior anlaysis. Lines 39 to 47 represent the FUEL group, giving the coal composition, moisture readjustments, ash rejection corrections, stoichiometry, etc. Lines 52 to 57 represent the NAMELIST input. Thus, the HP mode will be used with the desired pressures. The END keyword in line 51 indicates the end of the data that will be read-in in this call to NASAIN.

Lines 52 to 56 indicate the NAMELIST input necessary to carry out the thermodynamic properties calculations. Line 58 signifies the end for the second NASAIN call.

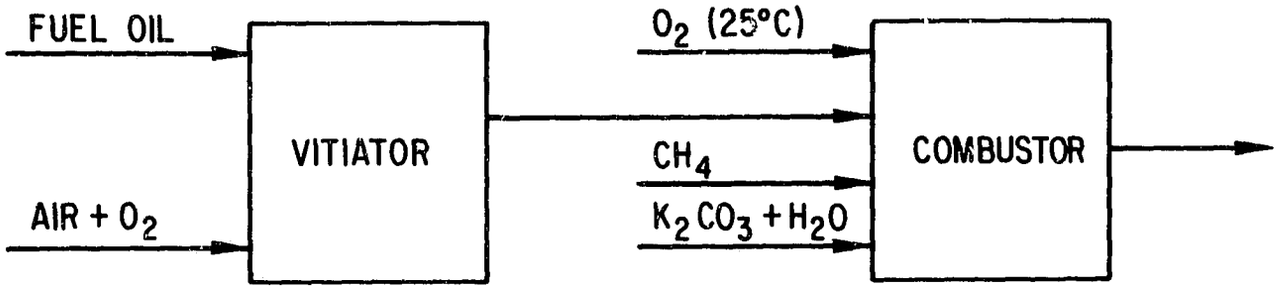

Fig. IV-2 Schematic diagram of proposed combination combustor

B. Example 2

1. Problem

Operate the combination combustor, depicted in Fig. IV-2, of a proposed experimental MHD facility. The vitiator burns a mixture of No. 2 fuel oil and preheated oxygen-enriched air. Oxygen is added to the air to establish 30 mass % O_2. In the combustor, the output of the vitiator is combined with additional, room-temperature oxygen, with methane, and with a one-to-one mixture of potassium carbonate and water. Potassium is to form 1 mass % of the total reactant mixture.

The composition of No. 2 fuel oil will be taken as follows:

C	86.4%
H	12.7%
S	0.7%, and
O	0.2%,

with a higher heating value of 10,877.3 cal/kg.

For a number of different air preheat temperatures and a number of different (total) oxygen enrichment levels, it is desirable to know the relative amounts of oil and methane necessary to achieve stated flame temperatures at 3 atm pressure, 7% system heat loss. Specifically, for

T preheat = 700, 800, 900, 1000 K, and

02 enrichment = 0.30, 0.35, 0.40,

we wish to obtain,

T flame = 2900, 3000, 3100 K.

It is required, further, that these temperatures be achieved with the minimum possible amount of oil, i.e., an optimal stoichiometry will be found simultaneously.

2. Analysis

As will be seen, the availability of GPSAP code-creation and optimization capabilities allows this entire study to be performed in a single computer job. A small amount of preliminary analysis is necessary, however.

Note, first, that only the final state of the combustion products is of interest. This final state is unaffected by the fact that combustion is carried out in a two-stage process. We will, accordingly, merely compute the equilibrium state that exists when all reactants are combined. Second, note that the thermodynamic properties under investigation are intrinsic quantities, unaffected by the total reactant mass. Therefore, all reactants will be scaled to 100 grams of methane.

The heating value for methane is not stated and, presumably, is not known. Conversely, the heating value for fuel oil is given, and we wish to avoid calculating the corresponding 'Hf.' As now composed, subroutine SETUP (which translates the FUEL groups into NASA input arrays) is rather awkward for this sort of FUEL/REACTANTS mixture. Therefore, it is easiest to input only the fuel oil through the FUEL group, and to adjust the amounts of air, O_2 (hot and cold), K_2CO_3, and H_2O explicitly from the input structure.

The question that must be answered is, given,

CH = 100 grams,

oil = X grams,

stoichiometry ratio = ST,

O_2 enrichment = O2_ENRICH,

T-preheat = AIRT,

seed fraction = 0.01, and

K_2CO_3/H_2O = 1.0,

find the weight of K_2CO_3, H_2O, O_2 (hot), air, and O_2 (cold). Once stated the problem is answered fairly easily. The total weight of oxygen necessary (air and pure oxygen) is

$$O2TOT = ST * \left\{[2* \frac{100}{16.043} + \frac{0.864*X}{12.011} + \frac{1}{2} \frac{0.127*X}{2.016} + \frac{0.007*X}{32.066}] * 32 - 0.002*X\right\}$$

$$= ST * [398.928 + 3.315 * X],$$

where, in the first entry, the four terms within the square brackets are, in order, the moles of methane and the moles of C, H, and S in the oil; the last term is the mass of oxygen already found in the fuel oil. From this, the weight of the air is

AIRW = O2TOT/O2_ENRICH.

The hot O_2-plus-air is to contain 30 mass % O_2; therefore the weight of hot O_2 is

O2_HOT = 0.3*AIRW,

and the weight of cold O_2 is

O2_COLD = O2TOT - O2_HOT.

Finally, the weight of potassium carbonate and of its water of hydration are determined by the requirement that potassium, which constitutes

0.5658 of the weight of K_2CO_3, is to comprise 0.01 of the total weight. The seed weight and the weight of H_2O are, thus, each

SW = 0.01*(100 + X + AIRW + O2_HOT + O2_COLD)/0.5658.

These manipulations are, of course, slightly tedious. It should be noted, however, that this is all that is required for the entire study with the present form of the code. Under the old regime also, all the same steps were required. In addition, 'Hf' would have to be calculated. And, finally, all formulae would have to be evaluated for each set of the X, ST, and O_2 _ENRICH to be studied.

3. Input

Only the input structure on file STRUCIN and the input data to NASAIN on file CARDIN will be explained. The rest of the JCL is similar to that for Example 1. Again, the input, shown in Figure IV-3, will be discussed on the basis of the line numbers shown on the left.

The REACTANTS cards, introduced by line 52 and contained on lines 53 to 58, are the same as those in the previous version of the code (except that separation into 'fuels' and 'oxidants' has been eliminated). The CH_4, K_2CO_3, H_2O, preheated O_2, air, and cold O_2 are described in turn. These will be known to NASA as reactants 1 through 6. The relative weights of all but reactant 1 (CH_4), as well as the enthalpy and reference temperature of reactant 5 and the reference temperature of reactant 4, are dummies, because they will be changed by the MAIN Program (these numbers could, in fact, be deleted). The blank line (126) is necessary to indicate the end of the REACTANTS group.

The FUEL group, lines 60 through 63, defines the fuel oil and the relative weights of carbon, hydrogen, and oxygen. Because STOICH and SEED_FRAC default (see Section III) to 1.0 and 0.01, respectively, it is

Figure IV-3

```
//ONE.STRUCIN  DD  *
 MMM  NASAIN  ;
 BBB  A  AIRT = 700 800 900 1000  ;
    AIRH=-2059.76+AIRT*(6.713+
                   AIRT*(2.3485E-4 +
                    AIRT*(3.823E-7 -
                     AIRT*1.174E-10)));
    BBB  B  O2_ENRICH = 0.3  0.35  0.4  ;
       BBB  C  T0 = 2900  3000  3100  ;
          BBB  D  X  100  10  500
                  ST  0.9  0.75  1.15  ;
             O2TOT=ST*(398.928 + 3.315*X);
             AIRW=O2_ENRICH *O2TOT;
             O2_HOT=0.3*AIRW;
             O2_COID=MAX(0.001, O2TOT-O2_HOT);
             SW=(100+X+AIRW+O2_HOT+O2_COLD)/54.58;
          AAA  'FUEL.TOT_WT'  X
               'PECWTS(2)'    SW
               'PECWTS(3)'    SW
               'PECWTS(4)'    O2_HOT
               'RTEMP(4)'     AIRT
               'PECWTS(5)'    AIRW
               'ENTH(5)'      AIRH
               'RTEMP(5)'     AIRT
               'PECWTS(6)'    O2_COLD
               'HP'           '0'B
               'TP'           '1'B
               'FIT'          '0'B
               'CONDUC'       '0'B
               'PRINT'        0
               'REFH'         0.0
               'P(1)'         1.0
               'T(1)'         300.0
               ;
          MMM  NASA  ;

          AAA  'HP'           '1'B
               'TP'           '0'B
               'P(1)'         3.0
               'T(1)'         0.93
               'REFH'         NASAP->A(4,NASAP->IFIN) ;
          MMM  NASA  ;
          CCC  D  NASAP->A(2,1) = T0 ;
          EEE  D  X  MAXIT=150 ACC=1.0E-2 DEL=1.0E-3  ;
          PUT SKIP EDIT('AIRT=',AIRT,'ONO='ONO,'T0=',TO,
             'OIL WT=',X,'STOICH=',ST)
             (5 (A,E(12,5),X(5)));
          MMM  NASAOUT  ;
       EEE  C  ;
    EEE  B  ;
 EEE  A  ;
//CARDIN   DD   *
REACTANTS
C 1.00   H 4.00                          00        1.5000           G 298.1  F
K 2.00   C 1.00   O 3.00                           18.902           S 298.15 F
H 2.00   O 1.00                          00        18.902           L 298.15 F
O 2.00                                   00        238.177          G 1073.5 O
N 1.5618 O 0.4196 AR0.0093 C 0.0003                693.489 5730.34 G 1073.0 O
O 2.00                                   00        0.001            G 298.15 O

FUEL
  FUEL.C=86.4  FUEL.H=12.7  FUEL.S=0.7  FUEL.O=0.2
  FUEL.STOICH=0.0  FUEL.SEED_FRAC=0.0  FUEL.T=298.15
  FUEL.HHV=10877.3  ;

NAMELISTS
  PRINT=1 ;

END
```

necessary to zero them explicitly to avoid introducing additional air, oxygen, and seed. Input, here, is terminated by the semicolon; the blank line (64) is cosmetic only.

Nearly all of the information input in the NAMELISTS group will be controlled by the MAIN Program. An exceedingly abbreviated NAMELISTS is included to set the defaults and to establish the desired amount of output on the 'production' runs. The END card returns control to the MAIN program.

The MAIN Program, which will perform the desired study, is described by the GPSAP input structure, lines 2 to 50. Line 31 calls the input module, NASAIN, which reads file CARDIN. Note that the reactants cards are read directly into arrays NAME, NUM, PECWTS, ENTH, FAZ, and RTEMP. The information from the FUEL group, on the other hand, is not translated into these arrays at that time.

The three BBB loops-- lines 3 to 50, 8 to 49, and 9 to 48--sweep the desired parameter space in air temperature, oxygen enrichment, and flame temperature. Lines 4 to 7 calculate the air enthalpy for the specified temperature. The optimization loop (lines 10 to 43), carried out for each (AIRT,O2ENRICH,TO) combination, is actually the heart of the computations. The BBB statement in lines 10 and 11 states that an optimizaiton study is to be performed and that the independent variables are X (the weight of oil) and ST (the overall stoichiometry). The starting value of X is 100 (one-to-one CH and oil) and will be varied automatically between 10 and 500; ST begins at 0.9 and remains in the interval $0.75 < ST < 1.15$. For given values of X and ST, the amounts of air, hot oxygen, cold oxygen, seed, and water of hydration are calculated in lines 12 to 16.

The AAA statement, lines 17 to 34, alters a large number of parameters within the next calculational entry called--here, the NASA call in line 35.

The total weight of the fuel group (the oil) is adjusted to X in line 17. The seed weight, SW, is assigned to the potassium carbonate (line 18) and to the water (line 19). Reactant 4, the preheated oxygen, is assigned weight O2_HOT and temperature AIRT; the air (reactant 5) is given weight AIRW, enthalpy AIRH, and temperature AIRT, and the cold oxygen weight, O2_COLD, is assigned to reactant 6. Note that a reactant may not have negative or zero relative weight; accordingly, O2_COLD has been adjusted to remain > 0.001.

Lines 26 to 34 define a typical reference enthalpy run. TP is true ('1'B), because the enthalpy is to be derived at given pressure (1 atm) and temperature (300 K); FIT and CONDUC are false, because polynomial fitting is not required at this point and conductivity is not needed. REFH is zeroed, so that the derived enthalpy is not distorted in successive iterations by the reference value derived in the preceding iteration. The pressure P(1) is assigned to 1 atm, and the temperature T(1) to 300 K.

After the reference run in line 35, the AAA statement in lines 36 to 40 establishes an HP run at 3 atm and 7% heat loss. The value of the enthalpy at the last calculational point from the previous NASA call (i.e., at P = 1 atm, T = 300 K) is assigned to REFH.

In line 41, NASA is called to calculate the flame temperature at 3 atm, 7% heat loss. Line 42 states that the optimization in this BBB loop will be carried out under the constraint that this flame temperature be the given value TO. The EEE statement in line 43 identifies the end of the optimization loop and states that X and ST are to be varied so as to minimize X subject to the above-stated constraint on flame temperature. MAXIT identifies the maximum number of times that lines 10 to 43 may be

executed (for each value of AIRT, O2_ENRICH, and TO) in attempting to perform the optimization. DEL is the relative step size the optimizer uses for computing derivatives, and ACC is the minimum accuracy to which the constraint and optimization are to proceed. These last two are decreased from their defaults (10^{-6} and 10^{-4}), both to save computation time and to avoid numerical difficulties associated with the fact that NASA is a single precision routine.

Line 47 then calls the NASAOUT entry to print the thermodynamic properties table, which will consist, in this case, of only one line, representing the properties at the last call to NASA.

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APPENDIX

```
NAMELISTS

 HP='1'B  FIT='0'B  P(1)=8.0 P(2)=7.0 P(3)=6.0 P(4)=5.0 P(5)=4.0 ;

END
```

SPECIES BEING CONSIDERED

J12/65	AL(S)	J12/65	AL(L)	J12/65	AL	J 6/65	AL+	J 6/63	ALH
J12/62	ALN(S)	J 3/67	ALN	J 6/75	ALO	J 6/75	ALO+	J 12/7	ALO-
J12/67	ALOH	J12/67	ALOH+	J12/67	ALOH-	J12/75	ALO2	J 6/77	ALO2-
J12/68	ALO2H	J 6/75	AL2O	J 6/75	AL2O+	J12/75	AL2O2	J12/75	AL2O2+
J 6/75	AL2O3(S)	J 6/75	AL2O3(L)	L 5/66	AR	L12/66	AR+	J 3/61	C(S)
J 3/61	C	L12/66	C+	J 9/65	C-	J12/67	CH	J12/71	CH+
J12/72	CH2	J 3/61	CH2O	J 6/69	CH3	J 3/61	CH4	J 6/69	CN
J12/70	CN+	J12/70	CN-	J 6/66	CNN	J12/70	CN2	J 9/65	CO
J 3/61	COS	J 9/65	CO2	J12/62	CS	J 6/61	CS2	J12/69	C2
J12/69	C2-	J 3/67	C2H	J 3/61	C2H2	J 9/65	C2H4	L 5/72	C2H6
J 3/67	C2N	J 3/61	C2N2	J 9/66	C2O	J12/69	C3	J 6/68	C3O2
J12/69	C4	J12/69	C5	J12/68	CA(S)	J12/68	CA(S)	J12/68	CA(L)
J12/68	CA	J12/70	CA+	BAR 73	CACO3(S)	BAR 73	CACO3(S)	J 6/73	CAO(S)
J 6/73	CAO(L)	J12/74	CAO	J12/75	CAOH	J12/75	CAOH+	J12/75	CAO2H2(S)
J 12/7	CAO2H2	J12/71	CAS(S)	BAR 73	CASO4(S)	L02/67	E	J 3/65	FE(S)
J 3/65	FE(S)	J 3/65	FE(S)	J 3/65	FE(L)	J 3/65	FE	J 6/65	FEO(S)
J 6/65	FEO(L)	J 9/66	FEO	J 6/66	FEO2H2(S)	J12/66	FEO2H2	J 6/66	FEO3H3(S)
BAR 73	FES(S)	BAR 73	FES(S)	BAR 73	FES(S)	BAR 73	FES(L)	J 6/65	FESO4(S)
BAR 73	FES2(S)	J 6/65	FE2O3(S)	J 6/66	FE2S3O12(S)	J 6/65	FE3O4(S)	J 6/74	H
J 6/66	H+	J 9/65	H-	J 3/64	HALO	L12/69	HCN	J12/70	HCO
J12/70	HCO+	J12/70	HNCO	J 3/63	HNO	J 6/63	HNO2	J 6/63	HNO3
J 3/64	HO2	J 3/61	H2	L11/65	H2O(S)	L11/65	H2O(L)	J 3/61	H2O
L 2/69	H2O2	J12/65	H2S	J12/66	H2SO4(L)	J12/66	H2SO4	J12/61	K(S)
J12/61	K(L)	J 6/62	K	J 3/65	K+	J12/67	KO	J12/67	KO-
J12/70	KOH	J12/70	KOH(S)	J12/70	KOH(S)	J12/70	KOH(L)	J12/71	KOH+
J12/61	K2	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)	J 6/63	K2O(S)	J12/70	K2O2H2
J12/71	K2SO4(S)	J12/71	K2SO4(S)	J12/71	K2SO4(L)	J 3/61	N	J12/70	NCO
J12/71	NH	J12/65	NH2	J 9/65	NH3	J 6/63	NO	J 6/65	NO+
J 9/64	NO2	J 6/72	NO2-	J12/64	N2O3	J 9/65	N2	J12/65	N2H4
J12/64	N2O	J12/70	N2O+	J 9/64	N2O4	J12/64	N2O5	J12/70	N3
J 6/74	O	L12/66	O+	J 6/65	O-	J12/70	OH	J12/70	OH+
J12/70	OH-	J 9/65	O2	J12/65	O2-	J 6/61	O3	J12/65	S(S)
J12/65	S(L)	J 6/7	S	L12/65	S+	J 6/67	SH	J 6/61	SN
J 6/71	SO	J 6/61	SO2	J 9/65	SO3	J12/65	S2	J6/64	S3
J 3/67	SI(S)	J 3/67	SI(L)	J 3/67	SI	J12/71	SI+	J 3/67	SIC
J 3/67	SIC2	J12/69	SIH	J12/71	SIH+	J12/60	SIH4	J 3/67	SIN
J 9/67	SIO	J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(L)
J 9/67	SIO2	J12/71	SIS	J 3/67	SI2	J 3/67	SI2C	J 3/67	SI2N
J 3/67	SI3								

HSUB0 =-3.16014290E+00 (KG-MOL)(DEG K)/KG

KG-ATOMS/KG	B0
C	7.39486629E-03
H	7.19954345E-03
S	4.16722872E-05
N	4.30832562E-02
O	1.73517969E-02
SI	1.20364417E-05
AL	9.94325738E-06
CA	1.10272364E-05
FE	2.60952736E-06
K	2.55750519E-04
AR	2.56565336E-04
E	0.00000000E+00

THERMODYNAMIC PROPERTIES SUMMARY

P	T	MW	H	S	RHO	CP	GAM	SON VEL	SIG	NE
8.0000E+00	2.6932E+03	2.9776E+01	-2.6277E+04	8.9958E+03	1.0779E+00	2.8262E+03	1.1542E+00	9.3167E+02		
7.0000E+00	2.6861E+03	2.9753E+01	-2.6276E+04	9.0331E+03	9.4503E-01	2.8655E+03	1.1531E+00	9.3028E+02		
6.0000E+00	2.6778E+03	2.9737E+01	-2.6275E+04	9.0761E+03	8.1203E-01	2.9116E+03	1.1519E+00	9.2886E+02		
5.0000E+00	2.6679E+03	2.9712E+01	-2.6277E+04	9.1271E+03	6.7862E-01	2.9670E+03	1.1504E+00	9.2673E+02		
4.0000E+00	2.6556E+03	2.9681E+01	-2.6278E+04	9.1896E+03	5.4434E-01	3.0362E+03	1.1486E+00	9.2436E+02		

```
NAMELISTS

 TP='1'B,CONDUC='1'B,FIT='1'B,LONG=2
 P(1)=8. P(2)=7. P(3)=6. P(4)=5. P(5)=4. P(6)=3. P(7)=2. P(8)=1 P(9)=.5
 T(1)=3000  T(2)=2800  T(3)=2600  T(4)=2400  T(5)=2200 T(6)=2000
 T(7)=1800  T(8)=1600  T(9)=1400  T(10)=1200 T(11)=1000 T(12)=800 ;

END


 HSUB0 =-3.16014290E+00 (KG-MOL)(DEG K)/KG

KG-ATOMS/KG                B0
      C                7.39486629E-03
      H                7.19954345E-03
      S                4.16722872E-05
      N                4.30882562E-02
      O                1.73517959E-02
      SI               1.20364417E-05
      AL               9.94325738E-06
      CA               1.10272364E-05
      FE               2.60952736E-06
      K                2.55750519E-04
      AR               2.56555336E-04
      E                0.00000000E+00
```

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

CHEMICAL FORMULA						WT FRACTION	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
C 1.00000						0.087186	-9445.063	S	300.00	0.0000
H 2.00000						0.005545	13.478	G	300.00	0.0000
S 1.00000						0.001336	14.745	S	300.00	0.0000
N 2.00000						0.001336	12.814	G	300.00	0.0000
O 2.00000						0.018406	12.892	G	300.00	0.0000
H 2.00000	O 1.00000					0.006428	-68284.125	L	300.00	0.0000
SI 1.00000	O 2.00000					0.000723	-217679.188	S	300.00	0.0000
AL 2.00000	O 3.00000					0.000507	-400464.250	S	300.00	0.0000
CA 1.00000	O 1.00000					0.000618	-151768.500	S	300.00	0.0000
FE 2.00000	O 3.00000					0.000208	-197203.750	S	300.00	0.0000
K 2.00000	C 1.00000	O 3.00000				0.017674	-274845.188	S	300.00	0.0000
O 2.00000						0.054618	5426.996	G	1000.00	0.0000
N 1.56176	O 0.41959	AR 0.00932	C 0.00030			0.797369	5152.984	G	1000.00	0.0000
H 2.00000	O 1.00000					0.007973	-51585.422	G	1000.00	0.0000

REACTANT DENSITY = 0.0000

THERMAL PROPERTIES

P, ATM	8.0000	8.0000	8.0000	8.0000	8.0000	8.0000	8.0000	8.0000	8.0000	8.0000	8.0000	8.0000	7.0000
T, DEG K	3000.0	2800.0	2600.0	2400.0	2200.0	2000.0	1800.0	1600.0	1400.0	1200.0	1000.0	800.0	3000.0
RHO, KG/CU M	9.3880-4	1.0276-3	1.1234-3	1.2273-3	1.3426-3	1.4778-3	1.6424-3	1.8482-3	2.1266-3	2.4869-3	2.9855-3	3.7446-3	8.1953-4
H, CAL/G	236.8	70.3	-65.8	-171.9	-252.1	-321.9	-388.9	-454.9	-531.8	-599.8	-663.6	-728.1	247.1
S, CAL/(G)(K)	2.2353	2.1779	2.1276	2.0852	2.0503	2.0171	1.9818	1.9430	1.8915	1.8392	1.7811	1.7090	2.2479
M, MOL WT	28.888	29.513	29.959	30.212	30.295	30.315	30.323	30.331	30.538	30.609	30.622	30.727	28.820
(DLV/DLP)T	-1.01716	-1.01119	-1.00613	-1.00239	-1.00066	-1.00029	-1.00020	-1.00024	-1.00213	-1.00007	-1.00001	-1.00353	-1.01779
(DLV/DLT)P	1.3660	1.2565	1.1499	1.0600	1.0135	1.0034	1.0018	1.0036	1.0397	1.0017	1.0002	1.0636	1.3789
C, CAL/(G)(K)	0.9037	0.7585	0.6010	0.4529	0.3635	0.3393	0.3316	0.3293	0.3707	0.3184	0.3099	0.3740	0.9236
GAMMA (S)	1.1427	1.1480	1.1625	1.1916	1.2265	1.2410	1.2472	1.2502	1.2309	1.2570	1.2650	1.2378	1.1418
SON VEL M/SEC	993.3	951.6	915.9	887.1	860.5	825.1	784.6	740.5	685.0	640.1	586.0	517.6	994.1
SIGMA MHO/M	1.5052 1	7.3816 0	3.1884 0	1.2063 0	3.8965-1	9.8963-2	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.6511 1
BETA	1.0719-1	1.0022-1	9.2925-2	8.5397-2	7.7845-2	7.0164-2	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.2233-1
ELEC NUM DEN	8.777 20	4.603 20	2.145 20	8.829 19	3.128 19	8.816 18	1.857 18	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	8.436 20

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	7.0000	7.0000	7.0000	7.0000	7.0000	7.0000	7.0000	7.0000	7.0000	7.0000	7.0000	6.0000	6.0000
T, DEG K	2800.0	2600.0	2400.0	2200.0	2000.0	1800.0	1600.0	1400.0	1200.0	1000.0	800.0	3000.0	2800.0
RHO, KG/CU M	8.9782-4	9.8214-4	1.0735-3	1.1746-3	1.2930-3	1.4371-3	1.6171-3	1.8603-3	2.1760-3	2.6123-3	3.2750-3	7.0050-4	7.6814-4
H, CAL/G	76.9	-62.2	-170.6	-251.9	-321.8	-388.9	-454.8	-531.3	-599.8	-663.6	-727.6	259.4	84.9
S, CAL/(G)(K)	2.1893	2.1378	2.0945	2.0592	2.0259	1.9906	1.9517	1.9006	1.8479	1.7858	1.7181	2.2627	2.2025
M, MOL WT	29.468	29.933	30.202	30.292	30.314	30.322	30.330	30.529	30.609	30.622	30.713	28.740	29.414
(DLV/DLP)T	-1.01166	-1.00646	-1.00258	-1.00071	-1.00031	-1.00021	-1.00023	-1.00235	-1.00008	-1.00001	-1.00331	-1.01843	-1.01222
(DLV/DLT)P	1.2670	1.1579	1.0650	1.0147	1.0036	1.0019	1.0034	1.0439	1.0019	1.0002	1.0596	1.3912	1.2795
C, CAL/(G)(K)	0.7754	0.6146	0.4619	0.3658	0.3397	0.3316	0.3290	0.3759	0.3188	0.3099	0.3698	0.9410	0.7955
GAMMA (S)	1.1467	1.1606	1.1890	1.2254	1.2408	1.2471	1.2504	1.2290	1.2568	1.2650	1.2394	1.1413	1.1452
SON VEL M/SEC	951.8	915.5	886.3	860.2	825.0	784.6	740.6	684.5	640.0	586.1	518.1	995.2	952.1
SIGMA MHO/M	8.1362 0	3.5220 0	1.3308 0	4.2937-1	1.0908-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.8582 1	9.0894 0
BETA	1.1451-1	1.0624-1	9.7649-2	8.9016-2	8.0232-2	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.4232-1	1.3354-1
ELEC NUM DEN	4.441 20	2.072 20	8.518 19	3.015 19	8.498 18	1.789 18	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	8.161 20	4.254 20

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	6.0000	6.0000	6.0000	6.0000	6.0000	6.0000	6.0000	6.0000	6.0000	6.0000	5.0000	5.0000	5.0000
T, DEG K	2600.0	2400.0	2200.0	2000.0	1800.0	1600.0	1400.0	1200.0	1000.0	800.0	3000.0	2800.0	2600.0
RHO, KG/CU M	8.4097-4	9.1978-4	1.0067-3	1.1082-3	1.2317-3	1.3861-3	1.5939-3	1.8651-3	2.2391-3	2.8058-3	5.8174-4	6.3866-4	6.9990-4
H, CAL/G	-57.9	-169.0	-251.5	-321.8	-388.8	-454.8	-530.6	-599.7	-663.6	-727.2	274.5	94.8	-52.4
S, CAL/(G)(K)	2.1497	2.1053	2.0695	2.0360	2.0007	1.9619	1.9111	1.8579	1.7998	1.7287	2.2803	2.2184	2.1639
M, MOL WT	29.903	30.189	30.289	30.313	30.321	30.329	30.517	30.609	30.622	30.698	28.641	29.347	29.864
(DLV/DLP)T	-1.00685	-1.00282	-1.00077	-1.00033	-1.00022	-1.00023	-1.00265	-1.00009	-1.00001	-1.00302	-1.01934	-1.01290	-1.00733
(DLV/DLT)P	1.1674	1.0711	1.0162	1.0039	1.0020	1.0032	1.0496	1.0022	1.0001	1.0543	1.4097	1.2947	1.1791
C, CAL/(G)(K)	0.6307	0.4730	0.3687	0.3401	0.3317	0.3286	0.3829	0.3193	0.3099	0.3640	0.9693	0.8201	0.6505
GAMMA (S)	1.1584	1.1860	1.2239	1.2406	1.2471	1.2506	1.2265	1.2565	1.2650	1.2417	1.1401	1.1435	1.1559
SON VEL M/SEC	915.1	885.4	859.7	824.9	784.6	740.6	684.0	640.0	586.1	518.7	996.4	952.4	914.7
SIGMA MHO/M	3.9464 0	1.4896 0	4.7999-1	1.2200-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	2.1379 1	1.0339 1	4.5079 0
BETA	1.2400-1	1.1399-1	1.0392-1	9.3667-2	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.7003-1	1.6010-1	1.4885-1
ELEC NUM DEN	1.989 20	8.168 19	2.887 19	8.141 18	1.714 18	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	7.859 20	4.036 20	1.893 20

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	5.0000	5.0000	5.0000	5.0000	5.0000	5.0000	5.0000	5.0000	5.0000	4.0000	4.0000	4.0000	4.0000
T, DEG K	2400.0	2200.0	2000.0	1800.0	1600.0	1400.0	1200.0	1000.0	800.0	3000.0	2800.0	2600.0	2400.0
RHO, KG/CU M	7.6607-4	8.3830-4	9.2348-4	1.0264-3	1.1550-3	1.3276-3	1.5542-3	1.8656-3	2.3370-3	4.6333-4	5.0941-4	5.5897-4	6.1240-4
H, CAL/G	-166.8	-251.1	-321.7	-383.8	-454.7	-529.7	-599.7	-663.5	-726.7	294.1	107.7	-45.2	-163.8
S, CAL/(G)(K)	2.7182	2.0816	2.0480	2.0127	1.9739	1.9236	1.8693	1.8118	1.7411	2.3024	2.2381	2.1815	2.1342
M, MOL WT	30.173	30.284	30.311	30.320	30.328	30.501	30.608	30.616	30.682	28.514	29.260	29.813	30.151
(DLV/DLP)T	-1.00312	-1.00085	-1.00035	-1.00023	-1.00023	-1.00308	-1.00311	-1.00100	-1.00262	-1.02049	-1.01376	-1.00794	-1.00353
(DLV/DLT)P	1.0790	1.0181	1.0043	1.0021	1.0030	1.0578	1.0027	1.0126	1.0472	1.4332	1.3142	1.1940	1.0895
C, CAL/(G)(K)	0.4872	0.3726	0.3407	0.3317	0.3283	0.3930	0.3200	0.3200	0.3561	1.0056	0.8516	0.6759	0.5063
GAMMA (S)	1.1824	1.2221	1.2402	1.2471	1.2509	1.2231	1.2561	1.2610	1.2451	1.1388	1.1415	1.1529	1.1779
SON VEL M/SEC	884.3	859.1	824.9	784.6	740.7	683.2	639.9	585.2	519.5	998.1	953.0	914.3	882.9
SIGMA MHO/M	1.6991 0	5.4717-1	1.3917-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	2.5214 1	1.2062 1	5.2922 0	1.9951 0
BETA	1.3689-1	1.2480-1	1.1249-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	2.1114-1	1.9978-1	1.8609-1	1.7126-1
ELEC NUM DEN	7.758 19	2.740 19	7.732 18	1.628 18	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	7.464 20	3.774 20	1.777 20	7.281 19

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	3.0000	3.0000	3.0000	3.0000	3.0000
T, DEG K	2200.0	2000.0	1800.0	1600.0	1400.0	1200.0	1000.0	800.0	3000.0	2800.0	2600.0	2400.0	2200.0
RHO, KG/CU M	6.7091-4	7.3873-4	8.2107-4	9.2395-4	1.0612-3	1.2434-3	1.4922-3	1.8686-3	3.4538-4	3.8048-4	4.1822-4	4.5830-4	5.0303-4
H, CAL/G	-250.4	-321.5	-383.7	-454.6	-528.4	-599.7	-663.3	-726.2	321.2	125.6	-35.1	-159.4	-249.5
S, CAL/(G)(K)	2.0966	2.0627	2.0273	1.9885	1.9391	1.8843	1.8264	1.7562	2.3315	2.2641	2.2047	2.1550	2.1159
M, MOL WT	30.278	30.308	30.318	30.326	30.478	30.607	30.612	30.666	28.340	29.139	29.742	30.118	30.269
(DLV/DLP)T	-1.00096	-1.00038	-1.00025	-1.00023	-1.00375	-1.00014	-1.00001	-1.00211	-1.02208	-1.01493	-1.00877	-1.00411	-1.00112
(DLV/DLT)P	1.0209	1.0047	1.0022	1.0028	1.0706	1.0033	1.0001	1.0380	1.4653	1.3406	1.2142	1.1048	1.0251
C, CAL/(G)(K)	0.3780	0.3416	0.3319	0.3279	0.4086	0.3210	0.3098	0.3458	1.0552	0.8946	0.7104	0.5338	0.3863
GAMMA (S)	1.2195	1.2398	1.2471	1.2511	1.2182	1.2554	1.2652	1.2497	1.1571	1.1390	1.1493	1.1720	1.2158
SON VEL M/SEC	858.3	824.7	784.6	740.8	682.1	639.7	586.2	520.6	1000.4	953.9	914.0	881.2	857.1
SIGMA MHO/M	6.4152-1	1.6333-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	3.0352 1	1.4628 1	6.4804 0	2.4477 0	7.8591-1
BETA	1.5616-1	1.4077-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	2.7849-1	2.6549-1	2.4805-1	2.2857-1	2.0849-1
ELEC NUM DEN	2.568 19	7.252 18	1.527 18	2.096 17	0.0000 0	0.0000 0	0.0000 0	0.0000 0	6.924 20	3.444 20	1.633 20	6.693 19	2.356 19

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000
T, DEG K	2000.0	1800.0	1600.0	1400.0	1200.0	1000.0	800.0	3000.0	2800.0	2600.0	2400.0	2200.0	2000.0
RHO, KG/CU M	5.5398-4	6.1576-4	6.9292-4	7.9494-4	9.3247-4	1.1192-3	1.4007-3	2.2809-4	2.5203-4	2.7775-4	3.0530-4	3.3518-4	3.6925-4
H, CAL/G	-321.3	-388.7	-454.6	-526.3	-599.6	-663.3	-725.7	363.2	153.6	-18.9	-151.9	-247.8	-321.0
S, CAL/(G)(K)	2.0817	2.0462	2.0074	1.9594	1.9031	1.8450	1.7754	2.3741	2.3018	2.2380	2.1849	2.1433	2.1084
M, MOL WT	30.305	30.316	30.324	30.440	30.606	30.612	30.650	28.074	28.953	29.629	30.062	30.254	30.299
(DLV/DLP)T	-1.00042	-1.00027	-1.00024	-1.00492	-1.00019	-1.00000	-1.00149	-1.02451	-1.01671	-1.01001	-1.00505	-1.00139	-1.00048
(DLV/DLT)P	1.0054	1.0024	1.0027	1.0925	1.0045	1.0001	1.0268	1.5141	1.3805	1.2447	1.1297	1.0326	1.0066
C, CAL/(G)(K)	0.3428	0.3321	0.3276	0.4354	0.3227	0.3098	0.3331	1.1310	0.9601	0.7629	0.5788	0.4010	0.3451
GAMMA (S)	1.2390	1.2470	1.2514	1.2107	1.2544	1.2652	1.2558	1.1350	1.1358	1.1444	1.1637	1.2096	1.2378
SON VEL M/SEC	824.5	784.6	740.9	680.4	639.5	586.2	522.1	1004.2	955.6	913.8	878.9	855.2	824.2
SIGMA MHO/M	2.0043-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	4.0172 1	1.8979 1	8.5464 0	3.2480 0	1.0420 0	2.6654-1
BETA	1.8797-1	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	4.0958-1	3.9535-1	3.7144-1	3.4321-1	3.1331-1	2.8258-1
ELEC NUM DEN	6.665 18	1.405 18	1.937 17	0.0000 0	0.0000 0	0.0000 0	0.0000 0	6.130 20	3.001 20	1.438 20	5.915 19	2.079 19	5.895 18

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
T, DEG K	1800.0	1600.0	1400.0	1200.0	1000.0	800.0	3000.0	2800.0	2600.0	2400.0	2200.0	2000.0	1800.0
RHO, KG/CU M	4.1046-4	4.6190-4	5.2898-4	6.2159-4	7.4612-4	9.3338-4	1.1194-4	1.2442-4	1.3781-4	1.5207-4	1.6740-4	1.8456-4	2.0518-4
H, CAL/G	-388.5	-454.4	-523.1	-599.4	-663.3	-725.3	446.4	209.7	14.3	-136.2	-243.7	-320.3	-388.3
S, CAL/(G)(K)	2.0729	2.0341	1.9882	1.9296	1.8714	1.8022	2.4513	2.3697	2.2974	2.2374	2.1907	2.1543	2.1185
M, MOL WT	30.312	30.321	30.384	30.603	30.611	30.635	27.557	28.586	29.400	29.947	30.219	30.288	30.305
(DLV/DLP)T	-1.00031	-1.00025	-1.00115	-1.00028	-1.00000	-1.00081	-1.02931	-1.02018	-1.01238	-1.00621	-1.00203	-1.00061	-1.00033
(DLV/DLT)P	1.0028	1.0026	1.0250	1.0067	1.0001	1.0146	1.6086	1.4579	1.3032	1.1613	1.0507	1.0094	1.0034
C, CAL/(G)(K)	0.3324	0.3272	0.3563	0.3262	0.3098	0.3191	1.2794	1.0879	0.8643	0.6382	0.4368	0.3506	0.3332
GAMMA (S)	1.2469	1.2517	1.2372	1.2523	1.2651	1.2633	1.1319	1.1307	1.1369	1.1547	1.1964	1.2347	1.2466
SON VEL M/SEC	784.6	741.0	688.4	639.0	586.2	523.7	1012.2	959.6	914.3	877.2	851.0	823.3	784.6
SIGMA MHO/M	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	5.9911 1	2.8689 1	1.3365 1	5.1844 0	1.6677 0	4.2950-1	0.0000 0
BETA	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	7.8206-1	7.7423-1	7.3699-1	6.8647-1	6.2841-1	5.6750-1	0.0000 0
ELEC NUM DEN	1.246 18	1.729 17	0.0000 0	0.0000 0	0.0000 0	0.0000 0	4.788 20	2.316 20	1.133 20	4.720 19	1.659 19	4.730 18	1.007 18

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	1.0000	1.0000	1.0000	1.0000	1.0000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000
T, DEG K	1600.0	1400.0	1200.0	1000.0	800.0	3000.0	2800.0	2600.0	2400.0	2200.0	2000.0	1800.0	1600.0
RHO, KG/CU M	2.3091-4	2.6416-4	3.1063-4	3.7306-4	4.6654-4	5.4740-5	6.1263-5	6.8251-5	7.5661-5	8.3555-5	9.2234-5	1.0256-4	1.1543-4
H, CAL/G	-454.2	-520.6	-598.6	-663.3	-725.0	546.8	277.6	55.4	-115.7	-237.3	-319.3	-388.0	-454.0
S, CAL/(G)(K)	2.0796	2.0353	1.9753	1.9164	1.8476	2.5353	2.4426	2.3603	2.2920	2.2392	2.2003	2.1641	2.1252
M, MOL WT	30.316	30.347	30.586	30.611	30.626	26.951	28.151	29.122	29.800	30.167	30.273	30.296	30.309
(DLV/DLP)T	-1.00029	-1.00254	-1.00101	-1.00000	-1.00024	-1.03501	-1.02424	-1.01514	-1.00797	-1.00294	-1.00077	-1.00044	-1.00035
(DLV/DLT)P	1.0028	1.0558	1.0197	1.0001	1.0042	1.7180	1.5451	1.3712	1.2092	1.0775	1.0137	1.0042	1.0031
C, CAL/(G)(K)	0.3270	0.4017	0.3420	0.3099	0.3073	1.4540	1.2308	0.9835	0.7270	0.4898	0.3595	0.3342	0.3271
GAMMA (S)	1.2520	1.2183	1.2445	1.2651	1.2701	1.1295	1.1270	1.1303	1.1444	1.1809	1.2297	1.2461	1.2521
SON VEL M/SEC	741.2	683.6	637.2	586.2	525.2	1022.4	965.4	916.0	875.4	846.2	821.9	784.6	741.3
SIGMA MHO/M	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	8.4432 1	4.2799 1	2.0177 1	8.0746 0	2.6278 0	6.8051-1	0.0000 0	0.0000 0
BETA	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.4708 0	1.4903 0	1.4493 0	1.3675 0	1.2591 0	1.1397 0	0.0000 0	0.0000 0
ELEC NUM DEN	1.415 17	0.0000 0	0.0000 0	0.0000 0	0.0000 0	3.588 20	1.795 20	8.701 19	3.690 19	1.304 19	3.732 18	8.048 17	1.148 17

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

THERMAL PROPERTIES

P, ATM	0.5000	0.5000	0.5000	0.5000
T, DEG K	1400.0	1200.0	1000.0	800.0
RHO, KG/CU M	1.3199-4	1.5519-4	1.8653-4	2.3325-4
H, CAL/G	-519.2	-597.3	-663.3	-724.9
S, CAL/(G)(K)	2.0817	2.0214	1.9614	1.8927
M, MOL WT	30.325	30.562	30.611	30.623
(DLV/DLP)T	-1.00038	-1.00139	-1.00001	-1.00006
(DLV/DLT)P	1.0061	1.0296	1.0002	1.0011
C, CAL/(G)(K)	0.3273	0.3580	0.3101	0.3038
GAMMA (S)	1.2536	1.2363	1.2649	1.2723
SON VEL M/SEC	693.7	635.3	586.1	525.7
SIGMA MHO/M	0.0000 0	0.0000 0	0.0000 0	0.0000 0
BETA	0.0000 0	0.0000 0	0.0000 0	0.0000 0
ELEC NUM DEN	0.0000 0	0.0000 0	0.0000 0	0.0000 0

THERMODYNAMIC PROPERTIES SUMMARY

P	T	MW	H	S	RHO	CP	GAM	NU TOT	SIG	NE
8.0000E+00	3.0000E+03	2.8888E+01	9.9082E+05	9.3525E+03	9.3880E-01	3.7813E+03	1.1427E+00	1.6431E+12	1.5052E+01	8.7772E+00
8.0000E+00	2.8000E+03	2.9513E+01	2.9423E+05	9.1124E+03	1.0276E+00	3.1737E+03	1.1480E+00	1.7533E+12	7.3816E+00	4.6034E+00
8.0000E+00	2.6000E+03	2.9959E+01	-2.7520E+05	8.9017E+03	1.1234E+00	2.5146E+03	1.1625E+00	1.8902E+12	3.1884E+00	2.1445E+00
8.0000E+00	2.4000E+03	3.0212E+01	-7.1941E+05	8.7243E+03	1.2273E+00	1.8951E+03	1.1916E+00	2.0596E+12	1.2063E+00	8.8287E-01
8.0000E+00	2.2000E+03	3.0295E+01	-1.0549E+06	8.5786E+03	1.3426E+00	1.5211E+03	1.2265E+00	2.2650E+12	3.8965E-01	3.1285E-01
8.0000E+00	2.0000E+03	3.0315E+01	-1.3468E+06	8.4395E+03	1.4778E+00	1.4197E+03	1.2410E+00	2.5214E+12	9.8963E-02	8.8156E-02
8.0000E+00	1.8000E+03	3.0323E+01	-1.6272E+06	8.2919E+03	1.6424E+00	1.3873E+03	1.2472E+00	7.8455E+02	0.0000E+00	0.0000E+00
8.0000E+00	1.6000E+03	3.0331E+01	-1.9032E+06	8.1293E+03	1.8482E+00	1.3778E+03	1.2502E+00	7.4050E+02	0.0000E+00	0.0000E+00
8.0000E+00	1.4000E+03	3.0338E+01	-2.2249E+06	7.9142E+03	2.1266E+00	1.5512E+03	1.2309E+00	6.8498E+02	0.0000E+00	0.0000E+00
8.0000E+00	1.2000E+03	3.0609E+01	-2.5095E+06	7.6954E+03	2.4869E+00	1.3324E+03	1.2570E+00	6.4010E+02	0.0000E+00	0.0000E+00
8.0000E+00	1.0000E+03	3.0622E+01	-2.7766E+06	7.4521E+03	2.9855E+00	1.2967E+03	1.2650E+00	5.8605E+02	0.0000E+00	0.0000E+00
8.0000E+00	8.0000E+02	3.0727E+01	-3.0462E+06	7.1503E+03	3.7446E+00	1.5647E+03	1.2378E+00	5.1763E+02	0.0000E+00	0.0000E+00
7.0000E+00	3.0000E+03	2.8820E+01	1.0338E+06	9.4053E+03	8.1953E-01	3.8645E+03	1.1418E+00	1.4394E+12	1.6511E+01	8.4363E+00
7.0000E+00	2.8000E+03	2.9468E+01	3.2182E+05	9.1599E+03	8.9782E-01	3.2444E+03	1.1467E+00	1.5344E+12	8.1362E+00	4.4407E+00
7.0000E+00	2.6000E+03	2.9933E+01	-2.6037E+05	8.9445E+03	9.8214E-01	2.5714E+03	1.1606E+00	1.6532E+12	3.5220E+00	2.0719E+00
7.0000E+00	2.4000E+03	3.0202E+01	-7.1390E+05	8.7633E+03	1.0735E+00	1.9326E+03	1.1890E+00	1.8012E+12	1.3308E+00	8.5181E-01
7.0000E+00	2.2000E+03	3.0292E+01	-1.0538E+06	8.6157E+03	1.1746E+00	1.5306E+03	1.2254E+00	1.9808E+12	4.2937E-01	3.0148E-01
7.0000E+00	2.0000E+03	3.0314E+01	-1.3465E+06	8.4763E+03	1.2930E+00	1.4212E+03	1.2408E+00	2.2050E+12	1.0908E-01	8.4977E-02
7.0000E+00	1.8000E+03	3.0322E+01	-1.6270E+06	8.3286E+03	1.4371E+00	1.3874E+03	1.2471E+00	7.8456E+02	0.0000E+00	0.0000E+00
7.0000E+00	1.6000E+03	3.0330E+01	-1.9030E+06	8.1661E+03	1.6171E+00	1.3764E+03	1.2504E+00	7.4057E+02	0.0000E+00	0.0000E+00
7.0000E+00	1.4000E+03	3.0529E+01	-2.2228E+06	7.9521E+03	1.8603E+00	1.5726E+03	1.2290E+00	6.8455E+02	0.0000E+00	0.0000E+00
7.0000E+00	1.2000E+03	3.0609E+01	-2.5095E+06	7.7317E+03	2.1760E+00	1.3339E+03	1.2568E+00	6.4005E+02	0.0000E+00	0.0000E+00
7.0000E+00	1.0000E+03	3.0622E+01	-2.7766E+06	7.4884E+03	2.6123E+00	1.2966E+03	1.2650E+00	5.8605E+02	0.0000E+00	0.0000E+00
7.0000E+00	8.0000E+02	3.0713E+01	-3.0444E+06	7.1887E+03	3.2750E+00	1.5471E+03	1.2394E+00	5.1809E+02	0.0000E+00	0.0000E+00
6.0000E+00	3.0000E+03	2.8740E+01	1.0852E+06	9.4669E+03	7.0050E-01	3.9370E+03	1.1413E+00	1.2369E+12	1.8532E+01	8.1608E+00
6.0000E+00	2.8000E+03	2.9414E+01	3.5513E+05	9.2153E+03	7.6814E-01	3.3284E+03	1.1452E+00	1.3158E+12	9.0894E+00	4.2543E+00
6.0000E+00	2.6000E+03	2.9903E+01	-2.4225E+05	8.9943E+03	8.4097E-01	2.6389E+03	1.1584E+00	1.4165E+12	3.9464E+00	1.9892E+00
6.0000E+00	2.4000E+03	3.0189E+01	-7.0697E+05	8.8037E+03	9.1978E-01	1.9791E+03	1.1860E+00	1.5429E+12	1.4896E+00	8.1676E-01
6.0000E+00	2.2000E+03	3.0289E+01	-1.0523E+06	8.6587E+03	1.0067E+00	1.5427E+03	1.2239E+00	1.6967E+12	4.7999E-01	2.8869E-01
6.0000E+00	2.0000E+03	3.0313E+01	-1.3462E+06	8.5187E+03	1.1082E+00	1.4232E+03	1.2406E+00	1.8887E+12	1.2200E-01	8.1407E-02
6.0000E+00	1.8000E+03	3.0321E+01	-1.6269E+06	8.3709E+03	1.2317E+00	1.3877E+03	1.2471E+00	7.8457E+02	0.0000E+00	0.0000E+00
6.0000E+00	1.6000E+03	3.0329E+01	-1.9028E+06	8.2085E+03	1.3861E+00	1.3750E+03	1.2505E+00	7.4065E+02	0.0000E+00	0.0000E+00
6.0000E+00	1.4000E+03	3.0517E+01	-2.2200E+06	7.9960E+03	1.5939E+00	1.6020E+03	1.2265E+00	6.8398E+02	0.0000E+00	0.0000E+00
6.0000E+00	1.2000E+03	3.0609E+01	-2.5094E+06	7.7736E+03	1.8651E+00	1.3360E+03	1.2565E+00	6.3997E+02	0.0000E+00	0.0000E+00
6.0000E+00	1.0000E+03	3.0622E+01	-2.7766E+06	7.5303E+03	2.2391E+00	1.2965E+03	1.2650E+00	5.8605E+02	0.0000E+00	0.0000E+00
6.0000E+00	8.0000E+02	3.0693E+01	-3.0425E+06	7.2328E+03	2.8053E+00	1.5220E+03	1.2417E+00	5.1871E+02	0.0000E+00	0.0000E+00
5.0000E+00	3.0000E+03	2.8641E+01	1.1486E+06	9.5409E+03	5.8174E-01	4.0557E+03	1.1401E+00	1.0348E+12	2.1379E+01	7.8587E+00
5.0000E+00	2.8000E+03	2.9347E+01	3.9660E+05	9.2818E+03	6.3866E-01	3.4315E+03	1.1435E+00	1.0974E+12	1.0339E+01	4.0361E+00
5.0000E+00	2.6000E+03	2.9864E+01	-2.1941E+05	9.0533E+03	6.9993E-01	2.7219E+03	1.1559E+00	1.1800E+12	4.5079E+00	1.8929E+00
5.0000E+00	2.4000E+03	3.0173E+01	-6.9793E+05	8.8627E+03	7.6607E-01	2.0386E+03	1.1824E+00	1.2849E+12	1.6991E+00	7.7578E-01
5.0000E+00	2.2000E+03	3.0284E+01	-1.0505E+06	8.7096E+03	8.3380E-01	1.5538E+03	1.2221E+00	1.4128E+12	5.4717E-01	2.7402E-01
5.0000E+00	2.0000E+03	3.0311E+01	-1.3455E+06	8.5689E+03	9.2343E-01	1.4257E+03	1.2402E+00	1.5725E+12	1.3917E-01	7.7322E-02
5.0000E+00	1.8000E+03	3.0320E+01	-1.6267E+06	8.4210E+03	1.0264E+00	1.3880E+03	1.2471E+00	7.8453E+02	0.0000E+00	0.0000E+00
5.0000E+00	1.6000E+03	3.0328E+01	-1.9025E+06	8.2586E+03	1.1550E+00	1.3736E+03	1.2509E+00	7.4073E+02	0.0000E+00	0.0000E+00
5.0000E+00	1.4000E+03	3.0501E+01	-2.2163E+06	8.0483E+03	1.3276E+00	1.6444E+03	1.2231E+00	6.8320E+02	0.0000E+00	0.0000E+00
5.0000E+00	1.2000E+03	3.0608E+01	-2.5092E+06	7.8233E+03	1.5542E+00	1.3388E+03	1.2561E+00	6.3987E+02	0.0000E+00	0.0000E+00
5.0000E+00	1.0000E+03	3.0616E+01	-2.7759E+06	7.5804E+03	1.8656E+00	1.3388E+03	1.2610E+00	5.8519E+02	0.0000E+00	0.0000E+00
5.0000E+00	8.0000E+02	3.0682E+01	-3.0405E+06	7.2847E+03	2.3370E+00	1.4899E+03	1.2451E+00	5.1953E+02	0.0000E+00	0.0000E+00

4.0000E+00	3.0000E+03	2.8514E+01	1.2307E+06	9.6332E+03	4.6333E-01	4.2075E+03	1.1300E+00	8.3292E+11	2.5214E+01	7.4641E+00
4.0000E+00	2.8000E+03	2.9260E+01	4.5056E+05	9.3643E+03	5.0941E-01	3.5633E+03	1.1415E+00	8.7933E+11	1.2062E+01	3.7735E+00
4.0000E+00	2.6000E+03	2.9313E+01	-1.8926E+05	9.1276E+03	5.5897E-01	2.8238E+03	1.1529E+00	9.4337E+11	5.2922E+00	1.7774E+00
4.0000E+00	2.4000E+03	3.0151E+01	-6.8550E+05	8.9294E+03	6.1240E-01	2.1134E+03	1.1779E+00	1.0270E+12	1.9951E+00	7.2311E-01
4.0000E+00	2.2000E+03	3.0278E+01	-1.0478E+06	8.7721E+03	6.7091E-01	1.5014E+03	1.2195E+00	1.1291E+12	6.4152E-01	2.5676E-01
4.0000E+00	2.0000E+03	3.0300E+01	-1.3453E+06	8.6304E+03	7.3573E-01	1.4291E+03	1.2350E+00	1.2536E+12	1.6333E-01	7.2521E-02
4.0000E+00	1.8000E+03	3.0310E+01	-1.6235E+06	8.4923E+03	8.2107E-01	1.3035E+03	1.2471E+00	7.8459E+02	0.0000E+00	0.0000E+00
4.0000E+00	1.6000E+03	3.0326E+01	-1.9022E+06	8.3200E+03	9.2395E-01	1.3721E+03	1.2511E+00	7.4032E+02	0.0000E+00	0.0000E+00
4.0000E+00	1.4000E+03	3.0478E+01	-2.2109E+06	8.1131E+03	1.0612E+00	1.7038E+03	1.2102E+00	6.8200E+02	0.0000E+00	0.0000E+00
4.0000E+00	1.2000E+03	3.0607E+01	-2.5090E+06	7.8971E+03	1.2434E+00	1.3432E+03	1.2554E+00	6.3271E+02	0.0000E+00	0.0000E+00
4.0000E+00	1.0000E+03	3.0612E+01	-2.7754E+06	7.6415E+03	1.4922E+00	1.2961E+03	1.2652E+00	5.8620E+02	0.0000E+00	0.0000E+00
4.0000E+00	8.0000E+02	3.0666E+01	-3.0335E+06	7.3478E+03	1.8606E+00	1.4482E+03	1.2497E+00	5.2863E+02	0.0000E+00	0.0000E+00
3.0000E+00	3.0000E+03	2.8340E+01	1.3440E+06	9.7551E+03	3.4520E-01	4.4150E+03	1.1371E+00	6.3104E+11	3.0352E+01	6.9240E+00
3.0000E+00	2.8000E+03	2.9139E+01	5.2561E+05	9.4731E+03	3.8048E-01	3.7431E+03	1.1393E+00	6.6163E+11	1.4823E+01	3.4438E+00
3.0000E+00	2.6000E+03	2.9742E+01	-1.4665E+05	9.2243E+03	4.1822E-01	2.9725E+03	1.1493E+00	7.0313E+11	6.4804E+00	1.6329E+00
3.0000E+00	2.4000E+03	3.0118E+01	-6.6702E+05	9.0164E+03	4.5000E-01	2.2331E+03	1.1720E+00	7.6954E+11	2.4477E+00	6.6933E-01
3.0000E+00	2.2000E+03	3.0269E+01	-1.0439E+06	8.8529E+03	5.0303E-01	1.6181E+03	1.2153E+00	8.4571E+11	7.8591E-01	2.3560E-01
3.0000E+00	2.0000E+03	3.0305E+01	-1.3445E+06	8.7098E+03	5.5390E-01	1.4344E+03	1.2390E+00	9.4106E+11	2.0043E-01	6.6647E-02
3.0000E+00	1.8000E+03	3.0316E+01	-1.6261E+06	8.5614E+03	6.1576E-01	1.3893E+03	1.2470E+00	7.8430E+02	0.0000E+00	0.0000E+00
3.0000E+00	1.6000E+03	3.0324E+01	-1.9019E+06	8.3991E+03	6.9292E-01	1.3706E+03	1.2514E+00	7.4093E+02	0.0000E+00	0.0000E+00
3.0000E+00	1.4000E+03	3.0440E+01	-2.2020E+06	8.1930E+03	7.9494E-01	1.8217E+03	1.2107E+00	6.8041E+02	0.0000E+00	0.0000E+00
3.0000E+00	1.2000E+03	3.0606E+01	-2.5086E+06	7.9625E+03	9.3247E-01	1.3504E+03	1.2544E+00	6.3946E+02	0.0000E+00	0.0000E+00
3.0000E+00	1.0000E+03	3.0612E+01	-2.7754E+06	7.7197E+03	1.1192E+00	1.2961E+03	1.2652E+00	5.8620E+02	0.0000E+00	0.0000E+00
3.0000E+00	8.0000E+02	3.0650E+01	-3.0365E+06	7.4203E+03	1.4007E+00	1.3936E+03	1.2553E+00	5.2205E+02	0.0000E+00	0.0000E+00
2.0000E+00	3.0000E+03	2.8074E+01	1.5195E+06	9.9331E+03	2.2809E-01	4.7323E+03	1.1358E+00	4.2882E+11	4.0172E+01	6.1302E+00
2.0000E+00	2.8000E+03	2.8953E+01	6.4269E+05	9.6309E+03	2.5203E-01	4.0172E+03	1.1383E+00	4.4426E+11	1.8979E+01	3.0003E+00
2.0000E+00	2.6000E+03	2.9629E+01	-7.8959E+04	9.3639E+03	2.7775E-01	3.1920E+03	1.1444E+00	4.7293E+11	8.5464E+00	1.4381E+00
2.0000E+00	2.4000E+03	3.0062E+01	-6.3559E+05	9.1416E+03	3.0530E-01	2.4217E+03	1.1637E+00	5.1233E+11	3.2400E+00	5.9149E-01
2.0000E+00	2.2000E+03	3.0254E+01	-1.0336E+06	8.9675E+03	3.3518E-01	1.6778E+03	1.2096E+00	5.6279E+11	1.0420E+00	2.0786E-01
2.0000E+00	2.0000E+03	3.0299E+01	-1.3431E+06	8.8217E+03	3.6925E-01	1.4437E+03	1.2378E+00	6.2594E+11	2.6654E-01	5.8952E-02
2.0000E+00	1.8000E+03	3.0312E+01	-1.6256E+06	8.6729E+03	4.1046E-01	1.3907E+03	1.2469E+00	7.8461E+02	0.0000E+00	0.0000E+00
2.0000E+00	1.6000E+03	3.0321E+01	-1.9014E+06	8.5105E+03	4.6190E-01	1.3692E+03	1.2517E+00	7.4105E+02	0.0000E+00	0.0000E+00
2.0000E+00	1.4000E+03	3.0384E+01	-2.1805E+06	8.3134E+03	5.2838E-01	1.4906E+03	1.2372E+00	6.8044E+02	0.0000E+00	0.0000E+00
2.0000E+00	1.2000E+03	3.0503E+01	-2.5079E+06	8.0733E+03	6.2158E-01	1.3643E+03	1.2523E+00	6.3396E+02	0.0000E+00	0.0000E+00
2.0000E+00	1.0000E+03	3.0611E+01	-2.7754E+06	7.8293E+03	7.4612E-01	1.2952E+03	1.2651E+00	5.8619E+02	0.0000E+00	0.0000E+00
2.0000E+00	8.0000E+02	3.0536E+01	-3.0347E+06	7.5405E+03	9.3320E-01	1.3355E+03	1.2633E+00	5.2371E+02	0.0000E+00	0.0000E+00

1.0000E+00	3.0000E+03	2.7557E+01	1.8676E+06	1.0256E+04	1.1194E-01	5.3530E+03	1.1319E+00	2.2498E+11	5.9911E+01	4.7881E+00
1.0000E+00	2.8000E+03	2.8536E+01	8.7723E+05	9.9150E+03	1.2442E-01	4.5513E+03	1.1307E+00	2.2691E+11	2.8609E+01	2.3160E+00
1.0000E+00	2.6000E+03	2.9400E+01	5.9767E+04	9.6125E+03	1.3781E-01	3.6163E+03	1.1359E+00	2.3045E+11	1.3335E+01	1.1334E+00
1.0000E+00	2.4000E+03	2.9947E+01	-5.6969E+05	9.3611E+03	1.5207E-01	2.6704E+03	1.1547E+00	2.5632E+11	5.1844E+00	4.7203E-01
1.0000E+00	2.2000E+03	3.0219E+01	-1.0196E+06	9.1659E+03	1.6740E-01	1.8277E+03	1.1964E+00	2.8063E+11	1.6677E+00	1.6597E-01
1.0000E+00	2.0000E+03	3.0288E+01	-1.3401E+06	9.0134E+03	1.8456E-01	1.4667E+03	1.2347E+00	3.1167E+11	4.2950E-01	4.7303E-02
1.0000E+00	1.8000E+03	3.0305E+01	-1.6246E+06	8.8636E+03	2.0513E-01	1.3939E+03	1.2486E+00	7.8460E+02	0.0000E+00	0.0000E+00
1.0000E+00	1.6000E+03	3.0316E+01	-1.9006E+06	8.7011E+03	2.3091E-01	1.3683E+03	1.2520E+00	7.4120E+02	0.0000E+00	0.0000E+00
1.0000E+00	1.4000E+03	3.0347E+01	-2.1782E+06	8.5156E+03	2.6416E-01	1.6809E+03	1.2133E+00	6.8359E+02	0.0000E+00	0.0000E+00
1.0000E+00	1.2000E+03	3.0586E+01	-2.5045E+06	8.2645E+03	3.1063E-01	1.4319E+03	1.2465E+00	6.3715E+02	0.0000E+00	0.0000E+00
1.0000E+00	1.0000E+03	3.0611E+01	-2.7754E+06	8.0131E+03	3.7306E-01	1.2966E+03	1.2351E+00	5.8617E+02	0.0000E+00	0.0000E+00
1.0000E+00	8.0000E+02	3.0626E+01	-3.0334E+06	7.7303E+03	4.6654E-01	1.2859E+03	1.2701E+00	5.2522E+02	0.0000E+00	0.0000E+00
5.0000E-01	3.0000E+03	2.6951E+01	2.2377E+06	1.0309E+04	5.4740E-02	6.0037E+03	1.1295E+00	1.2078E+11	8.4432E+01	3.5930E+00
5.0000E-01	2.8000E+03	2.8151E+01	1.1616E+06	1.0220E+04	6.1263E-02	5.1495E+03	1.1270E+00	1.1320E+11	4.2799E+01	1.7919E+00
5.0000E-01	2.6000E+03	2.9122E+01	2.3198E+05	9.8757E+03	6.8251E-02	4.1149E+03	1.1303E+00	1.2140E+11	2.0177E+01	8.7013E-01
5.0000E-01	2.4000E+03	2.9800E+01	-4.8418E+05	9.5896E+03	7.5861E-02	3.0420E+03	1.1444E+00	1.2875E+11	8.0746E+00	3.6904E-01
5.0000E-01	2.2000E+03	3.0167E+01	-9.9304E+05	9.3603E+03	8.3555E-02	2.0493E+03	1.1809E+00	1.4011E+11	2.6273E+00	1.3045E-01
5.0000E-01	2.0000E+03	3.0273E+01	-1.3358E+06	9.2059E+03	9.2234E-02	1.5043E+03	1.2297E+00	1.5519E+11	6.8051E-01	3.7313E-02
5.0000E-01	1.8000E+03	3.0296E+01	-1.6233E+06	9.0546E+03	1.0256E-01	1.3933E+03	1.2461E+00	7.8455E+02	0.0000E+00	0.0000E+00
5.0000E-01	1.6000E+03	3.0309E+01	-1.8997E+06	8.8913E+03	1.1543E-01	1.3687E+03	1.2521E+00	7.4132E+02	0.0000E+00	0.0000E+00
5.0000E-01	1.4000E+03	3.0325E+01	-2.1724E+06	8.7097E+03	1.3199E-01	1.3692E+03	1.2535E+00	6.9368E+02	0.0000E+00	0.0000E+00
5.0000E-01	1.2000E+03	3.0562E+01	-2.4991E+06	8.4575E+03	1.5519E-01	1.4979E+03	1.2363E+00	6.3530E+02	0.0000E+00	0.0000E+00
5.0000E-01	1.0000E+03	3.0611E+01	-2.7753E+06	8.2064E+03	1.8653E-01	1.2975E+03	1.2649E+00	5.2614E+02	0.0000E+00	0.0000E+00
5.0000E-01	8.0000E+02	3.0623E+01	-3.0330E+06	7.9109E+03	2.3325E-01	1.2709E+03	1.2723E+00	5.2570E+02	0.0000E+00	0.0000E+00