NASA Technical Paper 3378

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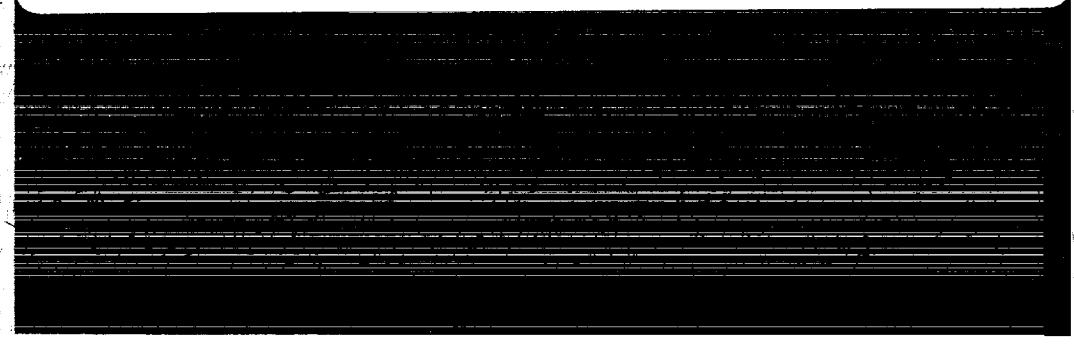
James T. Walton



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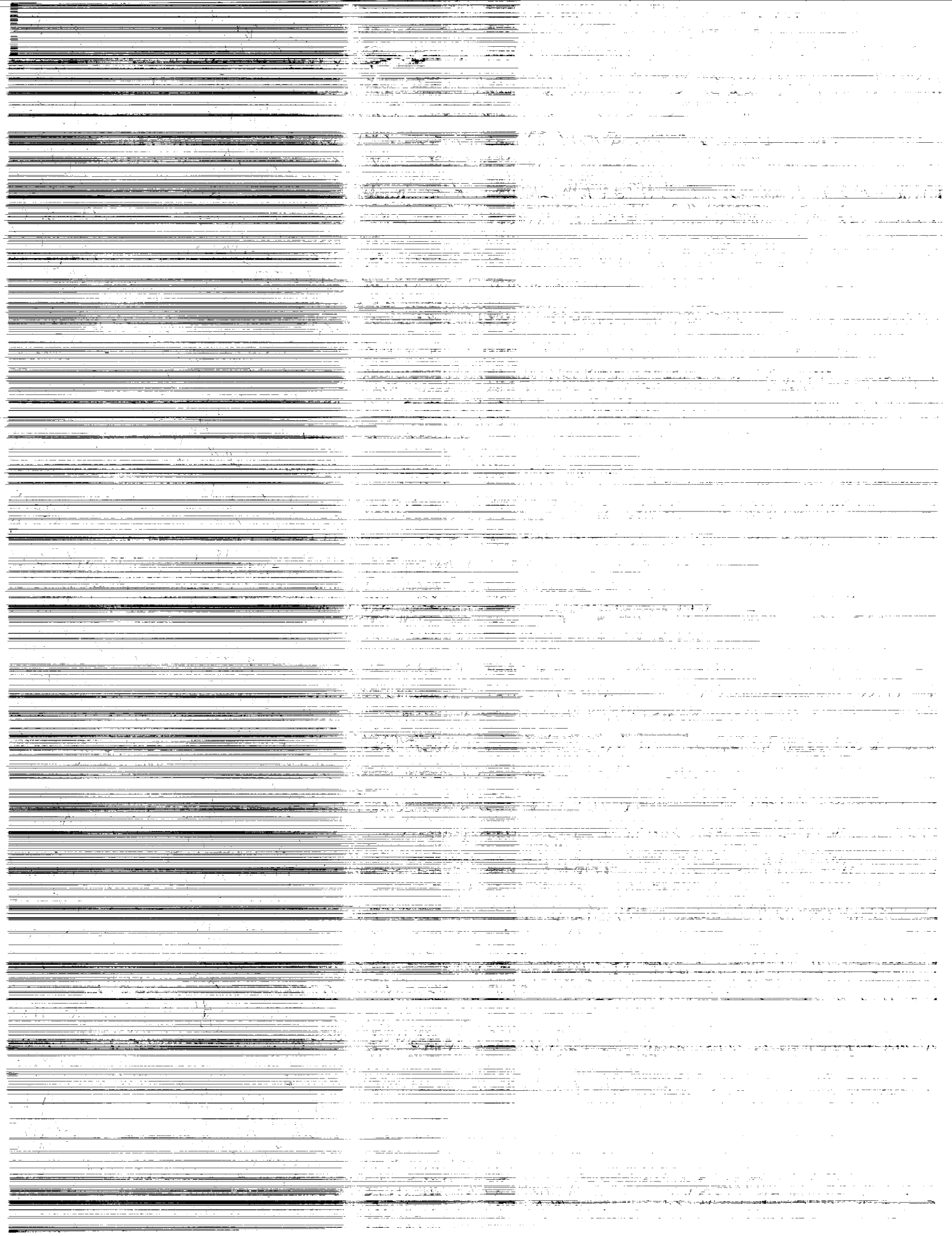

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Computer Program for Thermal and Transport Properties of Parahydrogen From 20 to 10 000 K

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NASA
National Aeronautics and Space Administration
Office of Management
Scientific and Technical Information Program

Summary

A computer program was recently developed to provide thermal and transport properties for parahydrogen across a wide temperature and pressure range. The program, $NBS^+\_pH_2$, matches the most recent parahydrogen property data from the National Bureau of Standards up to 3000 K and property data from the NASA Lewis Research Center's Chemical Equilibrium Computer Program up to 10 000 K. The pressure range of $NBS^+\_pH_2$ is from 1×10^4 to 1.6×10^7 Pa. The program was developed to meet the need for accurate parahydrogen properties from liquid to dissociated conditions as required by propulsion simulation programs being developed under the Space Exploration Initiative. $NBS^+\_pH_2$ is a machine-independent, standard Fortran 77 program which provides density, thermal conductivity, viscosity, Prandtl number, entropy, specific heats, and speed of sound given pressure and either temperature or enthalpy. This report describes this program and provides a comparison to programs previously available.

Statement of Need

Nuclear thermal propulsion (NTP) has been identified as an enabling technology for the manned Mars missions supported under the Space Exploration Initiative (ref. 1). In order to reduce the cost and time required to achieve a flight ready status, computer simulation of NTP systems will be relied upon heavily (ref. 2). In terms of efficiency, hydrogen is the best propellant for these systems, therefore, a model for the properties of hydrogen must be integrated with the NTP system simulations.

Within the system, the state of the hydrogen propellant varies dramatically. The pressure ranges from below 7×10^3 Pa (1 psia) at the nozzle exit to near 1.7×10^7 Pa (2500 psia) at the pump exit. The temperature ranges from 20 K (36 °R) at the pump inlet to up to 3000 K (5400 °R) in the nozzle chamber. Thus, the hydrogen properties model must provide a wide range of properties.

Nominally, hydrogen is a mixture of orthohydrogen and parahydrogen, which differ by the direction of the nuclear spin of the atoms within the molecule. The mixture compositions vary from 100 percent parahydrogen near liquid temperature to 25 percent parahydrogen near room temperature and above. Without a catalyst, conversion from parahydrogen to orthohydrogen at a given temperature variation can take days.

As a propellant for NTP systems, hydrogen is exposed to significant radiation fields. Experiments conducted during reactor tests in 1968 indicated that intense radiation fields hasten the conversion from parahydrogen to orthohydrogen (ref. 3). Because the properties of parahydrogen and orthohydrogen are significantly different between 56 K (100 °R) and 390 K (700 °R), the extent of conversion within the nozzle and reflector is important to their thermal design and nuclear analysis. The historical data indicate that in the range of power levels of interest, the parahydrogen content is above 85 percent, therefore, it would be a reasonable assumption to approximate the propellant as 100 percent parahydrogen.

The National Bureau of Standards (NBS), a branch of the U.S. Department of Commerce, is the source of the most recent compilation of parahydrogen properties data available in the Nation (ref. 4). The NBS data spans the temperature range from 13.8 K (24.8 °R) to 3000 K (5400 °R) and the pressure range from 1×10^4 MPa (1.5 psia) to 1×10^8 Pa (1.45×10^4 psia). Figures 1 to 9 reproduce the NBS tabular data and also list property uncertainty.

Fluid mechanics analysis of NTP systems will require both the thermal and transport properties of parahydrogen, including entropy, thermal conductivity, viscosity, enthalpy, Prandtl number, specific heats, and speed of sound. Moreover, owing to the numerical iterations for system analysis, the computational time required by the hydrogen properties model must be minimized.

Existing Hydrogen Models

Many programs have been developed to provide hydrogen properties, such as STATE, TAB, BW, PH, and MIPROPS. Although some of these programs match the 1981 NBS data within a few percent across limited ranges, none of the programs provide properties across the full range of temperature required for NTP system simulations (figs. 10 to 13).

STATE is a Fortran program for calculation of real fluid state relations, thermodynamic properties, and transport properties of molecular hydrogen in any fixed ortho-para combination (refs. 5, 6). Properties are obtained by combinations

of analytical and empirical formulations with tabulations of published data (refs. 7, 8). The range of the program is from 20 K (36 °R) to 5000 K (9000 °R) and from 10^4 Pa (1.5 psia) to 3.44×10^7 Pa (5000 psia); however, the equation of state (ref. 8) is only recommended for use up to 600 K (1080 °R), and above 2000 K (3600 °R), the gas is assumed to be in an ideal state where all properties are only a function of temperature. Program STATE was written to support heat transfer and fluid flow analyses of nuclear rockets at NASA Lewis Research Center.

TAB2 is a Fortran program which determines parahydrogen properties using a two-dimensional linear interpolation of thermodynamic and transport properties (refs. 7, 9 through 12). This program uses the same thermodynamic properties data as in the STATE program up to 600 K (1080 °R) (refs. 8, 13) and supplements this with dissociated hydrogen data up to 3333 K (6000 °R) (ref. 14). The pressure range is the same as STATE. Program TAB2 was written as a faster and wider range properties code for nuclear rocket propulsion analyses.

BW (ref. 15) is a Fortran program developed to solve a modified Benedict-Webb-Rubin equation of state (ref. 11) to provide para- and normal hydrogen properties up to 400 K (720 °R) and a modified Woolley equation of state (ref. 12) for properties up to 1500 K (2700 °R). The pressure range is from 10^4 Pa (1.5psia) to 3.44×10^7 Pa (5000 psia). This code has been incorporated into the GASPLUS Program (refs. 16, 17) which provides a user-friendly interface to a variety of pure fluid and mixture codes.

PH is a Fortran program developed by the National Bureau of Standards to provide parahydrogen properties (refs. 18 and 19). The program solves a 17 coefficient equation of state developed from data available up to 670 K (1200 °R). Extrapolation is used to provide a temperature range from the triple point to 2780 K (5000 °R). The source of experimental data for high temperature viscosity and thermal conductivity was not available to previous programs.

MIPROPS is a set of computer programs that gives the thermophysical and transport properties of selected fluids, including parahydrogen (ref. 20). These Fortran programs calculate the properties in both the liquid and vapor states but are limited to temperatures well below the dissociated gas region; the limit is 400 K (720 °R) for parahydrogen.

$NBS^+\_pH_2$ Program Structure

To remedy the deficiencies of the available programs, a new program was written to provide parahydrogen properties which matched the 1981 NBS data across the full range of temperatures required by propulsion simulations. This program is called $NBS^+\_pH_2$ (ref. 21). "NBS" refers to the program's ability to match the NBS data up to 3000 K (5400 °R) and the "+" signifies the program's extension beyond the NBS 3000 K (5400 °R) limit to 10000 K (18000 °R) using supplemental data. $NBS^+\_pH_2$ is a strict Fortran 77 program written to determine parahydrogen properties using a two-dimensional linear interpolation of 1981 NBS thermodynamic and transport tabular data (ref. 4). The pressure and temperature intervals of the tabular data are given in tables I and II.

$NBS^+\_pH_2$ is set up as a single Fortran subroutine in which pressure and temperature or enthalpy are sent to it through the Fortran call statement. In addition, the thermodynamic and transport properties at the given conditions are returned through the call statement. The coding in this single-precision subroutine (1) compares the input parameters to established boundaries, (2) locates the position of the input parameters in the data arrays, (3) interpolates between arrays if necessary, and (4) checks the interpolated properties with established boundaries. The property data is stored in arrays established in Fortran block data sections and integrated with the subroutine through a Fortran common block statement. By using tabular data, instead of solving an equation of state or minimization of Gibbs' free energy, $NBS^+\_pH_2$ minimizes run-time at the expense of code size. The subroutine coding is an 850 line source listing and requires 300 kilobytes. The executable code requires 310 kilobytes of memory on an IBM PC compatible. A sample control program is shown in appendix A.

The subroutine can be operated in four possible modes: (1) provide pressure and temperature, and return enthalpy along with all properties; (2) provide pressure and enthalpy, and return enthalpy along with all properties; (3) provide pressure and return saturated liquid enthalpy and temperature, along with all properties; (4) provide pressure and return saturated vapor enthalpy and temperature, along with all properties. The units of the input and output are shown in tables III and IV, respectively.

The temperature range of $NBS^+\_pH_2$ was extended beyond 3000 K (5400 °R) by using hydrogen properties data generated by Program CET89. Data from other sources was evaluated (refs. 22 to 26), however, it was either generated by earlier versions of the CET89 program, did not provide all the required properties, or provided data in intervals too large for accurate interpolation. CET89 is the most recent version of the Chemical Equilibrium Computer Program (refs. 27, 28). This Fortran program determines equilibrium composition through minimization of Gibbs free energy. CET89 assumes an ideal gas equation of state for all species. When modeling parahydrogen, the species considered include H_2, H^+, H, and electron gas. The properties of these species were gathered from references 29, 30, and31. The range is limited to gaseous temperatures.

Concluding Remarks

A Fortran computer program has been developed to provide thermodynamic and transport properties of parahydrogen across a wide range of pressure and temperature. $NBS^{+}\_pH_2$ has been successfully integrated into several NTP system simulations (refs. 32 to 34) resulting in higher fidelity solutions with reduced run time in most cases. Moreover, the use of a single parahydrogen properties code, with the most current data, reduces the number of variables when attempting to compare results between system simulations.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, April 1993

APPENDIX A
Control Program Listing

```
      PROGRAM NBS_TEST
CC
CC                    PROGRAM NBS-TEST
CC                    - - - - - - - - -
CC  THIS PROGRAM TESTS THE PARAHYDROGEN
      PROPERTIES SUBROUTINE, NBS_pH2,
CC  WHICH WAS DEVELOPED TO ACCESS THE NBS
      PARAHYDROGEN DATA.
CC
CC   PROGRAM:         LEW-15505
CC  AUTHOR:  JAMES T. WALTON, NASA LEWIS
      RESEARCH CENTER
CC   ORIGINATION:      APRIL 01, 1992
CC   LAST MODIFICATION: JANUARY 25, 1993
CC

      REAL K
      CHARACTER DATE*20
      DATA DATE/'JANUARY 25, 1993'/,VERSION/1.06/

      CALL BANNER(VERSION,DATE)

      WRITE(6,5)
    5 FORMAT(
     1' SELECT (1) PRESSURE & ENTHALPY OR (0)
PRESSURE & TEMPERA'
     2,'TURE INPUT FORMAT OR (-1) PRESSURE & EN-
TROPY: ')
      READ(5,*) IFLAG
    1 WRITE(6,10)
   10 FORMAT(25(/))
      WRITE(6,*)              ' ENTER PRESSURE (MPa):  '
      READ(5,*) P
      P = P*1000000
      IF (IFLAG.EQ.0) WRITE(6,*) ' ENTER TEMPERA-
TURE (K): '
      IF (IFLAG.EQ.0) READ(5,*) T
      IF (IFLAG.EQ.1) WRITE(6,*) ' ENTER ENTHALPY
(J/KG): '
      IF (IFLAG.EQ.1) READ(5,*) H
      IF (IFLAG.EQ.-1) WRITE(6,*) ' ENTER ENTROPY (J/
KG): '
      IF (IFLAG.EQ.-1) READ(5,*) S
                                                CALL
NBS_pH2(H,P,T,RHO,VIS,CP,PR,A,K,S,GAM,X,IFLAG)
      WRITE(6,10)
      WRITE(6,15)
   15 FORMAT(
     1 '              NASA LEWIS RESEARCH CENTER',/
     2 '                   LEW-15505',/,
     3 '                    NBS-PH2',/,/,/,/,/)
      WRITE(6,20) P,T,H,PR,VIS,CP,X,A,K,RHO,GAM,S
      WRITE(3,20) P,T,H,PR,VIS,CP,X,A,K,RHO,GAM,S
   20 FORMAT(
     1 ' PRESSURE =',E10.4,' Pa',1X,'TEMPER. =',E10.4,'
K   ',2X,
     2 'ENTHALPY =',E11.4,' J/kg',/,/,
     3 ' PRANDTL #=',E10.4,'  ',1X,'VISCOS. =',E10.4,'
kg/m-s',2X,
     4 'SPEC.HEAT=',E10.4,' J/kg-K',/,
     5 ' QUALITY  =',E10.4,'  ',1X,'SPD O SND=',E10.4,'
m/s  ',2X,
     6 'THER.COND=',E10.4,' W/K-m',/,/,
     7'         ',10X  ,'  ',1X,'DENSITY  =',E10.4,' kg/m3 ',/
,
     1 ' GAMMA    =',E10.4,'  ',1X,'ENTROPY  =',E10.4,'
J/KG-K',2X,
     2 '         ', 10X ,'     ',/)

      WRITE(6,30)
      WRITE(3,*)
      WRITE(3,*)
   30 FORMAT(/,/,/,/,/,/,/,/,' SELECT (1) TO REENTER OR
(0) TO QUIT: ')
      IZ = 0
      READ(5,40,END=9999) IZ
   40 FORMAT(I2)
      IF (IZ.EQ.1) GOTO 1
 9999 STOP
      END
```

```
      Subroutine Banner(Version, Date)
CC                    SUBROUTINE BANNER
CC                    ---------
CC
CC    THIS SUBROUTINE WRITES THE STANDARD
NASA PROGRAM BANNER PAGE
CC    TO THE TERMINAL SCREEN.
CC
CC    AUTHOR:          JAMES T. WALTON, NASA
LEWIS RESEARCH CENTER
CC    ORIGINATION:     MAY 13, 1991
CC    LAST MODIFICATION: NOVEMBER 02, 1992
CC
      CHARACTER JUNK*12,DATE*20,FILEOUT*12
      DATA FILEOUT/'NBS-PH2.OUT'/
      Write(6,100) Version, Date
  100 Format(24(/),' ',77('_'),' ',/,' |',77X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'NATIONAL AERONAUTICS & SPACE
ADMINISTRATION ',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'       Lewis Research Center  ',16X,'|'
     1,/,' |',17X,'         Cleveland, Ohio      ',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'                   PROGRAM NBS+pH2
',16X,'|'
     1,/,' |',17X,'            VERSION ',F4.2,'      ',20X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',18X,'NBS PARAHYDROGEN PROPERTIES
DATA BASE ACCESS',15X,'|'
     1,/,' |',17X,'              LEW-15505       ',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'         Author:    James T. Walton
',16X,'|'
     1,/,' |',17X,'                              ',16X,'|'
     1,/,' |',17X,'       Origination: MARCH 20, 1992
',16X,'|'
     1,/,' |',17X,'    Version Date: ',A20,      17X,'|'
     1,1(/,' |',77X,'|'),/,' |',77('_'),'|',/,' --> ')
      Read(5,101,end=9998) JUNK
  101 Format(A12)
                                                  OPEN
(UNIT=3,FILE=FILEOUT,STATUS='UNKNOWN')
      WRITE(3,100) VERSION,DATE
 9998 Return
      End
```

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TABLE I. – TABULAR DATA PRESSURE INTERVALS IN PASCALS

10000	600000	900000	3000000	8000000
200000	650000	950000	3500000	9000000
300000	700000	1000000	4000000	10000000
400000	750000	1500000	5000000	12000000
500000	800000	2000000	6000000	14000000
550000	850000	2500000	7000000	16000000

TABLE II. – TABULAR DATA TEMPERATURE INTERVALS IN KELVIN

14	26	42	90	280	1200	3750	6750
15	27	44	100	300	1400	4000	7000
16	28	46	110	350	1600	4250	7250
17	29	48	120	400	1800	4500	7500
18	30	50	130	450	2000	4750	7750
19	31	52	140	500	2200	5000	8000
20	32	56	160	550	2400	5250	8250
21	33	60	180	600	2600	5500	8500
22	34	65	200	700	2800	5750	8750
23	36	70	220	800	3000	6000	9000
24	38	75	240	900	3250	6250	9500
25	40	80	260	1000	3500	6500	10000

TABLE III. – NBS*–pH_2 INPUT PARAMETERS

P – pressure (Pa)

IFLAG – input mode selector
- (0) pressure and temperature are both required input
- (1) pressure and enthalpy are both required input
- (2) pressure at saturated liquid condition is required input
- (3) pressure at saturated vapor condition is required input

H – enthalpy; required if IFLAG = 1 (J/kg)

T – temperature; required if IFLAG = 0 (K)

TABLE IV. – NBS*–pH_2 OUTPUT PARAMETERS

H – enthalpy; output if IFLAG = 0 (J/kg)
T – temperature; output if IFLAG = 1 (K)
RHO – density (kg/m^3)
VIS – dynamic viscosity (kg/m-s)
Cp – constant pressure specific heat (J/kg-K)
Pr – Prandtl number
a – speed of sound (m/s)
k – thermal conductivity (W/K-m)
S – entropy (J/kg-K)
GAM – ratio of specific heats
X – quality
- 0: liquid
- 0 < X < 1 two-phase liquid and vapor
- 1; vapor

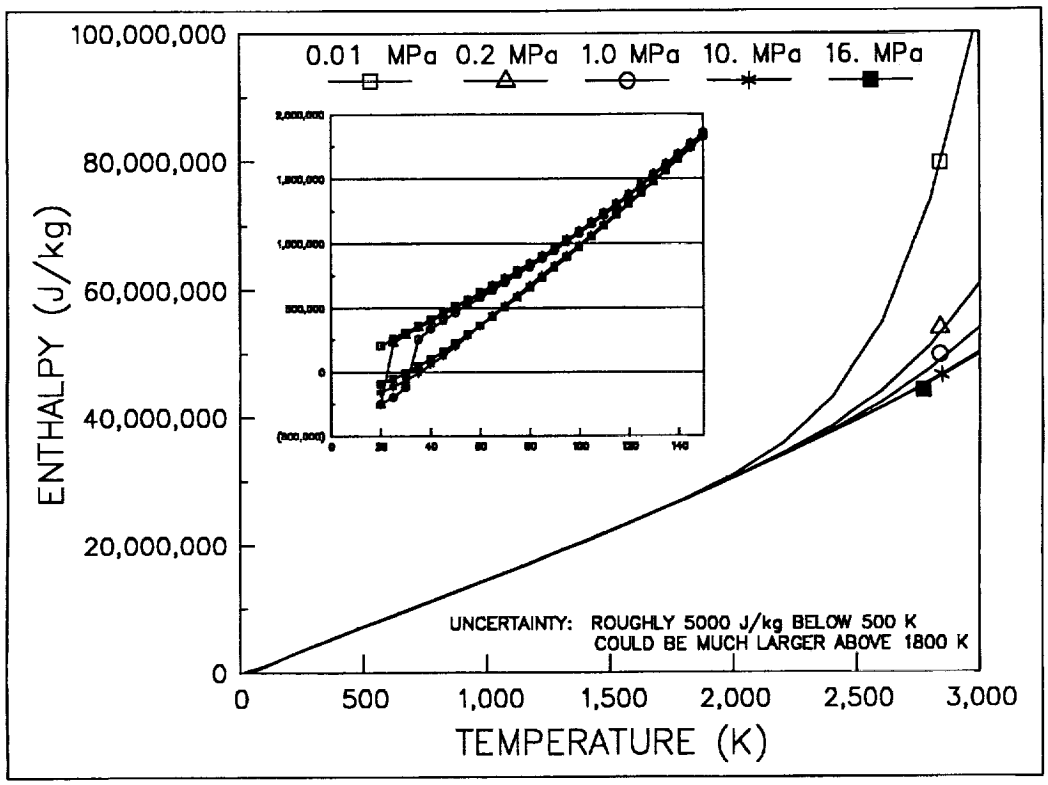

Figure 1. – Enthalpy of parahydrogen for selected pressures.

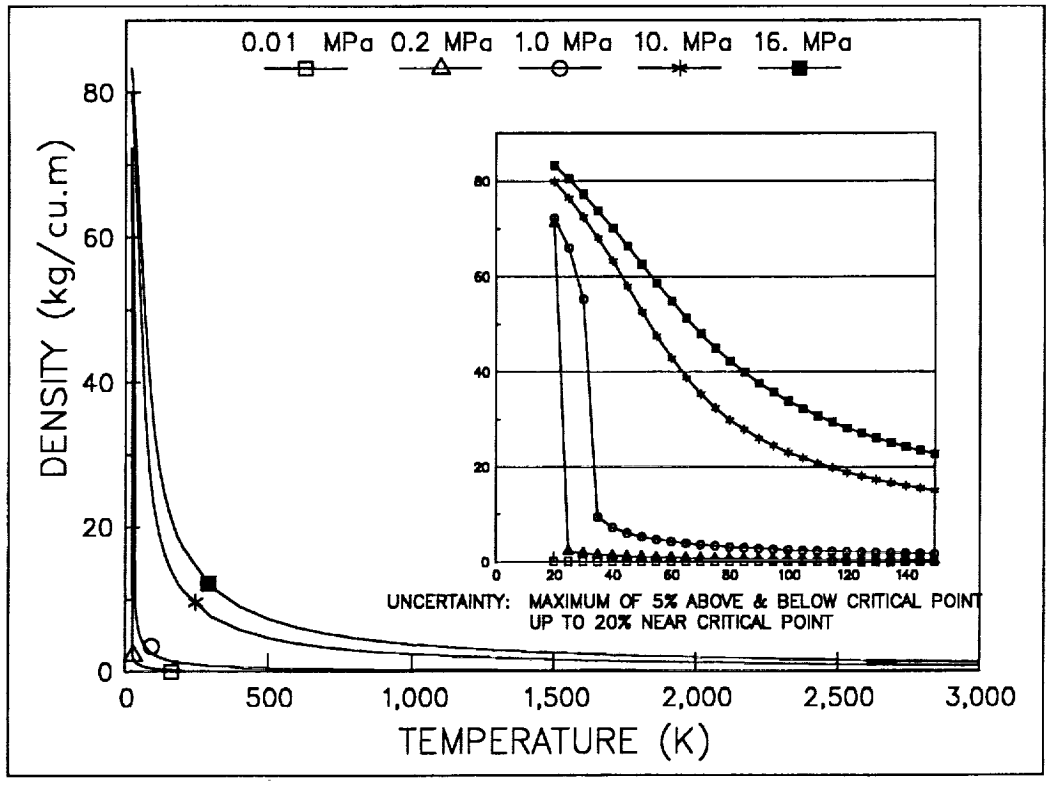

Figure 2. – Density of parahydrogen for selected pressures.

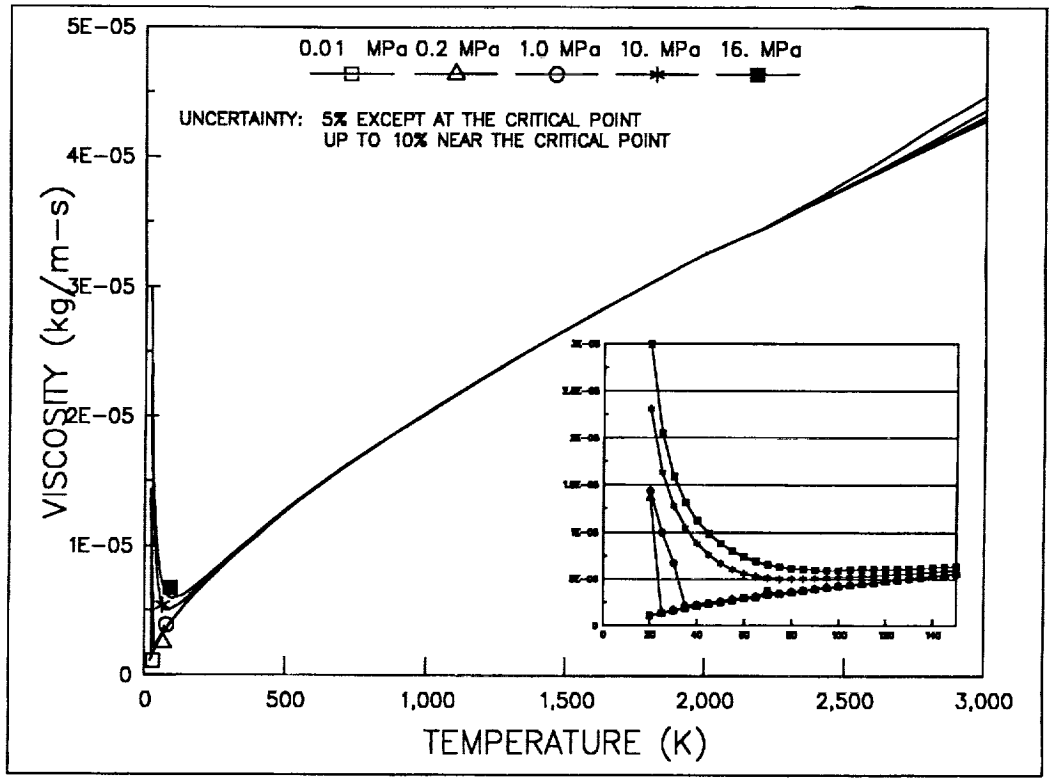

Figure 3. – Dynamic viscosity of parahydrogen for selected pressures.

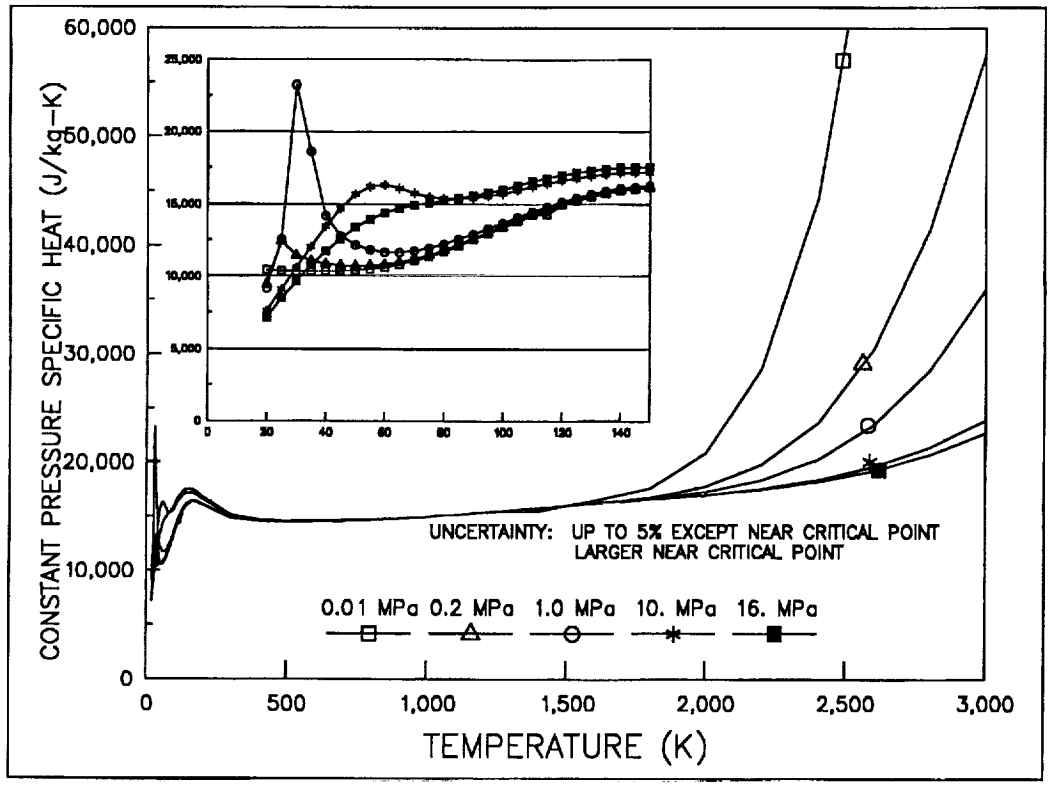

Figure 4. – Constant pressure specific heat of parahydrogen for selected pressures.

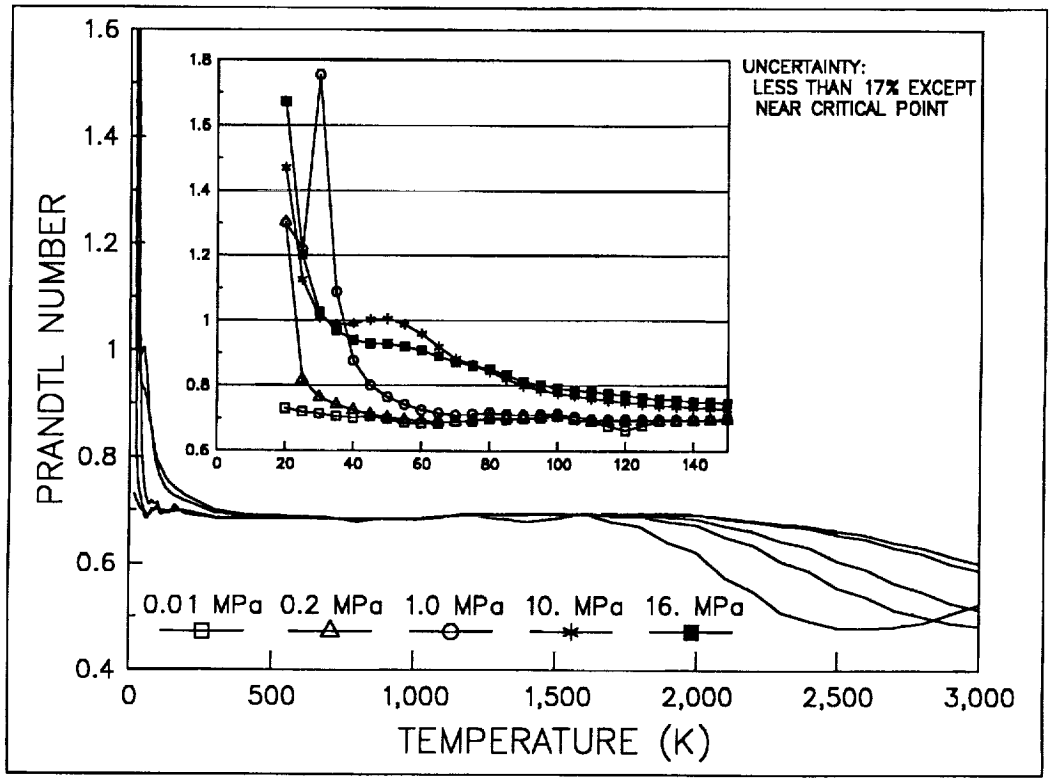

Figure 5. – Prandtl number of parahydrogen for selected pressures.

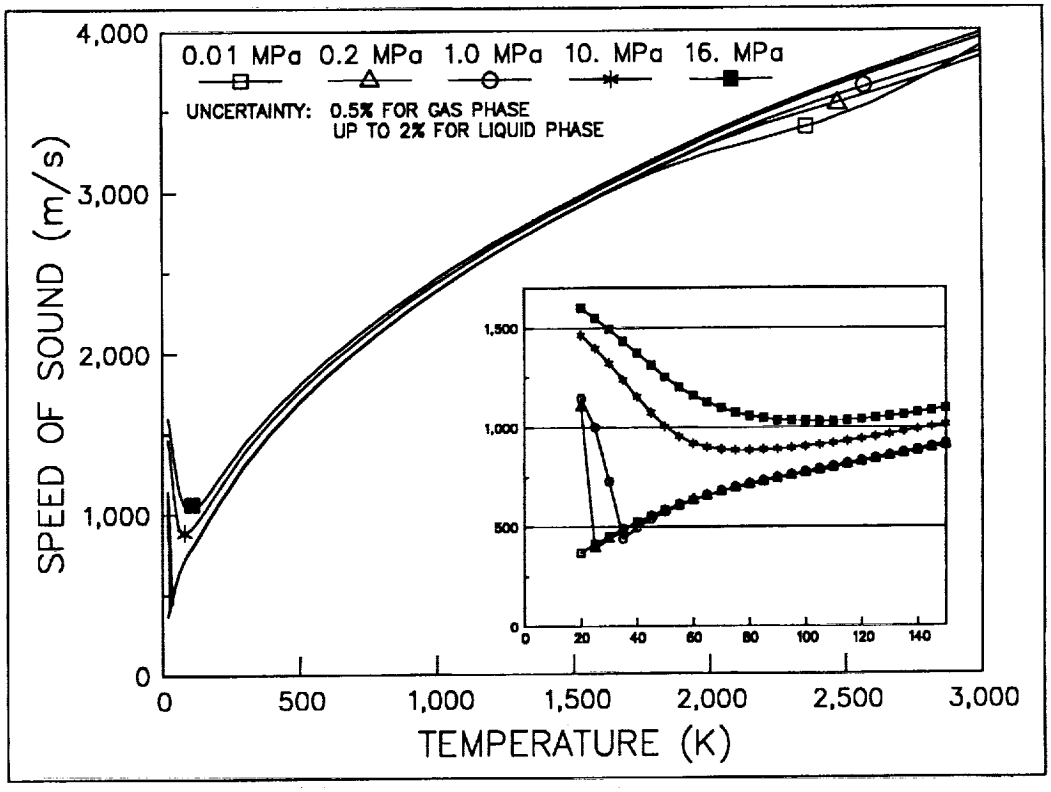

Figure 6.—Speed of sound of parahydrogen for selected pressures.

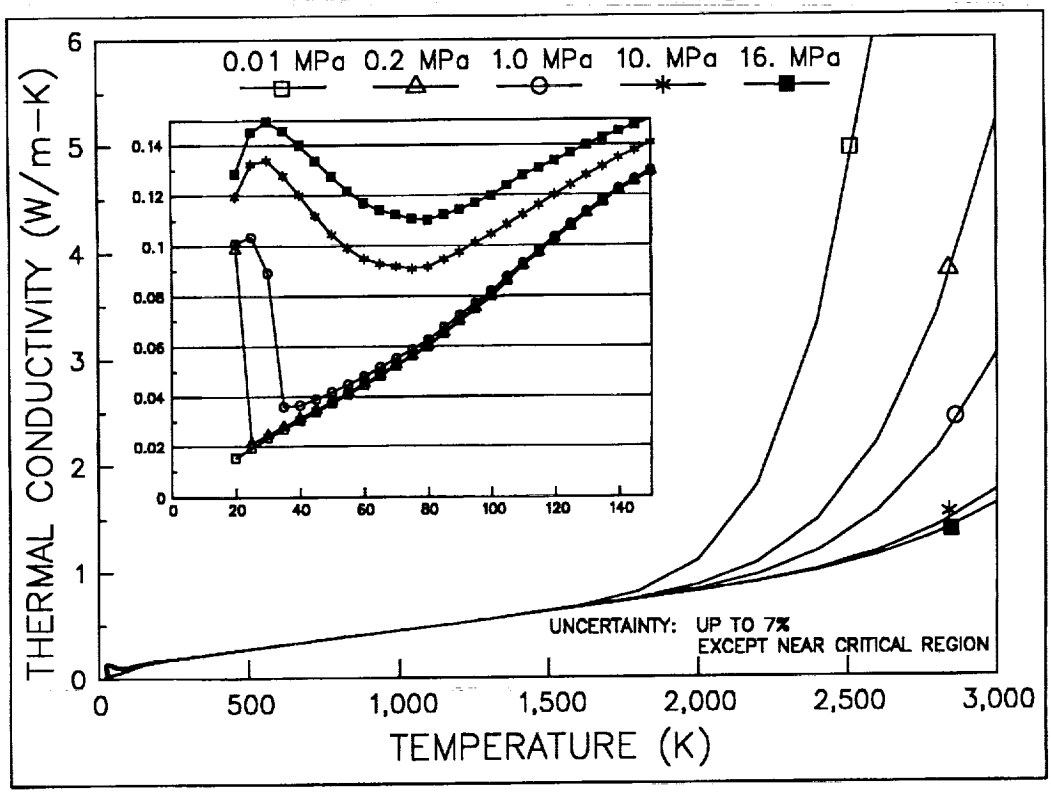

Figure 7.—Thermal conductivity of parahydrogen for selected pressures.

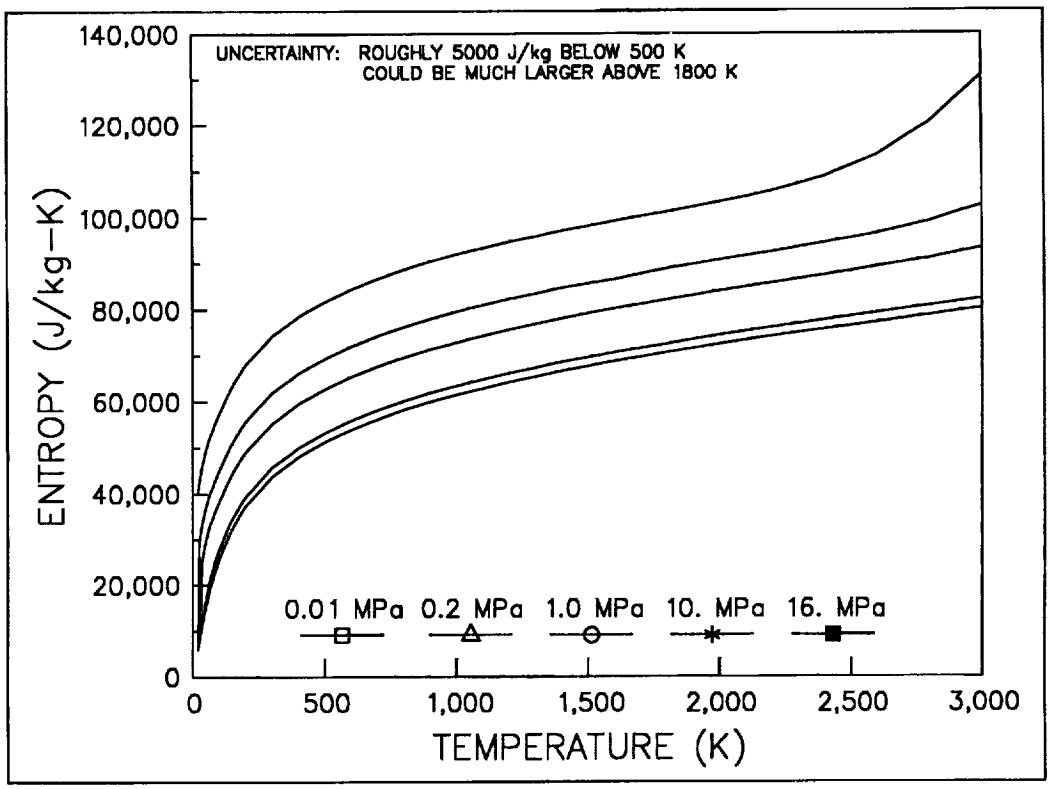

Figure 8.—Entropy of parahydrogen for selected pressures.

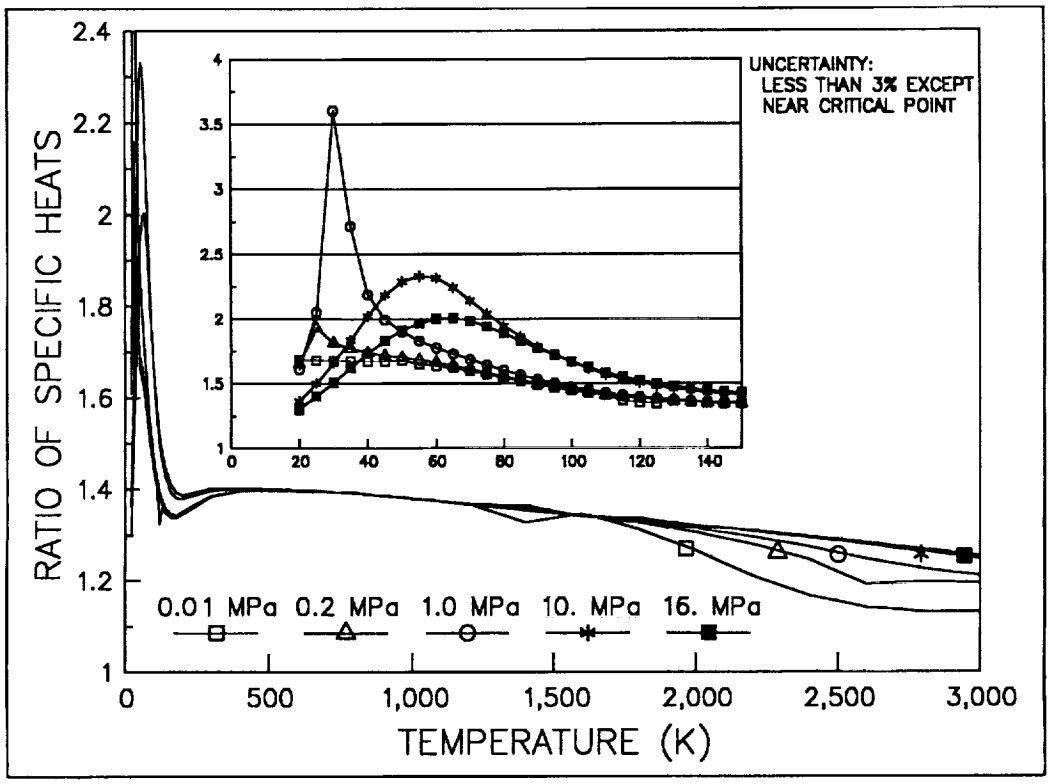

Figure 9.—Ratio of specific heats of parahydrogen for selected pressures.

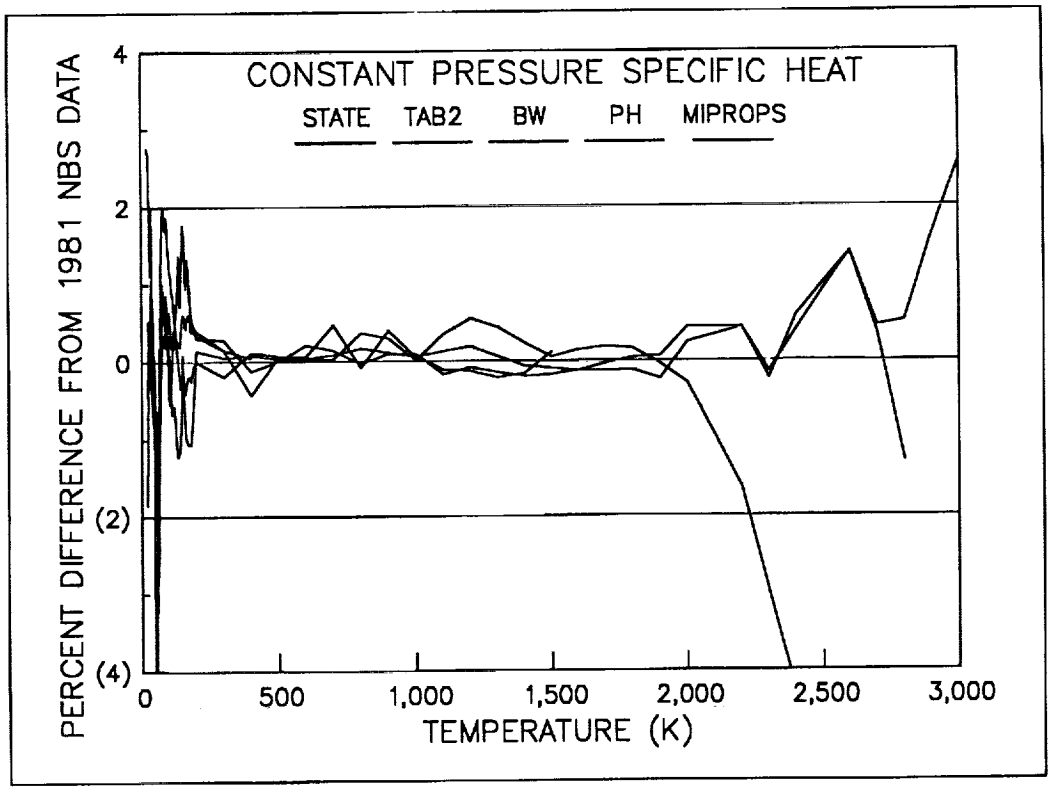

Figure 10.—Deviation of various programs to 1981 NBS specific heat data.

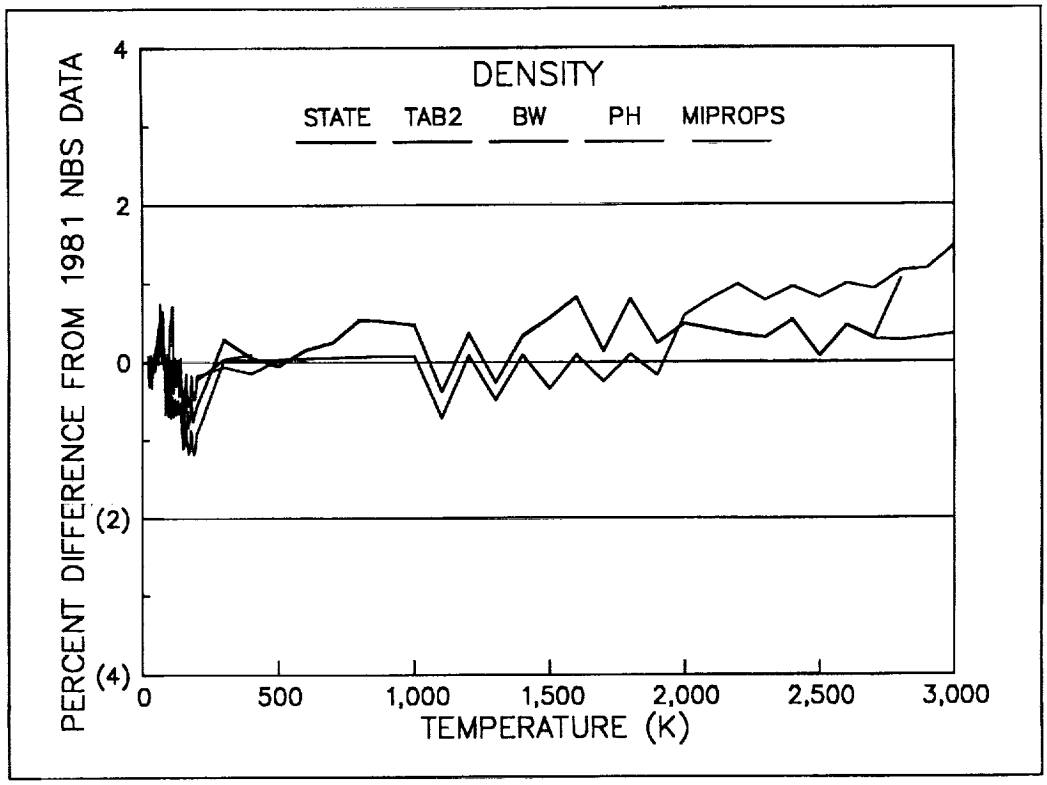

Figure 11.—Deviation of various programs to 1981 NBS density data.

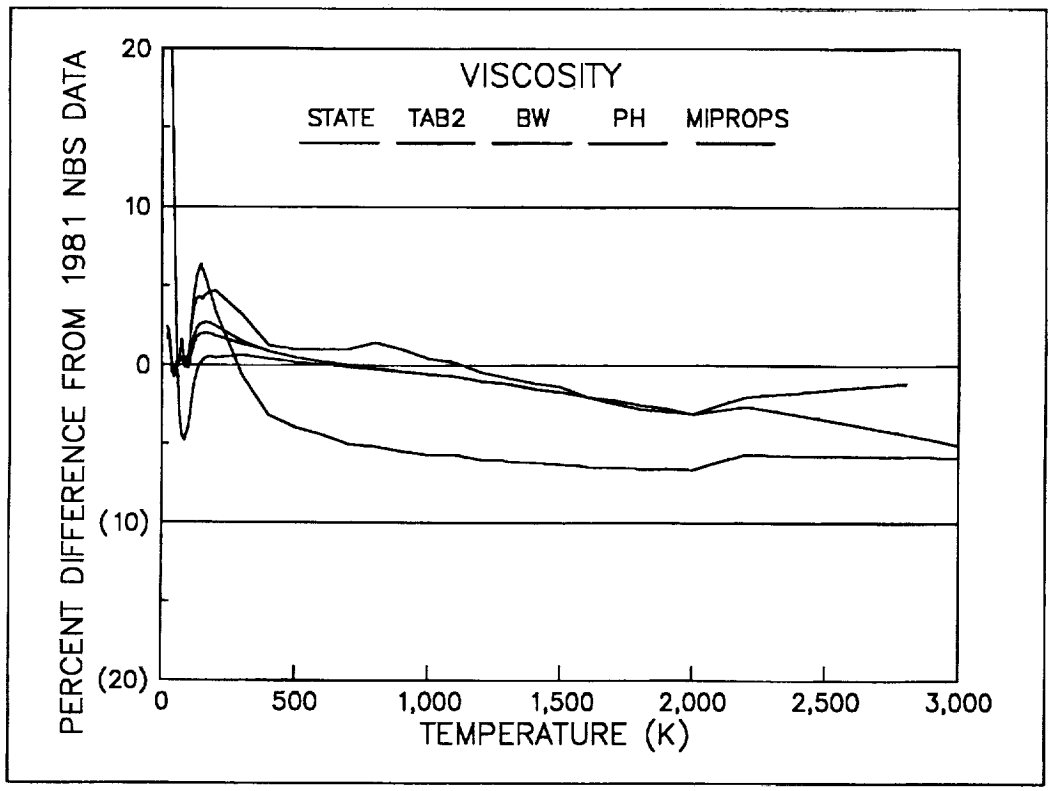

Figure 12.—Deviation of various programs to 1981 NBS viscosity data.

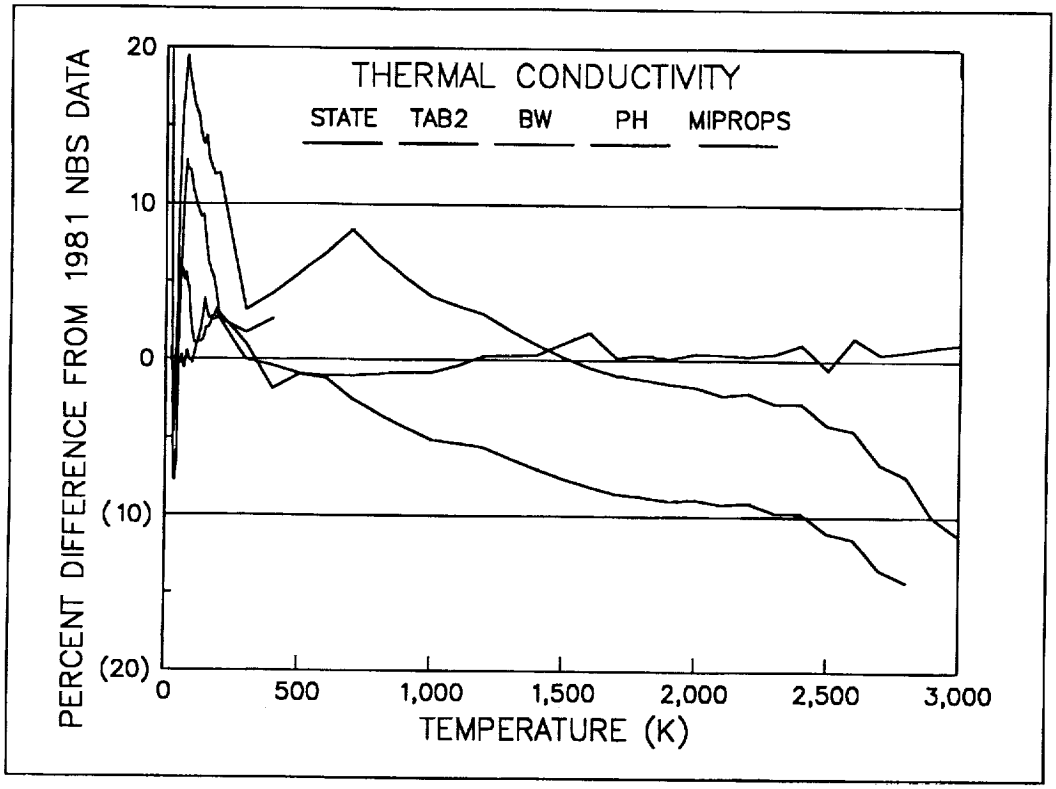

Figure 13.—Deviation of various programs to 1981 NBS thermal conductivity data.

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13. ABSTRACT (*Maximum 200 words*)

A computer program was recently developed to provide thermal and transport properties for parahydrogen across a wide temperature and pressure range. The program, NBS$^+$_pH_2, matches the most recent parahydrogen property data from the National Bureau of Standards up to 3000 K and property data from the NASA Lewis Research Center's Chemical Equilibrium Computer Program up to 10 000 K. The pressure range of NBS$^+$_pH_2 is from 1×10^4 to 1.6×10^7 Pa. The program was developed to meet the need for accurate parahydrogen properties from liquid to dissociated conditions as required by propulsion simulation programs being developed under the Space Exploration Initiative. NBS$^+$_pH_2 is a machine-independent, standard Fortran 77 program which provides density, thermal conductivity, viscosity, Prandtl number, entropy, specific heats, and speed of sound given pressure and either temperature or enthalpy. This report describes this program and provides a comparison to programs previously available.

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