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CALCULATION OF SUPERSONIC STREAM PARAMETERS OF A REAL GAS FROM MEASURABLE QUANTITIES USING FORTRAN IV ROUTINES

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16. Abstract

Two sets of routines are presented that calculate such real-gas supersonic stream properties as velocity, density, enthalpy, entropy, and isentropic exponent. Two alternative sets of measurements are assumed: (1) stagnation pressure, stagnation temperature, and the pressure on the surface of a static-pressure wedge; or (2) pressure and temperature in a plenum upstream of a supersonic nozzle and the stagnation pressure at the exit of this nozzle. The routines are applicable to any gas whose properties are known. Explicit routines are presented for determining these properties for air, nitrogen, oxygen, normal hydrogen, parahydrogen, helium, argon, steam, methane, and natural gas.

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SUMMARY

Two sets of FORTRAN IV routines are presented that calculate flow and thermodynamic properties of a supersonic stream from measurable quantities. These flow and thermodynamic properties include velocity, density, enthalpy, entropy, and isentropic exponent, both in the free stream and behind the normal shock. Two sets of measurements are considered. For one set, these measurements are the stagnation pressure, the stagnation temperature, and the pressure on the surface of a static-pressure wedge. For the other set, they are the pressure and temperature in a plenum upstream of the supersonic nozzle and the stagnation pressure at the exit of this nozzle. These routines apply to any undissociated gas whose real-gas properties are known. As examples, the routines are specifically applied to air, nitrogen, oxygen, normal hydrogen, parahydrogen, helium, argon, steam, methane, and natural gas.

INTRODUCTION

When the properties of a supersonic stream are to be determined from measured quantities, there are a number of sets of quantities that can be measured. For example, one set, which is useful when local stream properties are desired, could be the local stagnation pressure and temperature and the static pressure on the surface of a cone or wedge. (The term stagnation refers to total conditions downstream of the normal shock.) If the supersonic flow issues from a nozzle connected to an upstream plenum, another set of measurements is useful when the flow from the plenum to the nozzle exit can be considered isentropic and one dimensional (e.g., shock-free flow outside of the boundary layer). These measurements could be the pressure and temperature within the plenum and the stagnation pressure at the nozzle exit. From these measurements, such stream properties as Mach number, velocity, density, and temperature can be determined. However, since these stream properties are implicity rather than explicitly related to the measured quantities, iterative procedures must be used to make these determinations. For the case of a perfect gas, tables and graphs exist that simplify these calculations (e.g., ref. 1). In this report, a perfect gas is defined as one whose compressibility factor equals unity and whose specific heat is invariant. This perfect gas is to be distinguished from an ideal gas, which like a perfect gas is defined to have a compressibility factor of unity but, unlike a perfect gas, is defined to have a temperature-dependent specific heat. In the absence of dissociation, all gases approach this ideal-gas condition as the pressure is reduced. A nonperfect gas is called a real gas. For a gas such as air at room temperature and at pressures less than a few atmospheres, the perfect-gas assumption is adequate, at least for moderate Mach numbers. For gases at high pressures, and/or low temperatures, the perfect-gas assumption is not sufficiently valid for accurate computations, and real-gas computations should be made. Such calculations were made in reference 2, where high-pressure nitrogen was used to generate a Mach 3 stream.

In this report, the FORTRAN IV computer routines that were used to make the calculations in reference 2 are presented. In one set of routines, the independent variables are (1) the pressure and temperature such as would be measured by a stagnation pressure probe and a stagnation temperature probe and (2) the static pressure that would be measured on the surface of a wedge. In the other set of routines, the independent variables are (1) the total pressure and total temperature that would be measured in the subsonic plenum upstream of the supersonic nozzle and (2) the pressure that would be measured by a stagnation pressure probe at the exit of the nozzle. These routines apply to the following gases: air, nitrogen, oxygen, normal hydrogen, parahydrogen, helium, argon, steam, methane, and natural gas. The sections of the routines that have to do with the nature of the gas can also be used in conjunction with the routines given in reference 3. The combined set of routines can then be used to calculate the mass flow rate of these real gases through subsonic or sonic flow nozzles.

The pressure and temperature ranges for which these routines give accurate results depend on the pressure and temperature ranges of the state equations used to describe the behavior of the various gases. These ranges are given in table I for each gas. Generally, these routines are accurate at very low pressures, as long as the flow is in the continuum regime and no gas dissociation is present. Continuum flow exists when the mean free path is small compared to the probe dimensions. Dissociation is most liable to occur at high temperatures and low pressures. The lower limit of pressure is generally set by the criterion of continuum flow; the other limits of pressure and temperature are set by the range of validity of the state equations. In a supersonic stream, there can be a large pressure and temperature variation of the gas as it accelerates from a plenum, where the gas is at rest, to the exit of the supersonic nozzle. These pressures and temperatures should all be within the pressure and temperature ranges prescribed in table I.

TABLE I. - PRESSURE AND TEMPERATURE RANGES

FOR THE VARIOUS GASES

Gas	Pressure range, pascal	Temperature range, K
Air	100 to 100×10^5	150 to 1500
Nitrogen, range I	100 to 300×10^5	60 to 400
Nitrogen, range II	100 to 100×10^5	170 to 3000
Oxygen, range I	100 to 300×10^5	60 to 400
Oxygen, range II	100 to 100×10^5	180 to 3000
Normal hydrogen	100 to 100×10^5	70 to 600
Parahydrogen	100 to 300×10^5	13 to 100
	100 to 100×10^5	13 to 400
Helium	100 to 300×10^5	5.4 to 400
Argon	100 to 1000×10^5	80 to 400
Steam	100 to 1000×10^5	273 to 1600
Methane	100 to 400×10^5	70 to 600
Natural gas	100 to 100×10^5	200 to 400

In addition to such quantities as the free-stream velocity and density, additional thermodynamic quantities such as enthalpy, entropy, specific heat at constant pressure, specific-heat ratio, and isentropic exponent are calculated not only for free-stream conditions but also for plenum conditions, stagnation conditions behind the normal shock, free-stream conditions behind the normal shock, and (when applicable) free-stream conditions behind the oblique shock.

Both sets of routines are in two sections: one section is concerned with the iteration procedures, and the other section involves the specific behavior of the gas. The iteration routines that apply when the independent variables are the stagnation pressure, the stagnation temperature, and the static pressure at the surface of a wedge are described and presented in appendix B. The iteration routines that apply when the independent variables are the plenum pressure, the plenum temperature, and the stagnation pressure are described and presented in appendix C. For each of the gases, appendix D describes and presents the routines that have to do with the specific behavior of the gas. In addition, appendix D discusses the state equations that are involved in these routines. The routines in appendix D are used in conjunction with the routines in either appendix B or C and can also be used in conjunction with the iteration routines in reference 3 to calculate the mass flow rate of these gases through subsonic or sonic flow nozzles. Appendix E includes sample calculations for a supersonic air stream.

All symbols are defined in appendix A. The International System of Units (SI) is used throughout this report, except that appendix E illustrates the conversion from U.S. customary units to SI units in a practical example.

ANALYSIS

Basic Relations

The compressibility factor for all the gases involved in this report is given as a function of density and temperature. Therefore, this analysis requires that such thermodynamic functions as entropy, enthalpy, and specific heat also be expressed as a function of density and temperature. This involves the following compressibility-factor functions:

$$Z_I\ (\rho, T) = Z = \frac{p}{\rho RT} \tag{1}$$

$$Z_{II}(\rho, T) = Z + T\left(\frac{\partial Z}{\partial T}\right)_\rho = \frac{1}{R\rho}\left(\frac{\partial p}{\partial T}\right)_\rho \tag{2}$$

$$Z_{III}(\rho, T) = Z + \rho\left(\frac{\partial Z}{\partial \rho}\right)_T = \frac{1}{RT}\left(\frac{\partial p}{\partial \rho}\right)_T \tag{3}$$

$$Z_{IV}(\rho, T) = \int_0^\rho (Z_{II} - 1)\frac{d\rho}{\rho} \tag{4}$$

$$Z_V(\rho, T) = \int_0^\rho (Z_{II} - Z_I)\frac{d\rho}{\rho} \tag{5}$$

$$Z_{VI}(\rho, T) = T\left(\frac{\partial Z_{IV}}{\partial T}\right)_\rho \tag{6}$$

For an ideal gas, Z_I, Z_{II}, and Z_{III} equal 1 and Z_{IV}, Z_V, and Z_{VI} equal zero. In addition, for any real gas, Z_I, Z_{II}, and Z_{III} have to be positive.

In addition, the following functions of the ideal-gas specific heat $C_{v,id}$ are involved:

$$\xi_I(T) = \frac{C_{v,id}}{R} \tag{7}$$

$$\xi_{II}(T) = \int \frac{C_{v,id}}{R}\frac{dT}{T} = \frac{S_{id}}{R} + \ln\frac{p}{RT} \tag{8}$$

$$\xi_{III}(T) = \int \frac{C_{v,id}}{R}\, dT = \frac{H_{id}}{R} - T \tag{9}$$

In terms of the functions defined by equations (1) to (9), the following thermodynamic functions can now be expressed in terms of density and temperature:

$$\frac{p}{R} = Z_I \rho T \tag{10}$$

$$\frac{S}{R} = \xi_{II} - \ln \rho - Z_{IV} \tag{11}$$

$$\frac{H}{R} = \xi_{III} + T(Z_I - Z_V) \tag{12}$$

$$\frac{C_v}{R} = \xi_I - Z_{VI} \tag{13}$$

$$\frac{C_p}{R} = \frac{C_v}{R} + \frac{Z_{II}^2}{Z_{III}} \tag{14}$$

$$\gamma = \frac{C_p}{C_v} \tag{15}$$

$$k = \frac{\rho}{p}\left(\frac{\partial p}{\partial \rho}\right)_S = \gamma \frac{\rho}{p}\left(\frac{\partial p}{\partial \rho}\right)_T = \gamma \frac{Z_{III}}{Z_I} \tag{16}$$

where k is the isentropic exponent, and

$$\frac{\alpha^2}{R} = kZ_I T \tag{17}$$

Except for some symbol changes, equations (1) to (17) can be found in reference 4. The compressibility factor and the ideal-gas specific heat for the gases involved in this report are discussed in appendix D.

Now that the thermodynamic functions given by equations (10) to (17) are in terms of density and temperature, the procedures for calculating supersonic stream properties can be discussed. As indicated in the INTRODUCTION, there are two cases considered, and each one requires a different procedure. In the first case, measurements are made by a stagnation pressure probe, a stagnation temperature probe, and a wedge-type static-pressure probe. The quantities represented by these measurements are the total pressure and total temperature downstream of the normal shock (assuming that the recovery correction is applied to the temperature measurement) and the static pressure downstream of the oblique shock attached to the wedge. In the second case, the measurements are the pressure and temperature in the plenum upstream of a supersonic nozzle and the pressure indicated by a stagnation pressure probe at the nozzle exit. The quantities represented by these measurements are the free-stream total pressure and total temperature and the total pressure downstream of the normal shock.

These cases will be discussed separately. A word, first, about the notation. The subscript 1 refers to free-stream conditions, the subscript 2 refers to conditions downstream of the normal shock, and the subscript 3 refers to conditions downstream of the oblique shock that is attached to the wedge. The second subscript, t, when appended, refers to total conditions (i.e., conditions that would exist if the gas were brought to rest isentropically). Thus, a symbol like H_2 refers to the enthalpy downstream of the normal shock, and a symbol like $H_{2,t}$ refers to the total enthalpy downstream of the normal shock. The computational procedures for both of these cases involve solving nonlinear equations or sets of nonlinear equations. The Newton-Raphson iteration procedure is used in all cases.

Case I - given $p_{2,t}$, $T_{2,t}$, p_3, and δ. - Since the thermodynamic equations involve density and temperature rather than pressure and temperature, the following equation is implicity solved for $\rho_{2,t}$:

$$p_{2,t} = p(\rho_{2,t},\ T_{2,t}) \tag{18}$$

Next, there are two equations that relate total conditions to static conditions downstream of the normal shock. These are

$$S(\rho_{2,t},\ T_{2,t}) = S(\rho_2,\ T_2) \tag{19}$$

$$H(\rho_{2,t},\ T_{2,t}) = H(\rho_2,\ T_2) + \frac{1}{2}\ U_2^2 \tag{20}$$

Then, the energy, momentum, and continuity equations are written for the flow across the normal shock. These are

$$H(\rho_1,\ T_1) + \frac{1}{2}\ U_1^2 = H(\rho_2,\ T_2) + \frac{1}{2}\ U_2^2 \tag{21}$$

$$p(\rho_1,\ T_1) + \rho_1 U_1^2 = p(\rho_2,\ T_2) + \rho_2 U_2^2 \tag{22}$$

$$\rho_1 U_1 = \rho_2 U_2 \tag{23}$$

Next, energy, momentum, and continuity equations are written for the flow across the oblique shock attached to the static wedge whose half-angle is δ. These are

$$H(\rho_1, T_1) + \frac{1}{2}(U_1 \sin \theta)^2 = H(\rho_3, T_3) + \frac{1}{2}[U_3 \sin(\theta - \delta)]^2 \tag{24}$$

$$p(\rho_1, T_1) + \rho_1(U_1 \sin \theta)^2 = p(\rho_3, T_3) + \rho_3[U_3 \sin(\theta - \delta)]^2 \tag{25}$$

$$\rho_1 U_1 \sin \theta = \rho_3 U_3 \sin(\theta - \delta) \tag{26}$$

Since the tangential velocity just upstream of the shock equals the tangential velocity just downstream of the shock, there results

$$U_1 \cos \theta = U_3 \cos(\theta - \delta) \tag{27}$$

Next, the density and temperature on the wedge are related to the known pressure on the wedge by

$$p_3 = p(\rho_3, T_3) \tag{28}$$

The number of equations is reduced by using equation (23) to eliminate U_2 from equations (21) and (22) and by using equation (26) to eliminate U_3 from equations (24), (25), and (27). In order to more clearly distinguish between the known and unknown quantities, a subscripted variable, X_n, is used to indicate the unknown quantities. These are defined as follows;

$$X_1 = \rho_1 \qquad X_5 = \rho_3$$

$$X_2 = T_1 \qquad X_6 = T_3$$

$$X_3 = \rho_2 \qquad X_7 = \frac{U_1^2}{R}$$

$$X_4 = T_2$$

$$X_8 = \frac{(U_1 \sin \theta)^2}{R}$$

When these substitutions are made, the following eight equations result:

$$\frac{S(X_3, X_4)}{R} - \frac{S(\rho_{2,t}, T_{2,t})}{R} = 0 \tag{29}$$

$$\frac{H(X_3, X_4)}{R} - \frac{H(\rho_{2,t}, T_{2,t})}{R} + \frac{1}{2} X_7 \left(\frac{X_1}{X_3}\right)^2 = 0 \tag{30}$$

$$\frac{H(X_3, X_4)}{R} - \frac{H(X_1, X_2)}{R} + \frac{1}{2} X_7\left[\left(\frac{X_1}{X_3}\right)^2 - 1\right] = 0 \tag{31}$$

$$\frac{p(X_3, X_4)}{R} - \frac{p(X_1, X_2)}{R} + X_1X_7\left(\frac{X_1}{X_3} - 1\right) = 0 \tag{32}$$

$$\frac{H(X_5, X_6)}{R} - \frac{H(X_1, X_2)}{R} + \frac{1}{2} X_8\left[\left(\frac{X_1}{X_5}\right)^2 - 1\right] = 0 \tag{33}$$

$$\frac{p(X_5, X_6)}{R} - \frac{p(X_1, X_2)}{R} + X_1X_8\left(\frac{X_1}{X_5} - 1\right) = 0 \tag{34}$$

$$\text{arc sin}\sqrt{\frac{X_8}{X_7}} - \text{arc tan}\sqrt{\left(\frac{X_1}{X_5}\right)^2 \frac{X_8}{X_7 - X_8}} - \delta = 0 \tag{35}$$

$$\frac{p(X_5, X_6)}{R} - \frac{p_3}{R} = 0 \tag{36}$$

The solution of these equations requires an initial estimate of the X_n values that is close to the true X_n values. The initial values used herein are the result of a perfect-gas solution which is discussed as follows:

Equations (100) and (128) in reference 1 can be combined to yield

$$\frac{p_3}{p_{2,t}} = \left[\frac{4\gamma}{(\gamma + 1)^2}\right]^{\gamma/(\gamma-1)} \frac{(\eta - 1)^{1/(\gamma-1)}(\eta \sin^2\theta - 1)}{\eta^{\gamma/(\gamma-1)}} \tag{37}$$

where

$$\eta = \frac{2\gamma}{\gamma - 1} M_1^2 \tag{38}$$

The following equation is derived from equation (148 (a)) in reference 1

$$\frac{2\gamma}{\gamma - 1} \frac{\cos(\theta - \delta)}{\eta} = \frac{1}{2} \sin\theta\,[\sin(2\theta - \delta) - \gamma \sin\delta] \tag{39}$$

These equations are solved for M_1 and θ. From this, the initial estimates of $X_{n,i}$

are determined from equations found in reference 1. These estimates are

$$X_{3,i} = \frac{\rho_{2,t}}{\left(1 + \frac{\gamma - 1}{2} M_2^2\right)^{1/(\gamma - 1)}} \tag{40}$$

where

$$M_2^2 = \frac{M_1^2 + \frac{2}{\gamma - 1}}{\frac{2\gamma}{\gamma - 1} M_1^2 - 1} \tag{41}$$

$$X_{4,i} = \frac{T_{2,t}}{1 + \frac{\gamma - 1}{2} M_2^2} \tag{42}$$

$$X_{1,i} = \frac{M_1^2 + \frac{2}{\gamma - 1}}{\frac{\gamma + 1}{\gamma - 1} M_1^2} X_{3,i} \tag{43}$$

$$X_{2,i} = \frac{\left(\frac{\gamma + 1}{\gamma - 1}\right)^2 M_1^2}{\left(\frac{2\gamma}{\gamma - 1} M_1^2 - 1\right)\left(M_1^2 + \frac{2}{\gamma - 1}\right)} X_{4,i} \tag{44}$$

$$X_{5,i} = \frac{\frac{\gamma + 1}{\gamma - 1} (M_1 \sin \theta)^2}{(M_1 \sin \theta)^2 + \frac{2}{\gamma - 1}} X_{1,i} \tag{45}$$

$$X_{6,i} = \frac{\left[\frac{2\gamma}{\gamma - 1} (M_1 \sin \theta)^2 - 1\right]\left[(M_1 \sin \theta)^2 + \frac{2}{\gamma - 1}\right]}{\left(\frac{\gamma + 1}{\gamma - 1}\right)^2 (M_1 \sin \theta)^2} X_{2,i} \tag{46}$$

$$X_{7,i} = \gamma M_1^2 X_{2,i} \tag{47}$$

$$X_{8,i} = X_{7,i} \sin^2\theta \tag{48}$$

(Eqs. (37) to (48) apply only to a perfect gas. The value of γ in these equations is a perfect-gas value. The values assumed for these calculations are 5/3 for a monatomic gas, 7/5 for a diatomic gas, and 4/3 for a gas whose molecules contain three or more atoms.)

With these values of X_n as initial estimates, the procedure for solving equations (29) to (36) usually converges rapidly. At this point, flow properties and thermodynamic properties can be determined for total and static conditions downstream of the normal shock, for static conditions downstream of the oblique shock, and for free-stream conditions; however, they cannot yet be determined for total conditions in the free stream. To do this, the following equations have to be solved:

$$S(\rho_{1,t}, T_{1,t}) = S(\rho_1, T_1) \tag{49}$$

$$H(\rho_{1,t}, T_{1,t}) = H(\rho_1, T_1) + \frac{1}{2} U_1^2 \tag{50}$$

The initial estimate of $\rho_{1,t}$ and $T_{1,t}$ are obtained by assuming the gas to be perfect. The perfect-gas relations are

$$\rho_{1,t,i} = \rho_{2,t} e^{(S_2-S_1)/R} \tag{51}$$

$$T_{1,t,i} = T_{2,t} \tag{52}$$

When these initial values are used, the iteration procedure for solving equations (49) and (50) converges rapidly. Knowing $\rho_{1,t}$ and $T_{1,t}$ allows the thermodynamic properties to be determined for free-stream total conditions.

Case II - given $p_{1,t}$, $T_{1,t}$, and $p_{2,t}$. - First, the following equation has to be implicitly solved for $\rho_{1,t}$:

$$p_{1,t} = p(\rho_{1,t}, T_{1,t}) \tag{53}$$

Most of the equations that follow are given in case I, but they are repeated here for convenience. The two relations that relate total to static conditions upstream of the shock are

$$S(\rho_{1,t}, T_{1,t}) = S(\rho_1, T_1) \tag{49}$$

$$H(\rho_{1,t}, T_{1,t}) = H(\rho_1, T_1) + \frac{1}{2} U_1^2 \tag{50}$$

Next, the energy, momentum, and continuity equations are written for the flow across the normal shock.

$$H(\rho_1, T_1) + \frac{1}{2}U_1^2 = H(\rho_2, T_2) + \frac{1}{2}U_2^2 \tag{21}$$

$$p(\rho_1, T_1) + \rho_1 U_1^2 = p(\rho_2, T_2) + \rho_2 U_2^2 \tag{22}$$

$$\rho_1 U_1 = \rho_2 U_2 \tag{23}$$

Then the relations between total and static conditions downstream of the normal shock are

$$S(\rho_{2,t}, T_{2,t}) = S(\rho_2, T_2) \tag{19}$$

$$H(\rho_{2,t}, T_{2,t}) = H(\rho_2, T_2) + \frac{1}{2}U_2^2 \tag{20}$$

Then the equation that relates the total density and temperature to the known total pressure downstream of the normal shock is

$$p_{2,t} = p(\rho_{2,t}, T_{2,t}) \tag{18}$$

The number of equations is reduced by using equation (23) to eliminate U_2 from equations (20) to (22). In order to more clearly distinguish the known and unknown variables, a subscripted variable, X_n, is used to indicate the unknown variables. These are defined as follows:

$$X_1 = \rho_1 \qquad X_5 = \rho_{2,t}$$

$$X_2 = T_1 \qquad X_5 = T_{2,t}$$

$$X_3 = \rho_2 \qquad X_7 = \frac{U_1^2}{R}$$

$$X_4 = T_2$$

When these substitutions are made, the following equations can be written:

$$\frac{S(X_1, X_2)}{R} - \frac{S(\rho_{1,t}, T_{1,t})}{R} = 0 \tag{54}$$

$$\frac{H(X_1, X_2)}{R} - \frac{H(\rho_{1,t}, T_{1,t})}{R} + \frac{1}{2} X_7 = 0 \tag{55}$$

$$\frac{H(X_3, X_4)}{R} - \frac{H(X_1, X_2)}{R} + \frac{1}{2} X_7 \left[\left(\frac{X_1}{X_3}\right)^2 - 1\right] = 0 \tag{56}$$

$$\frac{p(X_3, X_4)}{R} - \frac{p(X_1, X_2)}{R} + X_1 X_7 \left(\frac{X_1}{X_3} - 1\right) = 0 \tag{57}$$

$$\frac{S(X_3, X_4)}{R} - \frac{S(X_5, X_6)}{R} = 0 \tag{58}$$

$$\frac{H(X_3, X_4)}{R} - \frac{H(X_5, X_6)}{R} + \frac{1}{2} X_7 \left(\frac{X_1}{X_3}\right)^2 = 0 \tag{59}$$

$$\frac{p(X_5, X_6)}{R} - \frac{p_{2,t}}{R} = 0 \tag{60}$$

The solution of these equations requires an initial estimate of the X_n values that is close to the true X_n values. A perfect-gas calculation is used to make this initial estimate. To do this, the following equation, derived from equation (99) in reference 1, has to be solved implicitly for M_1:

$$\frac{p_{2,t}}{p_{1,t}} = \left(\frac{\gamma + 1}{\gamma - 1}\right)^{(\gamma+1)/(\gamma-1)} \left(\frac{M_1^2}{M_1^2 + \frac{2}{\gamma - 1}}\right)^{\gamma/(\gamma-1)} \left(\frac{1}{\frac{2\gamma}{\gamma - 1} M_1^2 - 1}\right)^{1/(\gamma-1)} \tag{61}$$

Then, when the equations in reference 1 are used, the initial estimate for the X_n values is

$$X_{1,i} = \frac{\rho_{1,t}}{\left(1 + \frac{\gamma - 1}{2} M_1^2\right)^{1/(\gamma-1)}} \tag{62}$$

$$X_{2,i} = \frac{T_{1,t}}{\left(1 + \frac{\gamma - 1}{2} M_1^2\right)} \tag{63}$$

$$X_{3,i} = \frac{\frac{\gamma + 1}{\gamma - 1} M_1^2}{M_1^2 + \frac{2}{\gamma - 1}} X_{1,i} \tag{64}$$

$$X_{4,i} = \frac{\left(\frac{2\gamma}{\gamma - 1} M_1^2 - 1\right)\left(M_1^2 + \frac{2}{\gamma - 1}\right)}{\left(\frac{\gamma + 1}{\gamma - 1}\right)^2 M_1^2} X_{2,i} \tag{65}$$

$$X_{5,i} = \left(\frac{\frac{\gamma + 1}{\gamma - 1} M_1^2}{M_1^2 + \frac{2}{\gamma - 1}}\right)^{\gamma/(\gamma-1)} \left(\frac{\frac{\gamma + 1}{\gamma - 1}}{\frac{2\gamma}{\gamma - 1} M_1^2 - 1}\right)^{1/(\gamma-1)} \rho_{1,t} \tag{66}$$

$$X_{6,i} = T_{1,t} \tag{67}$$

$$X_{7,i} = X_{2,i} M_1^2 \tag{68}$$

(Eqs. (61) to (68) only apply for a perfect gas.) The use of these values of X_n as the initial estimates in equations (54) to (60) usually results in the iteration procedure converging rapidly. From the solution of these equations flow properties and thermodynamic properties can be determined for total and static conditions upstream and downstream of the normal shock.

Solution Criteria

The computer code for these equations includes certain tests to ensure that the solution is correct. First, all the iterative procedures used to solve the various equations and sets of equations have to converge to the prescribed degree. If this convergence is not obtained, the solution is flagged; and in some cases, the calculation is terminated. Second, even if the solution is mathematically valid, it may not be physically valid. For physical validity, the following have to be true:

(1) All the pressures and temperatures involved in the equations must be within range of the state equations. (This also ensures that the fluid is a gas.)

(2) The entropy of the gas must increase as the gas passes through a shock.

If these conditions are not satisfied, the solution is flagged; and in some cases, the calculation is terminated.

The following discussion applies only to case I. (This is the case where a wedge-type static-pressure probe is used.) For certain combinations of $p_{2,t}$, $T_{2,t}$, p_3, and δ, a solution is obtained which indicates that the oblique shock attached to the wedge is the strong shock, rather than the weak shock. Physically, this would be extremely unlikely. In fact, the true situation would probably be that the free stream is either subsonic or that the shock wave is not attached to the wedge. In either case, the solution is meaningless. The strong shock is recognized by the fact that a decrease in the wedge static pressure is accompanied by a decrease in the free-stream Mach number. Thus, the solution is tested by slightly decreasing p_3 and solving the equations again; if M_1 decreases, the oblique shock on the wedge is strong. If this happens, the solution is flagged. This test is performed only when the flow downstream of the shock is subsonic. Many trial calculations have shown no case in which the downstream real-gas flow was supersonic when the shock was strong.

RESULTS AND DISCUSSION

For both cases of the preceding analysis, the computer routines are in two sections. The routines in the first section include the necessary iteration procedures for solving the various sets of equations. The routines in the second section describe the specific behavior of the gas. The routines are written in the FORTRAN IV, version 13, language.

The routines that include the iteration procedures for case I (i.e., the case where the input is $p_{2,t}$, $T_{2,t}$, p_3, and δ) are given in appendix B. The routines that include the iteration procedures for case II (i.e., the case where the input is $p_{1,t}$, $T_{1,t}$, and $p_{2,t}$) are given in appendix C. The routines for either case have to be used in conjunction with one of the sets of routines in appendix D which describe the specific behavior of the gas. This appendix includes sets of routines of air, nitrogen, oxygen, normal hydrogen, parahydrogen, helium, argon, steam, methane, and natural gas. These routines can also be used in conjunction with the iteration routines in reference 3 to calculate the mass flow rate of these gases through nozzles.

In both cases, the output variables are M_1, $M_{1,P}$, U_1, $U_{1,P}$, M_2, and U_2. The second subscript P indicates the value that the variable would have if the gas were perfect. The perfect-gas calculation uses the same input as the real-gas calculation. Involved in this calculation is the perfect-gas specific-heat ratio. The following specific-heat ratios were chosen: 5/3 for helium and argon; 7/5 for air, nitrogen, oxygen, normal hydrogen, and parahydrogen; and 4/3 for steam, methane, and natural gas. In addition, thermodynamic state functions are calculated for static and total conditions upstream and downstream of the normal shock. These are p, ρ, T, H/R, S/R, C_p/R, γ, and k. Additional variables are calculated for case I. These have to do with the oblique shock attached to the static-pressure wedge. These are M_3, U_3, θ, θ_P, and the aforementioned thermodynamic state functions for the static conditions downstream of the

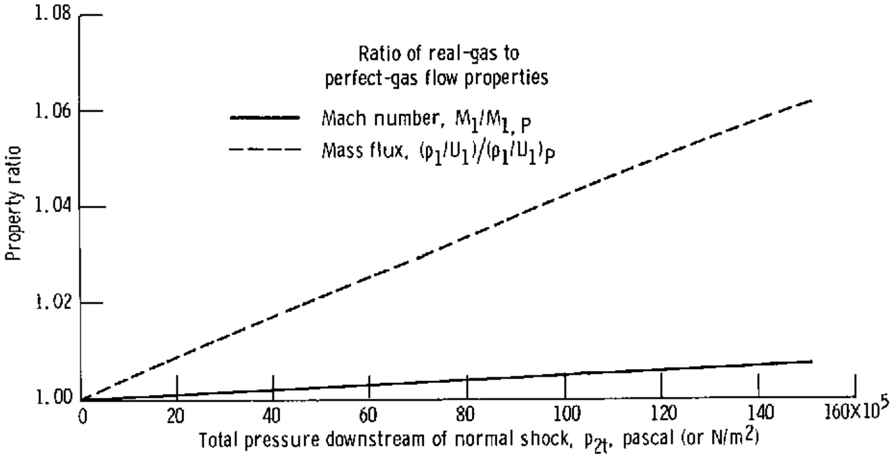

Figure 1. - Ratio of some real-gas flow properties to perfect-gas flow properties for nitrogen - case I. Total temperature downstream of normal shock, T_{2t}, 300 K; ratio of pressure downstream of oblique shock to total pressure downstream of normal shock, $p_3/p_{2,t}$, 0.1886; free-stream Mach number for a perfect gas, $M_{1,p}$, 2.5; specific-heat ratio for a perfect gas, γ_p, 1.4; half-angle of static-pressure wedge, δ, 7.5^0.

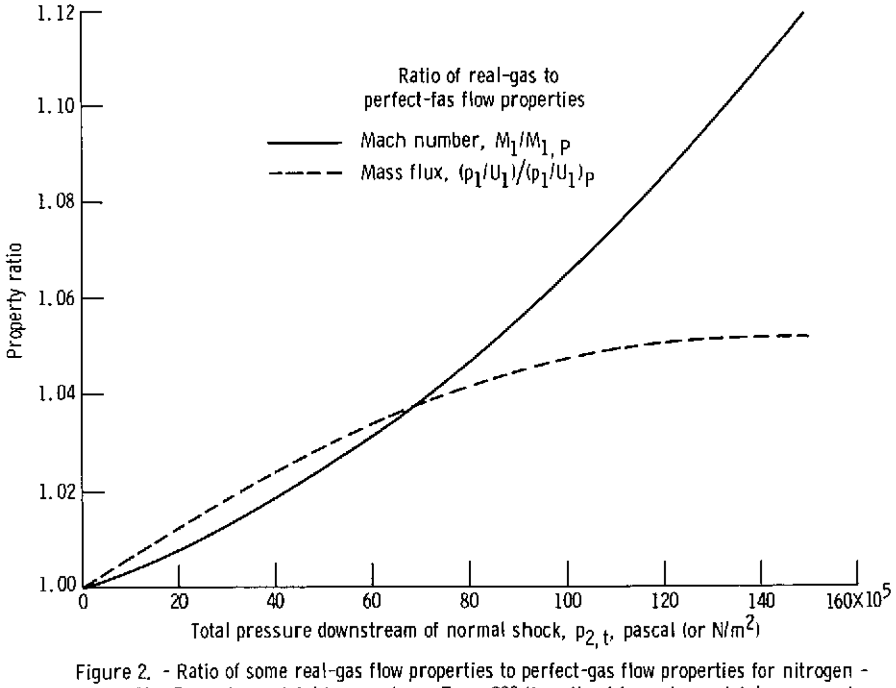

Figure 2. - Ratio of some real-gas flow properties to perfect-gas flow properties for nitrogen - case II. Free-stream total temperature, $T_{1,t}$, 300 K; ratio of free-stream total pressure to total pressure downstream of the normal shock, $p_{1,t}/p_{2,t}$, 2.004; free-stream Mach number for a perfect gas, $M_{1,p}$, 2.5; specific-heat ratio for a perfect gas, γ_p, 1.4.

oblique shock attached to the wedge.

Figures 1 and 2 are presented to illustrate the deviation of nitrogen from perfect-gas behavior. In figure 1, which applies to case I, two ratios are plotted against the measured $p_{2,t}$. These ratios are $M_1/M_{1,P}$ and $\rho_1 U_1/(\rho_1 U_1)_P$. The value of $M_{1,P}$ is 2.5, and the value of $p_3/p_{2,t}$ is constant. For a pressure of 150×10^5 pascals (newtons per square meter), the Mach number only deviates 0.8 percent from the perfect-gas value, while the mass flux deviates 6.1 percent. The results are different in figure 2. This figure applies to case II. The gas is again nitrogen and the perfect-gas Mach number is 2.5. This time $p_{1,t}/p_{2,t}$ is constant. For this case, for a pressure of 150×10^5 pascals, the Mach number deviates 12 percent from the perfect-gas value, and the mass flux deviates 5.2 percent. In both cases, these ratios approach unity as the pressure is reduced. This is because the ideal-gas specific-heat ratio of nitrogen is sensibly constant at room temperature. This relation is not true for a gas such as methane, whose ideal-gas specific heat is variable. Therefore, $M_1/M_{1,P}$ and $\rho_1 U_1/(\rho_1 U_1)_P$ would not approach unity, for methane, as the pressure is reduced.

These routines are designed to be incorporated as a set of subroutines in a main computer program. Appendix E includes two typical main programs for the routines contained in both appendixes B and C. In addition, the results of sample calculations are included. The exact storage requirements depend on the gas. On the average, the routines for case I require about 4200 storage locations and the routines for case II require about 3500. These stores include a necessary matrix inversion routine. This routine is called MINV and is provided by International Business Machines Corporation (IBM) in their Scientific Subroutine Package.

CONCLUDING REMARKS

Two sets of computer routines are presented that provide a means of calculating the properties of a supersonic stream from measured quantities. In the first set, the measurements are the total pressure and temperature downstream of a normal shock, and the pressure on the surface of a wedge-type static-pressure probe. In the second set, the measurements are the pressure and temperature in the plenum upstream of a supersonic nozzle and the total pressure behind the normal shock. These routines apply for 10 different undissociated gases.

The accuracy of these calculations depends primarily on the accuracy of the state equations that describe the gas. For a gas such as air at room temperature and at plenum pressures to 100 bar, the results would probably be accurate to within a percent. For a gas such as natural gas, which is a variable mixture of many components, the accuracy would not be as good.

In order to use these routines for gases other than those included in this report, only routines like those included in appendix D would have to be written. These routines are straightforward and require only appropriate state equations.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, January 16, 1974,
501-04.

APPENDIX A

SYMBOLS

C_p	specific heat at constant pressure, J/(kg)(K)
C_v	specific heat at constant volume, J/(kg)(K)
H	enthalpy, J/kg
k	isentropic exponent, eq. (16)
M	Mach number
p	pressure, Pa
R	gas constant, J/(kg)(K)
S	entropy, J/(kg)(K)
T	temperature, K
U	velocity, m/sec
X_n	unknown quantities in eqs. (29) to (36) where n runs from 1 to 8, and in eqs. (54) to (60) where n runs from 1 to 7
Z	compressibility factor
Z_I to Z_{VI}	functions of compressibility factor, eqs. (1) to (6)
α	speed of sound, m/sec
γ	specific-heat ratio
δ	half-angle of static-pressure wedge
θ	oblique shock angle
η	function of perfect-gas values of M_1 and γ, eq. (38)
ξ_I to ξ_{III}	functions of ideal-gas specific heat, eqs. (7) to (9)
ρ	density, kg/m^3

Subscripts:

i	initial estimate of a variable in an iteration process
id	ideal-gas condition
P	perfect-gas condition
t	total conditions

1 refers to free-stream conditions except when appended to X

2 refers to conditions downstream of normal shock except when appended to X

3 refers to conditions downstream of oblique shock except when appended to X

APPENDIX B

DESCRIPTION AND CARD LISTING OF COMPUTER ROUTINES

THAT APPLY TO CASE I

Case I applies to local measurements of stagnation pressure $p_{2,t}$, stagnation temperature $T_{2,t}$, and static pressure p_3 on a wedge of half-angle δ.

In order to make a workable set of routines, the routines in this section have to be combined with one of the sets of routines in appendix D. The particular set that is chosen depends on the type of gas. This combined set of routines is referenced in the main program by the following statement:

CALL RWEDG(PA2, TA2, PB3, DELTAS)

All the output is returned through labeled COMMON. Therefore, this COMMON statement has to be in the main program:

COMMON/OUTW/TP(8, 5), VM(10), CONV(12), Z(6, 5), KODE(11)

There are certain variables that have to do with the convergence requirements of the various iteration procedures in these routines. These variables are initialized in a BLOCK DATA subprogram. However, if the following COMMON statement is put in the main program, the value of these variables can be altered:

COMMON/LIMITW/EDA2, EMAT, EDTA1, EPWD

The symbols that apply to these routines are defined as follows:

PA2	Total pressure downstream of normal shock, $p_{2,t}$, Pa
TA2	Total temperature downstream of normal shock, $T_{2,t}$, K
PB3	Pressure downstream of oblique shock attached to wedge-type static-pressure probe, p_3, Pa
DELTAS	Half-angle of wedge-type static-pressure probe, δ, deg

The array TP(I, J) contains thermodynamic state functions. The subscript I identifies the function, and the subscript J identifies the region. The function definitions for the first subscript are as follows:

TP(1, J)	Pressure, p, Pa
TP(2, J)	Density, ρ, kg/m^3

TP(3,J)	Temperature, T,K
TP(4,J)	Enthalpy, H/R, K
TP(5,J)	Entropy, S/R
TP(6,J)	Specific heat, C_p/R
TP(7,J)	Specific-heat ratio, γ
TP(8,J)	Isentropic exponent, k

The region definitions for the second subscript are as follows:

TP(I, 1)	Total conditions in free stream
TP(I, 2)	Free-stream conditions
TP(I, 3)	Total conditions downstream of normal shock
TP(I, 4)	Conditions downstream of normal shock
TP(I, 5)	Conditions downstream of oblique shock attached to wedge-type static-pressure probe

(Thus, TP(3, 5) would be the temperature downstream of the oblique shock and TP(8, 2) would be the free-stream isentropic exponent.)

VM(1)	Free-stream Mach number, M_1
VM(2)	Perfect-gas calculation of free-stream Mach number, $M_{1,P}$
VM(3)	Free-stream velocity, U_1, m/sec
VM(4)	Perfect-gas calculation of free-stream velocity, $U_{1,P}$, m/sec
VM(5)	Mach number downstream of normal shock, M_2
VM(6)	Velocity downstream of normal shock, U_2, m/sec
VM(7)	Angle of oblique shock attached to wedge, θ, deg
VM(8)	Perfect-gas calculation of oblique shock angle, θ_P, deg
VM(9)	Mach number downstream of oblique shock, M_3
VM(10)	Velocity downstream of oblique shock, U_3

CONV(1) to CONV(8)
where

$$\mathrm{CONV(I)} = \frac{X_{I,n} - X_{I,n-1}}{X_{I,n-1}}$$

CONV(9) to CONV(12)
where

$$\mathrm{CONV}(9) = 1 - \frac{p_{2,t}}{Z_{2,t}\rho_{2,t}RT_{2,t}}$$

$$\mathrm{CONV}(10) = \frac{(\rho_{1,t})_n - (\rho_{1,t})_{n-1}}{(\rho_{1,t})_{n-1}}$$

$$\mathrm{CONV}(11) = \frac{(T_{1,t})_n - (T_{1,t})_{n-1}}{(T_{1,t})_{n-1}}$$

$$\mathrm{CONV}(12) = \frac{\left(\frac{p_3}{p_{2,t}}\right)_{\mathrm{eq.\ (37)}} - \left(\frac{p_3}{p_{2,t}}\right)_{\mathrm{given}}}{\left(\frac{p_3}{p_{2,t}}\right)_{\mathrm{given}}}$$

The array Z(I, J) contains the compressibility factor functions as represented by equations (1) to (6). The subscript I identifies the function, and the subscript J identifies the region. The second subscript definitions are the same as those for the array TP. The first subscript definition is

$$Z(1,J)\ .\ .\ .\ Z(6,J) \qquad \text{for } Z_I \text{ to } Z_{VI}$$

The following symbols represent integers to indicate various error conditions. If all the integers are zero, a valid calculation has been performed. If the integers are 1, errors exist. These errors are

KODE(1) Equals 1 if $p_{1,t}$ or $T_{1,t}$ is out of range of the state equations.

KODE(2) Equals 1 if $p_{2,t}$ or $T_{2,t}$ is out of range of the state equations. A value of 1 terminates the calculation.

KODE(3) Equals 1 if p_1 or T_1 is out of range of the state equations. A value of 1 terminates the calculation.

KODE(4) Equals 1 if p_2 or T_2 is out of range of the state equations. A value of 1 terminates the calculation.

KODE(5) Equals 1 if p_3 or T_3 is out of range of the state equations. A value of 1 terminates the calculation.

KODE(6) Equals 1 if the iterative procedures for the perfect-gas calculations for $M_{1,P}$, $M_{2,P}$, and θ_P fail to converge.

KODE(7) Equals 1 if the iterative procedures for calculating $\rho_{2,t}$ fails to converge.

KODE(8) Equals 1 if the iterative procedures for calculating X_1 to X_8 fail to converge.

KODE(9) Equals 1 if the iterative procedures for calculating $\rho_{1,t}$ and $T_{1,t}$ fail to converge.

KODE(10) Equals 1 if $S_1 > S_2$ or if $S_1 > S_3$.

KODE(11) Equals 1 if the shock attached to the wedge is the strong shock.

EDA2 Maximum value of $|CONV(9)|$ permitted. This is initialized at a value of 1×10^{-6}

EMAT Maximum value of $\sum_{I=1}^{8} |CONV(I)|$ permitted. This is initialized at a value of 1×10^{-5}.

EDTA1 Maximum value of $|CONV(10)| + |CONV(11)|$ permitted. This is initialized at a value of 2×10^{-6}.

EPWD Maximum value of $|CONV(12)|$ permitted. This is initialized at a value of 1×10^{-6}.

The routines that apply to case I are described briefly here. These routines are identified by their deck names.

Deck RGWED

This is the subroutine in which the output variables TP and VM are calculated. The iteration procedures for solving equations (18), (29) to (36), and (49) and (50) are in this routine.

Deck RGDFW

In this subroutine, the inverse of the derivative matrix, which is required to solve equations (29) to (36), is calculated. In addition, this routine requires the matrix inversion subroutine MINV supplied by IBM in their Scientific Subroutine Package.

Deck PGWED

This subroutine is used to calculate $M_{1,P}$, $M_{2,P}$, and θ_P. The iterative procedures necessary to solve equations (37) to (39) are in this subroutine.

Deck WDATA

This BLOCK DATA subprogram contains the initial values of the convergence limits for the various iterative procedures.

A workable set of routines includes not only these decks, but also one of the sets of decks in appendix D. The card listing of these decks follows.

```
C DECK RGWED
C
C  THIS IS THE SUBROUTINE WHERE THE FLOW FUNCTIONS AND THERMODYNAMIC
C  STATE FUNCTIONS OF A SUPERSONIC STREAM ARE CALCULATED FROM MEASURED
C  QUANTITIES.  THESE QUANTITIES ARE THE TOTAL PRESSURE AND TOTAL
C  TEMPERATURE DOWNSTREAM OF A NORMAL SHOCK, AND THE PRESSURE INDICATED
C  BY A WEDGE STATIC PRESSURE PROBE.
C
      SUBROUTINE RWEDG (PA2,TA2,PB3,DELTAS)
      COMMON /OUTW/ TP(8,5),VM(10),CONV(12),Z(6,5),KODE(11)
      COMMON /RDW/ W(8,8),X(8),X13,SQX13,X15,SQX15,V7,W7,CVB1,CVB2,CVB3
      COMMON /GDATW/ G1,G2,G3,G4,G5,G6,G7,G8,G9,G10
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      COMMON /LIMITW/ EDA2,EMAT,EDTA1,EPWD
      DIMENSION ZA1(6), ZB1(6), ZA2(6), ZB2(6), ZB3(6), F(8), OUT(103),
     1SAVE(103)
      EQUIVALENCE (TP(1),OUT(1)), (ZA1(1),Z(1)), (ZB1(1),Z(7)), (ZA2(1),
     1Z(13)), (ZB2(1),Z(19)), (ZB3(1),Z(25))
      DOUBLE PRECISION CP,CS,CH,DSA2,DHA2,DSA1,DHA1,DSB1,DHB1,DSB2,DHB2,
     1DHB3
      LOGICAL LGFN
      DATA RADIAN/.0174532925/
      DO 1 I=1,103
      SAVE(I)=0.0
1     OUT(I)=0.0
      DO 2 J=1,5
      DO 2 I=1,3
2     Z(I,J)=1.0
      DO 3 I=1,8
      X(I)=0.0
3     F(I)=0.0
      TP(1,3)=PA2
      TP(3,3)=TA2
      TP(1,5)=PB3
      NSAVE=0
```

```
C
C   THE PERFECT GAS VALUES OF THE SHOCK ANGLE, AND THE MACH NUMBER, BOTH
C   UPSTREAM AND DOWNSTREAM OF THE NORMAL SHOCK ARE CALCULATED IN PWEDG.
C
4      CALL PWEDG (TP(1,5)/TP(1,3),DELTAS,VM(2),XM2,VM(8),CONV(12),KODE(6
      1))
       IF (KODE(6).EQ.1) RETURN
       DELTA=DELTAS*RADIAN
       SQM1=VM(2)**2
       SQSM1=SQM1*SIN(VM(8)*RADIAN)**2
C
C   THE ITERATION PROCEDURE FOR CALCULATING THE TOTAL DENSITY DOWNSTREAM
C   OF THE NORMAL SHOCK STARTS HERE.
C
       A=TP(1,3)/(R*TP(3,3))
       TP(2,3)=A
       IF (LGFN(TP(1,3),TP(3,3),KODE(2),ZA2)) RETURN
       DO 5 I=1,20
       CALL ZETA (1,TP(2,3),TP(3,3),ZA2)
       CONV(9)=1.0-TP(1,3)/(ZA2(1)*R*TP(2,3)*TP(3,3))
       IF (ABS(CONV(9)).LT.EDA2) GO TO 6
5      TP(2,3)=TP(2,3)*(1.0-(ZA2(1)-A/TP(2,3))/ZA2(3))
C
       KODE(7)=1
       RETURN
6      CALL ZETA (3,TP(2,3),TP(3,3),ZA2)
       IF (LGFN(TP(1,3),TP(3,3),KODE(2),ZA2)) RETURN
       DSA2=CS(TP(3,3))-DLOG(DBLE(TP(2,3)))-ZA2(4)
       TP(5,3)=DSA2
       DHA2=CH(TP(3,3))+TP(3,3)*(ZA2(1)-ZA2(5))
       TP(4,3)=DHA2
       CV=CP(TP(3,3))-ZA2(6)
       GA=ZA2(3)+ZA2(2)**2/CV
       TP(7,3)=GA/ZA2(3)
       TP(8,3)=GA/ZA2(1)
       TP(6,3)=CV*TP(7,3)
       SQM2=(SQM1+G5)/(G7*SQM1-1.0)
C
C   THE INITIAL ESTIMATES OF THE VALUES OF X ARE CALCULATED BY THE
C   FOLLOWING STATEMENTS.
C
       A=1.0+G1*SQM2
       X(3)=TP(2,3)/A**G3
       X(4)=TP(3,3)/A
       X(1)=X(3)*(SQM1+G5)/(G6*SQM1)
       X(2)=TP(3,3)/(1.0+G1*SQM1)
       A=G6*SQSM1/(SQSM1+G5)
       X(5)=A*X(1)
       X(6)=X(2)*(G7*SQSM1-1.0)/(G6*A)
       X(7)=G2*SQM1*X(2)
       X(8)=G2*SQSM1*X(2)
C
       VM(4)=SQRT(R*X(7))
C
C   THE ITERATION PROCEDURE FOR CALCULATING THE VALUES OF X STARTS HERE.
C
       DO 11 I=1,20
       CALL ZETA (3,X(1),X(2),ZB1)
       CALL ZETA (3,X(3),X(4),ZB2)
```

```
      CALL ZETA (3,X(5),X(6),ZB3)
      TP(1,2)=ZB1(1)*X(1)*X(2)*R
      TP(1,4)=ZB2(1)*X(3)*X(4)*R
      IF (LGFN(TP(1,2),X(2),KODE(3),ZB1)) RETURN
      IF (LGFN(TP(1,4),X(4),KODE(4),ZB2)) RETURN
      IF (LGFN(TP(1,5),X(6),KODE(5),ZB3)) RETURN
      DSB2=CS(X(4))-DLOG(DBLE(X(3)))-ZB2(4)
      DHB1=CH(X(2))+X(2)*(ZB1(1)-ZB1(5))
      DHB2=CH(X(4))+X(4)*(ZB2(1)-ZB2(5))
      DHB3=CH(X(6))+X(6)*(ZB3(1)-ZB3(5))
      X13=X(1)/X(3)
      SQX13=X13**2
      X15=X(1)/X(5)
      SQX15=X15**2
      V7=SQRT(SQX15*X(8)/(X(7)-X(8)))
      W7=SQRT(X(8)/X(7))
      F(1)=DSB2-DSA2
      F(2)=DHB2-DHA2+SQX13*X(7)/2.0
      F(3)=DHB2-DHB1+X(7)*(SQX13-1.0)/2.0
      F(4)=DHB3-DHB1+X(8)*(SQX15-1.0)/2.0
      F1=TP(1,2)/R
      F3=TP(1,4)/R
      F5=X(5)*X(6)*ZB3(1)
      F(5)=F3-F1+X(1)*X(7)*(X13-1.0)
      F(6)=F5-F1+X(1)*X(8)*(X15-1.0)
      F(7)=ARSIN(W7)-ATAN(V7)-DELTA
      F(8)=F5-TP(1,5)/R
      IF (MOD(I,5).EQ.1) CALL RDFW
      DO 8 J=1,8
      CONV(J)=0.0
      DO 7 K=1,8
7     CONV(J)=CONV(J)+W(J,K)*F(K)
8     CONV(J)=CONV(J)/X(J)
      TEST=0.0
      DO 9 J=1,8
9     TEST=TEST+ABS(CONV(J))
      IF (TEST.LT.EMAT) GO TO 12
      DO 10 J=1,8
10    X(J)=X(J)*(1.0+CONV(J))
11    CONTINUE
C
      KODE(8)=1
12    CVB1=CP(X(2))-ZB1(6)
      GA=ZB1(3)+ZB1(2)**2/CVB1
      TP(7,2)=GA/ZB1(3)
      TP(8,2)=GA/ZB1(1)
      TP(6,2)=CVB1*TP(7,2)
      TP(3,2)=X(2)
      TP(2,2)=X(1)
      TP(4,2)=DHB1
      TP(5,5)=CS(X(6))-ALOG(X(5))-ZB3(4)
      TP(4,5)=DHB3
      TP(2,5)=X(5)
      TP(3,5)=X(6)
      GA=ZB3(3)+ZB3(2)**2/CVB3
      TP(7,5)=GA/ZB3(3)
      TP(8,5)=GA/ZB3(1)
      TP(6,5)=CVB3*TP(7,5)
      VM(3)=SQRT(R*X(7))
```

```
      VM(1)=VM(3)/SQRT(TP(8,2)*TP(1,2)/TP(2,2))
      VM(7)=ARSIN(SQRT(X(8)/X(7)))
      VM(10)=COS(VM(7))*SQRT(R*X(7))/COS(VM(7)-DELTA)
      VM(9)=VM(10)/SQRT(TP(8,5)*TP(1,5)/TP(2,5))
      IF (NSAVE.NE.1) GO TO 14
      IF(VM(1).LT.SAVE(41))KODE(11)=1
      DO 13 I=1,102
13    OUT(I)=SAVE(I)
      RETURN
14    DSB1=CS(TP(3,2))-DLOG(DBLE(TP(2,2)))-ZB1(4)
      TP(5,2)=DSB1
      VM(7)=VM(7)/RADIAN
      TP(3,4)=X(4)
      TP(2,4)=X(3)
      TP(4,4)=DHB2
      TP(5,4)=DSB2
      CVB2=CP(TP(3,4))-ZB2(6)
      GA=ZB2(3)+ZB2(2)**2/CVB2
      TP(7,4)=GA/ZB2(3)
      TP(8,4)=GA/ZB2(1)
      TP(6,4)=TP(7,4)*CVB2
      VM(6)=SQRT(2.0*R*(TP(4,3)-TP(4,4)))
      VM(5)=VM(6)/SQRT(TP(8,4)*TP(1,4)/TP(2,4))
      IF (TP(5,2).GT.TP(5,4).OR.TP(5,2).GT.TP(5,5)) KODE(10)=1
C
C  THE ITERATION PROCEDURE FOR CALCULATING THE TOTAL DENSITY AND
C  TEMPERATURE STARTS HERE.
C
      TP(3,1)=TP(3,3)
      TP(2,1)=TP(2,3)*EXP(SNGL(DSB2-DSB1))
      DO 15 I=1,20
      CALL ZETA (3,TP(2,1),TP(3,1),ZA1)
      TP(1,1)=TP(2,1)*TP(3,1)*R*ZA1(1)
      IF (LGFN(TP(1,1),TP(3,1),KODE(1),ZA1)) KODE(1)=1
      DSA1=CS(TP(3,1))-DLOG(DBLE(TP(2,1)))-ZA1(4)
      F1=DSB1-DSA1
      DHA1=CH(TP(3,1))+TP(3,1)*(ZA1(1)-ZA1(5))
      F2=X(7)/2.0+DHB1-DHA1
      F11=-ZA1(2)/TP(2,1)
      CVA1=CP(TP(3,1))-ZA1(6)
      F12=CVA1/TP(3,1)
      F21=TP(3,1)*(ZA1(3)-ZA1(2))/TP(2,1)
      F22=CVA1+ZA1(2)
      DET=F11*F22-F12*F21
      CONV(10)=(F1*F22-F2*F12)/(TP(2,1)*DET)
      CONV(11)=(F2*F11-F1*F21)/(TP(3,1)*DET)
      TEST=ABS(CONV(10))+ABS(CONV(11))
      IF (TEST.LT.EDTA1) GO TO 16
      TP(2,1)=TP(2,1)*(1.0+CONV(10))
15    TP(3,1)=TP(3,1)*(1.0+CONV(11))
C
      KODE(9)=1
16    TP(4,1)=DHA1
      TP(5,1)=DSA1
      GA=ZA1(3)+ZA1(2)**2/CVA1
      TP(7,1)=GA/ZA1(3)
      TP(8,1)=GA/ZA1(1)
      TP(6,1)=CVA1*TP(7,1)
      IF (VM(9).GT.1.0) RETURN
```

```
      NSAVE=1
      DO 17 I=1,103
17    SAVE(I)=OUT(I)
      TP(1,5)=TP(1,5)-0.001*(TP(1,3)-TP(1,5))
      GO TO 4
      END
```

```
C DECK RGDFW
C
C  THE INVERSE OF THE DERIVATIVE MATRIX REQUIRED FOR DETERMINING THE
C  VALUES OF X IS CALCULATED IN THIS SUBROUTINE.
C
      SUBROUTINE RDFW
      COMMON /RDW/ W(8,8),X(8),X13,SQX13,X15,SQX15,V7,W7,CVB1,CVB2,CVB3
      COMMON /OUTW/ E(62),ZA1(6),ZB1(6),ZA2(6),ZB2(6),ZB3(6),KODE(11)
      DIMENSION XW(8), YW(8)
      DOUBLE PRECISION CP
      DO 1 I=1,8
      DO 1 J=1,8
1     W(I,J)=0.0
      SV7=1.0+V7**2
      SW7=SQRT(1.0-W7**2)
      CVB1=CP(X(2))-ZB1(6)
      CVB2=CP(X(4))-ZB2(6)
      CVB3=CP(X(6))-ZB3(6)
      W(1,3)=ZB2(2)/X(3)
      W(1,4)=-CVB2/X(4)
      W(2,1)=-X(7)*SQX13/X(1)
      W(2,3)=(SQX13*X(7)-X(4)*(ZB2(3)-ZB2(2)))/X(3)
      W(2,4)=-CVB2-ZB2(2)
      W(2,7)=-SQX13/2.0
      A=X(2)*(ZB1(3)-ZB1(2))
      W(3,1)=(A-SQX13*X(7))/X(1)
      W(3,2)=CVB1+ZB1(2)
      W(3,3)=W(2,3)
      W(3,4)=W(2,4)
      W(3,7)=0.5+W(2,7)
      W(4,1)=(A-X(8)*SQX15)/X(1)
      W(4,2)=W(3,2)
      W(4,5)=(SQX15*X(8)-X(6)*(ZB3(3)-ZB3(2)))/X(5)
      W(4,6)=-CVB3-ZB3(2)
      W(4,8)=(1.0-SQX15)/2.0
      W(5,1)=X(2)*ZB1(3)-X(7)*(2.0*X13-1.0)
      W(5,2)=X(1)*ZB1(2)
      W(5,3)=X(7)*SQX13-X(4)*ZB2(3)
      W(5,4)=-X(3)*ZB2(2)
      W(5,7)=(1.0-X13)*X(1)
      W(6,1)=X(2)*ZB1(3)-X(8)*(2.0*X15-1.0)
      W(6,2)=W(5,2)
      W(6,5)=X(8)*SQX15-X(6)*ZB3(3)
      W(6,6)=-X(5)*ZB3(2)
      W(6,8)=X(1)*(1.0-X15)
      W(7,1)=V7/(SV7*X(1))
      W(7,5)=-W(7,1)*X15
```

```
      W(7,7)=W7/(2.0*X(7)*SW7)-V7/(2.0*SV7*(X(7)-X(8)))
      W(7,8)=(V7/(W7*SV7*(X(7)-X(8)))-1.0/(X(7)*SW7))/(2.0*W7)
      W(8,5)=-X(6)*ZB3(3)
      W(8,6)=-X(5)*ZB3(2)
      CALL MINV (W,8,DET,XW,YW)
C
C   MINV IS THE SUBROUTINE USED TO INVERT THE DERIVATIVE MATRIX. THIS
C   SUBROUTINE IS PART OF THE SCIENTIFIC SUBROUTINE PACKAGE SUPPLIED
C   BY I.B.M.
C
      RETURN
      END
```

```
C DECK PGWED
C
C   THE PERFECT GAS VALUES FOR VELOCITY, SHOCK ANGLE, AND THE MACH NUMBER
C   BOTH UPSTREAM AND DOWNSTREAM OF THE NORMAL SHOCK ARE CALCULATED IN
C   THIS SUBROUTINE.
C
      SUBROUTINE PWEDG (RATIO,DELTA,XM1,XM2,THETA,DELR,KK)
      COMMON /LDATA/ A(5),G
      COMMON /GDATW/ G1,G2,G3,G4,G5,G6,G7,G8,G9,G10
      COMMON /LIMITW/ EDA2,EMAT,EDTA1,EPWD
      DIMENSION DEL(3)
      DATA RADIAN,PI,KG/.0174532925,1.5707963,0/
      FF(A)=(1.0-1.0/A)**G3*(ST2-1.0/A)/G10-R
      XX(A)=G8*COS(A-D)/(ST*(SIN(2.0*A-D)-GSD))
      FFM(A)=SIN(A)**2/G10-R
      IF (KG.NE.0) GO TO 1
      G1=(G-1.0)/2.0
      G2=G
      G3=1.0/(G-1.0)
      G4=G*G3
      G5=2.0*G3
      G6=(G+1.0)*G3
      G7=2.0*G4
      G8=2.0*G7
      G9=G6**G6
      G10=((G+1.0)**2/(4.0*G))**G4
      KG=1
1     KKK=0
      DR=0.0
      R=RATIO
      D=DELTA*RADIAN
      GSD=G2*SIN(D)
      IF (D.LE.0.0.OR.GSD.GT.1.0) GO TO 11
      TMIN=(D+ARSIN(GSD))/2.0
      TMAX=PI+D-TMIN
      T1=TMIN+1.0E-4
      F1=FFM(TMIN)
      IF (F1.GT.0.0.OR.FFM(TMAX).LT.0.0) GO TO 11
      DEL(1)=(TMAX-TMIN-2.0E-4)/35.0
      DEL(2)=5.0*DEL(1)
      DEL(3)=DEL(1)
      DO 2 J=1,3
```

```
      DO 2 I=1,5
      T2=T1+DEL(J)
      ST=SIN(T2)
      ST2=ST**2
      X=XX(T2)
      F2=FF(X)
      IF (ABS(F1+F2).LT.ABS(F1)+ABS(F2)) GO TO 3
      F1=F2
2     T1=T2
      GO TO 11
3     IN=0
      DO 9 I=1,20
      DR=F2/R
      IF (ABS(DR).LT.EPWD) GO TO 10
      DT=(T2-T1)/(F1/F2-1.0)
      T1=T2
      F1=F2
      T2=T2+DT
      IF (T2-TMIN-1.0E-4) 4,4,5
4     T2=TMIN+1.0E-4
      GO TO 7
5     IF (TMAX-T2-1.0E-4) 6,6,8
6     T2=TMAX-1.0E-4
7     IF (IN.EQ.1) GO TO 11
      IN=1
8     ST=SIN(T2)
      ST2=ST**2
      X=XX(T2)
9     F2=FF(X)
      KKK=2
10    IF (X.GT.G7) GO TO 12
11    KKK=1
      X=0.0
      T2=0.0
      X2=0.0
12    DELR=DR
      IF (X.EQ.0.0) GO TO 13
      SX=ST2*X
      X2=(SX/G7+G5)/(SIN(T2-D)**2*(SX-1.0))
13    KK=KKK
      THETA=T2/RADIAN
      XM1=SQRT(X/G7)
      XM2=SQRT(X2)
      RETURN
      END
```

```
C DECK WDATA

      BLOCK DATA
      COMMON /LIMITW/ E(4)
      DATA E/1.0E-6,1.0E-5,2.0E-6,1.0E-6/
      END
```

APPENDIX C

DESCRIPTION AND CARD LISTING OF COMPUTER ROUTINES

THAT APPLY TO CASE II

Case II applies to measurements of nozzle flow using the upstream total pressure $p_{1,t}$, the upstream total temperature $T_{1,t}$, and the stagnation pressure $p_{2,t}$ at the nozzle exit.

In order to get a workable set of routines, the routines in this appendix have to be combined with one of the sets of routines in appendix D. The particular set that is chosen depends on the type of gas. This combined set of routines is referenced in the main program by the following statement:

```
CALL RNS(PA1,TA1,PA2)
```

All the output is returned through labeled COMMON. Therefore, this COMMON statement has to be in the main program:

```
COMMON/OUTNS/TP(8,4),VM(6),CONV(9),Z(6,4),KODE(8)
```

There are certain variables that have to do with the convergence requirements of the various iteration procedures in these routines. These variables are initialized in a BLOCK DATA subprogram. However, if the following COMMON statement is put in the main program, the value of these variables can be altered:

```
COMMON/LIMITN/EDA1,EMAT,EPNS
```

The symbols that apply to these routines are defined as follows:

PA1 Free-stream total pressure, $p_{1,t}$, Pa

TA1 Free-stream total temperature, $T_{1,t}$, K

PA2 Total pressure downstream of a normal shock, $p_{2,t}$, Pa

TP(I,J) Except for the fact that J does not assume the value of 5, the definition of the elements in this array is the same as that for the TP array in appendix B.

VM(I) Except for the fact that I does not exceed 6, the definition of the elements in this array is the same as that for the VM array in appendix B.

CONV(1) to CONV(7)
where

$$CONV(I) = \frac{X_{I,n} - X_{I,n-1}}{X_{I,n-1}}$$

CONV(8) and CONV(9)
where

$$CONV(8) = 1 - \frac{p_{1,t}}{Z_{1,t}\rho_{1,t}RT_{1,t}}$$

$$CONV(9) = \frac{\left(\frac{p_{2,t}}{p_{1,t}}\right)_{eq.\ (61)} - \left(\frac{p_{2,t}}{p_{1,t}}\right)_{given}}{\left(\frac{p_{2,t}}{p_{1,t}}\right)_{given}}$$

Z(I, J) Except for the fact that J does not assume the value of 5, the definition of the elements in this array are the same as that for Z in appendix B.

The following symbols represent integers to indicate various error conditions. If all the integers are zero, a valid calculation has been performed. If the integers are unity, errors exist. These errors are

KODE(1) Equals 1 if $p_{1,t}$ or $T_{1,t}$ are out of range of the state equations. A value of 1 terminates the calculation.

KODE(2) Equals 1 if $p_{2,t}$ or $T_{2,t}$ are out of range of the state equations. A value of 1 terminates the calculation.

KODE(3) Equals 1 if p_1 or T_1 are out of range of the state equation. A value of 1 terminates the calculation.

KODE(4) Equals 1 if p_2 or T_2 are out of range of the state equation. A value of 1 terminates the calculation.

KODE(5) Equals 1 if the iterative procedures for calculating $M_{1,P}$ fail to converge.

KODE(6) Equals 1 if the iterative procedures for calculating $\rho_{1,t}$ fails to converge.

KODE(7) Equals 1 if the iterative procedures for calculating X_1 to X_7 fails to converge.

KODE(8) Equals 1 if $S_1 > S_2$

EDA1 Maximum value of $|CONV(8)|$ permitted. This is initialized at 1×10^{-6}.

EMAT Maximum value of $\sum_{I=1}^{7} |CONV(I)|$. This is initialized at 1×10^{-5}.

EPNS Maximum value of $|CONV(9)|$ permitted. This is initialized at 1×10^{-6}.

The routines that apply to case II are described briefly here. These routines are identified by their deck names.

Deck RGNS

This is the subroutine in which the output variables TP and VM are calculated. The iteration procedure for solving equations (53) and (54) to (60) are in this routine.

Deck RGDFNS

In this subroutine, the inverse of the derivative matrix is calculated. This is required to solve equations (54) to (60). In addition, this routine requires the matrix inversion routine MINV supplied by IBM in their Scientific Subroutine Package.

Deck PGNS

This subroutine is used to calculate $M_{1,P}$. The iterative routine used to solve equation (61) is in this subroutine.

Deck NSDATA

The BLOCK DATA subprogram contains the initial values of the convergence limits for the various iterative procedures.

A workable set of routines has to include not only these decks, but also one of the sets of decks in appendix D. The card listing of these decks follows.

```
C DECK RGNS
C
C  THIS IS THE SUBROUTINE WHERE THE FLOW PROPERTIES AND THERMODYNAMIC
C  STATE FUNCTIONS OF A SUPERSONIC STREAM ARE CALCULATED FROM MEASURED
C  QUANTITIES.  THESE QUANTITIES ARE THE PRESSURE AND TEMPERATURE IN A
C  PLENUM UPSTREAM OF A SUPERSONIC NOZZLE, AND THE TOTAL PRESSURE
C  DOWNSTREAM OF A NORMAL SHOCK AT THE NOZZLE EXIT.
C
      SUBROUTINE RNS (PA1,TA1,PA2)
      COMMON /OUTNS/ TP(8,4),VM(6),CONV(9),Z(6,4),KODE(8)
      COMMON /RDNS/ W(7,7),X(7),X13,SQX13
      COMMON /GDATNS/ G1,G2,G3,G4,G5,G6,G7,G8,G9,G10,G11
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      COMMON /LIMITN/ EDA1,EMAT,EPNS
      DIMENSION ZA1(6), ZB1(6), ZA2(6), ZB2(6), F(7), OUT(79)
      EQUIVALENCE (TP(1),OUT(1)), (ZA1(1),Z(1)), (ZB1(1),Z(7)), (ZA2(1),
     1Z(13)), (ZB2(1),Z(19))
      DOUBLE PRECISION CP,CS,CH,DSA1,DSA2,DSB1,DSB2,DHA1,DHA2,DHB1,DHB2
      LOGICAL LGFN
      DO 1 I=1,79
1     OUT(I)=0.0
      DO 2 J=1,4
      DO 2 I=1,3
2     Z(I,J)=1.0
      DO 3 I=1,7
      X(I)=0.0
3     F(I)=0.0
      TP(1,1)=PA1
      TP(3,1)=TA1
      TP(1,3)=PA2
C
C  THE PERFECT GAS VALUES OF THE MACH NUMBER, BOTH UPSTREAM AND
C  DOWNSTREAM OF THE NORMAL SHOCK ARE CALCULATED IN PNS.
C
      CALL PNS (TP(1,3)/TP(1,1),VM(2),VM(5),CONV(9),KODE(5))
      IF (LGFN(TP(1,1),TP(3,1),KODE(1),ZA1)) RETURN
C
C  THE ITERATION PROCEDURE FOR CALCULATING THE PLENUM DENSITY STARTS
C  HERE.
C
      A=TP(1,1)/(R*TP(3,1))
      TP(2,1)=A
      DO 4 I=1,20
      CALL ZETA (1,TP(2,1),TP(3,1),ZA1)
      CONV(8)=1.0-TP(1,1)/(ZA1(1)*R*TP(2,1)*TP(3,1))
      IF (ABS(CONV(8)).LT.EDA1) GO TO 5
      AA=(ZA1(1)-A/TP(2,1))/ZA1(3)
4     TP(2,1)=TP(2,1)*(1.0-AA)
C
      KODE(6)=1
5     CALL ZETA (3,TP(2,1),TP(3,1),ZA1)
      IF (LGFN(TP(1,1),TP(3,1),KODE(1),ZA1)) RETURN
      DHA1=CH(TP(3,1))+TP(3,1)*(ZA1(1)-ZA1(5))
      TP(4,1)=DHA1
      DSA1=CS(TP(3,1))-DLOG(DBLE(TP(2,1)))-ZA1(4)
      TP(5,1)=DSA1
      CV=SNGL(CP(TP(3,1)))-ZA1(6)
      GA=ZA1(3)+ZA1(2)**2/CV
      TP(7,1)=GA/ZA1(3)
      TP(8,1)=GA/ZA1(1)
```

```
      TP(6,1)=CV*TP(7,1)
      IF (KODE(5).EQ.1) RETURN
C
C   THE INITIAL ESTIMATES OF THE VALUES OF X ARE CALCULATED BY THE
C   FOLLOWING STATEMENTS.
C
      SQM1=VM(2)**2
      AA=(1.D+G1*SQM1)
      X(1)=A/AA**G3
      X(2)=TP(3,1)/AA
      AA=G6*SQM1/(SQM1+G5)
      X(3)=X(1)*AA
      AAA=(G7*SQM1-1.D)/G6
      X(4)=X(2)*AAA/AA
      X(5)=A*AA**G4/AAA**G3
      X(6)=TP(3,1)
      X(7)=G2*X(2)*SQM1
C
      VM(4)=SQRT(X(7)*R)
C
C   THE ITERATION PROCEDURE FOR CALCULATING THE VALUES OF X STARTS HERE.
C
      DO 10 I=1,20
      CALL ZETA (3,X(1),X(2),ZB1)
      CALL ZETA (3,X(3),X(4),ZB2)
      CALL ZETA (3,X(5),X(6),ZA2)
      TP(1,2)=ZB1(1)*R*X(1)*X(2)
      TP(1,4)=ZB2(1)*R*X(3)*X(4)
      IF (LGFN(TP(1,2),X(2),KODE(3),ZB1)) RETURN
      IF (LGFN(TP(1,4),X(4),KODE(4),ZB2)) RETURN
      IF (LGFN(TP(1,3),X(6),KODE(2),ZA2)) RETURN
      DSA2=CS(X(6))-DLOG(DBLE(X(5)))-ZA2(4)
      DSB1=CS(X(2))-DLOG(DBLE(X(1)))-ZB1(4)
      DSB2=CS(X(4))-DLOG(DBLE(X(3)))-ZB2(4)
      DHA2=CH(X(6))+X(6)*(ZA2(1)-ZA2(5))
      DHB1=CH(X(2))+X(2)*(ZB1(1)-ZB1(5))
      DHB2=CH(X(4))+X(4)*(ZB2(1)-ZB2(5))
      F(1)=DSB1-DSA1
      F(2)=DHB1-DHA1+X(7)/2.0
      X13=X(1)/X(3)
      SQX13=X13**2
      F(3)=TP(1,4)/R-TP(1,2)/R-X(1)*X(7)*(1.0-X13)
      F(4)=DHB2-DHB1-X(7)*(1.0-SQX13)/2.0
      F(5)=DHB2-DHA2+X(7)*SQX13/2.0
      F(6)=DSB2-DSA2
      F(7)=ZA2(1)*X(5)*X(6)-TP(1,3)/R
      IF (MOD(I,5).EQ.1) CALL RDFNS
      DO 7 J=1,7
      CONV(J)=0.0
      DO 6 K=1,7
6     CONV(J)=CONV(J)+W(J,K)*F(K)
7     CONV(J)=CONV(J)/X(J)
      TEST=0.0
      DO 8 J=1,7
8     TEST=TEST+ABS(CONV(J))
      IF (TEST.LT.EMAT) GO TO 11
      DO 9 J=1,7
9     X(J)=X(J)*(1.0+CONV(J))
10    CONTINUE
```

```
C
      KODE(7)=1
11    TP(4,2)=DHB1
      TP(5,2)=DSB1
      TP(2,2)=X(1)
      TP(3,2)=X(2)
      CV=SNGL(CP(TP(3,2)))-ZB1(6)
      GA=ZB1(3)+ZB1(2)**2/CV
      TP(7,2)=GA/ZB1(3)
      TP(8,2)=GA/ZB1(1)
      TP(6,2)=CV*TP(7,2)
      VM(3)=SQRT(X(7)*R)
      VM(1)=VM(3)/SQRT(TP(8,2)*TP(1,2)/TP(2,2))
      TP(3,3)=X(6)
      TP(2,3)=X(5)
      TP(4,3)=DHA2
      TP(5,3)=DSA2
      CV=SNGL(CP(TP(3,3)))-ZA2(6)
      GA=ZA2(3)+ZA2(2)**2/CV
      TP(7,3)=GA/ZA2(3)
      TP(8,3)=GA/ZA2(1)
      TP(6,3)=CV*TP(7,3)
      TP(2,4)=X(3)
      TP(3,4)=X(4)
      TP(4,4)=DHB2
      TP(5,4)=DSB2
      IF (TP(5,2).GT.TP(5,4)) KODE(8)=1
      CV=SNGL(CP(TP(3,4)))-ZB2(6)
      GA=ZB2(3)+ZB2(2)**2/CV
      TP(7,4)=GA/ZB2(3)
      TP(8,4)=GA/ZB2(1)
      TP(6,4)=CV*TP(7,4)
      VM(6)=SQRT(2.0*R*(TP(4,3)-TP(4,4)))
      VM(5)=VM(6)/SQRT(TP(8,4)*TP(1,4)/TP(2,4))
      RETURN
      END


C DECK RGDFNS
C
C  THE INVERSE OF THE DERIVATIVE MATRIX REQUIRED FOR DETERMINING THE
C  VALUES OF X IS CALCULATED IN THIS SUBROUTINE.
C
      SUBROUTINE RDFNS
      COMMON /OUTNS/ E(47),ZA1(6),ZB1(6),ZA2(6),ZB2(6),KODE(8)
      COMMON /RDNS/ W(7,7),X(7),X13,SQX13
      DIMENSION XW(7), YW(7)
      DOUBLE PRECISION CP
      DO 1 I=1,7
      DO 1 J=1,7
1     W(I,J)=0.0
      CVB1=SNGL(CP(X(2)))-ZB1(6)
      CVB2=SNGL(CP(X(4)))-ZB2(6)
      CVA2=SNGL(CP(X(6)))-ZA2(6)
      W(1,1)=ZB1(2)/X(1)
      W(1,2)=-CVB1/X(2)
      W(2,1)=(ZB1(2)-ZB1(3))*X(2)/X(1)
      W(2,2)=-(CVB1+ZB1(2))
      W(2,7)=-0.5
      W(3,1)=X(2)*ZB1(3)+X(7)*(1.0-2.0*X13)
```

```
      W(3,2)=X(1)*ZB1(2)
      W(3,3)=X(7)*SQX13-X(4)*ZB2(3)
      W(3,4)=-X(3)*ZB2(2)
      W(3,7)=X(1)*(1.0-X13)
      W(4,1)=-W(2,1)-X(7)*X13/X(3)
      W(4,2)=-W(2,2)
      W(4,3)=(X(7)*SQX13-X(4)*(ZB2(3)-ZB2(2)))/X(3)
      W(4,4)=-(CVB2+ZB2(2) )
      W(4,7)=(1.0-SQX13)/2.0
      W(5,1)=W(2,1)+W(4,1)
      W(5,3)=W(4,3)
      W(5,4)=W(4,4)
      W(5,5)=X(6)*(ZA2(3)-ZA2(2))/X(5)
      W(5,6)=CVA2+ZA2(2)
      W(5,7)=W(4,7)-0.5
      W(6,3)=ZB2(2)/X(3)
      W(6,4)=-CVB2/X(4)
      W(6,5)=-ZA2(2)/X(5)
      W(6,6)=CVA2/X(6)
      W(7,5)=-X(6)*ZA2(3)
      W(7,6)=-X(5)*ZA2(2)
      CALL MINV (W,7,DET,XW,YW)
C
C  MINV IS THE SUBROUTINE USED TO INVERT THE DERIVATIVE MATRIX. THIS
C  SUBROUTINE IS PART OF THE SCIENTIFIC SUBROUTINE PACKAGE SUPPLIED
C  BY I.B.M.
C
      RETURN
      END
```

```
C DECK PGNS
C
C  THE PERFECT GAS VALUES FOR THE MACH NUMBER, BOTH UPSTREAM AND
C  DOWNSTREAM OF THE NORMAL SHOCK ARE CALCULATED IN THIS SUBROUTINE.
C
      SUBROUTINE PNS (RATIO,XM1,XM2,DELR,KK)
      COMMON /LDATA/ A(5),G
      COMMON /GDATNS/ G1,G2,G3,G4,G5,G6,G7,G8,G9,G10,G11
      COMMON /LIMITN/ EDA1,EMAT,EPNS
      DATA KG/0/
      F(A)=G8*(A/(A+G5))**G4/(G7*A-1.0)**G3
      IF (KG.NE.0) GO TO 1
      G1=(G-1.0)/2.0
      G2=G
      G3=1.0/(G-1.0)
      G4=G*G3
      G5=2.0*G3
      G6=(G+1.0)*G3
      G7=2.0*G4
      G8=G6**G6
      G9=1.5*(G+1.0)**2/G
      G10=F(4.0)
      G11=F(5.0)
      KG=1
1     R=RATIO
```

```
      KKK=0
      DR=0.0
      IF (R.LE.0.0.OR.R.GT.1.0) GO TO 4
      IF (R.LT.0.9999) GO TO 2
      X2=1.0+(G9*(1.0-R))**0.33333333
      GO TO 5
2     X1=4.0
      F1=G10-R
      X2=5.0
      F2=G11-R
      DO 3 I=1,20
      DR=F2/R
      IF (ABS(DR).LT.EPNS) GO TO 5
      DX=(X2-X1)/(F1/F2-1.0)
      X1=X2
      F1=F2
      X2=X2+DX
3     F2=F(X2)-R
      KKK=2
      GO TO 5
4     KKK=1
      X2=0.0
      Y2=0.0
      GO TO 6
5     Y2=(X2+G5)/(G7*X2-1.0)
6     XM1=SQRT(X2)
      XM2=SQRT(Y2)
      DELR=DR
      KK=KKK
      RETURN
      END
```

```
C DECK NSDATA

      BLOCK DATA
      COMMON /LIMITN/ E(3)
      DATA E/1.0E-6,1.0E-5,1.0E-6/
      END
```

APPENDIX D

DESCRIPTION AND CARD LISTING OF THE COMPUTER ROUTINES THAT DESCRIBE THE VARIOUS GASES

Any one of the sets of routines in this appendix is used with the routines in either appendix B or C. In addition, this set can also be used with the routines in reference 3 whose deck names are RGASC1 and RDATA. This combination extends the applicability of reference 3 to include all the gases in this report.

The deck names for these sets of routines consist of a one- or two-letter prefix identifying the gas and a root identifying the routine's purpose.

GENERAL PURPOSE OF ROUTINES

Deck --ZETA

In this subroutine, the compressibility-factor functions defined by equations (1) to (6) are calculated. With the exceptions of methane and natural gas, this subroutine can be used independently of the other routines. These points will be noted when the individual gases are discussed. Because of this independence, the use of this routine is described briefly here. This routine is referenced as follows:

CALL ZETA(K, RHO, T, Z)

where

RHO	Density, kg/m^3
T	Temperature, K
Z	This is a six-element array. These elements are, in order, Z_I to Z_{VI}.
K	If K = 1, only Z(1) and Z(3) are calculated. If K = 2, only Z(2) and Z(4) are calculated. If K = 3, Z(1) to Z(6) are calculated. For the case of steam, Z(1) to Z(6) are calculated regardless of the value of K.

Deck --TEMP

The ideal-gas specific-heat functions defined by equations (7) to (9) are calculated in this routine. Except for natural gas, whose ideal-gas specific heat is composition dependent, this routine can be used independently of the other routines. Because of this, the use of this routine is described briefly here.

This is a double-precision function routine with three entry points - CP, CS, and CH. All three entry points use a single-precision argument, which is temperature. The function definitions are

$$CP(T) = \xi_I(T) = \frac{C_{v,id}}{R} \tag{D1}$$

$$CS(T) = \xi_{II}(T) = \frac{S_{id}}{R} + \ln\left(\frac{p}{RT}\right) \tag{D2}$$

$$CH(T) = \xi_{III}(T) = \frac{H_{id}}{R} - T \tag{D3}$$

From equations (8) and (9), it is seen that ξ_{II} and ξ_{III} involve indefinite temperature integrals. The constants of integration for these integrals are included in this routine. The value of these constants is chosen such that the enthalpy and entropy equal zero at some reference thermodynamic state. Except for natural gas, steam, and low-temperature nitrogen, this reference state is that of the ideal gas at a temperature of 0 K and a pressure of 1×10^5 pascals. The reference state for natural gas, steam, and low-temperature nitrogen will be given when these gases are discussed.

Deck --LOG

This is a logical function that tests whether or not the pressure and temperature lie within the range of the state equations. If the temperature range extends below critical, the vapor pressure relation is used to determine whether or not the fluid is a gas. Because of the computational procedure, the lower pressure limit of the state equation for all gases has to be a nonzero positive number; this number is arbitrarily set at 0.1 pascal.

Deck --DATA

This is a BLOCK DATA subprogram that supplies gas-dependent constants for the other routines. Among these constants are the molecular weight, the gas constant, and the perfect-gas specific-heat ratio.

While the procedures in this report do not require this subroutine, the procedures in reference 3 do. The inclusion of this subroutine permits the application of the procedures in reference 3 to all the gases in this report. If necessary, this subroutine changes the temperature such that the fluid is a gas and lies within range of the state equation.

ROUTINES APPLIED TO VARIOUS GASES

Air

The equations for the compressibility factor and the ideal-gas specific heat for air are the result of a curve fit of the data in reference 5. The temperature range of these curve fits is from 150 to 1500 K. The pressure range extends to 100×10^5 pascals. These equations only apply to undissociated air.

In order to check the accuracy of these fits, the values of Z and C_p calculated by these routines were compared with those tabulated in reference 5. Over most of the pressure and temperature range, Z agrees to within 0.1 percent and C_p agrees to within 0.3 percent. The maximum disagreement is 0.3 percent for Z and 3 percent for C_p.

The card listing of these routines follows. The prefix for the deck names is AI.

```
C DECK AIZETA

      SUBROUTINE ZETA(KK,PP,TT,Z)
      DIMENSION Z(6),A(10,3,2),B(10,3,2)
      DATA A/0.0,9.7429208E-13,-4.2565612E-9,1.1837564E-7,-1.1911556E-6,
     14.2969317E-6,8.1108983E-6,-1.322802E-4,-1.402926E-4,1.194593E-3,5.
     28580855E-14,-6.0441752E-13,-1.2888247E-13,4.6020856E-11,-9.9022657
     3E-10,7.8369336E-9,-1.9986894E-8,-5.5490372E-8,4.8502964E-7,6.55400
     416E-7,0.0,2.4610094E-16,2.0018081E-14,-7.0226616E-13,7.7383923E-12
     5,-3.0953497E-11,-2.6931749E-11,5.104152E-10,-5.6194899E-10,1.36719
     633E-10,0.0,-6.82004456E-12,2.55393672E-8,-5.918782E-7,4.7646224E-6
     7,-1.28907951E-5,-1.62217966E-5,1.322802E-4,0.0,1.194593E-3,-4.6864
     8684E-13,4.23092264E-12,7.7329482E-13,-2.3010428E-10,3.96090628E-9,
     9-2.35108008E-8,3.9973788E-8,5.5490372E-8,0.0,6.5540016E-7,0.0,-1.7
     A2270658E-15,-1.20108486E-13,3.5113308E-12,-3.09535692E-11,9.286049
     B1E-11,5.3863498E-11,-5.104152E-10,0.0,1.3671933E-10/
      DATA B/0.0,-7.79433664E-12,2.97959284E-8,-7.1025384E-7,5.955778E-6
     1,-1.71877268E-5,-2.43326949E-5,2.645604E-4,1.402926E-4,0.0,-2.6361
     23848E-13,2.41767008E-12,4.51088645E-13,-1.38062568E-10,2.47556642E
     3-9,-1.56738672E-8,2.9980341E-8,5.5490372E-8,-2.4251482E-7,2*0.0,-6
     4.56269173E-16,-4.67088557E-14,1.40453232E-12,-1.28973205E-11,4.127
     513293E-11,2.6931749E-11,-3.402768E-10,1.8731633E-10,2*0.0,5.456035
     665E-11,-1.7877557E-7,3.5512692E-6,-2.3823112E-5,5.15631804E-5,4.86
     7653898E-5,-2.645604E-4,2*0.0,2.10891078E-12,-1.69236906E-11,-2.706
     853187E-12,6.9031284E-10,-9.9022657E-9,4.70216016E-8,-5.9960682E-8,
     9-5.5490372E-8,3*0.0,4.59388421E-15,2.80253134E-13,-7.0226616E-12,5
     A.1589282E-11,-1.23813988E-10,-5.3863498E-11,3.402768E-10,2*0.0/
```

```
      K= KK
      P= PP
      S=  1000.0/TT
      IF(K.EQ.2)  GO TO 2
      BB= A(1,1,1)
      CC= A(1,2,1)
      DD= A(1,3,1)
      DO 1  N=2,10
      BB= BB*S+A(N,1,1)
      CC= CC*S+A(N,2,1)
    1 DD= DD*S+A(N,3,1)
      Z(1)= 1.0+(BB+(CC+DD*P)*P)*P
      Z(3)= 1.0+(2.0*BB+(3.0*CC+4.0*DD*P)*P)*P
      IF(K.EQ.1) RETURN
    2 BB= A(1,1,2)
      CC= A(1,2,2)
      DD= A(1,3,2)
      DO 3  N=2,10
      BB= BB*S+A(N,1,2)
      CC= CC*S+A(N,2,2)
    3 DD= DD*S+A(N,3,2)
      Z(2)= 1.0+(BB+(CC+DD*P)*P)*P
      Z(4)= (BB+(CC/2.0+DD*P/3.0)*P)*P
      IF(K.EQ.2)  RETURN
      BB= B(1,1,1)
      BBB= B(1,1,2)
      CC= B(1,2,1)
      CCC= B(1,2,2)
      DD= B(1,3,1)
      DDD= B(1,3,2)
      DO 4  N=2,10
      BB= BB*S+B(N,1,1)
      BBB= BBB*S+B(N,1,2)
      CC= CC*S+B(N,2,1)
      CCC= CCC*S+B(N,2,2)
      DD= DD*S+B(N,3,1)
    4 DDD= DDD*S+B(N,3,2)
      Z(5)= (BB+(CC+DD*P)*P)*P
      Z(6)= (BBB+(CCC+DDD*P)*P)*P
      RETURN
      END
```

```
C DECK AITEMP
      DOUBLE PRECISION FUNCTION CP(T)
      DIMENSION A(8,3,2)
      DOUBLE PRECISION HI(2),SI(2),S
      DATA A/0.0,1.3466662E-5,-3.1114986E-4,2.4129691E-3,-6.332279E-3,5.
     14472783E-3,1.4259098E-3,2.4886014,0.0,2.24444367E-6,-6.2229972E-5,
     26.03242275E-4,-2.11075967E-3,2.72363915E-3,1.4259098E-3,2.4886014,
     30.0,1.92380886E-6,-5.185831E-5,4.8259382E-4,-1.58306975E-3,1.81575
     4943E-3,7.129549E-4,2.4886014,-1.752035E-8,6.3994684E-7,-6.2254094E
     5-6,3.4966174E-5,-1.8261613E-3,3.2562223E-2,-1.272201E-1,2.6256356,
     6-2.50290714E-9,1.06657807E-7,-1.24508188E-6,8.7415435E-6,-6.087204
     733E-4,1.62811115E-2,-1.272201E-1,2.6256356,-2.19004375E-9,9.142097
```

```
 871E-8,-1.03756823E-6,6.9932348E-6,-4.56540325E-4,1.08540743E-2,-6.
 9361005E-2,2.6256356/
  DATA HI,SI/-.8930568474993379,-8.369606556481244,21.32793295150501
 1,21.43850926781483/
  L=1
1 S=T/1.0D2
  K=1
  IF(S.GT.5.12397093D0)K=2
  CP=A(1,L,K)
  DO 2 N=2,7
2 CP=CP*S+A(N,L,K)
  GO TO (3,4,5),L
3 CP=CP*S+A(8,1,K)
  RETURN
  ENTRY CS(T)
  L=2
  GO TO 1
4 CP=CP*S+A(8,2,K)*DLOG(S)+SI(K)
  RETURN
  ENTRY CH(T)
  L=3
  GO TO 1
5 CP=T*(CP*S+A(8,3,K))+HI(K)
  RETURN
  END
```

```
C DECK AILOG

      LOGICAL FUNCTION LGFN (P,T,J,Z)
      DIMENSION Z(6)
      J=1
      LGFN=.TRUE.
      IF (P.LT.0.1.OR.P.GT.1.1E7.OR.T.LT.149.0.OR.T.GT.1510.0.OR.Z(1).LE
     1.0.0.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK AIDATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,287.0588,28.9641,1.633314E-3,5.6,1.4/
      END
```

```
C DECK AITLG

      SUBROUTINE TLOGIC(P,T)
      IF(T.LT.149.0)T=149.0
      RETURN
      END
```

Nitrogen

There are two sets of nitrogen routines: one covers the cryogenic temperature range, and the other covers the high-temperature range.

Nitrogen, range I. - The equations for the compressibility factor and the ideal-gas specific heat for nitrogen (range I) are from reference 6. This reference claims a temperature range from 64 to 350 K and a pressure range to 300×10^5 pascals. This report assumes a temperature range from 60 to 400 K and a pressure range to 300×10^5 pascals. These are the same ranges that were assumed in reference 7.

The values of Z and C_p calculated by these routines (using the state equations of ref. 6) were compared with those tabulated in reference 5. Over most of the pressure and temperature range where comparisons are possible, Z agrees to within 0.2 percent and C_p agrees to within 1 percent. The maximum disagreement was 0.4 percent for Z and 2 percent for C_p.

The reference state for the enthalpy and entropy is that of the saturated liquid at the triple point.

The card listing of these routines follows. The prefix for the deck names is N.

```
C DECK NZETA

      SUBROUTINE ZETA(KK,PP,TT,Z)
      DIMENSION Z(6)
      DATA A,B1,B2,B3,B4,B5,B6,B7,B8,B9,B10,B11,B12,B13,B14,B15/-7.135E-
     16,1.2034917E-3,-2.510789E-1,-4.9681584E1,3.7073373E2,1.496473E6,
     22.1027719E-6,-2.4516046E-4,2.3102822E-9,4.9866482,1.6771286E3,
     3-1.656225E5,-6.5374809E-5,2.4209108E-2,-1.126389,1.1829604E-12/
      CO(X,Y,Z)=X*S3+Y*S4+Z*S5
      K=KK
      P=PP
      T=TT
      S1=1.0/T
      S2=S1*S1
      S3=S1*S2
      S4=S1*S3
      S5=S1*S4
      P2=P*P
      EXPO=EXP(A*P2)
      AA=1.0/(2.0*A)
      BB=1.0/A
      C1=CO(B9,B10,B11)
      C2=CO(B12,B13,B14)
```

```
      IF (K.EQ.2) GO TO 1
      BA1=B1+B2*S1+B3*S2+B4*S3+B5*S5
      BA2=B6+B7*S1
      ZA=1.0+(BA1+(BA2+(B8+B15*S1*P2)*P)*P)*P
      ZB=EXPO*P2*(C1+C2*P2)
      Z(1)= ZA+ZB
      ZA=1.0+(2.0*BA1+(3.0*BA2+(4.0*B8+6.0*B15*S1*P2)*P)*P)*P
      ZB=P2*EXPO*(3.0*C1+(2.0*A*C1+5.0*C2+2.0*C2*P2*A)*P2)
      Z(3)= ZA+ZB
      IF (K.EQ.1) RETURN
1     BT=B1-B3*S2-2.0*B4*S3-4.0*B5*S5
      C1P=-CO(3.0*B9,4.0*B10,5.0*B11)
      C2P=-CO(3.0*B12,4.0*B13,5.0*B14)
      CC1=C1+C1P
      CC2=C2+C2P
      ZA=1.0+(BT+(B6+B8*P)*P)*P
      ZB=P2*EXPO*(CC1+CC2*P2)
      Z(2)= ZA+ZB
      ZA=(BT+(B6/2.0+B8*P/3.0)*P)*P
      ZB=AA*(EXPO*(CC1+(P2-BB)*CC2)+BB*CC2-CC1)
      Z(4)= ZA+ZB
      IF (K.EQ.2) RETURN
      C1PP=CO(9.0*B9,16.0*B10,25.0*B11)
      C2PP=CO(9.0*B12,16.0*B13,25.0*B14)
      ZA=-((B2*S1+2.0*B3*S2+3.0*B4*S3+5.0*B5*S5)+(B7*S1/2.0+B15*S1*P**3/
     15.0)*P)*P
      ZB=AA*(EXPO*(C1P+(P2-BB)*C2P)+BB*C2P-C1P)
      Z(5)= ZA+ZB
      CC1P=C1P+C1PP
      CC2P=C2P+C2PP
      ZA=(2.0*B3*S2+6.0*B4*S3+20.0*B5*S5)*P
      ZB=AA*(EXPO*(CC1P+(P2-BB)*CC2P)+CC2P*BB-CC1P)
      Z(6)= ZA+ZB
      RETURN
      END
```

```
C DECK NTEMP
      DOUBLE PRECISION FUNCTION CP(T)
      DOUBLE PRECISION A(5,3), S,HI,SI
      DATA A,SI,HI /2.501146D0,-9.720581D-5,1.036056D-6, -4.437258D-9,
     16.825596D-12,2.501146D0,-9.720581D-5,5.18028D-7,-1.479086D-9,
     21.706399D-12,2.501146D0,-4.8602905D-5,3.45352D-7,-1.1093145D-9,
     31.3651192D-12,7.7124D-1,5.0831D2/
      K=1
    1 S=T
      CP = A(5,K)
      DO 2  I=1,3
      M= 5-I
    2 CP= CP*S+A(M,K)
      GO TO (3,4,5),K
    3 CP= CP*S+A(1,1)
      RETURN
      ENTRY CS(T)
      K=2
```

```
      GO TO 1
    4 CP= CP*S+A(1,2)*DLOG(S)+SI
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
    5 CP= (CP*S+A(1,3)) *S+HI
      RETURN
      END
```

```
C DECK NLOG
      LOGICAL FUNCTION LGFN (P,T,J,Z)
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      DIMENSION Z(6)
      S=T
      J=1
      LGFN=.TRUE.
      IF (P.LT.0.1.OR.P.GT.3.1E7.OR.S.GT.410.0.OR.S.LT.59.0.OR.Z(1).LE.0
     1.0.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      IF (S.GT.126.26) GO TO 1
      PS=10.0**(-305.07339/S+5.5335216+(.16441101+(-3.1389205E-3+(2.9857
     1103E-5+(-1.4238458E-7+2.7375282E-10*S)*S)*S)*S)*S)
      IF (P.GT.XKV*PS) RETURN
1     J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK NDATA
      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,296.8008,28.0134,1.579703E-3,5.6,1.4/
      END
```

```
C DECK NTLG
      SUBROUTINE TLOGIC(P,T)
      DIMENSION A(7)
      DATA A/5.8435156E-6,-9.6521356E-5,3.2061122E-3,-8.1845679E-2,
     11.2169069,-5.2033603,50.343493/
      IF(T.GT.126.26) RETURN
      V= ALOG(P)
      S= A(1)
```

```
      DO 1  N=2,7
    1 S= S*V+A(N)
      IF(T.LT.S)  T=S
      IF(T.LT.59.0) T=59.0
      RETURN
      END
```

Nitrogen, range II. - The equations for the compressibility factor and the ideal-gas specific heat for nitrogen (range II) are the result of a curve fit of the data in reference 5. The temperature ranges of these fits is from 170 to 3000 K. The pressure range extends to 110×10^5 pascals. These equations only apply to undissociated nitrogen.

In order to check the accuracy of these curve fits, the values of Z and C_p calculated by these routines were compared with the values tabulated in reference 5. Over most of the range, Z agrees to within 0.1 percent, and C_p agrees to within 0.5 percent. The maximum disagreement is 0.7 percent for Z and 2 percent for C_p.

The card listing of these routines follows. The prefix for the deck names is HN.

```
C DECK HNZETA
      SUBROUTINE ZETA (KK,PP,TT,Z)
      DIMENSION BB(11,4), CC(11,4), DD(11,4), BCD(11,4,3), Z(6), A(4,3)
      EQUIVALENCE (BB(1),BCD(1)), (CC(1),BCD(45)), (DD(1),BCD(89))
      DATA BB/0.,1.338343E-9,-6.4553708E-9,-1.3807339E-7,1.0851228E-6,-1
     1.4108547E-7,-1.8585143E-5,3.0153933E-5,-4.9439856E-4,1.6440824E-3,
     2-1.0717843E-4,0.,-9.368401E-9,3.8732225E-8,6.9036695E-7,-4.3404912
     3E-6,4.2325641E-7,3.7170286E-5,-3.0153933E-5,0.,1.6440824E-3,-2.143
     45686E-4,0.,-1.0706744E-8,4.5187596E-8,8.2844034E-7,-5.425614E-6,5.
     56434188E-7,5.5755429E-5,-6.0307866E-5,4.9439856E-4,0.,-1.0717843E-
     64,0.,7.4947208E-8,-2.7112557E-7,-4.1422017E-6,2.1702456E-5,-1.6930
     7256E-6,-1.1151086E-4,6.0307866E-5,2*0.,-2.1435686E-4/
      DATA CC/0.,-1.4161135E-11,-1.8207963E-10,-9.1721547E-10,5.3411861E
     1-8,-2.000952E-7,-8.9753116E-7,6.4975889E-6,-1.1598976E-5,1.0653882
     2E-5,-2.7372964E-6,0.,8.496681E-11,9.1039815E-10,3.6688619E-9,-1.60
     323558E-7,4.001904E-7,8.9753116E-7,0.,-1.1598976E-5,2.1307764E-5,-8
     4.2118892E-6,0.,4.9563972E-11,5.4623889E-10,2.2930387E-9,-1.0682372
     5E-7,3.001428E-7,8.9753116E-7,-3.2487944E-6,0.,5.326941E-6,-2.73729
     664E-6,0.,-2.9738384E-10,-2.7311944E-9,-9.1721547E-9,3.2047117E-7,-
     76.002856E-7,-8.9753116E-7,2*0.,1.0653882E-5,-8.2118892E-6/
      DATA DD/8.9688983E-14,3.7837236E-13,-6.3374971E-12,4.2678663E-11,-
     19.4492282E-10,3.5667223E-9,2.0223068E-8,-1.3522968E-7,2.6433166E-7
     2,-2.0382481E-7,4.9983348E-8,-5.381339E-13,-1.8918618E-12,2.5349988
     3E-11,-1.2803599E-10,1.8898456E-9,-3.5667223E-9,0.,-1.3522968E-7,5.
     42866332E-7,-6.1147443E-7,1.9993339E-7,-2.0927429E-13,-7.567447E-13
     5,1.0562495E-11,-5.6904884E-11,9.4492282E-10,-2.3778149E-9,-6.74102
     627E-9,0.,8.8110553E-8,-1.3588321E-7,4.9983348E-8,1.2556458E-12,3.7
     77837236E-12,-4.2249981E-11,1.7071465E-10,-1.8898456E-9,2.3778149E-9
     8,2*0.,1.7622111E-7,-4.0764962E-7,1.9993339E-7/
      S=1000.0/TT
      P=PP/S
      K=KK
      DO 3 J=1,4
```

```
      IF (K.EQ.2.AND.J.NE.2) GO TO 3
      DO 2 I=1,3
      A(J,I)=BCD(1,J,I)
      DO 1 M=2,11
1     A(J,I)=A(J,I)*S+BCD(M,J,I)
2     CONTINUE
      IF (K.EQ.1.AND.J.EQ.1) GO TO 4
3     CONTINUE
      Z(2)=1.0+(A(2,1)+(A(2,2)+A(2,3)*P)*P)*P
      Z(4)=(A(2,1)+(A(2,2)/2.0+A(2,3)*P/3.0)*P)*P
      IF (K.EQ.2) RETURN
      Z(5)=(A(3,1)+(A(3,2)+A(3,3)*P)*P)*P
      Z(6)=(A(4,1)+(A(4,2)+A(4,3)*P)*P)*P
4     Z(1)=1.0+(A(1,1)+(A(1,2)+A(1,3)*P)*P)*P
      Z(3)=1.0+(2.0*A(1,1)+(3.0*A(1,2)+4.0*A(1,3)*P)*P)*P
      RETURN
      END
```

```
C DECK HNTEMP

      DOUBLE PRECISION FUNCTION CP (T)
      DIMENSION A(8,3,2)
      DOUBLE PRECISION CS,CH,S,HI(2),SI(2)
      DATA A/19.204975,-43.37888,31.583231,-6.7699321,-5.2724127E-3,6.42
     163567E-2,1.431144E-2,2.4986544,2.7435679,-7.2298135,6.3166462,-1.6
     292483,-1.7574709E-3,3.2131784E-2,1.431144E-2,2.4986544,2.4006219,-
     36.196983,5.2638718,-1.3539864,-1.3181032E-3,2.1421189E-2,7.15572E-
     43,2.4986544,1.2274093E-3,-6.9024646E-4,-9.3697914E-2,.5882261,-1.4
     5746878,1.4646469,.2916646,2.1558557,1.7534419E-4,-1.1504108E-4,-1.
     687395583E-2,.14705652,-.4915626,.73232345,.2916646,2.1558557,1.5342
     7616E-4,-9.8606637E-5,-1.5616319E-2,.11764522,-.36867195,.48821563,
     88.1458323,2.1558557/
      DATA HI,SI/-.9236215400014771,100.9379426775437,26.17073912726212,
     1125.67762552153525/
      K=1
1     J=1
      S=T/1.0D3
      IF (S.GT..8119820835) J=2
      CP=A(1,K,J)
      DO 2 N=2,7
2     CP=CP*S+A(N,K,J)
      GO TO (3,4,5),K
3     CP=CP*S+A(8,1,J)
      RETURN
      ENTRY CS(T)
      K=2
      GO TO 1
4     CP=CP*S+A(8,2,J)*DLOG(S)+SI(J)
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
5     CP=T*(CP*S+A(8,3,J))+HI(J)
      RETURN
      END
```

```
C DECK HNLOG

      LOGICAL FUNCTION LGFN (P,T,J,Z)
      DIMENSION Z(6)
      J=1
      LGFN=.TRUE.
      IF (P.LT.0.1.OR.P.GT.1.1E7.OR.T.LT.169.0.OR.T.GT.3010.0.OR.Z(1).LE
     1.0.0.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK HNDATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,296.8008,28.0134,1.579703E-3,5.6,1.4/
      END
```

```
C DECK HNTLG

      SUBROUTINE TLOGIC (P,T)
      IF (T.LT.169.0) T=169.0
      RETURN
      END
```

Oxygen

There are two sets of routines for oxygen: one covers the cryogenic temperature range, and the other covers the high-temperature range.

Oxygen, range I. - The equation for the compressibility factor for oxygen (range I) is from reference 8, and the equation for the ideal-gas specific heat is the result of a curve fit of the data in reference 5. Reference 8 claims a temperature range from 65 to 300 K and a pressure range to 300×10^5 pascals. This report assumes a temperature range from 60 to 400 K and a pressure range to 300×10^5 pascals.

The values of Z and C_p calculated by the routines in this report (using the state equation of ref. 8) were compared with those tabulated in reference 5. Over most of the pressure and temperature range where comparisons can be made, Z agrees to within

0.2 percent and C_p agrees to within 1 percent. The maximum disagreement is 3 percent for Z and 3 percent for C_p; the maximum disagreement in Z occurs at 170 K and 70 bars.

The card listing of these routines follows. The prefix for the deck names is O.

```
C DECK OZETA
      SUBROUTINE ZETA(KK,PP,TT,Z)
      DIMENSION Z(6),A(3,3,4),F1(3),F2(3)
      DATA A1,A2,A3,A32,A35,A36,A4,A42,A45,A46,A5,A52,A55,A56,A6,A62,A65
     1,A7,A8,A85,A9,A10,A102,A105,A106,A11,A12,A125,A13,A135,A14,A145,A2
     24,A244,A25,A26,A27,A29,A28,A30,A31,ALPHA,TC/1.29024534E-3,-.501253
     3921,-2814.00595,5628.01189,8442.01784,-16884.0357,7314650.15,-2925
     48600.6,-36573250.7,146293003.,-1.10552497E10,6.63314981E10,7.73867
     5478E10,-4.64320487E11,-6.78596713E-10,-1.35719343E-9,-3.39298357E-
     610,9.48465081E-7,7.22544527E-5,-3.61272264E-5,-3.22597218E-2,-.427
     7820494,.855640987,.64173074,-1.28346148,3.80215484E-10,7.08483179E
     8-8,-2.3616106E-8,1.41493762E-10,-3.53734405E-11,2.83963097E-8,-1.4
     91981549E-8,-5.46946646E-6,-1.09389329E-5,2.37789478E-5,-3.0667678E
     A-4,-.35,-.7,.9,6.02168773E-8,3.01534684E-2,232.832966,154.77/
      DATA A/2.06703766,3591.79212,-416047.043,1.03087315E-5,-3.113551E-
     13,1.22849158,6.40142244E-11,-1.27186613E-8,1.66719727E-6,-4.134075
     231,-10775.3764,1664188.17,-2.06174629E-5,9.34065301E-3,-4.91396632
     3,-1.28028449E-10,3.81559839E-8,-6.66878909E-6,-6.20111297,-14367.1
     4685,2080235.22,-3.09261944E-5,1.2454204E-2,-6.1424579,-1.92042673E
     5-10,5.08746452E-8,-8.33598636E-6,12.4022259,43101.5054,-8320940.86
     6,6.18523888E-5,-3.7362612E-2,24.5698316,3.84085346E-10,-1.52623935
     7E-7,3.33439455E-5/
      AF(P)=(B1+(B2+(B3+B4*P)*P)*P)*P
      BF1(A,B,C)=(A+(B+C*P2)*P2)*P2*EXPB
      BF2(A,B,C)=A*S3+B*S4+C*S5
      BF3(A,B,C,D)=((A+(B+C*P2)*P2-(B+D*P2-D/A24)/A24)*EXPB-A+(B-D/A24)/
     1A24)/A244
      K=KK
      P=PP
      T=TT
      S=1.0/T
      S2=S*S
      S3=S2*S
      S4=S3*S
      S5=S4*S
      S7=S5*S2
      P2=P*P
      APB=A24*P2
      EXPB=EXP(APB)
      P28=P**A28
      PALPHA=P28-ALPHA
      APC=A25*PALPHA**2
      EXPPC=EXP(APC)
      TTC=T-TC
      ATC=A27*TTC**2
      EXPTC=EXP(ATC)
      ZC1=A25*S*P28*PALPHA*EXPPC*EXPTC
      IF(K.EQ.2)GO TO 2
      B1=A1+A2*S+A3*S3+A4*S5+A5*S7
      B2=A6*T+A7+A8*S+A9*S2+A10*S3
      B3=A11+A12*S
      B4=A13*S+A14*S2
```

```
      ZA=1.0+AF(P)
      DO 1 N=1,3
    1 F1(N)=BF2(A(1,N,1),A(2,N,1),A(3,N,1))
      ZB=BF1(F1(1),F1(2),F1(3))
      Z(1)=ZA+ZB+ZC1
      IF(K.EQ.0)RETURN
      B1=2.0*B1
      B2=3.0*B2
      B3=4.0*B3
      B4=5.0*B4
      ZA=AF(P)+1.0
      ZB=(1.0+A244*P2)*ZB+BF1(2.0*F1(1),4.0*F1(2),6.0*F1(3))
      ZC=(1.0+A28*(1.0+P28*(1.0+2.0*APC)/PALPHA))*ZC1
      Z(3)=ZA+ZB+ZC
      IF(K.EQ.1)RETURN
    2 B1=A1+A32*S3+A42*S5+A52*S7
      B2=A62*T+A7-A9*S2+A102*S3
      B3=A11
      B4=-A14*S2
      ZA=1.0+AF(P)
      DO 3 N=1,3
    3 F1(N)=BF2(A(1,N,2),A(2,N,2),A(3,N,2))
      ZB=BF1(F1(1),F1(2),F1(3))
      ZC=A29*T*TTC*ZC1
      Z(2)=ZA+ZB+ZC
      B2=B2/2.0
      B3=B3/3.0
      B4=B4/4.0
      ZA=AF(P)
      ZB=BF3(F1(1),F1(2),F1(3),2.0*F1(3))
      ZC=A31*TTC*EXPTC*(EXPPC-A30)
      Z(4)=ZA+ZB+ZC
      IF(K.EQ.2)RETURN
      B1=A36*S3+A46*S5+A56*S7
      B2=A6*T+A9*S2+A106*S3
      B3=0.0
      B4=-A145*S2
      ZA=AF(P)
      DO 4 N=1,3
      F1(N)=BF2(A(1,N,3),A(2,N,3),A(3,N,3))
    4 F2(N)=BF2(A(1,N,4),A(2,N,4),A(3,N,4))
      ZB=BF3(F2(1),F2(2),F2(3),2.0*F2(3))
      ZC=T*ZC*(1.0+2.0*ATC)/TTC
      Z(6)=ZA+ZB+ZC
      B1=-A2*S+A35*S3+A45*S5+A55*S7
      B2=A65*T+A85*S-A9*S2+A105*S3
      B3=A125*S
      B4=A135*S+A145*S2
      ZA=AF(P)
      ZB=BF3(F1(1),F1(2),F1(3),2.0*F1(3))
      ZC=A31*(TTC-S/A29)*EXPTC*(EXPPC-A30)
      Z(5)=ZA+ZB+ZC
      RETURN
      END
```

C DECK OTEMP

```
      DOUBLE PRECISION FUNCTION CP(T)
      DOUBLE PRECISION A(9,3),HI,SI,S
      DATA A,HI,SI/3.0576085D-5,-3.6230043D-4,1.3986432D-3,-1.8234602D-3
     1,2.5741335D-3,-1.361753D-2,3.2534205D-2,-3.2270317D-2,2.5128273D0,
     23.82201062D-6,-5.17572043D-5,2.331072D-4,-3.6469204D-4,6.43533375D
     3-4,-4.53917667D-3,1.62671025D-2,-3.2270317D-2,2.5128273D0,3.397342
     478D-6,-4.52875538D-5,1.99806171D-4,-3.03910033D-4,5.148267D-4,-3.4
     50043825D-3,1.0844735D-2,-1.61351585D-2,2.5128273D0,-1.5155486D0,22.
     6202656124D0/
      K=1
    1 S=T/100.0D0
      CP=A(1,K)
      DO 2 N=2,8
    2 CP=CP*S+A(N,K)
      GO TO (3,4,5),K
    3 CP=CP*S+A(9,1)
      RETURN
      ENTRY CS(T)
      K=2
      GO TO 1
    4 CP=CP*S+A(9,2)*DLOG(S)+SI
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
    5 CP=T*(CP*S+A(9,3))+HI
      RETURN
      END
```

C DECK OLOG

```
      LOGICAL FUNCTION LGFN (P,T,J,Z)
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      DIMENSION Z(6), A(9)
      DATA A/.5115947,-1.469853,-1.8221345,11.180811,-13.613856,3.313939
     13,3.3609539,19.85226,-8.8689461/
      S=T/100.0
      J=1
      LGFN=.TRUE.
      IF (P.LT.0.1.OR.P.GT.3.1E7.OR.S.LT.0.59.OR.S.GT.4.1.OR.Z(1).LE.0.0
     1.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      IF (S.GT.1.5477) GO TO 2
      X=A(1)
      DO 1 N=2,8
1     X=X*S+A(N)
      X=EXP(X+A(9)/S)
      IF (P.GT.XKV*X) RETURN
2     J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK ODATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,259.8347,31.9988,1.804444E-3,5.6,1.4/
      END
```

```
C DECK OTLG

      SUBROUTINE TLOGIC(P,T)
      DIMENSION A(8)
      DATA A/1.5415673E-7,-5.58328E-6,2.7328988E-4,-3.4963316E-3,-1.5388
     1068E-4,5.487465E-1,-1.4597974,49.35502/
      IF(T.GT.154.77)RETURN
      V=ALOG(P)
      S=A(1)
      DO 1 N=2,8
    1 S=S*V+A(N)
      IF(T.LT.S) T=S
      IF(T.LT.59.0)T=59.0
      RETURN
      END
```

Oxygen, range II. - The equations for the compressibility factor and the ideal-gas specific heat for oxygen (range II) are the result of a curve fit of the data in reference 5. The temperature range of these fits is from 180 to 3000 K. The pressure range extends to 100×10^5 pascals. These equations only apply to undissociated oxygen.

In order to check the accuracy of these curve fits, the values of Z and C_p calculated by these routines were compared with those tabulated in reference 5. Over most of the temperature and pressure range, Z agrees to within 0.1 percent and C_p agrees to within 0.5 percent. The maximum disagreement is 0.3 percent for Z and 16 percent for C_p. This 16 percent disagreement in C_p occurred at a temperature of 180 K and a pressure of 40 bar.

The card listing of these routines follows. The prefix for the deck names is HO.

```
C DECK HOZETA

      SUBROUTINE ZETA (KK,PP,TT,Z)
      DIMENSION BB(11,4), CC(11,4), DD(11,4), BCD(11,4,3), Z(6), A(4,3)
      EQUIVALENCE (BB(1),BCD(1)), (CC(1),BCD(45)), (DD(1),BCD(89))
      DATA BB/-6.0201768E-10,3.97764E-9,3.1681402E-8,-2.5592444E-7,-8.15
     113199E-8,7.9876699E-7,2.4938354E-5,-1.6164074E-4,-1.606299E-4,1.06
     21436E-3,-2.8220151E-5,4.8161414E-9,-2.784348E-8,-1.9008841E-7,1.27
     396222E-6,3.260528E-7,-2.396301E-6,-4.9876708E-5,1.6164074E-4,0.,1.
     4061436E-3,-5.6440302E-5,5.4181591E-9,-3.182112E-8,-2.2176981E-7,1.
```

```
     55355466E-6,4.07566E-7,-3.195068E-6,-7.4815062E-5,3.2328148E-4,1.60
     66299E-4,0.,-2.8220151E-5,-4.3345273E-8,2.2274784E-7,1.3306189E-6,-
     77.6777332E-6,-1.630264E-6,9.5852039E-6,1.4963012E-4,-3.2328148E-4,
     82*0.,-5.6440302E-5/
      DATA CC/2*0.,3.0082239E-11,-3.4381911E-9,3.3326542E-8,-9.0112977E-
     18,3.5646415E-7,-2.4130715E-6,6.4195294E-6,-4.0224821E-6,9.912137E-
     27,2*0.,-1.5041119E-10,1.3752764E-8,-9.9979626E-8,1.8022595E-7,-3.5
     3646415E-7,0.,6.4195294E-6,-8.0449642E-6,2.9736411E-6,2*0.,-9.02467
     417E-11,8.5954778E-9,-6.6653084E-8,1.3516947E-7,-3.5646415E-7,1.206
     55358E-6,0.,-2.011241E-6,9.912137E-7,2*0.,4.5123358E-10,-3.4381911E
     6-8,1.9995925E-7,-2.7033893E-7,3.5646415E-7,2*0.,-4.0224821E-6,2.97
     736411E-6/
      DATA DD/3*0.,1.6667272E-10,-1.9308409E-9,5.4868082E-9,3.0655349E-9
     1,-7.5825703E-9,-5.6411225E-8,8.3326385E-8,-2.6382638E-8,3*0.,-5.00
     201816E-10,3.8616818E-9,-5.4868082E-9,0.,-7.5825703E-9,-1.1282245E-
     37,2.4997916E-7,-1.0553055E-7,3*0.,-2.2223029E-10,1.9308409E-9,-3.6
     4578721E-9,-1.021845E-9,0.,-1.8803742E-8,5.5550923E-8,-2.6382638E-8
     5,3*0.,5.6669088E-10,-3.8616818E-9,3.6578721E-9,2*0.,-3.7607483E-8,
     61.6665277E-7,-1.0553055E-7/
      S=1000.0/TT
      P=PP/S
      K=KK
      DO 3 J=1,4
      IF (K.EQ.2.AND.J.NE.2) GO TO 3
      DO 2 I=1,3
      A(J,I)=BCD(1,J,I)
      DO 1 M=2,11
1     A(J,I)=A(J,I)*S+BCD(M,J,I)
2     CONTINUE
      IF (K.EQ.1.AND.J.EQ.1) GO TO 4
3     CONTINUE
      Z(2)=1.0+(A(2,1)+(A(2,2)+A(2,3)*P)*P)*P
      Z(4)=(A(2,1)+(A(2,2)/2.0+A(2,3)*P/3.0)*P)*P
      IF (K.EQ.2) RETURN
      Z(5)=(A(3,1)+(A(3,2)+A(3,3)*P)*P)*P
      Z(6)=(A(4,1)+(A(4,2)+A(4,3)*P)*P)*P
4     Z(1)=1.0+(A(1,1)+(A(1,2)+A(1,3)*P)*P)*P
      Z(3)=1.0+(2.0*A(1,1)+(3.0*A(1,2)+4.0*A(1,3)*P)*P)*P
      RETURN
      END
```

```
C DECK HOTEMP

      DOUBLE PRECISION FUNCTION CP (T)
      DOUBLE PRECISION HI(2),SI(2),S
      DIMENSION A(9,3,2)
      DATA A/-223.15231,414.9894,-195.44586,-64.414824,67.444744,-5.4398
     1936,-3.9799316,0.8979885,2.4467825,-27.894039,59.2842,-32.57431,-1
     22.882965,16.861186,-1.8132979,-1.9899658,.8979885,2.4467825,-24.79
     34701,51.873675,-27.920837,-10.735804,13.488949,-1.3599734,-1.32664
     439,.44899425,2.4467825,-2.9168448E-4,3.1868334E-3,-6.6988664E-3,-2
     5.453835E-2,3.4493468E-2,.5086266,-1.9280242,2.9076944,1.6993272,-3
     6.646055E-5,4.5526191E-4,-1.1164777E-3,-4.90767E-3,8.623367E-3,.169
     75422,-.9640121,2.9076944,1.6993272,-3.2409387E-5,3.9835418E-4,-9.5
     8698091E-4,-4.089725E-3,6.8986936E-3,.12715665,-.64267473,1.4538472
     9,1.6993272/
```

```
      DATA HI,SI/1.17612602704J027,135.0144920564057,27.74745767553619,2
     16.21635718674784/
      K=1
1     J=1
      S=T/1.JD3
      IF (S.GT.5.34052860-1) J=2
      CP=A(1,K,J)
      DO 2 N=2,8
2     CP=CP*S+A(N,K,J)
      GO TO (3,4,5),K
3     CP=CP*S+A(9,1,J)
      RETURN
      ENTRY CS(T)
      K=2
      GO TO 1
4     CP=CP*S+A(9,2,J)*DLOG(S)+SI(J)
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
5     CP=T*(CP*S+A(9,3,J))+HI(J)
      RETURN
      END
```

```
C DECK HOLOG
      LOGICAL FUNCTION LGFN (P,T,J,Z)
      DIMENSION Z(6)
      J=1
      LGFN=.TRUE.
      IF (P.LT.D.1.OR.P.GT.1.1E7.OR.T.LT.179.0.OR.T.GT.3010.0.OR.Z(1).LE
     1.0.0.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK HODATA
      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,259.8347,31.9988,1.804444E-3,5.6,1.4/
      END
```

```
C DECK HOTLG
      SUBROUTINE TLOGIC (P,T)
      IF (T.LT.179.0) T=179.0
      RETURN
      END
```

Normal Hydrogen

For normal hydrogen, the equations for the compressibility factor and the ideal-gas specific heat are the result of curve fits of the data in reference 5. These equations cover a temperature range from 70 to 600 K. The pressure range extends to 100×10^5 pascals.

In order to check the accuracy of these curve fits, the values of Z and C_p calculated by these routines were compared with those tabulated in reference 5. Over most of the temperature and pressure range, Z agrees to within 0.1 percent and C_p agrees to within 1 percent. The maximum disagreement is 0.2 percent for Z and 5 percent for C_p.

The card listing for these routines follows. The prefix for the deck names is NH.

```
C DECK NHZETA
      SUBROUTINE ZETA (KK,PP,TT,Z)
      DIMENSION Z(6), BCD(6,4,2), A(4,2)
      DATA BCD/2.8086554E-3,-1.5620062E-2,3.377657E-2,-3.6316204E-2,5.87
     14617E-3,8.1391454E-3,-1.1234621E-2,4.6860185E-2,-6.7553139E-2,3.63
     216204E-2,0.,8.1391454E-3,-1.4043277E-2,6.2480247E-2,-.10132971,7.2
     3632409E-2,-5.874617E-3,0.,5.6173107E-2,-.18744074,.20265942,-7.263
     42409E-2,2*0.,-3.4569934E-5,1.5821139E-4,-2.2152582E-4,5.7982627E-5
     5,1.5996837E-4,4.0524086E-5,1.3827974E-4,-4.7463417E-4,4.4305163E-4
     6,-5.7982627E-5,0.,4.0524086E-5,8.6424835E-5,-3.1642278E-4,3.322887
     72E-4,-5.7982627E-5,-7.9984186E-5,0.,-3.4569934E-4,9.4926833E-4,-6.
     864577745E-4,5.7982627E-5,2*0./
      S=100.0/TT
      P=PP
      K=KK
      DO 3 J=1,4
      IF (K.EQ.2.AND.J.NE.2) GO TO 3
      DO 2 I=1,2
      A(J,I)=BCD(1,J,I)
      DO 1 M=2,6
1     A(J,I)=A(J,I)*S+BCD(M,J,I)
2     CONTINUE
      IF (K.EQ.1.AND.J.EQ.1) GO TO 4
3     CONTINUE
      Z(2)=1.0+(A(2,1)+A(2,2)*P)*P
      Z(4)=(A(2,1)+A(2,2)*P/2.0)*P
      IF (K.EQ.2) RETURN
      Z(5)=(A(3,1)+A(3,2)*P)*P
      Z(6)=(A(4,1)+A(4,2)*P)*P
```

```
4       Z(1)=1.0+(A(1,1)+A(1,2)*P)*P
        Z(3)=1.0+(2.0*A(1,1)+3.0*A(1,2)*P)*P
        RETURN
        END
```

```
C DECK NHTEMP

        DOUBLE PRECISION FUNCTION CP (T)
        DIMENSION A(8,3,2)
        DOUBLE PRECISION CS,CH,S,HI(2),SI(2)
        DATA A/4.4152734E-3,-5.1779658E-2,.1990402,-9.9781436E-2,-1.259836
       13,3.271702,-2.4018526,2.0533733,6.3075334E-4,-8.629943E-3,3.980804
       2E-2,-2.4945359E-2,-.41994543,1.635851,-2.4018526,2.0533733,5.51909
       318E-4,-7.397094E-3,3.3173367E-2,-1.9956287E-2,-.31495908,1.0905673
       4,-1.2009263,2.0533733,1.4719026E-6,-2.5457897E-5,-1.6392986E-4,4.5
       5782095E-3,-1.8045494E-2,-6.6869337E-2,.5687798,1.5362018,2.102718E
       6-7,-4.2429828E-6,-3.2785972E-5,1.1445524E-3,-6.0151647E-3,-3.34346
       769E-2,.5687798,1.5362018,1.8398783E-7,-3.6368424E-6,-2.7321643E-5,
       89.1564192E-4,-4.5113735E-3,-2.2289779E-2,.2843899,1.5362018/
        DATA HI,SI/118.5090360344103,85.18245132337324,12.03503970042298,1
       10.19779192852219/
        K=1
1       J=1
        S=T/1.0D2
        IF (S.GT.3.30230786D0) J=2
        CP=A(1,K,J)
        DO 2 N=2,7
2       CP=CP*S+A(N,K,J)
        GO TO (3,4,5),K
3       CP=CP*S+A(8,1,J)
        RETURN
        ENTRY CS(T)
        K=2
        GO TO 1
4       CP=CP*S+A(8,2,J)*DLOG(S)+SI(J)
        RETURN
        ENTRY CH(T)
        K=3
        GO TO 1
5       CP=T*(CP*S+A(8,3,J))+HI(J)
        RETURN
        END
```

```
C DECK NHLOG

        LOGICAL FUNCTION LGFN (P,T,J,Z)
        DIMENSION Z(6)
        J=1
        LGFN=.TRUE.
        IF (P.LT.0.1.OR.P.GT.1.1E7.OR.T.LT.69.D.OR.T.GT.610.D.OR.Z(1).LE.0
```

```
     1.O.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK NHDATA
      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,4124.33,2.01594,1.136808E-4,5.6,1.4/
      END
```

```
C DECK NHTLG
      SUBROUTINE TLOGIC (P,T)
      IF (T.LT.69.0) T=69.0
      RETURN
      END
```

Parahydrogen

For parahydrogen, the equation for the compressibility factor is from reference 9. For temperatures below 100 K, this equation is based on the parahydrogen data of reference 10. For temperatures above 100 K, this equation is based on normal-hydrogen data such as that found in reference 5. The equation for the ideal-gas specific heat is the result of a curve fit of the data in reference 11. For temperatures from 13 to 100 K, the pressure range extends to 300×10^5 pascals. For temperatures from 100 to 400 K, the pressure range extends to 100×10^5 pascals.

Except for the critical region, reference 9 estimates the mean error in Z to be 0.3 percent. Over most of the range from 100 to 400 K, the values of Z calculated by these routines agree with those tabulated in reference 5 to within 0.1 percent. No comparison of C_p was made.

The card listing of these routines follows. The prefix for the deck names is PH.

```
C DECK PHZETA
      SUBROUTINE ZETA(KK,PP,TT,Z)
      DIMENSION Z(6)
      DATA A,B1,B2,B3,B4,B5,B6,B7,B8,B9,B10,B11,B12,B13,B14,B15/-4.42910
     1289E-4,1.0229558E-2,-7.81250336E-1,-43.7354838,700.54484,-61088.73
     208,7.81519168E-5,7.73767544E-3,3.58441339E-7,-32.0855334,3046.6492
     34,-58106.0523,2.84494816E-3,-4.98394981E-1,10.7837894,1.9225229E-8
     4/
      CO(X,Y,Z)=X*S3+Y*S4+Z*S5
      K=KK
      P=PP
      T=TT
      S1=1.0/T
      S2=S1*S1
      S3=S1*S2
      S4=S1*S3
      S5=S1*S4
      P2=P*P
      EXPO=EXP(A*P2)
      AA=1.0/(2.0*A)
      BB=1.0/A
      C1=CO(B9,B10,B11)
      C2=CO(B12,B13,B14)
      IF (K.EQ.2) GO TO 1
      BA1=B1+B2*S1+B3*S2+B4*S3+B5*S5
      BA2=B6+B7*S1
      ZA=1.0+(BA1+(BA2+(B8+B15*S1*P2)*P)*P)*P
      ZB=EXPO*P2*(C1+C2*P2)
      Z(1)= ZA+ZB
      ZA=1.0+(2.0*BA1+(3.0*BA2+(4.0*B8+6.0*B15*S1*P2)*P)*P)*P
      ZB=P2*EXPO*(3.0*C1+(2.0*A*C1+5.0*C2+2.0*C2*P2*A)*P2)
      Z(3)= ZA+ZB
      IF (K.EQ.1) RETURN
1     BT=B1-B3*S2-2.0*B4*S3-4.0*B5*S5
      C1P=-CO(3.0*B9,4.0*B10,5.0*B11)
      C2P=-CO(3.0*B12,4.0*B13,5.0*B14)
      CC1=C1+C1P
      CC2=C2+C2P
      ZA=1.0+(BT+(B6+B8*P)*P)*P
      ZB=P2*EXPO*(CC1+CC2*P2)
      Z(2)= ZA+ZB
      ZA=(BT+(B6/2.0+B8*P/3.0)*P)*P
      ZB=AA*(EXPO*(CC1+(P2-BB)*CC2)+BB*CC2-CC1)
      Z(4)= ZA+ZB
      IF (K.EQ.2) RETURN
      C1PP=CO(9.0*B9,16.0*B10,25.0*B11)
      C2PP=CO(9.0*B12,16.0*B13,25.0*B14)
      ZA=-((B2*S1+2.0*B3*S2+3.0*B4*S3+5.0*B5*S5)+(B7*S1/2.0+B15*S1*P**3/
     15.0)*P)*P
      ZB=AA*(EXPO*(C1P+(P2-BB)*C2P)+BB*C2P-C1P)
      Z(5)= ZA+ZB
      CC1P=C1P+C1PP
      CC2P=C2P+C2PP
      ZA=(2.0*B3*S2+6.0*B4*S3+20.0*B5*S5)*P
      ZB=AA*(EXPO*(CC1P+(P2-BB)*CC2P)+CC2P*BB-CC1P)
      Z(6)= ZA+ZB
      RETURN
      END
```

C DECK PHTEMP

```
      DOUBLE PRECISION FUNCTION CP(T)
      DIMENSION A(6,3,4)
      DOUBLE PRECISION SL(3),SI(4),HI(4),S
      DATA A/5*0.0,1.5,5*0.0,1.5,5*0.0,1.5,0.0,-5.477243,14.151817,-10.9
     192694,3.4450167,1.1181079,0.0,-1.36931075,4.71727233,-5.496347,3.4
     2450167,1.1181079,0.0,-1.0954486,3.53795425,-3.66423133,1.72250835,
     31.1181079,-.9606211,8.1602445,-26.350196,39.1680848,-25.0299192,7.
     426108881,-.19212422,2.04006112,-8.78339867,19.5840424,-25.0299192,
     57.26108881,-.160103517,1.6320489,-6.587549,13.0560283, -12.5149596
     6,7.26108881,2*0.0,-2.3415379E-2,.3216503,-1.4584629,4.7141156,2*0.
     70,-7.80512633E-3,.16082515,-1.4584629,4.7141156,2*0.0,-5.85384475E
     8-3,.107216767,-.72923145,4.7141156/
      DATA SI,HI/9.982774057901375,8.867877636855692,22.54596376458948,
     111.14950174192363,-.02542447420268701,3.222638996244185,-103.53218
     278709574,-282.1978829444169/
      DATA SL/.299951327D0,.80208227D0,2.00239831D0/
      K=1
    1 S=T/1.0D2
      IF(S.GT.SL(1))GO TO 2
      N=1
      GO TO 5
    2 IF(S.GT.SL(2))GO TO 3
      N=2
      GO TO 5
    3 IF(S.GT.SL(3))GO TO 4
      N=3
      GO TO 5
    4 N=4
    5 CP=A(1,K,N)
      DO 6 I=2,5
    6 CP=CP*S+A(I,K,N)
      GO TO (7,8,9),K
    7 CP=CP*S+A(6,1,N)
      RETURN
      ENTRY CS(T)
      K=2
      GO TO 1
    8 CP=CP*S+A(6,2,N)*DLOG(S)+SI(N)
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
    9 CP=T*(CP*S+A(6,3,N))+HI(N)
      RETURN
      END
```

C DECK PHLOG

```
      LOGICAL FUNCTION LGFN (P,T,J,Z)
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      DIMENSION Z(6), A(8)
      DATA A/2080.3847,-2120.5641,878.06684,-213.15163,41.218448,-2.0944
     1688,16.331473,-1.054106/
```

```
      S=T/100.0
      J=1
      LGFN=.TRUE.
      IF (P.LT.0.1.OR.P.GT.3.1E7.OR.S.GT.4.1.OR.S.LT.0.13.OR.Z(1).LE.0.0
     1.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0.OR.(P.GT.1.1E7.AND.S.GT.1.1)) RETUR
     2N
      IF (S.GT.0.32976) GO TO 2
      PL=A(1)
      DO 1 N=2,7
    1 PL=PL*S+A(N)
      PL=XKV*EXP(PL+A(8)/S)
      IF (P.GT.PL) RETURN
    2 J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK PHDATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,4124.33,2.01594,1.136808E-4,5.6,1.4/
      END
```

```
C DECK PHTLG

      SUBROUTINE TLOGIC(P,T)
      DIMENSION A(6)
      DATA A/5.6592537E-5,-3.5285986E-4,-5.8183381E-3,9.6000865E-2,6.523
     13288E-1,3.618144/
      IF(T.GT.32.976)RETURN
      V=ALOG(P)
      S=A(1)
      DO 1 N=2,6
    1 S=S*V+A(N)
      IF(T.LT.S)T=S
      IF(T.LT.13.0)T=13.0
      RETURN
      END
```

For helium, the equation for the compressibility factor is from reference 12. Since helium is a monatomic gas, the value of the ideal-gas specific heat at constant volume $C_{v,id}/R$ is 1.5. Reference 12 claims a temperature range from 3 to 300 K and a pressure range extending to 101×10^5 pascals. This report assumes a temperature range from 5.4 to 400 K and a pressure range extending to 300×10^5 pascals. These are the same ranges assumed in reference 6, which uses the same equations.

For pressures to 101×10^5 pascals and temperatures from 10 to 300 K, reference 12 estimates that the calculated values of ρ, H, and S are accurate to within 3 percent and that the values of C_p are accurate to within 5 percent.

The card listing of these routines follows. The prefix for the deck names is HE.

```
C DECK HEZETA
      SUBROUTINE ZETA(KK,PP,TT,Z)
      DIMENSION Z(6)
      DATA A,B1,B2,B3,B4,B5,B6,B7,B8,B9,B10,B11,B12,B13,B14,B15,B16/
     1-4.057E-4,4.0665013E-3,-1.1267764E-1,2.3039266E-2,-5.7468818E-2,
     21.3691368E-1,9.7390626E-6,7.0543876E-4,-5.3854984E-6,-3.8053762E-3
     3,2.625179E-2,7.674266E-2,-8.7904911E-7,1.9960611E-6,-8.1300167E-6,
     43.6743583E-8,-3.4049435E-11/
      CO(X,Y,Z)=X*S3+Y*S4+Z*S5
      K=KK
      P=PP
      T=TT
      S1=1.0/T
      S2=S1*S1
      S3=S2*S1
      S4=S3*S1
      S5=S4*S1
      AA=A*S1
      P2=P*P
      EXPO=EXP(AA*P2)
      C1=CO(B9,B10,B11)
      C2=CO(B12,B13,B14)
      IF (K.EQ.2) GO TO 1
      BA1=B1+B2*S1+B3*S2+B4*S3+B5*S5
      BA2=B6+B7*S1
      ZA=1.0+(BA1+(BA2+(B8*S1+(B15*S1+B16*S1*P)*P)*P)*P)*P
      ZB=(C1+C2*P2)*P2*EXPO
      Z(1)= ZA+ZB
      ZA=1.0+(2.0*BA1+(3.0*BA2+(4.0*B8*S1+(5.0*B15*S1+6.0*B16*S1*P)*P)*P
     1)*P)*P
      ZB=(3.0*C1+(2.0*AA*C1+5.0*C2+2.0*AA*C2*P2)*P2)*P2*EXPO
      Z(3)= ZA+ZB
      IF (K.EQ.1) RETURN
1     BT=B1-B3*S2-2.0*B4*S3-4.0*B5*S5
      C1P=-CO(3.0*B9,4.0*B10,5.0*B11)
      C2P=-CO(3.0*B12,4.0*B13,5.0*B14)
      C11=(2.0*C1+C1P)/AA
      C22=(3.0*C2+C2P)/AA
      ZA=1.0+(BT+B6*P)*P
      ZB=P2*EXPO*(C1+C1P+(-AA*C1+C2+C2P-AA*C2*P2)*P2)
```

```
      Z(2)= ZA+ZB
      ZA=(BT+B6*P/2.0)*P
      ZB=0.5*(EXPO*(C11-C22/AA+(-C1+C22-C2*P2)*P2)-C11+C22/AA)
      Z(4)= ZA+ZB
      IF (K.EQ.2) RETURN
      C11=(C1+C1P)/AA
      C22=(2.0*C2+C2P)/AA
      ZA=(-(B2*S1+2.0*B3*S2+3.0*B4*S3+5.0*B5*S5)+(-B7*S1/2.0+(-B8*S1/3.0
     1+(-B15*S1/4.0-B16*S1*P/5.0)*P)*P)*P)*P
      ZB=0.5*(EXPO*(C11-C22/AA+(-C1+C22-C2*P2)*P2)-C11+C22/AA)
      Z(5)= ZA+ZB
      C1PP=C0(9.0*B9,16.0*B10,25.0*B11)
      C2PP=C0(9.0*B12,16.0*B13,25.0*B14)
      C11=(2.0*C1+3.0*C1P+C1PP)/AA
      C22=(6.0*C2+5.0*C2P+C2PP)/AA
      ZA=(2.0*B3*S2+6.0*B4*S3+20.*B5*S5)*P
      ZB=0.5*(EXPO*(C11-C22/AA+(-2.0*(C1+C1P)+C22+(AA*C1-3.0*C2-2.0*C2P+
     1AA*C2*P2)*P2)*P2)-C11+C22/AA)
      Z(6)= ZA+ZB
      RETURN
      END
```

```
C DECK HETEMP
      DOUBLE PRECISION FUNCTION CP(T)
      DOUBLE PRECISION S,C15,SI,HI
      DATA C15,SI,HI/1.5D0,4.75063D0,6.98973D0 /
      CP= C15
      RETURN
      ENTRY CS(T)
      S=T
      CP= C15*DLOG(S)+SI
      RETURN
      ENTRY CH(T)
      S=T
      CP= C15*S+HI
      RETURN
      END
```

```
C DECK HELOG
      LOGICAL FUNCTION LGFN(P, T,J,Z)
      DIMENSION Z(6)
      J=1
      LGFN= .TRUE.
      IF (P.LT.0.1.OR.P.GT.3.1E7.OR.T.LT.5.4.OR.T.GT.410.0.OR.Z(1).LE.0.
     10.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      J=0
      LGFN= .FALSE.
      RETURN
      END
```

```
C DECK HEDATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,2077.25,4.0026,2.538663E-4,.3333,1.6666667/
      END
```

```
C DECK HETLG

      SUBROUTINE TLOGIC(P,T)
      IF(T.LT.5.4) T=5.4
      RETURN
      END
```

Argon

For argon, the equation for the compressibility factor is from reference 13. Since argon is monatomic, the value of the ideal-gas specific heat at constant volume $C_{v,id}/R$ is 1.5. Reference 13 claims a temperature range from 86 to 300 K and a pressure range extending to 1010×10^5 pascals. This report assumes a temperature range from 80 to 400 K and a pressure range extending to 1000×10^5 pascals.

The values of Z and C_p calculated by these routines (using the state equation of ref. 13) were compared with those tabulated in reference 5. Over most of the temperature range 200 to 400 K and for pressures under 101×10^5 pascals, Z agrees to within 0.1 percent and C_p agrees to within 1 percent. The maximum disagreement (at about 200 K and 100 bar) was 2.4 percent in Z and 15 percent in C_p.

The card listing of these routines follows. The prefix for the deck names is AR.

```
C DECK ARZETA

      SUBROUTINE ZETA(KK,PP,TT,Z)
      DIMENSION Z(6)
      DATA A,B1,B2,B3,B4,B5,B6,B7,B8,B9,B10,B11,B12,B13,B14,B15/-3.00798
     1368E-6,7.92559677E-4,-2.73770136E-1,-20.5241378,-808.296022,297857
     26.6,5.382625E-7,-3.57177204E-5,4.32857895E-10,3.67665496,493.10182
     35,-87715.9942,-3.10301696E-6,2.22667069E-3,5.23279441E-2,8.3194622
     47E-14/
      CO(X,Y,Z)=X*S3+Y*S4+Z*S5
      K=KK
      P=PP
      T=TT
      S1=1.0/T
      S2=S1*S1
      S3=S1*S2
      S4=S1*S3
```

```
      S5=S1*S4
      P2=P*P
      EXPO=EXP(A*P2)
      AA=1.0/(2.0*A)
      BB=1.0/A
      C1=CO(B9,B10,B11)
      C2=CO(B12,B13,B14)
      IF (K.EQ.2) GO TO 1
      BA1=B1+B2*S1+B3*S2+B4*S3+B5*S5
      BA2=B6+B7*S1
      ZA=1.0+(BA1+(BA2+(B8+B15*S1*P2)*P)*P)*P
      ZB=EXPO*P2*(C1+C2*P2)
      Z(1)= ZA+ZB
      ZA=1.0+(2.0*BA1+(3.0*BA2+(4.0*B8+6.0*B15*S1*P2)*P)*P)*P
      ZB=P2*EXPO*(3.0*C1+(2.0*A*C1+5.0*C2+2.0*C2*P2*A)*P2)
      Z(3)= ZA+ZB
      IF (K.EQ.1) RETURN
1     BT=B1-B3*S2-2.0*B4*S3-4.0*B5*S5
      C1P=-CO(3.0*B9,4.0*B10,5.0*B11)
      C2P=-CO(3.0*B12,4.0*B13,5.0*B14)
      CC1=C1+C1P
      CC2=C2+C2P
      ZA=1.0+(BT+(B6+B8*P)*P)*P
      ZB=P2*EXPO*(CC1+CC2*P2)
      Z(2)= ZA+ZB
      ZA=(BT+(B6/2.0+B8*P/3.0)*P)*P
      ZB=AA*(EXPO*(CC1+(P2-BB)*CC2)+BB*CC2-CC1)
      Z(4)= ZA+ZB
      IF (K.EQ.2) RETURN
      C1PP=CO(9.0*B9,16.0*B10,25.0*B11)
      C2PP=CO(9.0*B12,16.0*B13,25.0*B14)
      ZA=-((B2*S1+2.0*B3*S2+3.0*B4*S3+5.0*B5*S5)+(B7*S1/2.0+B15*S1*P**3/
     15.0)*P)*P
      ZB=AA*(EXPO*(C1P+(P2-BB)*C2P)+BB*C2P-C1P)
      Z(5)= ZA+ZB
      CC1P=C1P+C1PP
      CC2P=C2P+C2PP
      ZA=(2.0*B3*S2+6.0*B4*S3+20.0*B5*S5)*P
      ZB=AA*(EXPO*(CC1P+(P2-BB)*CC2P)+CC2P*BB-CC1P)
      Z(6)= ZA+ZB
      RETURN
      END
```

```
C DECK ARTEMP
      DOUBLE PRECISION FUNCTION CP(T)
      DOUBLE PRECISION S,C15,SI
      DATA C15,SI/1.5D0,1D.54223318/
      CP=C15
      RETURN
      ENTRY CS(T)
      CP=C15*DLOG(DBLE(T))+SI
      RETURN
```

```
      ENTRY CH(T)
      CP=C15*T
      RETURN
      END
```

```
C DECK ARLOG
      LOGICAL FUNCTION LGFN (P,T,J,Z)
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      DIMENSION Z(6)
      S=T/100.0
      J=1
      LGFN=.TRUE.
      IF (P.LT.0.1.OR.P.GT.1.1E8.OR.S.GT.4.1.OR.S.LT.0.8.OR.Z(1).LE.0.0.
     1OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      IF (S.GT.1.5086) GO TO 1
      PL=XKV*EXP(-9.3287334/S+24.471369+(-3.5108148+1.0598825*S)*S)
      IF (P.GT.PL) RETURN
1     J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK ARDATA
      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,208.1306,39.948,2.533716E-3,5.6,1.6666667/
      END
```

```
C DECK ARTLG
      SUBROUTINE TLOGIC(P,T)
      DIMENSION A(5)
      DATA A/6.4612535E-3,-1.3007385E-1,3.9880245E-1,12.49659,-24.58815/
      IF(T.GT.150.86)RETURN
      V=ALOG(P)
      S=A(1)
      DO 1 N=2,5
    1 S=S*V+A(N)
      IF(T.LT.S)T=S
      IF(T.LT.80.)T=80.
      RETURN
      END
```

Steam

For steam, the equations for the compressibility factor and the ideal-gas specific heat are derived from equations (1) to (3) in reference 14. The temperature range for these equations is from 273 to 1600 K. The pressure range extends to 1000×10^5 pascals.

It is estimated, that except for the critical region, the values of Z are accurate to within 0.2 percent.

The reference state for the internal energy and entropy is that of the liquid at the triple point. (The value of the enthalpy at this state is 0.6 joules per kilogram.)

The card listing of these routines follows. The prefix for the deck names is ST. In this case, Z(1) to Z(6) are calculated in subroutine ZETA regardless of the value of K.

```
C DECK STZETA
      SUBROUTINE ZETA (K,PP,TT,Z)
      DIMENSION Z(6), A(8,7), D(7,7), PJ(10,2), PAJ(2), FI(7,3)
      DOUBLE PRECISION D,PD
      DATA A/29.492937,-132.13917,274.64632,-360.93828,342.18431,-244.50
     1042,155.18535,5.9728487,-5.1985860,7.7779182,-33.301902,-16.254622
     2,-177.31074,127.48742,137.46153,155.97836,6.8335354,-26.149751,65.
     3326396,-26.181978,4*0.0,-.15641040,-.72546108,-9.2734289,4.3125840
     4,4*0.0,-6.3972405,26.409282,-47.740374,56.323130,4*0.0,-3.9661401,
     515.453061,-29.142470,29.568796,4*0.0,-.69048554,2.7407416,-5.10280
     670,3.9536085,4*D.0/
      DATA D/-410.30848D0,337.31180D0,-137.46618D0,6.7874983D0,136.87317
     1D0,79.847970D0,13.041253D0,-416.05860D0,-209.88866D0,-733.96848D0,
     210.401717D0,645.81880D0,399.17570D0,71.531353D0,1137.363504,-2038.8
     373960,-808.0992960,-11.77655784,634.6463840,415.0811440,80.4646916
     40,1997.081280,1007.465568,3523.048704,-49.92824160,-3099.930240,-1
     5916.043360,-343.3504944,3106.844208,-3657.97060D0,-148.2616320,-44.
     635654958,-22.344832D0,31.810888D0,17.86667720,-1465.1822592,11801.
     7526144,10924.9740288,-43.329005568,-9246.1631232,-5824.4762112,-10
     872.93150848,-9585.990144,-4835.8347264,-16910.6337792,239.65555968
     9,14879.665152,9197.008128,1648.08237312/
      DATA TC,E,PAJ,PJ/1.5449120,-4.8,.634,1.0,20*1.0/
      P=PP/1.0E3
      T=1.0E3/TT
      DO 1 N=1,2
      PJ(4,N)=P-PAJ(N)
      PJ(2,N)=1.0/PJ(4,N)
      PJ(1,N)=PJ(2,N)**2
      DO 1 I=5,10
    1 PJ(I,N)=PJ(I-1,N)*PJ(4,N)
      EXPO=EXP(P*E)
      PD=DBLE(P)
      N=1
      DO 3 J=1,7
      FI(J,1)=EXPO*(SNGL(D(J,1)+D(J,2)*PD))
      FI(J,2)=EXPO*(SNGL(D(J,1)+(D(J,3)+D(J,4)*PD)*PD))
      FI(J,3)=EXPO*(SNGL(D(J,5)+(D(J,6)+D(J,7)*PD)*PD))
      DO 2 I=1,8
      IF (J.GT.2.AND.I.GT.4) GO TO 3
      FI(J,1)=FI(J,1)+A(I, J)*PJ(I+2,N)
      XI=I
```

```
      FI(J,2)=FI(J,2)+A(I,J)*(XI*P-PAJ(N))*PJ(I+1,N)
2     FI(J,3)=FI(J,3)+A(I,J)*(XI-1.0)*(XI*P-2.0*PAJ(N))*PJ(I,N)
3     N=2
      PT=P*T
      SC=T-TC
      Q=FI(1,1)+FI(2,1)*SC
      PQ=FI(1,2)+FI(2,2)*SC
      PPQ=FI(1,3)+FI(2,3)*SC
      VV=SC
      V=1.0
      S=T-2.5
      S2=S*S
      TQ=FI(2,1)
      TTQ=0.0
      PTQ=FI(2,2)
      DO 4 J=3,7
      V=V*S
      VV=VV*S
      Q=Q+VV*FI(J,1)
      PQ=PQ+VV*FI(J,2)
      PPQ=PPQ+VV*FI(J,3)
      XJ=J-2
      T1=(XJ*SC+S)*V/S
      TQ=TQ+T1*FI(J,1)
      PTQ=PTQ+T1*FI(J,2)
4     TTQ=TTQ+XJ*((XJ-1.0)*SC+2.0*S)*V*FI(J,1)/S2
      Z(1)=1.0+P*PQ
      Z(3)=2.0*Z(1)-1.0+P*P*PPQ
      Z(2)=Z(1)-PT*PTQ
      Z(5)=-PT*TQ
      Z(4)=P*Q+Z(5)
      Z(6)=T*PT*TTQ
      RETURN
      END
```

```
C DECK STTEMP

      DOUBLE PRECISION FUNCTION CP(T)
      DIMENSION A(6,3)
      DOUBLE PRECISION S
      DATA A/-.21028060,.53437455,-.47667309,1.8177938,2.1911746,.099672
     1813,-.052570150,.17812485,-.23833655,1.8177938,2.1911746,-.0996728
     213,-.342056120,.13359364,-.15889103,.90889688,2.1911746,99.672813/
      DATA HI,SI/4612.7316,17.238170/
      K=1
1     S=T/1.0E3
      CP=A(1,K)
      DO 2 I=2,4
2     CP=CP*S+A(I,K)
      GO TO (3,4,5),K
3     CP=CP*S+A(5,K)+A(6,K)/S
      RETURN
      ENTRY CS(T)
      K=2
      GO TO 1
```

```
4     CP=CP*S+A(5,2)*DLOG(S)+A(6,2)/S+SI
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
5     CP=T*(CP*S+A(5,3))+A(6,3)*DLOG(S)+HI
      RETURN
      END
```

```
C DECK STLOG

      LOGICAL FUNCTION LGFN (P,T,J,Z)
      DIMENSION Z(6), A(9)
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      DATA A/2.8281601E-5,-5.8328303E-4,4.084426E-3,-5.9629737E-3,-7.000
     13883E-2,5.6897698E-1,-3.091692,35.493889,-64.278808/
      S=T/100.0
      J=1
      LGFN=.TRUE.
      IF (P.GT.1.01E8.OR.P.LT.0.1.OR.S.GT.16.1.OR.S.LT.2.73.OR.Z(1).LE.0
     1.0.OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      IF (S.GT.6.47286) GO TO 2
      PL=A(1)
      DO 1 N=2,8
1     PL=PL*S+A(N)
      IF (P.GT.XKV*EXP(PL+A(9)/S)) RETURN
2     J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK STDATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,461.51,18.01534,9.82042E-4,5.6,1.3333333/
      END
```

```
C DECK STTLG

      SUBROUTINE TLOGIC (P,T)
      DATA A1,A2,A3,A4,A5,A6/2.6832873,-0.1739764,.038877378,-1.7257127E
     1-3,-9.1550282E-6,3.4056076E-6/
      S=T/100.0
      IF (S.GT.6.47286) RETURN
      V=ALOG(P)
      SS=A1+(A2+(A3+(A4+(A5+A6*V)*V)*V)*V)*V
```

```
      IF (S.LE.SS) S=SS
      IF (S.LT.2.73) S=2.73
      T=100.0*S
      RETURN
      END
```

Methane

The routines for methane are described and presented in reference 3. The compressibility-factor equation is from reference 15, and the ideal-gas specific-heat equation is the result of a curve fit of the data in reference 16. The temperature range is from 70 to 600 K and the pressure range extends to 400×10^5 pascals.

Even though the card listing of the methane routines is in reference 3, this listing is included in this report for convenience. The prefix for the deck names is ME. The subroutine ZETA is not independent, but the combination of subroutines ZETA and POLY is independent.

```
C DECK MEZETA
      SUBROUTINE ZETA (KK,PP,TT,Z)
      COMMON /VALUE/ F(4,4),G(6,4)
      DIMENSION Z(6)
      DOUBLE PRECISION F,G,B1,B2,B3,B4,B5,A1,A2,A3,A4,A5,E1,E2,PA,TA,TH1
     1,TH2,TH3,TH4,D1,D2,D3,D4,D5,F1,F2,UA,P,T,P1,P2,U,T1,RC,EXPC,RB,EXP
     2B,ZB1,ZC1,AB1,AB2,AB3,AB4,AB5,ZA,ZB,ZC,RB1,EXPB1,S,SS,PSI1,PSI2,PS
     3I3,PSI4,RC1,EXPC1,PSI5,PSI6,PSI7,PSI8
      DATA B1,B2,B3,B4,B5,A1,A2,A3,A4,A5,E1,E2,PA/4.91473574991686D-03,7
     1.37664223478550D-06,-1.14587843032923D-07,5.89510209511141D-10,-5.
     274382281343532D-13,-2.23983199201862D00,1.34331253741270D-03,2.759
     310182936551D-05,-1.65546977053542D-07,2.34124562687064D-10,-4.6002
     4000000000D-02,-2.11770000000000D-10,1.13318000000000D02/
      DATA TA,TH1,TH2,TH3,TH4,D1,D2,D3,D4,D5,F1,F2,UA/1.47710550000000D0
     12,1.09934666473654D-14,1.64873321284064D07,1.07243639762491D08,3.6
     264488882455140-15,-3.97760537104600D00,-1.50622516081086D-02,4.329
     340740732648D-04,-1.85355607372189D-06,2.05286315303314D-09,-1.3787
     4933000000D03,1.34418460000000D00,1.45511293919343D06/
      K=KK
      P=PP
      T=TT
      P1=P+PA
      P2=P1*P1
      U=P2*P1
      T1=T+TA
      RC=(F1+F2*P)/T
      EXPC=DEXP(RC)
      RB=(E1+E2*U)
      EXPB=DEXP(RB*T1)
      ZB1=(TH1*P*P2*(U-TH2)*(TH3-U)*EXPB)/T
      ZC1=(D1+(D2+(D3+(D4+D5*P)*P)*P)*P)*P*EXPC/T
      IF (K.EQ.2) GO TO 1
```

```
      AB1=B1+A1/T
      AB2=B2+A2/T
      AB3=B3+A3/T
      AB4=B4+A4/T
      AB5=B5+A5/T
      ZA=1.0D0+(AB1+(AB2+(AB3+(AB4+AB5*P)*P)*P)*P)*P
      Z(1)=ZA+ZB1+ZC1
      IF (K.EQ.0) RETURN
      ZA=1.0D0+(2.0D0*AB1+(3.0D0*AB2+(4.0D0*AB3+(5.0D0*AB4+6.0D0*AB5*P)*
     1P)*P)*P)*P
      ZB=ZB1*(2.0D0*(1.0D0+P/P1)+3.0D0*P*P2*(E2*T1+1.0D0/(U-TH3)+1.0D0/(
     1U-TH2)))
      ZC=(F2*P*ZC1+EXPC*(2.0D0*D1+(3.0D0*D2+(4.0D0*D3+(5.0D0*D4+6.0D0*D5
     1*P)*P)*P)*P)*P)/T
      Z(3)=ZA+ZB+ZC
      IF (K.EQ.1) RETURN
 1    RB1=E1+E2*UA
      EXPB1=DEXP(RB1*T1)
      ZA=1.0D0+(B1+(B2+(B3+(B4+B5*P)*P)*P)*P)*P
      ZB=RB*T*ZB1
      ZC=-RC*ZC1
      Z(2)=ZA+ZB+ZC
      S=E2*T1
      SS=F2/T
      CALL POLY (1,1,U,T,S)
      CALL POLY (1,2,P,T,SS)
      ZA=(B1+(B2/2.0D0+(B3/3.0D0+(B4/4.0D0+B5*P/5.0D0)*P)*P)*P)*P
      PSI1=F(1,1)-F(2,1)+F(3,1)-F(4,1)
      PSI2=F(1,2)-F(2,2)+F(3,2)-F(4,2)
      ZB=TH4*(PSI1*EXPB-PSI2*EXPB1)
      PSI3=G(1,1)-G(2,1)+G(3,1)-G(4,1)+G(5,1)-G(6,1)
      PSI4=G(1,2)-G(2,2)+G(3,2)-G(4,2)+G(5,2)-G(6,2)
      RC1=F1/T
      EXPC1=DEXP(RC1)
      ZC=(PSI4*EXPC1-PSI3*EXPC)/T**2
      Z(4)=ZA+ZB+ZC
      IF (K.EQ.2) RETURN
      CALL POLY (2,1,U,T,S)
      CALL POLY (2,2,P,T,SS)
      PSI5=F(1,3)-F(2,3)+F(3,3)-F(4,3)
      PSI6=F(1,4)-F(2,4)+F(3,4)-F(4,4)
      PSI7=G(1,3)-G(2,3)+G(3,3)-G(4,3)+G(5,3)-G(6,3)
      PSI8=G(1,4)-G(2,4)+G(3,4)-G(4,4)+G(5,4)-G(6,4)
      ZA=-(A1+(A2/2.0D0+(A3/3.0D0+(A4/4.0D0+A5*P/5.0D0)*P)*P)*P)*P/T
      ZB=TH4*(PSI5*EXPB-PSI6*EXPB1)
      ZC=(PSI8*EXPC1-PSI7*EXPC)/T**2
      Z(5)=ZA+ZB+ZC
      ZB=TH4*T*(EXPB*(RB*PSI1-(F(1,1)-2.0D0*F(2,1)+3.0D0*F(3,1)-4.0D0*F(
     14,1))/T1)-EXPB1*(RB1*PSI2-(F(1,2)-2.0D0*F(2,2)+3.0D0*F(3,2)-4.0D0*
     2F(4,2))/T1))
      ZC=(EXPC*((2.0D0+RC)*PSI3-G(1,1)+2.0D0*G(2,1)-3.0D0*G(3,1)+4.0D0*G
     1(4,1)-5.*G(5,1)+6.0D0*G(6,1))-EXPC1*((2.0D0+RC1)*PSI4-G(1,2)+2.0D0
     2*G(2,2)-3.0D0*G(3,2)+4.0D0*G(4,2)-5.0D0*G(5,2)+6.0D0*G(6,2)))/T**2
      Z(6)=ZB+ZC
      RETURN
      END
```

```
C DECK MEPOLY
      SUBROUTINE POLY (J,K,PP,TT,CC)
      COMMON /VALUE/ F(4,4),G(6,4)
      DIMENSION A(7,2), B(16,2)
      DOUBLE PRECISION PP,TT,CC,F,G,A,B,AA,AB,UA,D1,D2,D3,D4,D5,P,T,C1,C
     12,C3,C4,C5,C6,V1,V2,V3
      DATA B/5.48429563564224D03,1.54210957155370D01,-6.17182239272157D-
     101,3.13762297202746D-03,-5.32199549075239D-06,2.75942703621458D-09
     2,-1.23436447854431D00,9.41286891608238D-03,1.88257378321648D-02,-2
     3.12879819630095D-05,-6.38639458890286D-05,-1.27727891778057D-04,1.
     437971351810729D-08,5.51885407242917D-08,1.65565622172875D-07,3.311
     531244345750D-07,5*0.0D00,2.75942703621458D-09,6*0.0D00,1.379713518
     610729D-08,5.51885407242917D-08,1.65565622172875D-07,3.311312443457
     750D-07/
      DATA A,AA,AB,UA,D1,D2,D3,D4,D5,V1,V2,V3/8.13389656644895D13,-5.317
     142860649802D06,1.97994920826647D-02,2.11770000000000D-10,3.9598984
     21653293D-02,6.35310000000000D-10,1.27062000000000D-09,3*0.0D00,2.1
     31770000000000D-10,0.0D00,6.35310000000000D-10,1.27062000000000D-09
     4,1.76816150742336D15,1.23730971890897D08,1.45511293919343D06,-3.97
     576053710460D00,-1.50622516081086D-02,4.32940740732648D-04,-1.8535
     656073721890D-06,2.05286315303314D-09,7.36440814840596D13,-5.2584624
     73630271D06,4.14478797681273D-02/
      P=PP
      T=TT
      C1=CC
      C2=C1*C1
      C3=C1*C2
      C4=C1*C3
      GO TO (1,7),K
1     GO TO (2,3),J
2     N=1
      GO TO 4
3     A(1,2)=A(1,1)+AA/T
      A(2,2)=A(2,1)-AB/T
      A(3,2)=A(3,1)+1.0D0/T
      A(5,2)=2.0D0*A(3,2)
      N=2
4     DO 5 I=1,2
      M=2*N-2+I
      IF (M.EQ.2) GO TO 6
      F(1,M)=(A(1,N)+(A(2,N)+(A(3,N)+A(4,N)*P)*P)*P)/C1
      F(2,M)=(A(2,N)+(A(5,N)+A(6,N)*P)*P)/C2
      F(3,M)=(A(5,N)+A(7,N)*P)/C3
      F(4,M)=A(7,N)/C4
5     P=UA
      RETURN
6     F(1,2)=V1/C1
      F(2,2)=V2/C2
      F(3,2)=V3/C3
      F(4,2)=F(4,1)
      RETURN
7     C5=C4*C1
      C6=C5*C1
      GO TO (8,9),J
8     N=1
      GO TO 10
9     B(1,2)=B(1,1)+T*D1
      B(2,2)=B(2,1)+T*D2
      B(3,2)=B(3,1)+T*D3
```

```
      B(4,2)=B(4,1)+T*D4
      B(5,2)=B(5,1)+T*D5
      B(7,2)=B(3,2)*2.0D0
      B(8,2)=B(4,2)*3.0D0
      B(9,2)=B(8,2)*2.0D0
      B(10,2)=B(5,2)*4.0D0
      B(11,2)=B(10,2)*3.0D0
      B(12,2)=B(11,2)*2.0D0
      N=2
10    M=2*N-1
      G(1,M)=(B(1,N)+(B(2,N)+(B(3,N)+(B(4,N)+(B(5,N)+B(6,N)*P)*P)*P)*P)*
     1P)/C1
      G(2,M)=(B(2,N)+(B(7,N)+(B(8,N)+(B(10,N)+B(13,N)*P)*P)*P)*P)/C2
      G(3,M)=(B(7,N)+(B(9,N)+(B(11,N)+B(14,N)*P)*P)*P)/C3
      G(4,M)=(B(9,N)+(B(12,N)+B(15,N)*P)*P)/C4
      G(5,M)=(B(12,N)+B(16,N)*P)/C5
      G(6,M)=B(16,N)/C6
      M=M+1
      G(1,M)=B(1,N)/C1
      G(2,M)=B(2,N)/C2
      G(3,M)=B(7,N)/C3
      G(4,M)=B(9,N)/C4
      G(5,M)=B(12,N)/C5
      G(6,M)=B(16,N)/C6
      RETURN
      END
```

```
C DECK METEMP
      DOUBLE PRECISION FUNCTION CP(T)
      DOUBLE PRECISION SI(2),HI(2),S
      DIMENSION A(9,3,2)
      DATA A/2.5771104E-6,-2.240781E-4,-4.6776567E-4,7.7524692E-3,1.0207
     1347E-3,-5.9827343E-2,.1053479,-6.7124682E-2,3.0159729,3.221388E-7,
     2-3.2011157E-5,-7.7960945E-5,1.5504938E-3,2.5518368E-4,-1.9942448E-
     32,5.267395E-2,-6.7124682E-2,3.0159729,2.863456E-7,-2.8009762E-5,-6
     4.6823557E-5,1.2920782E-3,2.0414694E-4,-1.4956836E-2,3.5115967E-2,-
     53.3562341E-2,3.0159729,2.1771302E-6,-3.6924768E-5,1.2048213E-4,1.7
     66546467E-3,-1.7244897E-2,1.8825512E-2,.4503988,-1.6311027,4.5834702
     7,2.7214128E-7,-5.2749669E-6,2.0080355E-5,3.5092934E-4,-4.3112242E-
     83,6.2751707E-3,.2251994,-1.6311027,4.5834702,2.4190336E-7,-4.61559
     96E-6,1.7211733E-5,2.9244112E-4,-3.4489794E-3,4.706378E-3,.15013293
     $,-.81555135,4.5834702/
      DATA SI,HI/18.66792402732497,19.90897487890906,-2.176323905587196,
     1-110.4372755187238/
      K=1
1     N=1
      IF(T.GE.259.78828)N=2
      S=T/1.0D2
      CP=A(1,K,N)
      DO 2 J=2,8
2     CP=CP*S+A(J,K,N)
      GO TO (3,4,5),K
3     CP=CP*S+A(9,1,N)
      RETURN
```

```
      ENTRY CS(T)
      K=2
      GO TO 1
4     CP=CP*S+A(9,2,N)*DLOG(S)+SI(N)
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
5     CP=T*(CP*S+A(9,3,N))+HI(N)
      RETURN
      END
```

```
C DECK MELOG

      LOGICAL FUNCTION LGFN(P,T,J,Z)
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      DIMENSION Z(6)
      S=T/100.0
      J=1
      LGFN=.TRUE.
      IF (P.GT.4.1E7.OR.P.LT.0.1.OR.S.LT..69.OR.S.GT.6.1.OR.Z(1).LE.0.0.
     1OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      IF (S.GT.1.9077) GO TO 1
      PLOG=8.30516+(-2.961-0.8/S)/S
      IF (S.GE.1.1883) PLOG=PLOG+0.257*(S/1.1883-1.0)**1.32
      IF (P.GT.XKV*EXP(2.3025851*PLOG)) RETURN
1     J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK MEDATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R/1.0,518.2562,16.04303,8.745139E-4,5.6,1.3333333/
      END
```

```
C DECK METLG

      SUBROUTINE TLOGIC (P,T)
      DATA A1,A2,A3,A4,A5, A6,A7,A8,A9/53.88758,1.8253577,0.18723912,1.57
     10661E-5,-8.7451662E-4,1.2470553E-4,9.4808617E-6,-1.280319E-6,4.544
     26557E-8/
      IF (T.GT.190.77) RETURN
      V=ALOG(P)
```

```
S=A1+(A2+(A3+(A4+(A5+(A6+(A7+(A8+A9*V)*V)*V)*V)*V)*V)*V)*V
IF (T.LT.S) T=S
IF (T.LT.69.0) T=69.0
RETURN
END
```

Natural Gas

The routines for natural gas are described and presented in reference 3. The temperature is from 200 to 400 K, and the pressure range extends to 100×10^5 pascals. The composition of natural gas is assumed to consist of alkanes containing from one to six carbon atoms and the dilutant gases N_2 and CO_2. The alkanes C_4H_{10}, C_5H_{12}, and C_6H_{14} can have more than one molecular configuration. For these cases, the assumption is made that each molecular configuration, for a given gas, is equally probable.

The reference state for the enthalpy and entropy is that of the ideal gas at a temperature of 200 K and a pressure of 1×10^5 pascals.

Since natural gas is a mixture of many gases, an additional subroutine, whose deck name is NMCOMP, is necessary. This subroutine supplies composition-dependent constants to the other routines. For a given composition, this subroutine has to be referenced only once in the main program. This reference has to occur prior to a reference to either RWEDG or RNS. The reference to this subroutine is

CALL BDATA(X)

where X is an eight-element array whose elements are proportional to the mole fractions of the natural-gas components. The order in which these components appear in the array is as follows: CH_4, C_2H_6, C_3H_8, C_4H_{10}, C_5H_{12}, C_6H_{14}, N_2, and CO_2. The natural-gas routine, as distinguished from the other routines, requires input of these values of X as additional data.

Even though the card listing of these routines is in reference 3, this listing is repeated here for convenience. The prefix for the deck names is NM. The subroutine NMZETA is not independent; but the combination of NMZETA, NMPOLY, and NMCOMP is. The routine NMTEMP is not independent, but the combination of NMTEMP and NMCOMP is.

```
C DECK NMCOMP
      SUBROUTINE BDATA (X)
      DIMENSION X(8), MOL(8), XMOL(8), S(8), H(8), CP(8,8), T(8), P(8),
     1RHO(8)
      COMMON /LDATA/ XKV,R,MW,RC,D2,G
      COMMON /PDATA/ F(9)/ZDATA/PC,TC,RHOC/TDATA/A(8,3),HI,SI
      REAL MOL,MW
      DATA MOL,XMOL/16.043,30.07,44.097,58.124,72.151,86.178,28.013,44.0
     11,2.77527262,3.403528,3.78639175,4.06264748,4.27876115,4.45641492,
     23.33266869,3.78441688/
      DATA CP/2.7998255,.4284998,-.2751805,2.5821711E-2,2.4165792E-2,-2.
     15163737E-3,-8.2465805E-4,1.1523272E-4,-9.8533835,19.657673,-10.186
     2582,1.8267443,.2463681,-.1202048,1.0807487E-2,0.0,-16.796807,29.08
     34569,-13.810883,2.2198327,.3655141,-.1532602,1.296668E-2,0.0,-1.81
     422946,5.6640979,-.907714,.1435233,.034644782,-.017195974,1.7660626
     5E-3,0.0,-3.3598014,7.4196271,-.726671,.045531828,4*0.0,-.5379224,5
     6.6539353,.3607859,-.1684308,.015475231,3*0.0,2.501146,-9.720581E-3
     7,1.036056E-2,-4.437258E-3,6.825596E-4,3*0.0,2.5044684,-.5085567,.4
     8840302,-3.730571E-2,-2.522643E-2,6.1401476E-3,-4.1166357E-4,0.0/
      DATA S,H/-2.42592233,-16.722706,-24.4685144,-7.4352313,-9.71086973
     1,-9.62405754,-1.20430845,-.54815092,-794.255051,-224.353146,43.254
     2268,-792.772573,-836.398938,-1261.94398,-699.709835,-702.986595/
      DATA P,T,RHO/4.626E6,4.894E6,4.257E6,3.722E6,3.299E6,3.149E6,3.398
     1E6,7.368E6,190.77,305.56,369.97,416.7,454.6,499.7,126.135,304.20,1
     262.5,203.2,220.5,224.4,235.0,236.7,311.0,468.0/
      XX=0.0
      DO 1 N=1,8
1     XX=XX+X(N)
      DO 2 N=1,8
2     F(N)=X(N)/XX
      F(9)=F(8)-F(7)/2.0+F(2)+2.0*F(3)+3.0*F(4)+4.0*F(5)+5.0*F(6)
      PC=0.0
      TC=0.0
      RHOC=0.0
      SI=0.0
      HI=0.0
      MW=0.0
      DO 3 N=1,8
      SI=SI+F(N)*(S(N)-XMOL(N))
      HI=HI+F(N)*H(N)
      MW=MW+F(N)*MOL(N)
      PC=PC+F(N)*P(N)
      TC=TC+F(N)*T(N)
3     RHOC=RHOC+F(N)*RHO(N)
      SI=SI+ALOG(MW)
      PC=P(1)/PC
      TC=T(1)/TC
      RHOC=RHO(1)/RHOC
      DO 5 N=1,8
      NN=9-N
      A(NN,1)=0.0
      DO 4 M=1,8
4     A(NN,1)=A(NN,1)+F(M)*CP(N,M)
      XN=N-1
      IF (XN.EQ.0.0) XN=1.0
      A(NN,2)=A(NN,1)/XN
5     A(NN,3)=A(NN,1)/FLOAT(N)
```

```
      R=8314.41/MW
      RC=5.45105E-5*MW
      RETURN
      END
```

```
C DECK NMZETA
      SUBROUTINE ZETA (KK,PP,TT,Z)
      COMMON /VALUE/ F(4,4),G(6,4)
      COMMON /ZDATA/ PC,TC,RHOC
      DIMENSION Z(6)
      DOUBLE PRECISION F,G,B1,B2,B3,B4,B5,A1,A2,A3,A4,A5,E1,E2,PA,TA,TH1
     1,TH2,TH3,TH4,D1,D2,D3,D4,D5,F1,F2,UA,P,T,P1,P2,U,T1,RC,EXPC,RB,EXP
     2B,ZB1,ZC1,AB1,AB2,AB3,AB4,AB5,ZA,ZB,ZC,RB1,EXPB1,S,SS,PSI1,PSI2,PS
     3I3,PSI4,RC1,EXPC1,PSI5,PSI6,PSI7,PSI8
      DATA B1,B2,B3,B4,B5,A1,A2,A3,A4,A5,E1,E2,PA/4.91473574991686D-03,7
     1.37664223478550D-06,-1.14587843032923D-07,5.89510209511141D-10,-5.
     274382281343532D-13,-2.23983199201862D00,1.34331253741270D-03,2.759
     3101829J6551D-05,-1.65546977053542D-07,2.34124562687064D-10,-4.6002
     40000000J000D-02,-2.11770000000000D-10,1.13318000000000D02/
      DATA TA,TH1,TH2,TH3,TH4,D1,D2,D3,D4,D5,F1,F2,UA/1.47710550000000D0
     12,1.09934666473654D-14,1.64873321284064D07,1.07243639762491D08,3.6
     2644888245514D-15,-3.97760537104600D00,-1.50622516081086D-02,4.329
     3407407326480-04,-1.85355607372189D-06,2.05286315303314D-09,-1.3787
     49330003000003,1.34418460000000D00,1.45511293919343D06/
      K=KK
      P=PP*RHOC
      T=TT*TC
      P1=P+PA
      P2=P1*P1
      U=P2*P1
      T1=T+TA
      RC=(F1+F2*P)/T
      EXPC=DEXP(RC)
      RB=(E1+E2*U)
      EXPB=DEXP(RB*T1)
      ZB1=(TH1*P*P2*(U-TH2)*(TH3-U)*EXPB)/T
      ZC1=(D1+(D2+(D3+(D4+D5*P)*P)*P)*P)*P*EXPC/T
      IF (K.EQ.2) GO TO 1
      AB1=B1+A1/T
      AB2=B2+A2/T
      AB3=B3+A3/T
      AB4=B4+A4/T
      AB5=B5+A5/T
      ZA=1.0D0+(AB1+(AB2+(AB3+(AB4+AB5*P)*P)*P)*P)*P
      Z(1)=ZA+ZB1+ZC1
      IF (K.EQ.0) RETURN
      ZA=1.0D0+(2.0D0*AB1+(3.0D0*AB2+(4.0D0*AB3+(5.0D0*AB4+6.0D0*AB5*P)*
     1P)*P)*P)*P
      ZB=ZB1*(2.0D0*(1.0D0+P/P1)+3.0D0*P*P2*(E2*T1+1.0D0/(U-TH3)+1.0D0/(
     1U-TH2)))
      ZC=(F2*P*ZC1+EXPC*(2.0D0*D1+(3.0D0*D2+(4.0D0*D3+(5.0D0*D4+6.0D0*D5
     1*P)*P)*P)*P)*P)/T
      Z(3)=ZA+ZB+ZC
      IF (K.EQ.1) RETURN
```

```
1     RB1=E1+E2*UA
      EXPB1=DEXP(RB1*T1)
      ZA=1.0D0+(B1+(B2+(B3+(B4+B5*P)*P)*P)*P)*P
      ZB=RB*T*ZB1
      ZC=-RC*ZC1
      Z(2)=ZA+ZB+ZC
      S=E2*T1
      SS=F2/T
      CALL POLY (1,1,U,T,S)
      CALL POLY (1,2,P,T,SS)
      ZA=(B1+(B2/2.0D0+(B3/3.0D0+(B4/4.0D0+B5*P/5.0D0)*P)*P)*P)*P
      PSI1=F(1,1)-F(2,1)+F(3,1)-F(4,1)
      PSI2=F(1,2)-F(2,2)+F(3,2)-F(4,2)
      ZB=TH4*(PSI1*EXPB-PSI2*EXPB1)
      PSI3=G(1,1)-G(2,1)+G(3,1)-G(4,1)+G(5,1)-G(6,1)
      PSI4=G(1,2)-G(2,2)+G(3,2)-G(4,2)+G(5,2)-G(6,2)
      RC1=F1/T
      EXPC1=DEXP(RC1)
      ZC=(PSI4*EXPC1-PSI3*EXPC)/T**2
      Z(4)=ZA+ZB+ZC
      IF (K.EQ.2) RETURN
      CALL POLY (2,1,U,T,S)
      CALL POLY (2,2,P,T,SS)
      PSI5=F(1,3)-F(2,3)+F(3,3)-F(4,3)
      PSI6=F(1,4)-F(2,4)+F(3,4)-F(4,4)
      PSI7=G(1,3)-G(2,3)+G(3,3)-G(4,3)+G(5,3)-G(6,3)
      PSI8=G(1,4)-G(2,4)+G(3,4)-G(4,4)+G(5,4)-G(6,4)
      ZA=-(A1+(A2/2.0D0+(A3/3.0D0+(A4/4.0D0+A5*P/5.0D0)*P)*P)*P)*P/T
      ZB=TH4*(PSI5*EXPB-PSI6*EXPB1)
      ZC=(PSI8*EXPC1-PSI7*EXPC)/T**2
      Z(5)=ZA+ZB+ZC
      ZB=TH4*T*(EXPB*(RB*PSI1-(F(1,1)-2.0D0*F(2,1)+3.0D0*F(3,1)-4.0D0*F(
     14,1))/T1)-EXPB1*(RB1*PSI2-(F(1,2)-2.0D0*F(2,2)+3.0D0*F(3,2)-4.0D0*
     2F(4,2))/T1))
      ZC=(EXPC*((2.0D0+RC)*PSI3-G(1,1)+2.0D0*G(2,1)-3.0D0*G(3,1)+4.0D0*G
     1(4,1)-5.*G(5,1)+6.0D0*G(6,1))-EXPC1*((2.0D0+RC1)*PSI4-G(1,2)+2.0D0
     2*G(2,2)-3.0D0*G(3,2)+4.0D0*G(4,2)-5.0D0*G(5,2)+6.0D0*G(6,2)))/T**2
      Z(6)=ZB+ZC
      RETURN
      END
```

```
C DECK NMPOLY

      SUBROUTINE POLY (J,K,PP,TT,CC)
      COMMON /VALUE/ F(4,4),G(6,4)
      DIMENSION A(7,2), B(16,2)
      DOUBLE PRECISION PP,TT,CC,F,G,A,B,AA,AB,UA,D1,D2,D3,D4,D5,P,T,C1,C
     12,C3,C4,C5,C6,V1,V2,V3
      DATA B/5.484295635642240D03,1.54210957155370D01,-6.17182239272157D-
     101,3.13762297202746D-03,-5.32199549075239D-06,2.75942703621458D-09
     2,-1.23436447854431D00,9.41286891608238D-03,1.88257378321648D-02,-2
     3.12879819630095D-05,-6.38639458890286D-05,-1.27727891778057D-04,1.
     437971351810729D-08,5.51885407242917D-08,1.65565622172875D-07,3.311
     531244345750D-07,5*0.0D00,2.75942703621458D-09,6*0.0D00,1.379713518
     610729D-08,5.51885407242917D-08,1.65565622172875D-07,3.311312443457
```

```
      750D-07/
       DATA A,AA,AB,UA,D1,D2,D3,D4,D5,V1,V2,V3/8.13389656644895D13,-5.317
      142860649802D06,1.97994920826647D-02,2.11770000000000D-10,3.9598984
      21653293D-02,6.35310000000000D-10,1.27062000000000D-09,3*0.0D00,2.1
      3177000000000D-10,0.0D00,6.35310000000000D-10,1.27062000000000D-09
      4,1.76816150742336D15,1.23730971890897D08,1.45511293919343D06,-3.97
      576053710460D00,-1.50622516081086D-02,4.32940740732648D-04,-1.8535
      656073721 89D-06,2.05286315303314D-09,7.36440814840596D13,-5.2584624
      73630271D06,4.14478797681273D-02/
       P=PP
       T=TT
       C1=CC
       C2=C1*C1
       C3=C1*C2
       C4=C1*C3
       GO TO (1,7),K
1      GO TO (2,3),J
2      N=1
       GO TO 4
3      A(1,2)=A(1,1)+AA/T
       A(2,2)=A(2,1)-AB/T
       A(3,2)=A(3,1)+1.0D0/T
       A(5,2)=2.0D0*A(3,2)
       N=2
4      DO 5 I=1,2
       M=2*N-2+I
       IF (M.EQ.2) GO TO 6
       F(1,M)=(A(1,N)+(A(2,N)+(A(3,N)+A(4,N)*P)*P)*P)/C1
       F(2,M)=(A(2,N)+(A(5,N)+A(6,N)*P)*P)/C2
       F(3,M)=(A(5,N)+A(7,N)*P)/C3
       F(4,M)=A(7,N)/C4
5      P=UA
       RETURN
6      F(1,2)=V1/C1
       F(2,2)=V2/C2
       F(3,2)=V3/C3
       F(4,2)=F(4,1)
       RETURN
7      C5=C4*C1
       C6=C5*C1
       GO TO (8,9),J
8      N=1
       GO TO 10
9      B(1,2)=B(1,1)+T*D1
       B(2,2)=B(2,1)+T*D2
       B(3,2)=B(3,1)+T*D3
       B(4,2)=B(4,1)+T*D4
       B(5,2)=B(5,1)+T*D5
       B(7,2)=B(3,2)*2.0D0
       B(8,2)=B(4,2)*3.0D0
       B(9,2)=B(8,2)*2.0D0
       B(10,2)=B(5,2)*4.0D0
       B(11,2)=B(10,2)*3.0D0
       B(12,2)=B(11,2)*2.0D0
       N=2
10     M=2*N-1
       G(1,M)=(B(1,N)+(B(2,N)+(B(3,N)+(B(4,N)+(B(5,N)+B(6,N)*P)*P)*P)*P)*
      1P)/C1
       G(2,M)=(B(2,N)+(B(7,N)+(B(8,N)+(B(10,N)+B(13,N)*P)*P)*P)*P)/C2
       G(3,M)=(B(7,N)+(B(9,N)+(B(11,N)+B(14,N)*P)*P)*P)/C3
       G(4,M)=(B(9,N)+(B(12,N)+B(15,N)*P)*P)/C4
```

```
      G(5,M)=(B(12,N)+B(16,N)*P)/C5
      G(6,M)=B(16,N)/C6
      M=M+1
      G(1,M)=B(1,N)/C1
      G(2,M)=B(2,N)/C2
      G(3,M)=B(7,N)/C3
      G(4,M)=B(9,N)/C4
      G(5,M)=B(12,N)/C5
      G(6,M)=B(16,N)/C6
      RETURN
      END
```

```
C DECK NMTEMP

      DOUBLE PRECISION FUNCTION CP(T)
      DOUBLE PRECISION S
      COMMON/TDATA/A(8,3),HI,SI
      K=1
    1 S=T/1.0D2
      CP=A(1,K)
      DO 2 N=2,7
    2 CP=CP*S+A(N,K)
      GO TO (3,4,5),K
    3 CP=CP*S+A(8,1)
      RETURN
      ENTRY CS(T)
      K=2
      GO TO 1
    4 CP=CP*S+A(8,2)*DLOG(S)+SI
      RETURN
      ENTRY CH(T)
      K=3
      GO TO 1
    5 CP=T*(CP*S+A(8,3))+HI
      RETURN
      END
```

```
C DECK NMLOG

      LOGICAL FUNCTION LGFN(P,T,J,Z)
      COMMON /ZDATA/ PC,TC,RHOC
      COMMON /LDATA/ XKV,R,XMW,RC,D2,G
      DIMENSION Z(6)
      S=T/100.0
      J=1
      LGFN=.TRUE.
      IF (P.GT.1.1E7.OR.P.LT.0.1.OR.S.LT.1.9.OR.S.GT.4.1.OR.Z(1).LE.0.0.
     1OR.Z(2).LE.0.0.OR.Z(3).LE.0.0) RETURN
      S=S*TC
      IF (S.GT.1.9077) GO TO 1
      PLOG=8.30516+(-2.961-0.8/S)/S+.257*(S/1.1883-1.0)**1.32
```

```
      IF (P*PC.GT.XKV*EXP(2.3025851*PLOG)) RETURN
1     J=0
      LGFN=.FALSE.
      RETURN
      END
```

```
C DECK NMDATA

      BLOCK DATA
      COMMON /LDATA/ R(6)
      DATA R(1),R(5),R(6)/1.0,5.6,1.3333333/
      END
```

```
C DECK NMTLG

      SUBROUTINE TLOGIC (P,T)
      COMMON /ZDATA/ PC,TC,RHOC
      DIMENSION A(9)
      DATA A/4.5446557E-8,-1.280319E-6,9.4808617E-6,1.2470553E-4,-8.7451
     1662E-4,1.570661E-5,.18723912,1.8253577,53.88758/
      PP=P*PC
      TT=T*TC
      IF (TT.GT.190.77) RETURN
      V=ALOG(PP)
      S=0.0
      DO 1 N=1,9
1     S=S*V+A(N)
      IF (TT.LT.S) T=S/TC
      IF(T.LT.190.0)T=190.0
      RETURN
      END
```

APPENDIX E

SAMPLE CALCULATIONS

It is desired to determine the properties of a supersonic air stream. These properties are the velocity; the Mach number; and the pressure, density, and temperature under both total and static conditions. Two cases are considered: one uses the routines in appendix B, and the other uses the routines in appendix C. For both cases, the input and output variables are in U.S. customary units rather than SI units. That is, pressure is in psia, temperature in degrees F, density in lb/ft^3, and velocity in ft/sec. Appropriate conversion factors are included in the main computer programs.

CASE I

For case I, the measurements are

(1) The pressure indicated by a total-head tube. This is the total pressure downstream of the normal shock.

(2) The stagnation temperature, as indicated by thermocouple probe whose recovery factor is unity. This is the total temperature downstream of the normal shock.

(3) The pressure indicated by a wedge-type static-pressure probe whose total wedge angle is 15°. This is the pressure behind the oblique shock attached to the wedge.

These measurements are such that the routines in appendix B and the air routines in appendix D apply. However, in order to activate these routines, a main computer program must be written. A typical main program could be

```
$IBFTC MAINW
      COMMON/OUTW/TP(8,5),VM(10),CONV(12),Z(6,5),KODE(11)
      REAL M1
      NAMELIST/OUT/P2T,T2T,P3,DELTA2,U1,M1,P1T,RHO1T,T1T,P1,RHO1,
     1T1,KODE
1     READ(5,OUT)
      P=P2T*6894.73
      PP=P3*6894.73
      T=(T2T+459.67/1.8
      DELTA=DELTA2/2.0
      CALL RWEDG(P,T,PP,DELTA)
      U1=VM(3)*3.28083
      M1=VM(1)
      P1T=TP(1,1)/6894.73
```

```
P1=TP(1,2)/6894.73
RHO1T=TP(2,1)*0.0624284
RHO1=TP(2,2)*0.0624284
T1T=TP(3,1)*1.8-459.67
T1=TP(3,2)*1.8-459.67
WRITE(6,OUT)
GO TO 1
END
```

The decks that are loaded are as follows; MAINW, RGWED, RGDFW, PGWED, WDATA, AIZETA, AITEMP, AILOG, AIDATA, and the necessary matrix inversion routine deck called MINV which is supplied by IBM in their Scientific Subroutine Package.

The input for a typical case is

P2T	Pressure indicated by the total head tube, 1027 psia
T2T	Temperature indicated by a stagnation thermocouple, 83.4° F
P3	Pressure indicated by a wedge-type static-pressure probe, 354 psia
DELTA2	Wedge angle, 15°

The output for this case is

U1	Velocity, 1517 ft/sec
M1	Mach number, 1.702
P1T	Total pressure, 1186 psia
RHO1T	Total density, 5.902 lb/ft^3
T1T	Total temperature, 86.7° F
P1	Pressure, 241.1 psia
RHO1	Density, 2.005 lb/ft^3
T1	Temperature, -119.1° F

CASE II

For case II, the flow issues from a supersonic nozzle attached to a plenum. The assumption is made that the flow is isentropic and one dimensional from the plenum to the nozzle exit. The measurements are

(1) The pressure in the plenum. This is the total pressure.

(2) The temperature in the plenum. This is the total temperature.

(3) The pressure indicated by a total-head tube. This is the total pressure downstream of the normal shock.

The measurements are such that the routines in appendix C and the air routines in appendix D apply. However, in order to activate these routines, a main computer program must be written. A typical main program, which is similar to that in case I, could be

```
$IBFTC MAINNS
      COMMON/OUTNS/TP(8,4),VM(6),CONV(9),Z(6,4),KODE(8)
      REAL M1
      NAMELIST/OUT/P1T,T1T,P2T,U1,M1,RHO1T,P1,RHO1,T1,KODE
1     READ(5,OUT)
      P=P1T*6894.73
      PP=P2T*6894.73
      T=(T1T+459.67)/1.8
      CALL RNS(P,T,PP)
      U1=VM(3)*3.28083
      M1=VM(1)
      P1=TP(1,2)/6894.73
      RHO1T=TP(2,1)*0.0624284
      RHO1=TP(2,2)*0.0624284
      T1=TP(3,2)*1.8-459.67
      WRITE(6,OUT)
      GO TO 1
      END
```

The decks that are loaded are as follows: MAINNS, RGNS, RGDFNS, PGNS, NSDATA, AIZETA, AITEMP, AILOG, AIDATA, and the necessary matrix inversion deck called MINV supplied by IBM in their Scientific Subroutine Package.

The input for this case is

P1T	Plenum pressure, 1186 psia
T1T	Plenum temperature 86.7° F
P2T	Pressure indicated by a total head tube, 1027 psia

The values of P1T and T1T are given the same as those calculated in the previous case, also the value of P2T is the same as in the previous case.

The output for this case is

U1	Velocity, 1517 ft/sec

M1	Mach number, 1.702
RHO1T	Total density, 5.902 lb/ft^3
P1	Pressure, 241.1 psia
RHO1	Density, 2.005 lb/ft^3
T1	Temperature, -119.1° F

The results for this case are the same as in the previous case, as would be expected from the input. This similarity constitutes a good check on the validity of the routines in appendixes B and C.

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