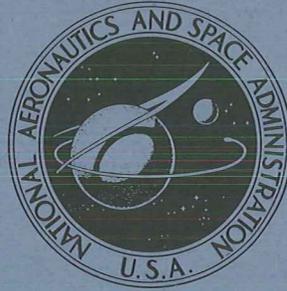


5-6

NASA TECHNICAL
MEMORANDUM



NASA TM X-2240

NASA TM X-2240

NASA FILE COPY

Return to
NASA HQ. LIBRARY (KSS-10)
WASHINGTON, D. C. 20546 STOP 85

HQ. LIBRARY (KSS-10)

A SET OF FORTRAN IV ROUTINES
USED TO CALCULATE THE MASS FLOW RATE
OF NATURAL GAS THROUGH NOZZLES

by Robert C. Johnson
Lewis Research Center
Cleveland, Ohio 44135

1. Report No. NASA TM X-2240	2. Government Accession No.	3. Recipient's Catalog No.	
4. Title and Subtitle. A SET OF FORTRAN IV ROUTINES USED TO CALCULATE THE MASS FLOW RATE OF NATURAL GAS THROUGH NOZZLES		5. Report Date April 1971	6. Performing Organization Code
		8. Performing Organization Report No. E-6086	
7. Author(s) Robert C. Johnson		10. Work Unit No. 720-03	11. Contract or Grant No.
9. Performing Organization Name and Address Lewis Research Center National Aeronautics and Space Administration Cleveland, Ohio 44135		13. Type of Report and Period Covered Technical Memorandum	
		14. Sponsoring Agency Code	
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D. C. 20546		15. Supplementary Notes	
16. Abstract A set of FORTRAN IV subroutines is presented that calculates the isentropic mass flow rate of natural gas through nozzles and also thermodynamic functions such as compressibility factor, entropy, enthalpy, and specific heat. The pressure range for these routines is 0.1 to 100×10^5 newtons per square meter, and the temperature range is from 200 to 400 Kelvin. Three sets of independent variables are permitted. In addition to the plenum pressure and plenum temperature, the other independent variable may be either the nozzle-exit pressure, the nozzle-exit Mach number, or the nozzle-exit temperature.			
17. Key Words (Suggested by Author(s)) Mass flow rate Real gas Natural gas Isentropic processes		18. Distribution Statement Unclassified - unlimited	
19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No. of Pages 36	22. Price* \$3.00

ERRATA

NASA Technical Memorandum X-2240

A SET OF FORTRAN IV ROUTINES USED TO CALCULATE THE MASS FLOW RATE OF NATURAL GAS THROUGH NOZZLES

by Robert C. Johnson

April 1971

Page 11: Equation (42) should be

$$\Delta \left(\frac{S_0 - S_e}{R} \right) = \frac{S(\rho_{e,n-1}, T_e) - S(\rho_0, T_0)}{R}$$

Page 12: The equation numbers in the fifth line from the bottom should be (30), (31), and (32).

Page 14: Equation (53) should be

$$T_{e,1} = T_0 \left(1 + \frac{1}{6} M_e^2 \right)^{-1}$$

Page 23: The definition of EDB should read "Maximum value of $(S_e - S_0)/R$ permitted. Unless otherwise specified, EDB equals 1×10^{-6} ."

Page 24: The equation defining CONV(4) should be

$$\text{CONV}(4) = \frac{S_e - S_0}{R}$$

Issued August 1973

A SET OF FORTRAN IV ROUTINES USED TO CALCULATE THE MASS FLOW RATE OF NATURAL GAS THROUGH NOZZLES

by Robert C. Johnson

Lewis Research Center

SUMMARY

A set of FORTRAN IV subroutines is presented that calculates the isentropic mass flow rate of natural gas through nozzles and also thermodynamic functions such as compressibility factor, entropy, enthalpy, and specific heat. The pressure range for these routines is 0.1 to 100×10^5 newtons per square meter, and the temperature range is from 200 to 400 Kelvin. Three sets of independent variables are permitted. In addition to the plenum pressure and plenum temperature, the other independent variable may be either the nozzle-exit pressure, the nozzle-exit Mach number, or the nozzle-exit temperature.

INTRODUCTION

When nozzles are used for measuring the mass flow rate of natural gas, the conventional isentropic flow equations do not apply. These equations only apply to a perfect gas. A perfect gas is defined as one whose compressibility factor is invariant, with a value of 1, and whose specific heat is invariant. This ideal condition is closely approximated by a gas such as air at room temperature and at pressures up to a few atmospheres. Natural gas, on the other hand, cannot be considered perfect even at atmospheric pressure because of the specific-heat variation with temperature. At higher pressures, the compressibility factor variation also becomes important.

Since natural gas is being considered as a fuel for aircraft, as well as for other propulsion and power systems, an accurate method for making mass flow rate calculations is necessary for gas metering.

In reference 1, isentropic flow calculations were made for natural gas using the Benedict-Webb-Rubin state equation (refs. 2 to 4). The result of these calculations was a critical-flow factor. By using this factor, the isentropic mass flow rate of natural

gas through critical-flow nozzles can be calculated. A critical-flow nozzle is one that operates with a throat Mach number of 1. The output of FORTRAN IV routines used to make the calculations in reference 1 includes more than the isentropic mass flow rate of natural gas. In fact, a set of thermodynamic point functions are evaluated at both the plenum and the nozzle exit. These functions include compressibility factor, specific heat, isentropic exponent, and specific-heat ratio.

In all these calculations, the plenum independent variables are pressure and temperature. The nozzle-exit independent variable is either pressure, Mach number, or temperature.

Because of the versatility of these routines as previously indicated, they are presented in this report. The routines operate over a temperature range from 199 to 401 K and a pressure range from 0.1 to 101×10^5 newtons per square meter. For a successful calculation, the components of the natural gas mixture have to remain in the gaseous state.

BASIC EQUATIONS

The routines in this report use three basic relations. The first describes the pressure-temperature-density behavior of natural gas. This relation is referred to as the state equation. The second describes the ideal-gas, specific-heat variation with temperature. The third describes the saturated-vapor-pressure variation with temperature. This last relation is used to determine that the fluid is a gas. These three relations are discussed in detail in the following sections.

State Equation

Since natural gas is a mixture of many gases, it is useful to have a state equation whose coefficients can be determined from the coefficients of the individual components. Such an equation is that developed by Benedict, Webb, and Rubin in reference 2. This equation is as follows:

$$Z = \frac{p}{\rho RT} = 1 + \left(a_2 - \frac{a_3}{T} - \frac{a_4}{T^3} \right) \rho + \left(a_5 - \frac{a_6}{T} \right) \rho^2 + \frac{a_6 a_8}{T} \rho^5 + \frac{a_7 \rho^2 (1 + a_1 \rho^2) e^{-a_1 \rho^2}}{T^3} \quad (1)$$

where

$$R = \frac{8314.41}{m} \quad m^2/(\text{sec}^2)(K) \quad (2)$$

and

$$m = \sum_{i=1}^N x_i m_i \quad (3)$$

(All symbols are defined in appendix A.)

In reference 3, a set of rules is presented that permits the coefficients of equation (1) to be determined for a gas mixture when the coefficients for the component gases are known. These mixing rules are

$$a_1 = \frac{1}{m^2} \left[\sum_{i=1}^N x_i (a_{1,i} m_i^2)^{1/2} \right]^2 \quad (4)$$

$$a_2 = \frac{1}{8m} \sum_{i=1}^N \sum_{j=1}^N x_i x_j \left[(a_{2,i} m_i)^{1/3} + (a_{2,j} m_j)^{1/3} \right]^3 \quad (5)$$

$$a_3 = \frac{1}{m} \left[\sum_{i=1}^N x_i (a_{3,i} m_i)^{1/2} \right]^2 \quad (6)$$

$$a_4 = \frac{1}{m} \left[\sum_{i=1}^N x_i (a_{4,i} m_i)^{1/2} \right]^2 \quad (7)$$

$$a_5 = \frac{1}{m^2} \left[\sum_{i=1}^N x_i (a_{5,i} m_i^2)^{1/3} \right]^3 \quad (8)$$

$$a_6 = \frac{1}{m^2} \left[\sum_{i=1}^N x_i (a_{6,i} m_i^2)^{1/3} \right]^3 \quad (9)$$

$$a_7 = \frac{1}{m^2} \left[\sum_{i=1}^N x_i (a_{7,i} m_i^2)^{1/3} \right]^3 \quad (10)$$

$$a_8 = \frac{1}{m^3} \left[\sum_{i=1}^N x_i (a_{8,i} m_i^3)^{1/3} \right]^3 \quad (11)$$

In table I, the appropriate functions of the Benedict-Webb-Rubin coefficients and the molecular weight that permit easy use of the mixing rules (eqs. (4) to (11)) are presented for hydrocarbons with up to four carbon atoms, and for the dilutant gases, nitrogen and carbon dioxide. Hydrocarbons having more than four carbon atoms are not included. For pipeline natural gas, the presence of appreciable amounts of the higher hydrocarbons would be unusual.

TABLE I. - FUNCTIONS OF BENEDICT-WEBB-RUBIN COEFFICIENTS FOR NATURAL GAS COMPONENTS

Function	Methane	Ethane	Propane	Butane	2-Methyl propane	Nitrogen	Carbon dioxide
	Molecular weight, m						
	16.043	30.07	44.097	58.124	58.124	28.013	44.01
$(a_1 m^2)^{1/2}$	0.0774618	0.108631	0.148328	0.184396	0.184396	0.08660497	0.1264947
$(a_2 m)^{1/3}$.3492534	.3974298	.459968	.4991506	.5162001	.3577881	.3667953
$(a_3 m)^{1/2}$	4.754745	7.116558	9.140405	11.0863	11.16732	3.81227	5.79486
$(a_4 m)^{1/2}$	524.4702	1479.446	2488.837	3478.505	3218.478	267.9035	1273.766
$(a_5 m^2)^{1/3}$.1500773	.2232212	.2823162	.3419966	.3488057	.1256056	.1324808
$(a_6 m^2)^{1/3}$.8444029	1.614287	2.260465	2.841437	2.869004	.5662865	.926749
$(a_7 m^2)^{1/3}$	31.41978	73.64101	116.2798	156.8145	151.624	18.83293	53.5166
$(a_8 m^3)^{1/3}$.04991572	.0624375	.08454082	.1032721	.1024136	.06631022	.09234484

The coefficients for the hydrocarbons were calculated from the Benedict-Webb-Rubin coefficients tabulated in references 2 and 4. The nitrogen coefficients were calculated from the Benedict-Webb-Rubin coefficients tabulated in reference 5. Benedict-Webb-Rubin coefficients for carbon dioxide were calculated by a least-squares technique using the compressibility data in reference 6. From these, the coefficients for table I were calculated. The coefficients a_1 to a_8 are consistent with temperature in Kelvin and density in kilograms per cubic meter. Because of the use of these density units

rather than the molar density units used in references 2, 4, and 5, molecular weight is involved in the mixing equations (eqs. (4) to (11)), while molecular weight is not involved in the mixing equations given in reference 3. Computationally, equations (1) to (11) are equivalent to those given in references 2 to 4.

Ideal-Gas Specific Heat

The ideal-gas specific heat of a natural gas mixture is represented by

$$\frac{C_{v, \text{ideal}}}{R} = \beta_0 + \sum_{k=1}^7 \beta_k \left(\frac{T}{100}\right)^k \quad (12a)$$

The ideal-gas specific heat of the natural gas components is given by

$$\left(\frac{C_{v, \text{ideal}}}{R}\right)_i = \beta_{0, i} + \sum_{k=1}^7 \beta_{k, i} \left(\frac{T}{100}\right)^k \quad (12b)$$

(An "ideal gas" is defined as a gas that has an invariant compressibility factor whose value is 1. However, unlike a perfect gas, the specific heat varies with temperature. Real gases approach the ideal-gas condition as the pressure assumes lower and lower values, providing no dissociation takes place.)

For a natural-gas mixture, the ideal-gas specific heat can be expressed in terms of the ideal-gas specific heat of the components as follows:

$$\frac{C_{v, \text{ideal}}}{R} = \sum_{i=1}^7 x_i \left(\frac{C_{v, \text{ideal}}}{R}\right)_i \quad (13)$$

From this, it is evident that

$$\beta_k = \sum_{i=1}^7 x_i \beta_{k, i} \quad (14)$$

TABLE II. - COEFFICIENTS FOR IDEAL-GAS, SPECIFIC-HEAT EQUATION FOR COMPONENTS OF NATURAL GAS

Coefficient	Methane	Ethane	Propane	Butane	2-Methyl propane	Nitrogen	Carbon dioxide
β_0	2.79983	-9.85338	-16.7968	-1.0068	-3.06092	2.50115	2.50447
β_1	.4285	19.6577	29.0846	4.60962	6.08128	-9.72058×10^{-3}	-.508557
β_2	-.27518	-10.1866	-13.8109	-.235295	-.593889	1.03606×10^{-2}	.48403
β_3	2.58217×10^{-2}	1.82674	2.21984	4.87536×10^{-3}	1.34513×10^{-2}	-4.43726×10^{-3}	-3.73057×10^{-2}
β_4	2.41658×10^{-2}	.246368	.365514	0	1.07774×10^{-2}	6.8256×10^{-4}	-2.52264×10^{-2}
β_5	-2.51637×10^{-3}	-.120205	-.15326	↓	-1.31759×10^{-3}	0	6.14015×10^{-3}
β_6	-8.24658×10^{-4}	1.08075×10^{-2}	1.29667×10^{-2}	↓	0	0	-4.11664×10^{-4}
β_7	1.15233×10^{-4}	0	0	↓	0	0	0

The values of $\beta_{k,i}$ are presented in table II for the seven gases that comprise the components of natural gas. These values were obtained by a least-squares fit of tabulated data. These fits are valid for a temperature range of 200 to 400 K. The methane data are from reference 7. These data are the result of an analysis of spectroscopic data and agree with the data of the American Petroleum Institute (ref. 8) to within 1 percent. The ethane and propane data below 273 K are from reference 9. The ethane and propane data above 273 K are from reference 8, as are the butane and 2-methyl propane data. The nitrogen data are from reference 10 and the carbon dioxide data are from reference 6.

Saturated Vapor Pressure

The equation used to express the vapor pressure as a function of temperature is

$$\ln p_{\text{sat}} = b_0 + \sum_{k=1}^6 b_k \left(\frac{T}{100} \right)_{\text{sat}}^k \quad (15)$$

The coefficients for ethane, propane, and butane were determined by a least-squares fit of the data in reference 9. The coefficients for 2-methyl propane were determined by a least-squares fit of the data in reference 8, and the coefficients for carbon dioxide were determined by a least-squares fit of the data in reference 6. The vapor pressure of nitrogen and methane need not be considered since the temperatures considered in these routines are all above critical. Table III lists the coefficients involved in equation (15).

TABLE III. - COEFFICIENTS FOR EQUATION FOR SATURATED VAPOR
PRESSURE AS FUNCTION OF TEMPERATURE

Coefficient	Ethane	Propane	Butane	2-Methyl propane	Carbon dioxide
b ₀	-8.76886	-13.83014	-19.89223	-10.14642	-65.13333
b ₁	18.78746	16.45255	18.41968	8.17872	48.09596
b ₂	-5.205866	-.765418	-.787275	2.679815	30.296025
b ₃	.538879	-1.080231	-.980618	-.944109	-34.13448
b ₄	0	.0642219	-.0129045	-.275245	10.442646
b ₅	0	.0667237	.0766147	.128236	-1.071251
b ₆	0	-.0097026	-.0094861	-.0124255	0

In addition to equation (15), the routines require direct representation of temperature in terms of pressure; that is,

$$\left(\frac{T}{100}\right)_{\text{sat}} = c_0 + \sum_{k=1}^5 c_k (\ln p_{\text{sat}})^k \quad (16)$$

Table IV lists the coefficients for equation (16).

TABLE IV. - COEFFICIENTS FOR EQUATION FOR TEMPERATURE AS FUNCTION
OF SATURATED VAPOR PRESSURE

Coefficient	Ethane	Propane	Butane	2-Methyl propane	Carbon dioxide
c ₀	0.107196	0.729923	1.51144	-5.888696	7.571723
c ₁	.134425	9.58931×10 ⁻²	-4.29761×10 ⁻³	2.473601	-1.022272
c ₂	9.57502×10 ⁻³	6.82915×10 ⁻³	7.92127×10 ⁻³	-.291051	4.65321×10 ⁻²
c ₃	-1.26548×10 ⁻³	-4.18242×10 ⁻⁴	6.85975×10 ⁻⁴	1.49661×10 ⁻²	0
c ₄	2.14075×10 ⁻⁵	-3.12624×10 ⁻⁵	-1.14435×10 ⁻⁴	-2.41504×10 ⁻⁴	0
c ₅	2.33577×10 ⁻⁶	3.74086×10 ⁻⁶	5.80657×10 ⁻⁶	0	0

CALCULATION PROCEDURE

For these calculations, six functions of the compressibility factor are used:

$$Z_I(\rho, T) = Z = \frac{p}{\rho RT} \quad (17)$$

$$Z_{\text{II}}(\rho, T) = Z + T \left(\frac{\partial Z}{\partial T} \right)_{\rho} = \frac{1}{R\rho} \left(\frac{\partial p}{\partial T} \right)_{\rho} \quad (18)$$

$$Z_{\text{III}}(\rho, T) = Z + \rho \left(\frac{\partial Z}{\partial \rho} \right)_{T} = \frac{1}{RT} \left(\frac{\partial p}{\partial \rho} \right)_{T} \quad (19)$$

$$Z_{\text{IV}}(\rho, T) = \int_0^{\rho} (Z_{\text{II}} - 1) \frac{d\rho}{\rho} \quad (20)$$

$$Z_{\text{V}}(\rho, T) = \int_0^{\rho} (Z_{\text{II}} - Z_{\text{I}}) \frac{d\rho}{\rho} \quad (21)$$

$$Z_{\text{VI}}(\rho, T) = T \left(\frac{\partial Z_{\text{IV}}}{\partial T} \right)_{\rho} = \frac{C_{v, \text{ideal}} - C_v}{R} \quad (22)$$

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, two functions of the ideal-gas specific heat are used in these calculations. These are

$$\xi_{\text{I}}(T) = \int \frac{C_{v, \text{ideal}}}{R} \frac{dT}{T} = \beta_0 \ln \left(\frac{T}{100} \right) + \sum_{k=1}^7 \frac{\beta_k}{k} \left(\frac{T}{100} \right)^k + K_{\text{S}} \quad (23)$$

$$\xi_{\text{II}}(T) = \int \frac{C_{v, \text{ideal}}}{R} dT = 100 \left[\sum_{k=0}^7 \frac{\beta_k}{k+1} \left(\frac{T}{100} \right)^{k+1} \right] + K_{\text{H}} \quad (24)$$

In terms of ξ_{I} and ξ_{II} , the ideal-gas entropy and enthalpy are given by

$$\frac{S_{\text{ideal}}}{R} = \xi_{\text{I}}(T) - \ln \left(\frac{p}{RT} \right) \quad (25)$$

$$\frac{H_{\text{ideal}}}{R} = \xi_{\text{II}}(T) + T \quad (26)$$

TABLE V. - VALUE OF INTEGRATION CONSTANTS USED IN EQUATIONS (23) AND (24)

Component	Constant K_S	Constant K_H
Methane	-2.42592233	-794.255051
Ethane	-16.722706	-224.353146
Propane	-24.4685144	43.254680
Butane	-6.81234692	-859.768636
2-Methyl propane	-7.67222838	-656.575168
Nitrogen	-1.20430845	-699.709835
Carbon dioxide	-.54815092	-702.986595

The terms K_S and K_H in equations (23) and (24) are constants of integration for the indefinite temperature integrals in these equations. The constant K_S is chosen such that the ideal-gas entropy equals zero at a temperature of 200 K and a pressure of 1×10^5 newtons per square meter. The constant K_H is chosen such that the ideal-gas enthalpy equals zero at a temperature of 200 K. Table V lists the values of K_S and K_H for the components of natural gas. The values of K_S and K_H for natural gas mixtures are given by

$$K_S = \ln m + \sum_{i=1}^7 x_i (K_{S,i} - \ln m_i) \quad (27)$$

$$K_H = \sum_{i=1}^7 x_i K_{H,i} \quad (28)$$

In terms of these compressibility-factor and ideal-gas specific-heat functions, the following thermodynamic quantities can be expressed in terms of density and temperature:

$$\frac{S}{R} = \xi_I - \ln \rho - Z_{IV} \quad (29)$$

$$\frac{H}{R} = \xi_{II} + T(Z_I - Z_V) \quad (30)$$

$$\frac{C_p}{R} = \frac{C_{v,ideal}}{R} - Z_{VI} + \frac{Z_{II}^2}{Z_{III}} \quad (31)$$

$$\gamma = \frac{C_p}{C_v} = \frac{1}{Z_{III}} \left(Z_{III} + \frac{Z_{II}^2}{\frac{C_{v,ideal}}{R} - Z_{VI}} \right) \quad (32)$$

$$k = \frac{\rho}{p} \left(\frac{\partial p}{\partial \rho} \right)_S = \gamma \frac{\rho}{p} \left(\frac{\partial p}{\partial \rho} \right)_T = \gamma \times \frac{Z_{III}}{Z_I} \quad (33)$$

With minor modifications, equations (29) to (33) are from reference 11. The gas is assumed to flow from a plenum, where the gas is at rest, to the exit of the nozzle, where the gas velocity can either be subsonic or supersonic. This flow is assumed to be isentropic and one dimensional. The independent variables in the plenum are pressure and temperature. The independent variable at the nozzle exit can be either pressure, Mach number, or temperature. The first case to be considered is where the nozzle-exit independent variable is temperature.

Since the thermodynamic functions are in terms of density and temperature, it is first necessary to solve the following equation for the plenum density:

$$\rho_0 = \frac{p_0}{Z_0(\rho_0, T_0)RT_0} \quad (34)$$

Since ρ_0 is involved implicitly in equation (34), an iterative solution for ρ_0 is necessary. This solution is as follows:

First estimate of ρ_0 :

$$\rho_{0,1} = \frac{p_0}{RT_0} \quad (35)$$

Succeeding estimates:

$$\rho_{0,n} = \rho_{0,n-1} + \left(\frac{\partial \rho}{\partial p} \right)_T (p_0 - p_{0,n-1}) \quad (36)$$

where

$$\left(\frac{\partial \rho}{\partial f}\right)_T = \frac{1}{RT_0 \times Z_{III}(\rho_0, n-1, T_0)} \quad (37)$$

When $p_{0,n-1}$ and p_0 differ by less than 1 part per million, the computation is considered complete.

The condition that the flow is isentropic leads to the following equation:

$$\frac{S_0 - S_e}{R} = 0 = \xi_I(T_0) - \xi_I(T_e) - \ln \frac{\rho_0}{\rho_e} - Z_{IV}(\rho_0, T_0) + Z_{IV}(\rho_e, T_e) \quad (38)$$

Since this equation is implicit in ρ_e , an iterative solution for ρ_e is necessary. This solution is as follows:

First estimate of ρ_e :

$$\ln \rho_{e,1} = \ln \rho_0 - \xi_I(T_0) + \xi_I(T_e) \quad (39)$$

Succeeding estimates:

$$\ln \rho_{e,n} = \ln \rho_{e,n-1} + \left[\frac{\partial(\ln \rho_e)}{\partial \left(\frac{S_0 - S_e}{R}\right)} \right]_T \Delta \left(\frac{S_0 - S_e}{R}\right) \quad (40)$$

where

$$\left[\frac{\partial(\ln \rho_e)}{\partial \left(\frac{S_0 - S_e}{R}\right)} \right]_T = \frac{1}{Z_{II}(\rho_{e,n-1}, T_e)} \quad (41)$$

and

$$\Delta \left(\frac{S_0 - S_e}{R}\right) = S(\rho_{e,n-1}, T_e) - S(\rho_0, T_0) \quad (42)$$

When the S_e and S_0 differ by less than 1×10^{-6} , the computation is considered complete.

For physically valid solutions of ρ_0 and ρ_e , it is necessary that Z_I , Z_{II} , and Z_{III} be positive; that is, the density must be positive, the pressure must increase with temperature at constant density, and the pressure must increase with density at constant temperature. In addition, the partial pressure of each natural gas component has to be less than a constant times the saturation pressure of that component. The value of this constant is initially 1, but it can be set to other values under program control.

At this point, the thermodynamic states at both the plenum and the nozzle exit are defined. Again, because of equation (38), the plenum and nozzle-exit entropy are equal. In order to calculate the mass flow rate per unit area at the nozzle exit, the nozzle-exit velocity has to be determined. This can be calculated by means of the following equation:

$$V_e = \left\{ 2 \left[H(\rho_0, T_0) - H(\rho_e, T_e) \right] \right\}^{1/2} \quad (43)$$

The enthalpies in this equation are calculated from equation (30). The mass flow rate per unit area is then given by

$$G_e = \rho_e \times V_e \quad (44)$$

If it is desired to calculate the Mach number at the nozzle exit, the speed of sound at the nozzle exit has to be calculated. The equation for the speed of sound is

$$\alpha_e = \left[k(\rho_e, T_e) \times Z_I(\rho_e, T_e) \times R \times T_e \right]^{1/2} \quad (45)$$

Then the Mach number becomes

$$M_e = \frac{V_e}{\alpha_e} \quad (46)$$

Other quantities such as enthalpy, specific heat, and specific-heat ratio are calculated at both the plenum and nozzle exit by using equations (30), (31), and (33).

If the nozzle-exit independent variable is either pressure or Mach number, a nozzle-exit temperature has to be estimated such that the calculated nozzle-exit pressure or Mach number agrees with the prescribed nozzle-exit pressure or Mach number. To do this, a series of temperature estimates is usually required. Each estimate is used in

equations (39) to (42). This ensures that the flow is isentropic. The procedure for estimating the nozzle-exit temperature for these two cases is now described.

If the nozzle-exit pressure is the independent variable, the first estimate of the nozzle-exit temperature has to satisfy the following conditions:

$$T_{e,1} < T_0 \quad (47)$$

$$T_{e,1} > T_{\text{sat}} \quad (48)$$

Condition (48) holds for each and every component of the natural gas mixture. These conditions take precedence over the following equation for the first estimate of the nozzle-exit temperature:

$$T_{e,1} = T_0 \left(\frac{p_e}{p_0} \right)^{1/4} \quad (49)$$

Equation (49) is what would result if natural gas were perfect, with γ equal to 4/3. The second temperature estimate is given by

$$T_{e,2} = T_{e,1} + \left[\left(\frac{\partial T}{\partial p} \right)_S \right]_{\text{perf}} \times (p_e - p_{e,1}) \quad (50)$$

where

$$\left[\left(\frac{\partial T}{\partial p} \right)_S \right]_{\text{perf}} = \frac{1}{4} \frac{T_{e,1}}{p_{e,1}} \quad (51)$$

Equation (51) is based on a γ of 4/3. The other estimates are given by

$$T_{e,n} = T_{e,n-1} + \left(\frac{T_{e,n-1} - T_{e,n-2}}{p_{e,n-1} - p_{e,n-2}} \right) \times (p_e - p_{e,n-1}) \quad (52)$$

When the calculated nozzle-exit pressure agrees with the prescribed nozzle-exit pressure to within 1 part per million, the nozzle-exit temperature is considered to be determined.

If the nozzle-exit Mach number is the independent variable, the first estimate of the

nozzle-exit temperature has to satisfy conditions (47) and (48). These conditions take precedence over the following equation for the first nozzle-exit temperature estimate:

$$T_{e,1} = T_0 \left(1 - \frac{1}{6} M_{e,1}^2 \right)^{-1} \quad (53)$$

Equation (53) is what would result if natural gas were perfect with γ equal to 4/3. The second estimate is given by

$$T_{e,2} = T_{e,1} + \left[\left(\frac{\partial T}{\partial M} \right)_{e,1} \right]_{\text{perf}} \times (M_e - M_{e,1}) \quad (54)$$

where

$$\left[\left(\frac{\partial T}{\partial M} \right)_{e,1} \right]_{\text{perf}} = -\frac{1}{3} \left(\frac{T_{e,1}^2}{T_0} \right) \times M_e \quad (55)$$

Equation (55) is based on a γ of 4/3. The other estimates are given by

$$T_{e,n} = T_{e,n-1} + \left(\frac{T_{e,n-1} - T_{e,n-2}}{M_{e,n-1} - M_{e,n-2}} \right) \times (M_e - M_{e,n-1}) \quad (56)$$

When the calculated nozzle-exit Mach number agrees with the prescribed nozzle-exit Mach number to within 1 part in 10 thousand, the nozzle-exit temperature is considered to be determined.

RESULTS AND DISCUSSION

Using the equations and iterative procedures given in the previous section, a set of computer routines written in the FORTRAN IV version 13 language were developed to calculate the isentropic flow properties that would result from flow through a nozzle. A brief description of these routines follows. These routines are identified by their deck name. Routines whose names start with the letters "NG" depend on the nature of natural gas. The other routines are general and can be used for any real gas whose compressibility factor is a function of density and temperature.

Deck NGCOMP

This subroutine calculates composition-dependent constants required by the other routines. These constants are

- (1) Gas constant, R (eq. (2))
- (2) Molecular weight, m (eq. (3))
- (3) Benedict-Webb-Rubin coefficients a_1 to a_8 (eqs. (4) to (11))
- (4) Ideal-gas, specific-heat coefficients, β_0 to β_7 (eq. (14))
- (5) Integration constant for entropy, K_S (eq. (27))
- (6) Integration constant for enthalpy, K_H (eq. (28))

Deck RGASC

This is the subroutine that includes the iteration procedures necessary to calculate the isentropic mass flow rate of natural gas through a nozzle. These procedures are represented by equations (34) to (56). The procedures are general and would apply for most real gases whose compressibility factor is given as a function of density and temperature. Naturally, it is necessary to provide the other routines with the appropriate basic equations. In other words, as far as this particular subroutine is concerned, it could be used for other gases. In addition to the mass flow rate per unit area, the output of this subroutine includes entropy, enthalpy, specific heat, and compressibility factor.

Deck RDATA

This is a block data subprogram that supplies constants that mainly have to do with the convergence limits of the various iteration procedures in RGASC. These constants do not depend on the nature of the gas.

Deck NGZETA

The compressibility-factor functions Z_I to Z_{VI} , as defined by equations (17) to (22), are calculated in this subroutine.

Deck NGTEMP

The nondimensional ideal-gas specific heat ($C_{v, \text{ideal}}/R$) and the related functions ξ_I and ξ_{II} , as given by equations (12a), (23), and (24), are calculated in this routine.

Deck NGLOG

This is a logical function that tests whether the pressure and temperature lie within the range of the state equation (eq. (1)) and within the range of the ideal-gas, specific-heat equation (eq. (12a)). In addition, this routine also tests whether all the natural gas components are in the gaseous state.

Deck NGTLG

This routine, if necessary, will change the temperature such that it is above the condensation temperature of each and every natural gas component.

Deck NGDATA

This is a block data subprogram that supplies constants for the other routines. These constants depend on the nature of the gas.

This set of routines requires 2137 storage locations, not including the library routines. The execution time for a typical case on an IBM 7094-7044 direct couple computer is of the order of 0.04 second.

In appendix B, the rules for using these routines are described; and, in addition, the input and output computer variables are defined. The card listing of these routines is given in appendix C.

As an example of the results obtainable by these routines, two figures are presented. These figures apply to a typical natural gas mixture. The mole fraction of the components of this mixture are 0.9272 methane, 0.0361 ethane, 0.0055 propane, 0.001 butane, 0.0007 2-methyl propane, 0.0218 nitrogen, and 0.0077 carbon dioxide. Figure 1 illustrates the mass flow rate deviation from perfect-gas behavior. In order to compress the scale of the ordinate, the ratio of real-gas to perfect-gas mass flow rate per unit area is multiplied by the square root of the plenum compressibility factor. This assures that the value of this expression approaches 1 as the pressure drop across the nozzle approaches zero. This occurrence is independent of plenum pressure and temperature.

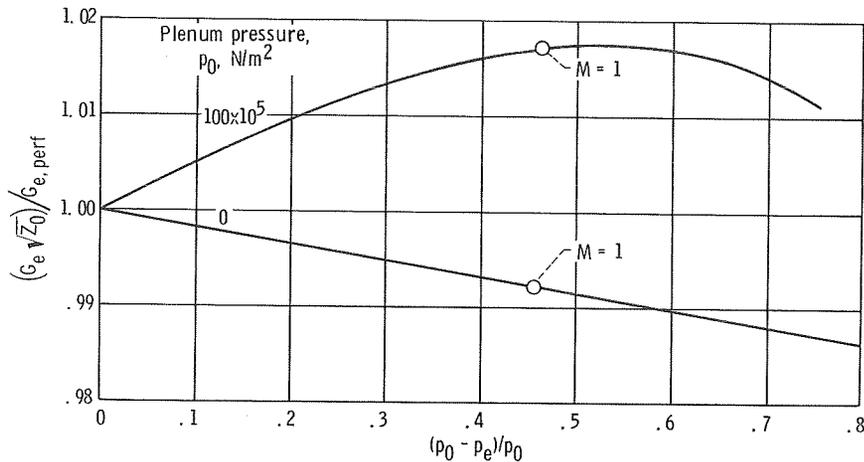


Figure 1. - Mass-flow-rate deviation from perfect-gas behavior for a natural gas mixture. Plenum temperature, 300 K.

The expression for the perfect-gas mass flow rate per unit area is as follows:

$$G_{e, \text{perf}} = \frac{p_0}{\sqrt{RT_0}} \left\{ \delta \left(\frac{p_e}{p_0} \right)^{3/2} \left[1 - \left(\frac{p_e}{p_0} \right)^{1/4} \right] \right\}^{1/2} \quad (57)$$

Equation (57) assumes a γ of 4/3. Even at a pressure level of zero, where the compressibility factor is 1; the mass flow ratio is not constant. The reason for this is that as the nozzle-exit pressure is reduced, the gas speeds up and its temperature drops. This drop in temperature causes the ideal-gas specific heat to vary. This is not perfect-gas behavior and equation (57) does not apply. At a plenum pressure of 100×10^5 newtons per square meter, the gas is neither perfect nor ideal. The value of the plenum compressibility factor under these conditions is 0.8366. So, while the ordinate of figure 1 is 1.017 at a Mach number of 1, the actual mass flow rate ratio $G_e / G_{e, \text{perf}}$ is equal to 1.112.

In figure 2, two quantities are plotted. One is the specific-heat ratio, and the other is the isentropic exponent as defined by equation (33). At very low pressures these quantities are equal to each other. At the higher pressures they are not equal, but differ by as much as 12 percent. This illustrates that, for this case, errors of as much as 6 percent would be involved if the specific-heat ratio rather than the isentropic exponent were used to calculate the speed of sound.

It should be pointed out that although these routines calculate thermodynamic functions that, for the most part, are more accurate than the functions that would be calculated using the perfect-gas assumption, errors are still present. The principal sources

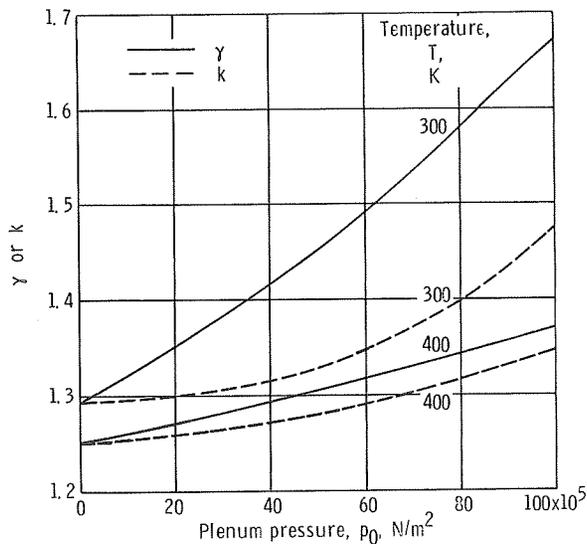


Figure 2. - Specific-heat ratio γ and isentropic exponent k as function of plenum pressure for a natural gas mixture.

of these errors are inaccuracies in the Benedict-Webb-Rubin state equation. Some estimate of these errors can be made for the case of pure methane. Reference 12 presents a state equation for pure methane that is probably accurate to within 0.1 percent over the range of pressures and temperatures covered by the routines in this report. Using this state equation, the compressibility factor, the specific heat, and the critical mass flow rate were calculated. The details of these calculations are beyond the scope of this report. A comparison of the highly accurate values obtained by the state equation in reference 12 with the values obtained by the Benedict-Webb-Rubin state equation used in this report is shown in table VI. Except for the low-temperature region, the compressibility factors differ by less than 0.5 percent. The specific heats differ by as much as 12 percent at a pressure of 50×10^5 newtons per square meter and a temperature of 200 K. However, for most of the range, the deviation is under 1 percent. The mass-flow-rate deviation seems to be under 1 percent over the permissible range of the calculations. It should be pointed out that these comparisons do not apply exactly for natural gas mixtures. However, since natural gas consists primarily of methane, these comparisons should still apply approximately.

TABLE VI. - COMPARISON OF THERMODYNAMIC FUNCTIONS FOR METHANE CALCULATED BY EQUATION (1) WITH THESE SAME FUNCTIONS CALCULATED BY THE STATE EQUATION IN REFERENCE 12^a

Plenum station temperature, T_0 , K	Plenum station pressure, P_0 , N/m ²	Compressibility factor		$\frac{Z_0 - Z_0^*}{Z_0^*}$	Ratio of specific heat to gas constant		$\frac{C_p - C_p^*}{C_p^*}$	Mass-flow-rate ratio at Mach 1		$\frac{G - G^*}{G^*}$
		Z_0	Z_0^*		$C_{p,0}/R$	$C_{p,0}^*/R$		$\frac{G}{G_{\text{perf}}}$	$\frac{G^*}{G_{\text{perf}}}$	
		200	50×10 ⁵ 100	0.560 .367	0.549 .362	0.020 .014	12.82 10.50	14.66 10.54	-0.126 -.004	Conditions at the nozzle exit are such that condensation could occur.
250	50×10 ⁵ 100	0.836 .689	0.835 .686	0.001 .004	5.51 7.97	5.39 7.94	0.022 .004	1.095 1.262	1.098 1.273	-0.003 -.009
300	50×10 ⁵ 100	0.918 .854	0.919 .855	-0.001 -.001	4.96 5.79	4.93 5.75	0.006 .007	1.042 1.103	1.047 1.110	-0.005 -.006
350	50×10 ⁵ 100	0.957 .928	0.958 .930	-0.001 -.002	4.96 5.39	4.97 5.41	-0.002 -.004	1.017 1.048	1.020 1.050	-0.003 -.002
400	50×10 ⁵ 100	0.978 .966	0.980 .970	-0.002 -.004	5.14 5.41	5.16 5.45	-0.004 -.007	1.000 1.018	1.000 1.020	0 -.002

^aThe asterisk denotes the quantity obtained by using the state equation in ref. 12.

CONCLUDING REMARKS

A set of computer routines are presented that provide a means of calculating the one-dimensional, isentropic mass flow rate of natural gas through a nozzle, and also such thermodynamic functions as the compressibility factor, specific heat, entropy, and enthalpy. The results indicate that the inaccuracy of these calculations is less than 1 percent over most of the permissible pressure and temperature range.

The design of the routines is such that it is easy to modify them for other gases.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, January 15, 1971,
720-03.

APPENDIX A

SYMBOLS

a_1, a_2, \dots, a_8	coefficients for the Benedict-Webb-Rubin state equation (eq. (1))
b_0, b_1, \dots, b_6	coefficients for saturation-pressure-against-temperature equation (eq. (15))
C_p	specific heat at constant pressure, $m^2/(\text{sec}^2)(K)$
C_v	specific heat at constant volume, $m^2/(\text{sec}^2)(K)$
c_0, c_1, \dots, c_5	coefficients for saturation-temperature-against-pressure equation (eq. (16))
G	mass flow rate per unit area, $kg/(m^2)(\text{sec})$
H	enthalpy, m^2/sec^2
K_H	constant of integration involved in equation (24), K
K_S	constant of integration involved in equation (23)
M	Mach number
m	molecular weight
N	number of components in natural gas mixture
p	pressure, N/m^2
p_{sat}	minimum pressure at which condensation takes place at a given temperature, N/m^2
R	gas constant, $m^2/(\text{sec}^2)(K)$
S	entropy, $m^2/(\text{sec}^2)(K)$
T	temperature, K
T_{sat}	maximum temperature at which condensation takes place for a given pressure; K
V	velocity, m/sec
x	mole fraction of a natural gas component
Z	compressibility factor
$Z_I, Z_{II}, \dots, Z_{VI}$	functions of the compressibility factor as defined by equations (17) to (22)
α	speed of sound, m/sec

$\beta_0, \beta_1, \dots, \beta_7$	coefficients for ideal-gas, specific-heat equation (eq. (12a))
γ	specific-heat ratio
ξ_I, ξ_{II}	functions of ideal-gas specific heat as defined by equations (23) and (24)
ρ	density, kg/m^3
Subscripts:	
e	nozzle-exit station
i	species
ideal	ideal gas
j	species
k	running index
n	n^{th} estimate in iteration procedure
perf	perfect gas
0	plenum station

APPENDIX B

DESCRIPTION OF NATURAL GAS ROUTINES

Since natural gas is a gas mixture whose composition is not fixed, the first subroutine that is referenced is one that calculates a set of composition-dependent constants for use in the other routines. For a given composition, this only has to be called once in a given run. The following statement references this routine:

```
CALL BDATA(X)
```

The subroutine used to calculate the thermodynamic properties of natural gas is referenced by the following statement.

```
CALL RGAS (KK, PA, TA, AM, PB, TB, FLOW, KODE)
```

For a valid computation, the following conditions have to be satisfied:

(1) $199 \text{ K} < T < 401 \text{ K}$

(2) $0.1 \text{ N/m}^2 \leq p \leq 101 \times 10^5 \text{ N/m}^2$

(3) The partial pressure of any component has to be less than a constant times the saturation pressure. Unless specified otherwise, this constant will have the value of 1.

Some of the variables in these programs are entered or returned through labeled common. Therefore, the following common statements should be in the main program.

```
COMMON/LDATA/XKV, R, XMW
```

```
COMMON/LIMIT/EDA, EDB, ETP, ETM
```

```
COMMON/OUTPUT/OUT(9), CONV(4), ZA(6), ZB(6), KOD1(5)
```

The following symbols apply to these routines:

- X This is a seven-element array. The elements in this array are proportional to the mole fraction of the natural gas components. The order in which the gases appear are as follows: (1) methane, (2) ethane, (3) propane, (4) butane, (5) 2-methyl propane, (6) nitrogen, and (7) carbon dioxide.
- KK Controls entry to, and exit from, the subroutine. If $KK = 0$, just the plenum properties are calculated. If $KK = 2$, both the plenum and the nozzle-exit properties are calculated. If $KK = 1$, just the nozzle-exit properties are calculated. For a given set of plenum conditions, at least one reference has to be made for $KK = 0$ or $KK = 2$ before a reference can be made for $KK = 1$.
- PA Plenum pressure, p_0 , N/m^2

TA	Plenum temperature, T_0 , K
AM	Nozzle-exit Mach number, M_e
PB	Nozzle-exit pressure, p_e , N/m^2
TB	Nozzle-exit temperature, T_e , K
FLOW	Nozzle-exit mass flow rate per unit area, G_e , $kg/(m^2)(sec)$
KODE	Indicates the independent variables to the subroutine. If KODE = 1, these variables are PA, TA, and PB. If KODE = 2, these variables are PA, TA, and AM. If KODE = 3, these variables are PA, TA, and TB.
XKV	Constant referred to in condition (3). Unless specified otherwise, the value of this constant is 1.
R	Gas constant, R , $m^2/(sec^2)(K)$
XMW	Molecular weight, m
EDA	Maximum fractional difference permitted between calculated plenum pressure and prescribed plenum pressure. Unless otherwise specified, EDA equals 1×10^{-6} .
EDB	Maximum difference permitted between the nozzle-exit entropy and the plenum entropy. Unless otherwise specified, EDB equals 1×10^{-6} .
ETP	This is pertinent when the nozzle-exit independent variable is pressure, and represents the maximum fractional difference permitted between the calculated nozzle-exit pressure and the prescribed nozzle-exit pressure. Unless otherwise specified, ETP equals 1×10^{-6} .
ETM	This is pertinent when the nozzle-exit independent variable is Mach number, and represents the maximum fractional difference permitted between the calculated nozzle-exit Mach number and the prescribed nozzle-exit Mach number. Unless otherwise specified, ETM equals 1×10^{-4} .
OUT(1)	Actual mass flow rate G_e divided by the perfect-gas mass flow rate $G_{e,perf}$. The perfect-gas mass flow rate is defined as follows:

$$G_{e,perf} = \frac{p_0}{\sqrt{RT_0}} \left\{ 8 \left(\frac{p_e}{p_0} \right)^{3/2} \left[1 - \left(\frac{p_e}{p_0} \right)^{1/4} \right] \right\}^{1/2} \quad \text{for } M_e \neq 1 \quad (57)$$

$$G_{e,perf} = 0.6732 \frac{p_0}{\sqrt{RT_0}} \quad \text{for } M = 1 \quad (B1)$$

- OUT(2) Nozzle-exit specific heat, $C_{p,e}/R$
- OUT(3) Nozzle-exit specific-heat ratio, γ_e
- OUT(4) Nozzle-exit isentropic exponent, k_e
- OUT(5) Plenum enthalpy, H_0/R , K
- OUT(6) Plenum entropy, S_0/R
- OUT(7) Plenum specific heat, $C_{p,0}/R$
- OUT(8) Plenum specific-heat ratio, γ_0
- OUT(9) Plenum isentropic exponent, k_0
- CONV(1) Plenum pressure as calculated by the plenum density. This pressure should equal PA.
- CONV(2) For KODE = 1, this is the nozzle-exit pressure as calculated from the nozzle-exit density. This pressure should equal PB. For KODE = 2, this is the nozzle-exit Mach number as calculated from the nozzle-exit velocity and speed of sound. CONV(2) should equal AM. For KODE = 3, CONV(2) is equal to zero.
- CONV(3) Indicates the degree of convergence achieved in calculating the plenum density

$$\text{CONV(3)} = 1 - \frac{p_0}{Z_0 \rho_0 R T_0}$$

- CONV(4) Indicates the degree to which the nozzle-exit entropy equals the plenum entropy.

$$\text{CONV(4)} = S_e - S_0$$

- ZA(1) $Z_I(\rho_0, T_0)$
- ZA(2) $Z_{II}(\rho_0, T_0)$
- ZA(3) $Z_{III}(\rho_0, T_0)$
- ZA(4) $Z_{IV}(\rho_0, T_0)$
- ZA(5) $Z_V(\rho_0, T_0)$
- ZA(6) $Z_{VI}(\rho_0, T_0)$
- ZB(1) $Z_I(\rho_e, T_e)$

ZB(2)	$Z_{II}(\rho_e, T_e)$
ZB(3)	$Z_{III}(\rho_e, T_e)$
ZB(4)	$Z_{IV}(\rho_e, T_e)$
ZB(5)	$Z_V(\rho_e, T_e)$
ZB(6)	$Z_{VI}(\rho_e, T_e)$

The following symbols represent integers that are used to indicate if the calculation is valid. If all the integers are zero, a valid calculation has been performed. If these are not zero, the conditions are as follows:

- KOD1(1) Equals 1 if the plenum conditions are out of range in either pressure or temperature. A value of 1 terminates the calculation.
- KOD1(2) Equals 1 if the nozzle-exit conditions are out of range in either pressure or temperature. A value of 1 terminates the calculation.
- KOD1(3) If $KODE = 1$, this quantity equals 1 if the nozzle-exit pressure fails to converge to the prescribed nozzle-exit pressure. If $KODE = 2$, this quantity equals 1 if the nozzle-exit Mach number fails to converge to the prescribed nozzle-exit Mach number.
- KOD1(4) Equals 1 if the iteration procedure for the calculation of the plenum density fails to converge.
- KOD1(5) Equals 1 if the iteration procedure for the calculation of the nozzle-exit density fails to converge.

APPENDIX C

CARD LISTING OF NATURAL GAS COMPUTER PROGRAM

SRBFTC NGCOMP

C
 C THE FOLLOWING SUBROUTINE CALCULATES THE COMPOSITION DEPENDENT
 C CONSTANTS THAT ARE USED BY THE OTHER ROUTINES. THIS SUBROUTINE HAS
 C TO BE CALLED BEFORE A CALL TO RGAS CAN BE MADE.
 C

```

SUBROUTINE BDATA (X)
  DIMENSION X(7), MOL(7), XMOL(7), S(7), H(7), BE(8), BWR(8,7), CP(8
1,7)
  COMMON /LDATA/ XKV,R,MW
  COMMON /GDATA/ RC,D2,GAMA,GAMB,GAMC,GAMD,GAME
  COMMON /PDATA/ F(7)/ZDATA/Z(8)/TDATA/A(8),HI,SI
  REAL MOL,MW,MW2
  EQUIVALENCE (A(1),BE(1))
  DATA MOL,XMOL/16.043,39.07,44.097,2*58.124,28.013,44.01,2.77527262
1,3.403528,3.78639175,2*4.06264748,3.33266869,3.78441688/
  DATA S,H/-2.42592233,-16.722706,-24.4685144,-6.81234692,-7.6722283
18,-1.20430845,-0.54815092,-794.255051,-224.353146,43.25468,-859.76
28636,-656.575166,-699.709835,-702.986595/
  DATA CP/2.7998255,4.284998E-1,-2.751805E-1,2.5821711E-2,2.4165792E
1-2,-2.5163737E-3,-8.2465805E-4,1.1523272E-4,-9.8533835,19.657673,-
210.186582,1.8267443,0.2463681,-0.1252048,1.0807487E-2,0.0,-16.7968
307,29.084569,-13.810883,2.2198327,0.3655141,-0.1532602,1.296668E-2
4,0.0,-1.0067996,4.609619,-0.2352952,4.8753558E-3,4*0.0,-3.0609193,
56.0812842,-0.5938891,1.345131E-2,1.077738E-2,-1.3175933E-3,2*0.0,2
6.501145,-9.720581E-3,1.036056E-2,-4.437258E-3,6.825596E-4,3*0.0,2.
75044684,-0.5085567,0.4840302,-3.730571E-2,-2.522643E-2,6.1401476E-
83,-4.1166357E-4,0.0/
  DATA BWR/.0774618,.3492534,4.754745,524.4702,.1500773,.8444029,31.
141978,.04991572,.108631,.3974298,7.116558,1479.446,.2232212,1.6142
287,73.64101,.0624375,.148328,.459968,9.140405,2488.837,.2823162,2.
3260465,116.2798,.08454082,.184396,.4991506,11.0863,3478.505,.34199
466,2.841437,156.8145,.1032721,.184396,.5162001,11.16732,3218.478,.
53488057,2.369004,151.624,.1024136,.08660497,.3577881,3.81227,267.9
6035,.1256056,.5662865,18.83293,.06631022,.1264947,.3667953,5.79486
7,1273.766,.1324808,.926749,53.5166,.09234484/
  XX=0.0
  DO 1 N=1,7
1  XX=XX+X(N)
  DO 2 N=1,7
  BE(N)=0.0
2  F(N)=X(N)/XX
  BE(8)=0.0
  SI=0.0
  HI=0.0
  MW=0.0
  DO 3 N=1,7
  SI=SI+F(N)*(S(N)-XMOL(N))
  HI=HI+F(N)*H(N)
  MW=MW+F(N)*MOL(N)
  BE(1)=BE(1)+F(N)*BWR(1,N)
  
```

```

DO 3 I=3,8
3 BE(I)=BE(I)+F(N)*BWR(I,N)
SI=SI+ALOG(MW)
DO 4 N=1,7
DO 4 M=1,7
4 BE(2)=BE(2)+F(N)*F(M)*(BWR(2,N)+BWR(2,M))*3
MW2=MW**2
Z(1)=-BE(1)**2/MW2
Z(2)=BE(2)/(8.0*MW)
Z(3)=-BE(3)**2/MW
Z(4)=-BE(4)**2/MW
Z(5)=BE(5)**3/MW2
Z(6)=-BE(6)**3/MW2
Z(7)=(BE(6)*BE(8))**3/(MW*MW2**2)
Z(8)=BE(7)**3/MW2
DO 5 N=1,8
A(N)=0.0
DO 5 M=1,7
5 A(N)=A(N)+F(M)*CP(N,M)
R=8314.41/MW
RC=5.45105E-5*MW
RETURN
END

```

\$IBFTC RGASC

C
C THE THERMODYNAMIC PROPERTIES OF A NON IDEAL GAS ARE CALCULATED IN
C THIS SUBROUTINE.
C

```

SUBROUTINE RGAS (KK,PAA,TAA,AMM,PBB,TBB,FLOW,KO)
COMMON /OUTPUT/ OUT(9),CONV(4),ZA(6),ZB(6),KOD1(5)
COMMON /LDATA/ XKV,R,XMW
COMMON /LIMIT/ EDA,EDB,ETP,ETM
COMMON/GDATA/RC,D2,GAMA,GAMB,GAMC,GAMD,GAME,GAMF
DOUBLE PRECISION CP,CS,CH,CHA,CSA,CSB,CAB,LRHUA,LRHOB,DZA,DZB
LOGICAL LGFN
PA=PAA
TA=TAA
KKK=KK
KODE=KO
GO TO (1,2,3),KODE
1 PB=PBB
GO TO 4
2 AM=AMM
GO TO 4
3 TB=TBB
4 IF (KKK.EQ.1) GO TO 17
DO 5 N=1,3
ZA(N)=1.0
5 ZB(N)=1.0
DO 6 N=4,6
ZA(N)=0.0
6 ZB(N)=0.0
DO 7 N=1,5

```

```

7   KOD1(N)=0
   DO 8 N=1,9
8   OUT(N)=C.0
   DO 9 N=1,4
9   CONV(N)=0.0
   IF (LGFN(PA,TA,KOD1(1),ZA)) RETURN

```

```

C
C THE ITERATION PROCESS FOR CALCULATING THE PLENUM DENSITY FOLLOWS.
C

```

```

   A=PA/(R*TA)
   RHOA=A
   KN=0
10  DO 13 MM=1,50
   CALL ZETA (1,RHOA,TA,ZA)
   IF (ZA(3).LE.0.0) GO TO 14
   CONV(3)=1.0-(PA/RHOA)/(ZA(1)*R*TA)
   IF (ABS(CONV(3)).LT.EDA) GO TO 16
   AAA=(ZA(1)-A/RHOA)/ZA(3)
11  IF (1.0-AAA) 12,12,13
12  AAA=AAA/2.0
   GO TO 11
13  RHOA=RHOA*(1.0-AAA)
14  IF (KN.EQ.1) GO TO 15
   RHOA=D2*A
   KN=1
   GO TO 10
15  KOD1(4)=1
16  CALL ZETA (3,RHOA,TA,ZA)
   IF (LGFN(PA,TA,KOD1(1),ZA)) RETURN

```

```

C
C THE PLENUM THERMODYNAMIC FUNCTIONS ARE CALCULATED BY THE FOLLOWING
C STATEMENTS.
C

```

```

   CV=CP(TA)-ZA(6)
   GA=ZA(3)+ZA(2)**2/CV
   OUT(8)=GA/ZA(3)
   OUT(9)=GA/ZA(1)
   OUT(7)=CV*OUT(8)
   CHA=CH(TA)+DBLE(TA*(ZA(1)-ZA(5)))
   CUT(5)=CHA
   CSA=CS(TA)
   LRHOA=DLOG(DBLE(RHOA))
   DZA=DBLE(ZA(4))
   OUT(6)=CSA-LRHOA-DZA
   CONV(1)=ZA(1)*TA*R*RHOA

```

```

C
   IF (KKK.EQ.0) RETURN
17  GO TO (18,19,20),KODE
18  AM=0.0
C

```

```

C THE INITIAL ESTIMATE OF THE NOZZLE EXIT TEMPERATURE WHEN THE NOZZLE
C EXIT PRESSURE IS GIVEN IS MADE BY THE FOLLOWING STATEMENTS.
C

```

```

   TB=TA*(PB/PA)**GAMA
   GO TO 21
C

```

```

C THE INITIAL ESTIMATE OF THE NOZZLE EXIT TEMPERATURE WHEN THE NOZZLE
C EXIT MACH NUMBER IS GIVEN IS MADE BY THE FOLLOWING STATEMENTS.
C

```

```

19  TRAT=1.0+GAMB*AN**2
    PB=PA/TRAT**GAMF
    TB=TA/TRAT
C
    GO TO 21
20  PB=PA*(TB/TA)**GAMF
    GO TO 22
21  CALL TLOGIC (PB,TB)
22  IF (TB.LT.TA.AND.PB.LT.PA) GO TO 23
    KOD1(2)=1
    RETURN
23  TB1=TB
    KOD1(3)=0
    AN=1
    DO 24 N=1,4
24  OUT(N)=0.0
    CONV(2)=0.0
    CONV(4)=0.0
    DO 25 N=1,3
25  ZB(N)=1.0
    FLOW=0.0
    DO 26 N=4,6
26  ZB(N)=0.0
27  KOD1(5)=0
    IF (NN.EQ.1) GO TO 28
    IF (LGFN(PB,TB,KOD1(2),ZB)) RETURN
C
C  THE ITERATION PROCESS FOR CALCULATING THE NOZZLE EXIT DENSITY
C  FOLLOWS.
C
28  CSB=CS(TB)
    CAB=CSB-CSA+LRHOA+DZA
    LRHOB=LRHOA+CSB-CSA
    DO 29 M=1,50
    RHOB=DEXP(LRHOB)
    CALL ZETA (2,RHOB,TB,ZB)
    DZB=DBLE(ZB(4))
    CONV(4)=CAB-DZB-LRHOB
    IF (ABS(CONV(4)).LT.EDB) GO TO 30
29  LRHOB=LRHOB+CONV(4)/ZB(2)
    KOD1(5)=1
30  IF (RHOA-RHOB) 31,31,32
31  KOD1(2)=1
    RETURN
32  CALL ZETA (3,RHOB,TB,ZB)
C
C  THE THERMODYNAMIC FUNCTIONS AT THE NOZZLE EXIT CONDITIONS ARE
C  CALCULATED BY THE FOLLOWING STATEMENTS.
C
    VV=2.0DD*(CHA-CH(TB)-DBLL(TB*(ZB(1)-ZB(5))))
    CV=CP(TB)-ZB(6)
    GA=ZB(3)+ZB(2)**2/CV
    OUT(4)=GA/ZB(1)
C
    GO TO (33,37,41),KODE
33  AM=ASQRT(VV/(ZB(1)*OUT(4)*TB))
    IF (NN.NE.1) B1=CONV(2)
    CONV(2)=RHOB*ZB(1)*R*TB
    PERR=PB/CONV(2)-1.0

```

```
IF (ABS(PERR).LT.ETP) GO TO 42
IF (NN.GT.20) GO TO 36
NN=NN+1
```

```
C
C THE SUCCEEDING ESTIMATES OF THE NOZZLE EXIT TEMPERATURE ARE MADE
C BY THE FOLLOWING STATEMENTS FOR THE CASE OF A GIVEN NOZZLE EXIT
C PRESSURE.
```

```
C
34 IF (NN-2) 35,34,35
   TB=TB*(1.0+GAMA*PERR)
   IF (TB.GE.TA) TB=0.999*TA
   TB2=TB
   GO TO 27
35 TB=TB+(TB2-TB1)*(PB-CONV(2))/(CONV(2)-B1)
   TB1=TB2
   TB2=TB
   GO TO 27
```

```
C
36 KOD1(3)=1
   GO TO 42
37 PB=ZB(1)*TB*R*RHOB
   IF (NN.NE.1) B1=CONV(2)
   CONV(2)=ASQRT(VV/(ZB(1)*TB*OUT(4)))
   IF (ABS(1.0-CONV(2)/AM).LT.ETM) GO TO 42
   IF (NN.GT.20) GO TO 40
   NN=NN+1
```

```
C
C THE SUCCEEDING ESTIMATES OF THE NOZZLE EXIT TEMPERATURE ARE MADE
C BY THE FOLLOWING STATEMENTS FOR THE CASE OF A GIVEN NOZZLE EXIT
C MACH NUMBER.
```

```
C
38 IF (NN-2) 39,38,39
   TB=TB*(1.0-GAMD*TB*AM*(AM-CONV(2))/TA)
   IF (TB.GE.TA) TB=0.999*TA
   TB2=TB
   GO TO 27
39 TB=TB+(TB2-TB1)*(AM-CONV(2))/(CONV(2)-B1)
   TB1=TB2
   TB2=TB
   GO TO 27
```

```
C
40 KOD1(3)=1
   GO TO 42
41 AM=ASQRT(VV/(ZB(1)*OUT(4)*TB))
   PB=ZB(1)*R*RHGB*TB
   CONV(2)=0.0
42 IF (LSFN(PB,TB,KOD1(2),ZB)) RETURN
   IF (VV.GT.0.0) GO TO 43
   KOD1(2)=1
   RETURN
```

```
C
C THE ISENTROPIC FLOW PROPERTIES ARE CALCULATED BY THE FOLLOWING
C STATEMENTS.
```

```
C
43 FLOW=PB*SQRT(VV/R)/(ZB(1)*TB)
   OUT(3)=GA/ZB(3)
   OUT(2)=CV*OUT(3)
   TBF=(PB/PA)**GAMA
   IF ((AM.EQ.1.0).AND.(KODE.EQ.2)) GO TO 44
```

```

FLOWI=PA*SQRT(GAME*(PB/PA)**GAMC*(1.0-TBF)/(R*TA))
GO TO 45
44 FLOWI=PA*SQRT(RC/TA)
45 OUT(1)=FLOW/FLOWI
C
GO TO (46,47,48),KODE
46 AMM=AM
TBR=TB
RETURN
47 PBB=PB
TBB=TB
RETURN
48 AMM=AM
PBB=PB
RETURN
END

```

\$IBFTC RDATA

```

BLOCK DATA
COMMON /LDATA/ XKV,R,XMW
COMMON /LIMIT/ FDA,EDB,ETP,ETM
DATA XKV,EDA,EDS,ETP,ETM/1.0,3*1.0E-6,1.0E-4/
END

```

\$IBFTC NGZETA

```

C
C THE FUNCTIONS OF THE COMPRESSIBILITY FACTOR ARE CALCULATED IN THE
C FOLLOWING SUBROUTINE.
C

```

```

SUBROUTINE ZETA (KK,PA,TA,Z)
COMMON /ZDATA/ A,B1,B2,B3,B4,B5,B6,B7
DIMENSION Z(6)
K=KK
P=PA
T=TA
T3=T**3
B7T3=B7/T3
P2=P*P
P4=P2*P2
P5=P4*P
AP2=A*P2
PEXP=EXP(AP2)
IF (K.EQ.2) GO TO 1
BT1=(B1+B2/T+B3/T3)*P
BT2=(B4+B5/T)*P2
BT5=B6*P5/T
ZA=1.0+BT1+BT2+BT5
ZB=B7T3*P2*(1.0-AP2)*PEXP
Z(1)=ZA+ZB

```

```

ZA=1.0+2.0*BT1+3.0*BT2+6.0*BT5
ZB=B7T3*P2*PEXP*(3.0*(1.0-AP2)-2.0*AP2**2)
Z(3)=ZA+ZB
IF (K.EQ.1) RETURN
1 BT1=(B1-2.0*B3/T3)*P
BT2=B4*P2
ZA=1.0+BT1+BT2
ZB=-2.0*B7T3*P2*PEXP*(1.0-AP2)
Z(2)=ZA+ZB
ZA=BT1+BT2/2.0
ZB=-B7T3*(2.0*(PEXP-1.0)/A-P2*PEXP)
Z(4)=ZA+ZB
IF (K.EQ.2) RETURN
ZA=-(B2/T+3.0*B3/T3)*P-0.5*B5*P2/T-0.2*B6*P5/T
ZB=1.5*ZB
Z(5)=ZA+ZB
ZA=6.0*B3*P/T3
ZB=-2.0*ZB
Z(6)=ZA+ZB
RETURN
END

```

\$IBFTC NGTEMP

C
C THE IDEAL GAS SPECIFIC HEAT AND FUNCTIONS OF THE IDEAL GAS SPECIFIC
C HEAT ARE CALCULATED BY THE FOLLOWING ROUTINE.
C

```

DOUBLE PRECISION FUNCTION CP(T)
COMMON /TDATA/ A(8),HT,SI
DOUBLE PRECISION S,XN,CS,CH
K=1
1 S=T/100.000
GO TO (2,4,6),K
2 CP=A(8)
DO 3 N=1,7
NN=8-N
3 CP=CP*S+A(NN)
RETURN
ENTRY CS(T)
K=2
GO TO 1
4 CP=A(8)/7.0
DO 5 N=1,6
NN=8-N
XN=7-N
5 CP=CP*S+A(NN)/XN
CP=CP*S+A(1)*ALOG(S)+SI
RETURN
ENTRY CH(T)
K=3
GO TO 1
6 CP=A(8)/8.0
DO 7 N=1,7
NN=8-N
XN=NN

```

```

7 CP=CP*S+A(NN)/XN
  CP=CP*T+HI
  RETURN
  END

```

\$IBFTC NGLOG

```

C
C THE FOLLOWING FUNCTION IS USED TO DETERMINE WHETHER OR NOT THE FLUID
C COMPONENTS ARE A GAS AND WHETHER OR NOT THE PRESSURE AND TEMPERATURE
C OF THE FLUID LIES WITHIN THE RANGE OF THE STATE EQUATION.
C

```

```

  LOGICAL FUNCTION LGFN(P,T,J,Z)

```

```

  COMMON /PDATA/ X(7)

```

```

  COMMON /LDATA/ XKV,R,XMW

```

```

  COMMON /PMTM/ TMAX(5),PMIN(5)

```

```

  DIMENSION Z(6), F(5), A(7,5)

```

```

  DATA A/ -8.7688639,18.787464,-5.2058657,0.5388787,3*0.0,-13.830142,
116.452554,-0.7654184,-1.9802311,6.4221948E-2,6.67237E-2,-9.702621E
2-3,-19.892234,18.419682,-0.7872747,-.9806178,-1.2904525E-2,7.66146
367E-2,-9.4861348E-3,-10.146418,8.1787204,2.6798147,-.9441094,-.275
42447,.128236,-1.242546E-2,-65.133331,48.095955,30.296025,-34.13448
5,10.442646,-1.071251,0.0/

```

```

  S=T/100.0

```

```

  J=1

```

```

  LGFN=.TRUE.

```

```

  IF (P.GT.101.0E5.OR.P.LT.0.1.OR.S.LT.1.99.OR.S.GT.4.01.OR.Z(1).LE.
10.0.OR.Z(2).LE.0.0.OR.Z(3).LE.C.0) RETURN

```

```

  F(1)=X(2)

```

```

  F(2)=X(3)

```

```

  F(3)=X(4)

```

```

  F(4)=X(5)

```

```

  F(5)=X(7)

```

```

  DO 2 I=1,5

```

```

  PX=P*F(I)

```

```

  IF (PX.LT.PMIN(I).OR.S.GT.TMAX(I)) GO TO 2

```

```

  PLOG=A(7,I)

```

```

  DO 1 N=1,6

```

```

  V=7-N

```

```

1 PLOG=PLOG*S+A(M,I)

```

```

  IF (PX.GT.XKV*EXP(PLOG)) RETURN

```

```

2 CONTINUE

```

```

  J=0

```

```

  LGFN=.FALSE.

```

```

  RETURN

```

```

  END

```

\$IBFTC NGTLG

C
C THIS SUBROUTINE WILL, IF NECESSARY, CHANGE THE VALUE OF TA SO THAT IT
C IS ABOVE THE CONDENSATION TEMPERATURE OF EACH AND EVERY FLUID
C COMPONENT.
C

```
      SUBROUTINE TLOGIC (PA,TA)
      COMMON /PDATA/ X(7)
      COMMON /PMTM/ TMAX(5),PMIN(5)
      DIMENSION F(5), A(6,5), SS(5)
      DATA A/.1071958,.1344249,9.5750167E-3,-1.2654772E-3,2.1407483E-5,2
1.335769E-6,.7299231,9.5893073E-2,6.8291523E-3,-4.1824175E-4,-3.126
22431E-5,3.7408577E-6,1.5114395,-4.2976141E-3,7.9212714E-3,6.859754
32E-4,-1.1443498E-4,5.8065712E-6,-5.8886957,2.4736013,-.291051,1.49
466109E-2,-2.4150376E-4,0.0,7.5717232,-1.0222722,4.6532148E-2,3*0.0
5/
      P=PA
      S=TA/100.0
      F(1)=X(2)
      F(2)=X(3)
      F(3)=X(4)
      F(4)=X(5)
      F(5)=X(7)
      DO 3 N=1,5
      PX=P*F(N)
      IF (PX.LT.PMIN(N).OR.S.GT.TMAX(N)) GO TO 2
      PLX=ALDG(PX)
      SS(N)=A(6,N)
      DO 1 M=1,5
      MX=6-M
1      SS(N)=SS(N)*PLX+A(MX,N)
      GO TO 3
2      SS(N)=S
3      CONTINUE
      TA=100.0*AMAX1(SS(1),SS(2),SS(3),SS(4),SS(5),S)
      IF (TA.LT.199.0) TA=199.01
      RETURN
      END
```

\$IBFTC NGDATA

```
      BLOCK DATA
      COMMON /PMTM/ TMAX(5),PMIN(5)
      COMMON/GDATA/RC,D2,GAMA,GAMB,GAMC,GAMD,GAME,GAMF
      DATA TMAX,PMIN/3.0555,3.6996,2*4.01,3.04,218300.,20100.,1981.,3906
1.,157800./
      DATA GAMA,GAMB,GAMC,GAMD,GAME,GAMF,D2/.25,.160666667,1.5,.33333333
13,8.0,4.0,5.6/
      END
```

REFERENCES

1. Johnson, R. C.: Calculations of the Flow of Natural Gas Through Critical-Flow Nozzles. *J. Basic Eng.*, vol. 92, no. 3, Sept. 1970, pp. 580-589.
2. Benedict, Manson; Webb, George B.; and Rubin, Louis C.: An Empirical Equation for Thermodynamic Properties of Light Hydrocarbons and Their Mixtures. I. Methane, Ethane, Propane and n-Butane. *J. Chem. Phys.*, vol. 8, no. 4, Apr. 1940, pp. 334-345.
3. Benedict, Manson; Webb, George B.; and Rubin, Louis C.: An Empirical Equation for Thermodynamic Properties of Light Hydrocarbons and Their Mixtures. II. Mixtures of Methane, Ethane, Propane, and n-Butane. *J. Chem. Phys.*, vol. 10, no. 12, Dec. 1942, pp. 747-758.
4. Benedict, Manson; Webb, George B.; and Rubin, Louis C.: An Empirical Equation for Thermodynamic Properties of Light Hydrocarbons and Their Mixtures - Constants for Twelve Hydrocarbons. *Chem. Eng. Progr.*, vol. 47, no. 8, Aug. 1951, pp. 419-422.
5. Hirschfelder, Joseph O.; Curtiss, Charles F.; and Bird, R. Byron: *Molecular Theory of Gases and Liquids*. John Wiley & Sons, Inc., 1954, p. 260.
6. Hilsenrath, Joseph; et al.: *Tables of Thermodynamic and Transport Properties of Air, Argon, Carbon Dioxide, Carbon Monoxide, Hydrogen, Nitrogen, Oxygen, and Steam*. Pergamon Press, 1960.
7. McDowell, Robin S.; and Kruse, F. H.: Thermodynamic Functions of Methane. *J. Chem. Eng. Data*, vol. 8, no. 4, Oct. 1963, pp. 547-548.
8. Anon.: *Technical Data Book - Petroleum Refining*. American Petroleum Institute, 1966.
9. Sciance, C. T.; Colver, C. P.; and Sliepcevich, C. M.: Bring Your C₁ - C₄ Data Up to Date. *Hydrocarbon Processing*, vol. 46, no. 9, Sept. 1967, pp. 173-182.
10. Strobbridge, Thomas R.: The Thermodynamic Properties of Nitrogen From 64 to 300 K Between 0.1 and 200 Atmospheres. Tech. Note 129, National Bureau of Standards, Jan. 1962.
11. Johnson, Robert C.: Real-Gas Effects in Critical Flow Through Nozzles and Thermodynamic Properties of Nitrogen and Helium at Pressures to 300×10^5 Newtons per Square Meter (Approx. 300 Atm.). NASA SP-3046, 1968.
12. Vennix, A. J.; and Kobayashi, Riki: An Equation of State for Methane in the Gas and Liquid Phases. *AIChE J.*, vol. 15, no. 6, Nov. 1969, pp. 926-931.

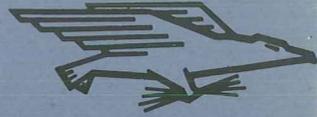
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

WASHINGTON, D. C. 20546

OFFICIAL BUSINESS

PENALTY FOR PRIVATE USE \$300

FIRST CLASS MAIL



POSTAGE AND FEES PAID
NATIONAL AERONAUTICS AND
SPACE ADMINISTRATION

POSTMASTER: If Undeliverable (Section 158
Postal Manual) Do Not Return

"The aeronautical and space activities of the United States shall be conducted so as to contribute . . . to the expansion of human knowledge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."

— NATIONAL AERONAUTICS AND SPACE ACT OF 1958

NASA SCIENTIFIC AND TECHNICAL PUBLICATIONS

TECHNICAL REPORTS: Scientific and technical information considered important, complete, and a lasting contribution to existing knowledge.

TECHNICAL NOTES: Information less broad in scope but nevertheless of importance as a contribution to existing knowledge.

TECHNICAL MEMORANDUMS: Information receiving limited distribution because of preliminary data, security classification, or other reasons.

CONTRACTOR REPORTS: Scientific and technical information generated under a NASA contract or grant and considered an important contribution to existing knowledge.

TECHNICAL TRANSLATIONS: Information published in a foreign language considered to merit NASA distribution in English.

SPECIAL PUBLICATIONS: Information derived from or of value to NASA activities. Publications include conference proceedings, monographs, data compilations, handbooks, sourcebooks, and special bibliographies.

TECHNOLOGY UTILIZATION PUBLICATIONS: Information on technology used by NASA that may be of particular interest in commercial and other non-aerospace applications. Publications include Tech Briefs, Technology Utilization Reports and Technology Surveys.

Details on the availability of these publications may be obtained from:

SCIENTIFIC AND TECHNICAL INFORMATION OFFICE

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Washington, D.C. 20546