Sandia National Laboratories
Waste Isolation Pilot Plant

# Technical Memorandum: Hydrogen Gas As Surrogate for Waste-Generated Gas Physical Properties in BRAGFLO

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# 1 Introduction

Sandia National Laboratories (SNL) has performed an impact assessment to determine the effects of supercompacted waste and heterogeneous waste emplacement on repository performance at the Waste Isolation Pilot Plant (WIPP) [9]. This impact assessment addressed the performance of supercompacted waste processed by the Idaho National Engineering and Environmental Laboratory's (INEEL) Advanced Mixed Waste Treatment Project (AMWTP). The results of the impact assessment were submitted to the US Environmental Protection Agency (EPA) by the Department of Energy (DOE) in order to obtain regulatory approval for disposal at WIPP of supercompacted AMWTP waste.

EPA's initial review [7] of the AMWTP impact assessment identified the gas properties used in the `bragflo` code as one area where additional information is required in order for EPA to properly evaluate the impact of supercompacted waste on the WIPP disposal system. The `bragflo` code implements a gas generation model in which the gas phase is assigned the properties of hydrogen ($H_2$). EPA has requested information on the sensitivity of the results to the use of $H_2$ as a surrogate for carbon dioxide ($CO_2$) and methane ($CH_4$) because methanogenesis is now thought to be an important gas generation process.

## 1.1 Objective

The work presented here provides additional information requested by the EPA regarding the use of $H_2$ as a surrogate for waste-generated gas in the `bragflo` calculations for the AMWTP supercompacted waste impact assessment.

## 1.2 Analysis Overview

The question of using $H_2$ as surrogate for waste-generated gas was addressed in Appendix MASS of the 1996 WIPP Compliance Certification Application (CCA) [6]. The analysis presented there compared the effects of variation in gas viscosity and compressibility on repository pressures and flow rates for $H_2$-$CO_2$ mixtures. This analysis extends that of the CCA to include $H_2$-$CH_4$ mixtures.

# 2 Background

Gas may be generated in the repository via several mechanisms. $H_2$ gas may be produced by the corrosion of steel in the repository by water or brine [14]. Microbial processes such as denitrification, sulfate reduction, fermentation and methanogenesis may also occur, producing nitrogen ($N_2$), $H_2$, hydrogen sulfide ($H_2S$), $CO_2$ and $CH_4$ [3]. If microbial degradation occurs, a significant amount of $CO_2$ and $CH_4$ may be generated by microbial degradation of cellulosics and, perhaps, plastics and rubbers in the waste [6]. Since almost all of the $CO_2$ produced will react with the magnesium oxide (MgO) backfill and cementous materials to form hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) and calcium carbonate ($CaCO_3$), the $CO_2$ fugacity in the repository is expected to be very low [6].

An analysis of the effects on repository pressures and flow velocities of using $H_2$ instead of an $H_2$-$CO_2$ mixture as the gas in `bragflo` was presented in Appendix MASS of the 1996 WIPP Compliance Certification Application (CCA) [6]. The CCA analysis considered saturated radial flow of a nonideal gas as described by the following formulation often used in the petroleum reservoir engineering literature [1]

$$q_b = 1.988 \times 10^{-5} \left[ \frac{T_b z_b}{P_b} \frac{kh\left(P_e^2 - P_w^2\right)}{\eta_{avg} z_{avg} \log\left(\frac{r_e}{r_w}\right)} \right] \tag{1}$$

where:

| | | |
|---|---|---|
| $b$ | = | quantity at base or reference condition for gas |
| $e$ | = | quantity at external boundary (repository) |
| $w$ | = | quantity at internal houndary (wellbore) |
| $avg$ | = | quantity averaged between internal and external boundaries |
| $q$ | = | gas flow rate (cubic feet per day) |
| $T$ | = | temperature (K) |
| $P$ | = | pressure (PSIA) |
| $k$ | = | permeability (millidarcys) |
| $h$ | = | height (feet) |
| $\eta$ | = | viscosity (centipoise) |
| $z$ | = | compressibility factor (dimensionless) |
| $r$ | = | radial distance from center of wellbore (consistent units) |

The effects on gas flow rate of varying viscosity or compressibility are easily deduced from Eq. (1). The flow rate is inversely related to viscosity and to compressibility. So increasing the viscosity by a factor of two should reduce the velocity by a factor of two. Similarly, reducing the compressibility factor will increase the gas flow rate.

The effects on repository pressure can be obtained by rearranging Eq. (1) as follows

$$P_e^2 - P_w^2 = \frac{q_b}{1.988 \times 10^{-5}} \left[ \frac{P_b}{T_b z_b} \frac{\eta_{avg} z_{avg} \log\left(\frac{r_e}{r_w}\right)}{kh} \right] \tag{2}$$

In this form, one can observe that the square of repository pressure is directly proportional to both viscosity and compressibility.

The CCA Appendix MASS analysis computed viscosity and compressibility factors for a range of $H_2$-$CO_2$ mixtures using the `supertrapp` thermophysical properties database [10]. $CH_4$ was not included in the analysis hecause it was assumed that the properties of $CH_4$ would be similar to that of $CO_2$. The `supertrapp` code was used to calculate gas viscosity and compressibility factor at pressures of 7 MPa and 15 Mpa for a range of gas compositions. Results of the supertrapp modeling showed that for a gas mixture consisting of equal parts $H_2$ and $CO_2$, at 15 Mpa, the viscosity would increase by a factor of approximately 2.3 compared to the viscosity of pure $H_2$. The compressibility factor would decrease by a factor of approximately 0.9. This means that the flow rate predicted by Eq. (1) would be half of that for pure $H_2$ while the square of the repository pressure would approximately double. Since the rock permeability, $k$, was expected to vary by four orders of magnitude, the CCA Appendix MASS analysis drew the conclusion that the potential factor of two variability in the square of repository pressure introduced by using pure $H_2$ properties in bragflo was not significant.

## 3 Approach

The approach used in this analysis is to repeat the calculations presented in CCA Appendix MASS, but include results for a range of $H_2$-$CH_4$ mixtures to determine if increased $CH_4$ production will change any of the conclusions drawn regarding the use of $H_2$ *gas as a surrogate* for waste-generated gas physical properties.

As in the CCA Appendix MASS calculations, the National Institute of Standards and Technology (NIST) Thermophysical Properties of Hydrocarhon Mixtures Datahase (supertrapp) is used to compute viscosity and compressibility factor for the gas mixtures.

Compressibility factor and viscosity of $H_2$-$CO_2$ and $H_2$-$CH_4$ mixtures are computed over a wide range of compositions. Calculations are performed at 300K for pressures of 7 MPa and 15 MPa. Eqs. (1)-(2) are used to estimate the effect that variability in compressibility and viscosity may have on repository pressures and flow rates.

Version 3.1 of the supertrapp database was used for these calculations. The calculations were performed on a PC workstation running the Windows XP operating system, Version 5.1.2600. Input files, recorded user interaction with the database, and output files for the supertrapp calculations are included in Appendix A.

Use of supertrapp database is treated as a routine calculation under Nuclear Waste Management Procedure (NWMP) NP 9-1 [4]. Comparisons of supertrapp results with experimental data and correlations reported in the scientific literature are used to verify the database for the purpose of these calculations. The verification procedure and results are detailed in Appendix B.

## 4 Results

Results of the supertrapp calculations for the $H_2$-$CO_2$ and $H_2$-$CH_4$ mixtures are shown in Tables 1 and 2, respectively. The results for both mixtures are summarized in Figure 1.

The results for the $H_2$-$CO_2$ mixtures are similar to the results shown in CCA Appendix MASS. At T=300K and P=15 Mpa, the viscosity of a 50% $H_2$ mole fraction $H_2$-$CO_2$ mixture is approximately 2.6 times higher than that of pure $H_2$ while the compressibility differs by a factor of about 0.9. Inserting these factors into Eqs. (1)-(2) indicates that the repository gas flow rate for the $H_2$-$CO_2$ mixture might be as much as 2.3 times slower than that for pure $H_2$ while the square of repository pressure might be up to 2.3 times higher.

It should be noted here that the `bragflo` code includes a pressure-induced fracture model [13] which will limit pressure increases in the repository. For example, at high repository pressures, the factor of 2.3 pressure increase predicted by the simplified radial flow model is unlikely to be seen in the `bragflo` results since fracturing will lead to increased permeability, effectively limiting pressure increases.

`supertrapp` results for the $H_2$-$CH_4$ mixtures show that excursions in velocity and pressure from the $H_2$ values are less than that observed for the $H_2$-$CH_4$ mixtures. At T=300K and P=15 Mpa, the viscosity of a 50% $H_2$ mole fraction $H_2$-$CH_4$ mixture is approximately 1.6 times higher than that of pure $H_2$ while the compressibility differs by a factor of about 0.94. Inserting these factors into Eqs. (1)-(2) indicates that the repository gas flow rate for the $H_2$-$CH_4$ mixture might about 1.5 times slower than that for pure $H_2$ while the square of repository pressure might be approximately 1.5 times higher.

Table 1: Predicted Compressibility and Viscosity of $H_2$-$CO_2$ Mixtures at 300K

| | $P = 7$ MPa | | | | $P = 15$ MPa | | | |
|---|---|---|---|---|---|---|---|---|
| $\chi_{H_2}$ (-) | $Z$ (-) | $Z/Z_{H_2}$ (-) | $\eta$ ($\mu$Pa s) | $\eta/\eta_{H_2}$ (-) | $Z$ (-) | $Z/Z_{H_2}$ (-) | $\eta$ ($\mu$Pa s) | $\eta/\eta_{H_2}$ (-) |
| 1.00 | 1.0655 | 1.0000 | 8.8860 | 1.0000 | 1.1335 | 1.0000 | 8.8860 | 1.0000 |
| 0.90 | 1.0659 | 1.0004 | 14.9953 | 1.6875 | 1.1358 | 1.0020 | 14.7648 | 1.6616 |
| 0.80 | 1.0612 | 0.9960 | 18.2596 | 2.0549 | 1.1291 | 0.9961 | 18.0631 | 2.0328 |
| 0.70 | 1.0498 | 0.9853 | 20.3486 | 2.2900 | 1.1103 | 0.9795 | 20.7417 | 2.3342 |
| 0.60 | 1.0308 | 0.9675 | 21.5629 | 2.4266 | 1.0775 | 0.9506 | 22.3739 | 2.5179 |
| 0.50 | 1.0035 | 0.9419 | 21.9005 | 2.4646 | 1.0288 | 0.9076 | 23.2925 | 2.6213 |
| 0.40 | 0.9655 | 0.9062 | 21.6284 | 2.4340 | 0.9586 | 0.8457 | 23.8523 | 2.6843 |
| 0.30 | 0.9139 | 0.8577 | 20.9860 | 2.3617 | 0.8581 | 0.7570 | 24.5776 | 2.7659 |
| 0.20 | 0.8420 | 0.7903 | 20.1960 | 2.2728 | *ng* | *ng* | *ng* | *ng* |
| 0.10 | 0.7280 | 0.6833 | 19.6289 | 2.2090 | *ng* | *ng* | *ng* | *ng* |

*ng* = mixture not a gas at this composition and pressure
$\chi$ = mole fraction
$Z$ = compressibility factor
$\eta$ = viscosity

Table 2: Predicted Compressibility and Viscosity of $H_2$-$CH_4$ Mixtures at 300K

| | $P = 7$ MPa | | | | $P = 15$ MPa | | | |
|---|---|---|---|---|---|---|---|---|
| $\chi_{H_2}$ | $Z$ | $Z/Z_{H_2}$ | $\eta$ ($\mu$Pa s) | $\eta/\eta_{H_2}$ | $Z$ | $Z/Z_{H_2}$ | $\eta$ ($\mu$Pa s) | $\eta/\eta_{H_2}$ |
| 1.00 | 1.0655 | 1.0000 | 8.8860 | 1.0000 | 1.1335 | 1.0000 | 8.8860 | 1.0000 |
| 0.90 | 1.0648 | 0.9993 | 10.5975 | 1.1926 | 1.1341 | 1.0005 | 10.5277 | 1.1848 |
| 0.80 | 1.0598 | 0.9947 | 11.6439 | 1.3104 | 1.1269 | 0.9942 | 11.8009 | 1.3280 |
| 0.70 | 1.0511 | 0.9865 | 12.5864 | 1.4164 | 1.1129 | 0.9818 | 13.0513 | 1.4688 |
| 0.60 | 1.0388 | 0.9750 | 13.2309 | 1.4890 | 1.0924 | 0.9637 | 13.9004 | 1.5643 |
| 0.50 | 1.0231 | 0.9602 | 13.5571 | 1.5257 | 1.0656 | 0.9401 | 14.4809 | 1.6296 |
| 0.40 | 1.0038 | 0.9421 | 13.6601 | 1.5373 | 1.0321 | 0.9106 | 14.8961 | 1.6764 |
| 0.30 | 0.9807 | 0.9204 | 13.6108 | 1.5317 | 0.9914 | 0.8746 | 15.2371 | 1.7147 |
| 0.20 | 0.9543 | 0.8956 | 13.4626 | 1.5150 | 0.9443 | 0.8331 | 15.5857 | 1.7540 |
| 0.10 | 0.9253 | 0.8684 | 13.2679 | 1.4931 | 0.8919 | 0.7869 | 16.0389 | 1.8050 |

$\chi$ = mole fraction
$Z$ = compressibility factor
$\eta$ = viscosity

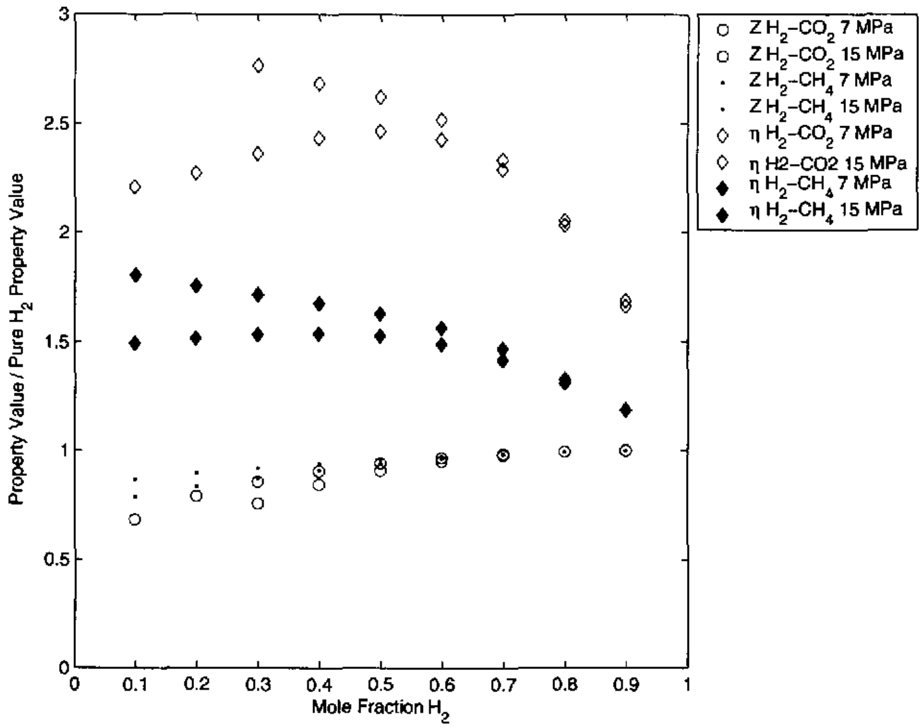


Figure 1: Predicted Compressibility ($Z$) and Viscosity ($\eta$) at $T = 300K$

# 5 Conclusions

The results of the supertrapp calculations indicate that the variability in gas flow rates and pressures due to differences in viscosity and compressibility of pure $H_2$ versus $H_2$-$CH_4$ is somewhat smaller than that seen for the $H_2$-$CO_2$ mixtures. Thus, the conclusion drawn in CCA Appendix MASS regarding the suitability of using $H_2$ gas properties in bragflo instead of actual waste gas properties should not be affected by the increased concentration of $CH_4$ in the repository that may result from emplacing the AMWTP supercompacted waste therein. Although not discussed in the CCA analysis, it is clear that the fracture model used in bragflo will not allow pressures to build within the repository to levels as large as those implied in this simplified radial flow analysis.

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# Appendix A: Input Files, User Interaction, and Output Files for supertrapp Calculations

## $H_2$-$CO_2$ Mixture supertrapp Input File (h2co2.inp)

```
COMP 1    HYDROGEN
COMP 2    CO2
FEED 1      1.0000
FEED 2       0.0000
FLTP      300        7.0
FEED 1      0.9000
FEED 2       0.1000
FLTP      300        7.0
FEED 1      0.8000
FEED 2       0.2000
FLTP      300        7.0
FEED 1      0.7000
FEED 2       0.3000
FLTP      300        7.0
FEED 1      0.6000
FEED 2       0.4000
FLTP      300        7.0
FEED 1      0.5000
FEED 2       0.5000
FLTP      300        7.0
FEED 1      0.4000
FEED 2       0.6000
FLTP      300        7.0
FEED 1      0.3000
FEED 2       0.7000
FLTP      300        7.0
FEED 1      0.2000
FEED 2       0.8000
FLTP      300        7.0
FEED 1      0.1000
FEED 2       0.9000
FLTP      300        7.0
FEED 1      1.0000
FEED 2       0.0000
FLTP      300        15.0
FEED 1      0.9000
FEED 2       0.1000
FLTP      300        15.0
FEED 1      0.8000
FEED 2       0.2000
FLTP      300        15.0
FEED 1      0.7000
FEED 2       0.3000
FLTP      300        15.0
FEED 1      0.6000
FEED 2       0.4000
FLTP      300        15.0
FEED 1      0.5000
FEED 2       0.5000
FLTP      300        15.0
FEED 1      0.4000
FEED 2       0.6000
FLTP      300        15.0
FEED 1      0.3000
FEED 2       0.7000
FLTP      300        15.0
FEED 1      0.2000
FEED 2       0.8000
FLTP      300        15.0
FEED 1      0.1000
FEED 2       0.9000
FLTP      300        15.0
$END
```

## User Interaction with supertrapp: $H_2$-$CO_2$ Mixture (Part 1/2)

```
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.

C:\PROGRA~1\NIST\sprtrap>strapp

          ************************************************************
          *         NIST Standard Reference Database 4               *
          *  NIST THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES  *
          *          Program SUPERTRAPP - Version 3.1                *
          *                                                          *
          *             Based on research sponsored by               *
          *              the NASA Lewis Research Center,             *
          *   the NIST Supercritical Fluid Property Consortium       *
          *              and Standard Reference Data                 *
          *                                                          *
          *                                                          *
          *     Physical and Chemical Properties Division            *
          *                                                          *
          *        Distributed by Standard Reference Data            *
          *     National Institute of Standards and Technology       *
          *            Gaithersburg, MD 20899 USA                    *
          *                                                          *
          *    Copyright 2003 by the U.S. Secretary of Commerce      *
          *        on behalf of the United States of America         *
          *                All rights reserved.                      *
          ************************************************************

For help in response to any question, enter "?".
For a brief description of SUPERTRAPP, enter "?".
Press enter to continue.

Do you want to use default settings? (Y/N)
(The default settings are whatever you last selected for units and file I/O.)
n

Do you want to input from a file (N/Y)? y
Please enter the name of the input file.  h2co2.inp
Do you want to output to a file (N/Y)? y
Please enter the output file name.  h2co2.out
Do you also want output to the terminal (Y/N) ? n

Do you want to change the units (N/Y) ? y



                           **************************
                           SUPERTRAPP 2.00 Property Unit Menu
                           **************************


Property    ***********************options********************** current

Temperature(K      ,R          ,C          ,F          ,          ,    ,   )K
Pressure   (atm    ,bar        ,MPa        ,Psig       ,Psia      ,mmHg,kpf)bar
Volume     (liter  ,m**3       ,cm**3      ,in**3      ,ft**3     ,    ,   )liter
Energy     (cal    ,J          ,btu        ,kcal       ,kJ        ,    ,   )kJ
Mass       (mol    ,lb-mol     ,kg         ,g          ,lb        ,    ,   )mol
Velocity   (m/s    ,cm/s       ,ft/s       ,in/s       ,          ,    ,   )m/s
Viscosity  (uP     ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,   ,    ,   )uP
Thm. Cond. (W/m.K  ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,    ,   )mW/m.K


default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/c  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )

Enter the new unit or default option (X to exit)?
```

## User Interaction with supertrapp: $H_2$-$CO_2$ Mixture (Part 2/2)

```
Enter the new unit or default option (X to exit)? 2


                                  ****************************
                                  SUPERTRAPP 2.00 Property Unit Menu
                                  ****************************

Property     ***************************options************************ current

Temperature(K       ,R          ,C          ,F          ,           ,     ,    )K
Pressure    (atm    ,bar        ,MPa        ,Psig       ,Psia       ,mmHg,kpf)MPa
Volume      (liter  ,m**3       ,cm**3      ,in**3      ,ft**3      ,     ,    )m**3
Energy      (cal    ,J          ,btu        ,kcal       ,kJ         ,     ,    )kJ
Mass        (mol    ,lb-mol     ,kg         ,g          ,lb         ,     ,    )kg
Velocity    (m/s    ,cm/s       ,ft/s       ,in/s       ,           ,     ,    )m/s
Viscosity   (uP     ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,         ,    )uPa.s
Thm. Cond.  (W/m.K  ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,     ,    )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )

Enter the new unit or default option (X to exit)? x


                                  ****************************
                                  SUPERTRAPP 2.00 Property Unit Menu
                                  ****************************

Property     ***************************options************************ current

Temperature(K       ,R          ,C          ,F          ,           ,     ,    )K
Pressure    (atm    ,bar        ,MPa        ,Psig       ,Psia       ,mmHg,kpf)MPa
Volume      (liter  ,m**3       ,cm**3      ,in**3      ,ft**3      ,     ,    )m**3
Energy      (cal    ,J          ,btu        ,kcal       ,kJ         ,     ,    )kJ
Mass        (mol    ,lb-mol     ,kg         ,g          ,lb         ,     ,    )kg
Velocity    (m/s    ,cm/s       ,ft/s       ,in/s       ,           ,     ,    )m/s
Viscosity   (uP     ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,         ,    )uPa.s
Thm. Cond.  (W/m.K  ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,     ,    )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )
The units have been reset as requested.

Do you want to enter compositions on a mass basis (N/Y)?n

Do you want to input composition as mole fractions
 (If the answer is no, input can be in moles)  (N/Y)?y


End-of-file encountered on input file
returing to interactive input mode
For a list of available options, type ? Otherwise
enter command or, if you wish to do a flash calculation,
enter T(K) and P(MPa) separated by a comma.
quit

 Program Terminated- Exiting NIST4

C:\PROGRA~1\NIST\sprtrap>_
```

## $H_2$-$CO_2$ Mixture supertrapp Output File (H2CO2.OUT)

```
 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen              1.00000     1.00000      1.06975
,Molar Basis
                       1.00000     1.00000      Feed Fraction
                       2.01588     2.01588      Molar Mass
                       1.06547     1.06547      Comp. Factor, Z
                       5.30972     5.30972      D, kg/m**3
                       105.994     105.994      H, kJ/kg
                       47.5940     47.5940      S, kJ/kg.K
                       15.5532     15.5532      Cp, kJ/kg.K
                                   1.36429      Cp/Cv
                                   1381.97      Sound Speed, m/s
                                 -0.685445      JT, K/MPa
                                   8.88598      Visc., uPa.s
                                  0.207163      Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.900000    0.900000     0.963460
 carbon dioxide       0.100000    0.100000     0.106332
,Molar Basis
                       1.00000     1.00000      Feed Fraction
                       6.21524     6.21524      Molar Mass
                       1.06586     1.06586      Comp. Factor, Z
                       16.3846     16.3846      D, kg/m**3
                      -6301.52    -6301.52      H, kJ/kg
                       17.1865     17.1865      S, kJ/kg.K
                       5.19483     5.19483      Cp, kJ/kg.K
                                   1.36054      Cp/Cv
                                   786.513      Sound Speed, m/s
                                 -0.562273      JT, K/MPa
                                   14.9953      Visc., uPa.s
                                  0.120653      Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.800000    0.800000     0.862734
 carbon dioxide       0.200000    0.200000     0.201542
,Molar Basis
                       1.00000     1.00000      Feed Fraction
                       10.4146     10.4146      Molar Mass
                       1.06118     1.06118      Comp. Factor, Z
                       27.5425     27.5425      D, kg/m**3
                      -7545.13    -7545.13      H, kJ/kg
                       11.1744     11.1744      S, kJ/kg.K
                       3.20290     3.20290      Cp, kJ/kg.K
                                   1.36268      Cp/Cv
                                   605.870      Sound Speed, m/s
                                 -0.280723      JT, K/MPa
                                   18.2596      Visc., uPa.s
                              0.932287E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.700000    0.700000     0.768031
 carbon dioxide       0.300000    0.300000     0.284669
,Molar Basis
                       1.00000     1.00000      Feed Fraction
                       14.6140     14.6140      Molar Mass
                       1.04979     1.04979      Comp. Factor, Z
                       39.0673     39.0673      D, kg/m**3
                      -8076.81    -8076.81      H, kJ/kg
                       8.57546     8.57546      S, kJ/kg.K
                       2.36564     2.36564      Cp, kJ/kg.K
                                   1.37143      Cp/Cv
                                   508.247      Sound Speed, m/s
                                  0.110189      JT, K/MPa
                                   20.3486      Visc., uPa.s
                              0.762434E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.600000    0.600000     0.677295
 carbon dioxide       0.400000    0.400000     0.358133
,Molar Basis
                       1.00000     1.00000      Feed Fraction
                       18.8133     18.8133      Molar Mass
                       1.03082     1.03082      Comp. Factor, Z
                       51.2191     51.2191      D, kg/m**3
                      -8373.46    -8373.46      H, kJ/kg
                       7.11116     7.11116      S, kJ/kg.K
                       1.91174     1.91174      Cp, kJ/kg.K
                                   1.38756      Cp/Cv
```

```
                                443.189     Sound Speed, m/s
                               0.651531     JT, K/MPa
                                21.5629     Visc., uPa.s
                               0.638032E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.500000     0.500000     0.588053
 carbon dioxide      0.500000     0.500000     0.424601
,Molar Basis
                      1.00000      1.00000     Feed Fraction
                      23.0127      23.0127     Molar Mass
                      1.00353      1.00353     Comp. Factor, Z
                      64.3556      64.3555     D, kg/m**3
                     -8563.97     -8563.97     H, kJ/kg
                      6.16202      6.16202     S, kJ/kg.K
                      1.63594      1.63594     Cp, kJ/kg.K
                                   1.41271     Cp/Cv
                                   384.407     Sound Speed, m/s
                                   1.34026     JT, K/MPa
                                   21.9005     Visc., uPa.s
                               0.540980E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.400000     0.400000     0.499117
 carbon dioxide      0.600000     0.600000     0.484253
,Molar Basis
                      1.00000      1.00000     Feed Fraction
                      27.2121      27.2121     Molar Mass
                     0.965513     0.965513     Comp. Factor, Z
                      79.0966      79.0956     D, kg/m**3
                     -8698.23     -8698.23     H, kJ/kg
                      5.48821      5.48821     S, kJ/kg.K
                      1.46683      1.46683     Cp, kJ/kg.K
                                   1.45209     Cp/Cv
                                   354.460     Sound Speed, m/s
                                   2.22665     JT, K/MPa
                                   21.6284     Visc., uPa.s
                               0.463975E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.300000     0.300000     0.410199
 carbon dioxide      0.700000     0.700000     0.537163
,Molar Basis
                      1.00000      1.00000     Feed Fraction
                      31.4114      31.4114     Molar Mass
                     0.913896     0.913896     Comp. Factor, Z
                      96.4583      96.4583     D, kg/m**3
                     -8799.78     -8799.78     H, kJ/kg
                      4.97597      4.97597     S, kJ/kg.K
                      1.38281      1.38281     Cp, kJ/kg.K
                                   1.51630     Cp/Cv
                                   319.364     Sound Speed, m/s
                                   3.36732     JT, K/MPa
                                   20.9860     Visc., uPa.s
                               0.403075E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.200000     0.200000     0.318836
 carbon dioxide      0.800000     0.800000     0.583846
,Molar Basis
                      1.00000      1.00000     Feed Fraction
                      35.6108      35.6108     Molar Mass
                     0.841994     0.841994     Comp. Factor, Z
                      118.692      118.692     D, kg/m**3
                     -8882.24     -8882.24     H, kJ/kg
                      4.56074      4.56074     S, kJ/kg.K
                      1.40443      1.40443     Cp, kJ/kg.K
                                   1.83707     Cp/Cv
                                   286.127     Sound Speed, m/s
                                   4.86347     JT, K/MPa
                                   20.1960     Visc., uPa.s
                               0.357280E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.100000     0.100000     0.215471
 carbon dioxide      0.900000     0.900000     0.624262
,Molar Basis
                      1.00000      1.00000     Feed Fraction
                      39.8101      39.8101     Molar Mass
                     0.728029     0.728029     Comp. Factor, Z
                      153.460      153.460     D, kg/m**3
```

```
                          -8957.33     -8957.33     H, kJ/kg
                           4.19172      4.19172     S, kJ/kg.K
                           1.69594      1.69594     Cp, kJ/kg.K
                                        1.96620     Cp/Cv
                                        250.333     Sound Speed, m/s
                                        6.91944     JT, K/MPa
                                        19.6289     Visc., uPa.s
                                      0.330200E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---    --Liquid--    ---Phi----
 hydrogen                1.00000      1.00000      1.15063
,Molar Basis
                           1.00000      1.00000     Feed Fraction
                           2.01588      2.01588     Molar Mass
                           1.13351      1.13351     Comp. Factor, Z
                           10.6950      10.6950     D, kg/m**3
                           189.082      189.082     H, kJ/kg
                           44.4270      44.4270     S, kJ/kg.K
                           15.6931      15.6931     Cp, kJ/kg.K
                                        1.36128     Cp/Cv
                                        1463.58     Sound Speed, m/s
                                      -0.648917     JT, K/MPa
                                        8.88598     Visc., uPa.s
                                       0.215994     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---    --Vapor---    ---Phi----
 hydrogen              0.900000     0.900000      1.03699
 carbon dioxide        0.100000     0.100000     0.114661
,Molar Basis
                           1.00000      1.00000     Feed Fraction
                           6.21524      6.21524     Molar Mass
                           1.13577      1.13577     Comp. Factor, Z
                           32.9085      32.9085     D, kg/m**3
                          -6278.55     -6278.55     H, kJ/kg
                           16.1448      16.1448     S, kJ/kg.K
                           5.27095      5.27095     Cp, kJ/kg.K
                                        1.36248     Cp/Cv
                                        838.552     Sound Speed, m/s
                                      -0.547614     JT, K/MPa
                                        14.7648     Visc., uPa.s
                                       0.129761     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---    --Vapor---    ---Phi----
 hydrogen              0.800000     0.800000     0.935108
 carbon dioxide        0.200000     0.200000     0.206505
,Molar Basis
                           1.00000      1.00000     Feed Fraction
                           10.4146      10.4146     Molar Mass
                           1.12908      1.12908     Comp. Factor, Z
                           55.4703      55.4703     D, kg/m**3
                          -7536.86     -7536.86     H, kJ/kg
                           10.5382      10.5382     S, kJ/kg.K
                           3.27749      3.27749     Cp, kJ/kg.K
                                        1.37363     Cp/Cv
                                        646.830     Sound Speed, m/s
                                      -0.346238     JT, K/MPa
                                        18.0631     Visc., uPa.s
                                       0.102604     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---    --Vapor---    ---Phi----
 hydrogen              0.700000     0.700000     0.846718
 carbon dioxide        0.300000     0.300000     0.274937
,Molar Basis
                           1.00000      1.00000     Feed Fraction
                           14.6140      14.6140     Molar Mass
                           1.11027      1.11027     Comp. Factor, Z
                           79.1558      79.1558     D, kg/m**3
                          -8077.44     -8077.44     H, kJ/kg
                           8.10684      8.10684     S, kJ/kg.K
                           2.44897      2.44897     Cp, kJ/kg.K
                                        1.39693     Cp/Cv
                                        544.019     Sound Speed, m/s
                                      -0.378833E-01 JT, K/MPa
                                        20.7417     Visc., uPa.s
                                      0.859313E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---    --Vapor---    ---Phi----
 hydrogen              0.600000     0.600000     0.768891
 carbon dioxide        0.400000     0.400000     0.325837
,Molar Basis
                           1.00000      1.00000     Feed Fraction
```

```
                     18.8133      18.8133     Molar Mass
                     1.07746      1.07746     Comp. Factor, Z
                     105.004      105.004     D, kg/m**3
                    -8381.43     -8381.43     H, kJ/kg
                     6.73085      6.73085     S, kJ/kg.K
                     2.01113      2.01113     Cp, kJ/kg.K
                                  1.43571     Cp/Cv
                                  474.970     Sound Speed, m/s
                                 0.376396     JT, K/MPa
                                  22.3739     Visc., uPa.s
                                 0.738962E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.500000     0.500000     0.698564
 carbon dioxide     0.500000     0.500000     0.364463
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     23.0127      23.0127     Molar Mass
                     1.02879      1.02879     Comp. Factor, Z
                     134.518      134.518     D, kg/m**3
                    -8579.08     -8579.08     H, kJ/kg
                     5.83281      5.83281     S, kJ/kg.K
                     1.76345      1.76345     Cp, kJ/kg.K
                                  1.49887     Cp/Cv
                                  422.589     Sound Speed, m/s
                                 0.898955     JT, K/MPa
                                  23.2925     Visc., uPa.s
                                 0.647554E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.400000     0.400000     0.637797
 carbon dioxide     0.600000     0.600000     0.390619
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     27.2121      27.2121     Molar Mass
                    0.958553     0.958553     Comp. Factor, Z
                     170.721      170.721     D, kg/m**3
                    -8721.68     -8721.68     H, kJ/kg
                     5.18658      5.18658     S, kJ/kg.K
                     1.65160      1.65160     Cp, kJ/kg.K
                                  1.60044     Cp/Cv
                                  378.972     Sound Speed, m/s
                                  1.55791     JT, K/MPa
                                  23.8523     Visc., uPa.s
                                 0.579651E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 hydrogen           0.300000     0.300000     0.599193
 carbon dioxide     0.700000     0.700000     0.402907
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     31.4114      31.4114     Molar Mass
                    0.858111     0.858111     Comp. Factor, Z
                     220.134      220.134     D, kg/m**3
                    -8834.83     -8834.83     H, kJ/kg
                     4.68060      4.68060     S, kJ/kg.K
                     1.70305      1.70305     Cp, kJ/kg.K
                                  1.79933     Cp/Cv
                                  340.060     Sound Speed, m/s
                                  2.34534     JT, K/MPa
                                  24.5776     Visc., uPa.s
                                 0.534817E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 No convergence at these conditions;        T(K)=          300.
                                            P(bar)=        150.

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 hydrogen           0.100000     0.100000      1.06878
 carbon dioxide     0.900000     0.900000     0.365127
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     39.8101      39.8101     Molar Mass
                    0.454068     0.454068     Comp. Factor, Z
                     527.248      527.248     D, kg/m**3
                    -9064.77     -9064.77     H, kJ/kg
                     3.74180      3.74180     S, kJ/kg.K
                     3.31037      3.31037     Cp, kJ/kg.K
                                  3.47846     Cp/Cv
                                  311.591     Sound Speed, m/s
                                  2.31189     JT, K/MPa
                                  40.6300     Visc., uPa.s
                                 0.655165E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)
```

## $H_2$-$CH_4$ Mixture supertrapp **Input File** (`h2ch4.inp`)

```
COMP 1      HYDROGEN
COMP 2      METHANE
FEED 1         1.0000
FEED 2          0.0000
FLTP        300          7.0
FEED 1         0.9000
FEED 2          0.1000
FLTP        300          7.0
FEED 1         0.8000
FEED 2          0.2000
FLTP        300          7.0
FEED 1         0.7000
FEED 2          0.3000
FLTP        300          7.0
FEED 1         0.6000
FEED 2          0.4000
FLTP        300          7.0
FEED 1         0.5000
FEED 2          0.5000
FLTP        300          7.0
FEED 1         0.4000
FEED 2          0.6000
FLTP        300          7.0
FEED 1         0.3000
FEED 2          0.7000
FLTP        300          7.0
FEED 1         0.2000
FEED 2          0.8000
FLTP        300          7.0
FEED 1         0.1000
FEED 2          0.9000
FLTP        300          7.0
FEED 1         1.0000
FEED 2          0.0000
FLTP        300          15.0
FEED 1         0.9000
FEED 2          0.1000
FLTP        300          15.0
FEED 1         0.8000
FEED 2          0.2000
FLTP        300          15.0
FEED 1         0.7000
FEED 2          0.3000
FLTP        300          15.0
FEED 1         0.6000
FEED 2          0.4000
FLTP        300          15.0
FEED 1         0.5000
FEED 2          0.5000
FLTP        300          15.0
FEED 1         0.4000
FEED 2          0.6000
FLTP        300          15.0
FEED 1         0.3000
FEED 2          0.7000
FLTP        300          15.0
FEED 1         0.2000
FEED 2          0.8000
FLTP        300          15.0
FEED 1         0.1000
FEED 2          0.9000
FLTP        300          15.0
$END
```

## User Interaction with supertrapp: $H_2$-$CH_4$ Mixture (Part 1/2)

```
C:\PROGRA~1\NIST\sprtrap>strapp

        ************************************************************
        *          NIST Standard Reference Database 4              *
        *  NIST THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES  *
        *           Program SUPERTRAPP - Version 3.1               *
        *                                                          *
        *            Based on research sponsored by                *
        *             the NASA Lewis Research Center,              *
        *   the NIST Supercritical Fluid Property Consortium       *
        *              and Standard Reference Data                 *
        *                                                          *
        *                                                          *
        *      Physical and Chemical Properties Division           *
        *                                                          *
        *         Distributed by Standard Reference Data           *
        *      National Institute of Standards and Technology      *
        *              Gaithersburg, MD 20899 USA                  *
        *                                                          *
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        *         on behalf of the United States of America        *
        *                  All rights reserved.                    *
        ************************************************************

For help in response to any question, enter "?".
For a brief description of SUPERTRAPP, enter "I".
Press enter to continue.

Do you want to use default settings? (Y/N)
(The default settings are whatever you last selected for units and file I/O.)
n

Do you want to input from a file (N/Y)? y
Please enter the name of the input file.  h2ch4.inp
Do you want to output to a file (N/Y)? y
Please enter the output file name.  h2ch4.out
Do you also want output to the terminal (Y/N) ? n

Do you want to change the units (N/Y) ? y



                           **************************
                           SUPERTRAPP 2.00 Property Unit Menu
                           **************************

Property     ************************options*********************** current

Temperature(K     ,R          ,C          ,F          ,          ,    ,    )K
Pressure   (atm   ,bar        ,MPa        ,Psig       ,Psia      ,mmHg,kpf)bar
Volume     (liter ,m**3       ,cm**3      ,in**3      ,ft**3     ,    ,    )liter
Energy     (cal   ,J          ,btu        ,kcal       ,kJ        ,    ,    )kJ
Mass       (mol   ,lb-mol     ,kg         ,g          ,lb        ,    ,    )mol
Velocity   (m/s   ,cm/s       ,ft/s       ,in/s       ,          ,    ,    )m/s
Viscosity  (uP    ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,       ,    )uP
Thm. Cond. (W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,       ,    )mW/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP      ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s   ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP      ,mW/m.K    )

Enter the new unit or default option (X to exit)?
```

```
Enter the new unit or default option (X to exit)? 2


                               ***************************
                               SUPERTRAPP 2.00 Property Unit Menu
                               ***************************

Property     ************************options**********************  current

Temperature(K      ,R         ,C          ,F          ,         ,     ,   >K
Pressure    (atm   ,bar       ,MPa        ,Psig       ,Psia     ,mmHg,kpf >MPa
Volume      (liter ,m**3      ,cm**3      ,in**3      ,ft**3    ,     ,   >m**3
Energy      (cal   ,J         ,btu        ,kcal       ,kJ       ,     ,   >kJ
Mass        (mol   ,lb-mol    ,kg         ,g          ,lb       ,     ,   >kg
Velocity    (m/s   ,cm/s      ,ft/s       ,in/s       ,         ,     ,   >m/s
Viscosity   (uP    ,cP        ,uPa.s      ,lb/ft.s    ,lb/ft.h, ,     ,   >uPa.s
Thm. Cond.  (W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,   ,     ,   >W/m.K

default set options

(1)  Scientific   (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP      ,cal/cm.s.K)
(2)  S.I.         (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s   ,W/m.K     )
(3)  Engineering  (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s ,btu/ft.h.F)
(4)  Mixed        (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP      ,mW/m.K    )

Enter the new unit or default option (X to exit)? x


                               ***************************
                               SUPERTRAPP 2.00 Property Unit Menu
                               ***************************

Property     ************************options**********************  current

Temperature(K      ,R         ,C          ,F          ,         ,     ,   >K
Pressure    (atm   ,bar       ,MPa        ,Psig       ,Psia     ,mmHg,kpf >MPa
Volume      (liter ,m**3      ,cm**3      ,in**3      ,ft**3    ,     ,   >m**3
Energy      (cal   ,J         ,btu        ,kcal       ,kJ       ,     ,   >kJ
Mass        (mol   ,lb-mol    ,kg         ,g          ,lb       ,     ,   >kg
Velocity    (m/s   ,cm/s      ,ft/s       ,in/s       ,         ,     ,   >m/s
Viscosity   (uP    ,cP        ,uPa.s      ,lb/ft.s    ,lb/ft.h, ,     ,   >uPa.s
Thm. Cond.  (W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,   ,     ,   >W/m.K

default set options

(1)  Scientific   (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP      ,cal/cm.s.K)
(2)  S.I.         (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s   ,W/m.K     )
(3)  Engineering  (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s ,btu/ft.h.F)
(4)  Mixed        (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP      ,mW/m.K    )

The units have been reset as requested.

Do you want to enter compositions on a mass basis (N/Y)?n

Do you want to input composition as mole fractions
 (If the answer is no, input can be in moles)  (N/Y)?y


End-of-file encountered on input file
returing to interactive input mode
For a list of available options, type ? Otherwise
enter command or, if you wish to do a flash calculation,
enter T(K) and P(MPa) separated by a comma.
quit

 Program Terminated- Exiting NIST4

C:\PROGRA~1\NIST\sprtrap>_
```

## $H_2$-$CH_4$ Mixture supertrapp Output File (H2CH4.OUT)

```
 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen              1.00000     1.00000      1.06975
,Molar Basis
                        1.00000      1.00000    Feed Fraction
                        2.01588      2.01688    Molar Mass
                        1.06547      1.06547    Comp. Factor, Z
                        5.30972      5.30972    D, kg/m**3
                        105.994      105.994    H, kJ/kg
                        47.5940      47.5940    S, kJ/kg.K
                        15.5532      15.5532    Cp, kJ/kg.K
                                     1.36429    Cp/Cv
                                     1381.97    Sound Speed, m/s
                                   -0.686445    JT, K/MPa
                                     8.88598    Visc., uPa.s
                                    0.207163    Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.900000    0.900000     0.962958
 methane              0.100000    0.100000     0.105464
,Molar Basis
                        1.00000      1.00000    Feed Fraction
                        3.41854      3.41854    Molar Mass
                        1.06475      1.06475    Comp. Factor, Z
                        9.01033      9.01033    D, kg/m**3
                       -2138.53     -2138.63    H, kJ/kg
                        30.4379      30.4379    S, kJ/kg.K
                        9.42530      9.42630    Cp, kJ/kg.K
                                     1.36416    Cp/Cv
                                     1060.98    Sound Speed, m/s
                                   -0.513224    JT, K/MPa
                                     10.5975    Visc., uPa.s
                                    0.152315    Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.800000    0.800000     0.858835
 methane              0.200000    0.200000     0.203645
,Molar Basis
                        1.00000      1.00000    Feed Fraction
                        4.82120      4.82120    Molar Mass
                        1.05982      1.05982    Comp. Factor, Z
                        12.7665      12.7665    D, kg/m**3
                       -3081.22     -3081.22    H, kJ/kg
                        23.0001      23.0001    S, kJ/kg.K
                        6.87312      6.87312    Cp, kJ/kg.K
                                     1.36679    Cp/Cv
                                     890.828    Sound Speed, m/s
                                   -0.270804    JT, K/MPa
                                     11.6439    Visc., uPa.s
                                    0.123805    Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.700000    0.700000     0.758297
 methane              0.300000    0.300000     0.296426
,Molar Basis
                        1.00000      1.00000    Feed Fraction
                        6.22385      6.22385    Molar Mass
                        1.05110      1.05110    Comp. Factor, Z
                        16.6174      16.6174    D, kg/m**3
                       -3601.95     -3601.95    H, kJ/kg
                        18.8236      18.8236    S, kJ/kg.K
                        5.47976      5.47976    Cp, kJ/kg.K
                                     1.37206    Cp/Cv
                                     779.918    Sound Speed, m/s
                                0.303452E-01    JT, K/MPa
                                     12.5864    Visc., uPa.s
                                    0.104744    Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen             0.600000    0.600000     0.654423
 methane              0.400000    0.400000     0.385164
,Molar Basis
                        1.00000      1.00000    Feed Fraction
                        7.62651      7.62651    Molar Mass
                        1.03884      1.03884    Comp. Factor, Z
                        20.6028      20.6028    D, kg/m**3
                       -3933.49     -3933.49    H, kJ/kg
                        16.1271      16.1271    S, kJ/kg.K
                        4.60756      4.60756    Cp, kJ/kg.K
                                     1.38002    Cp/Cv
```

```
                                 699.254      Sound Speed, m/s
                                0.384487      JT, K/MPa
                                 13.2309      Visc., uPa.s
                                0.904899E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.500000     0.500000     0.552381
 methane             0.500000     0.500000     0.470870
,Molar Basis
                      1.00000      1.00000      Feed Fraction
                      9.02917      9.02917      Molar Mass
                      1.02310      1.02310      Comp. Factor, Z
                      24.7674      24.7674      D, kg/m**3
                     -4164.05     -4164.05      H, kJ/kg
                      14.2261      14.2261      S, kJ/kg.K
                      4.01634      4.01634      Cp, kJ/kg.K
                                   1.39099      Cp/Cv
                                   636.366      Sound Speed, m/s
                                  0.790206      JT, K/MPa
                                   13.6571      Visc., uPa.s
                                  0.791983E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.400000     0.400000     0.449343
 methane             0.600000     0.600000     0.554345
,Molar Basis
                      1.00000      1.00000      Feed Fraction
                      10.4318      10.4318      Molar Mass
                      1.00378      1.00378      Comp. Factor, Z
                      29.1655      29.1655      D, kg/m**3
                     -4334.56     -4334.56      H, kJ/kg
                      12.8007      12.8007      S, kJ/kg.K
                      3.59665      3.59665      Cp, kJ/kg.K
                                   1.40555      Cp/Cv
                                   584.821      Sound Speed, m/s
                                   1.25009      JT, K/MPa
                                   13.6601      Visc., uPa.s
                                  0.699759E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.300000     0.300000     0.344342
 methane             0.700000     0.700000     0.636312
,Molar Basis
                      1.00000      1.00000      Feed Fraction
                      11.8345      11.8345      Molar Mass
                     0.980653     0.980653      Comp. Factor, Z
                      33.8675      33.8675      D, kg/m**3
                     -4466.64     -4466.64      H, kJ/kg
                      11.6796      11.6796      S, kJ/kg.K
                      3.29291      3.29291      Cp, kJ/kg.K
                                   1.42474      Cp/Cv
                                   540.953      Sound Speed, m/s
                                   1.77043      JT, K/MPa
                                   13.6108      Visc., uPa.s
                                  0.623318E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.200000     0.200000     0.235883
 methane             0.800000     0.800000     0.718648
,Molar Basis
                      1.00000      1.00000      Feed Fraction
                      13.2371      13.2371      Molar Mass
                     0.954269     0.954269      Comp. Factor, Z
                      38.9289      38.9289      D, kg/m**3
                     -4572.46     -4572.46      H, kJ/kg
                      10.7618      10.7618      S, kJ/kg.K
                      3.07309      3.07309      Cp, kJ/kg.K
                                   1.44921      Cp/Cv
                                   502.756      Sound Speed, m/s
                                   2.34073      JT, K/MPa
                                   13.4626      Visc., uPa.s
                                  0.559476E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  7.00000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen            0.100000     0.100000     0.121972
 methane             0.900000     0.900000     0.803363
,Molar Basis
                      1.00000      1.00000      Feed Fraction
                      14.6398      14.6398      Molar Mass
                     0.925288     0.925288      Comp. Factor, Z
                      44.4025      44.4025      D, kg/m**3
```

```
                    -4659.50      -4659.50     H, kJ/kg
                     9.97926       9.97926     S, kJ/kg.K
                     2.91788       2.91788     Cp, kJ/kg.K
                                   1.47981     Cp/Cv
                                   469.012     Sound Speed, m/s
                                   2.94702     JT, K/MPa
                                   13.2679     Visc., uPa.s
                               0.606119E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 hydrogen            1.00000       1.00000     1.15063
,Molar Basis
                     1.00000       1.00000     Feed Fraction
                     2.01588       2.01588     Molar Mass
                     1.13351       1.13351     Comp. Factor, Z
                     10.6950       10.6950     D, kg/m**3
                     189.082       189.082     H, kJ/kg
                     44.4270       44.4270     S, kJ/kg.K
                     15.6931       15.6931     Cp, kJ/kg.K
                                   1.36128     Cp/Cv
                                   1463.58     Sound Speed, m/s
                                 -0.648917     JT, K/MPa
                                   8.88598     Visc., uPa.s
                                  0.215994     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.900000      0.900000     1.03605
 methane            0.100000      0.100000    0.112889
,Molar Basis
                     1.00000       1.00000     Feed Fraction
                     3.41854       3.41854     Molar Mass
                     1.13406       1.13406     Comp. Factor, Z
                     18.1278       18.1278     D, kg/m**3
                    -2099.42      -2099.42     H, kJ/kg
                     28.5380       28.5380     S, kJ/kg.K
                     9.57208       9.57208     Cp, kJ/kg.K
                                   1.36764     Cp/Cv
                                   1129.02     Sound Speed, m/s
                                 -0.518252     JT, K/MPa
                                   10.5277     Visc., uPa.s
                                  0.161590     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.800000      0.800000    0.927053
 methane            0.200000      0.200000    0.210697
,Molar Basis
                     1.00000       1.00000     Feed Fraction
                     4.82120       4.82120     Molar Mass
                     1.12690       1.12690     Comp. Factor, Z
                     25.7284       25.7284     D, kg/m**3
                    -3064.35      -3064.35     H, kJ/kg
                     21.6248       21.6248     S, kJ/kg.K
                     7.03081       7.03081     Cp, kJ/kg.K
                                   1.37861     Cp/Cv
                                   951.142     Sound Speed, m/s
                                 -0.384229     JT, K/MPa
                                   11.8009     Visc., uPa.s
                                  0.133455     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.700000      0.700000    0.821487
 methane            0.300000      0.300000    0.297819
,Molar Basis
                     1.00000       1.00000     Feed Fraction
                     6.22385       6.22385     Molar Mass
                     1.11287       1.11287     Comp. Factor, 2
                     33.6322       33.6322     D, kg/m**3
                    -3600.12      -3600.12     H, kJ/kg
                     17.7324       17.7324     S, kJ/kg.K
                     5.65151       5.65151     Cp, kJ/kg.K
                                   1.39432     Cp/Cv
                                   834.657     Sound Speed, m/s
                                 -0.107154     JT, H/MPa
                                   13.0513     Visc., uPa.s
                                  0.114723     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.600000      0.600000    0.717578
 methane            0.400000      0.400000    0.377147
,Molar Basis
                     1.00000       1.00000     Feed Fraction
```

```
                     7.62651      7.62651     Molar Mass
                     1.09241      1.09241     Comp. Factor, Z
                     41.9840      41.9840     D, kg/m**3
                    -3943.49     -3943.49     H, kJ/kg
                     16.2116      16.2116     S, kJ/kg.K
                     4.79772      4.79772     Cp, kJ/kg.K
                                  1.41641     Cp/Cv
                                  749.466     Sound Speed, m/s
                                 0.157559     JT, K/MPa
                                  13.9004     Visc., uPa.s
                                 0.100770     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.500000     0.500000     0.613741
 methane            0.500000     0.500000     0.460669
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     9.02917      9.02917     Molar Mass
                     1.06558      1.06558     Comp. Factor, Z
                     50.9572      50.9572     D, kg/m**3
                    -4184.40     -4184.40     H, kJ/kg
                     13.4282      13.4282     S, kJ/kg.K
                     4.23169      4.23169     Cp, kJ/kg.K
                                  1.44313     Cp/Cv
                                  682.646     Sound Speed, m/s
                                 0.457869     JT, K/MPa
                                  14.4809     Visc., uPa.s
                                 0.897750E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 hydrogen           0.400000     0.400000     0.508339
 methane            0.600000     0.600000     0.519847
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     10.4318      10.4318     Molar Mass
                     1.03212      1.03212     Comp. Factor, Z
                     60.7814      60.7814     D, kg/m**3
                    -4364.71     -4364.71     H, kJ/kg
                     12.0841      12.0841     S, kJ/kg.K
                     3.84797      3.84797     Cp, kJ/kg.K
                                  1.47970     Cp/Cv
                                  627.590     Sound Speed, m/s
                                 0.794117     JT, K/MPa
                                  14.8961     Visc., uPa.s
                                 0.808683E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 hydrogen           0.300000     0.300000     0.399298
 methane            0.700000     0.700000     0.585920
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     11.8345      11.8345     Molar Mass
                    0.991397     0.991397     Comp. Factor, Z
                     71.7867      71.7867     D, kg/m**3
                    -4506.81     -4506.81     H, kJ/kg
                     11.0196      11.0196     S, kJ/kg.K
                     3.59774      3.59774     Cp, kJ/kg.K
                                  1.52896     Cp/Cv
                                  580.514     Sound Speed, m/s
                                  1.16777     JT, K/MPa
                                  15.2371     Visc., uPa.s
                                 0.735930E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 hydrogen           0.200000     0.200000     0.282715
 methane            0.800000     0.800000     0.652401
,Molar Basis
                     1.00000      1.00000     Feed Fraction
                     13.2371      13.2371     Molar Mass
                    0.944281     0.944281     Comp. Factor, Z
                     84.3015      84.3015     D, kg/m**3
                    -4623.10     -4623.10     H, kJ/kg
                     10.1401      10.1401     S, kJ/kg.K
                     3.46582      3.46582     Cp, kJ/kg.K
                                  1.59483     Cp/Cv
                                  539.661     Sound Speed, m/s
                                  1.56241     JT, K/MPa
                                  15.5857     Visc., uPa.s
                                 0.676295E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.0000     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
```

```
hydrogen            0.100000    0.100000    0.152954
methane             0.900000    0.900000    0.723259
,Molar Basis
                     1.00000     1.00000    Feed Fraction
                     14.6398     14.6398    Molar Mass
                    0.891926    0.891925    Comp. Factor, Z
                     98.7073     98.7073    D, kg/m**3
                    -4721.20    -4721.20    H, kJ/kg
                     9.38161     9.38161    S, kJ/kg.K
                     3.41044     3.41044    Cp, kJ/kg.K
                                 1.68229    Cp/Cv
                                 504.265    Sound Speed, m/s
                                 1.95136    JT, K/MPa
                                 16.0389    Visc., uPa.s
                                0.627646E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)
```

# Appendix B: supertrapp Code Verification

## B.1 Code Description

**Identification**

NIST Standard Reference Database 4
NIST Thermophysical Properties of Hydrocarbon Mixtures Database (SUPERTRAPP)
Version 3.1
February 2003

**Author**

M.L. Huber
National Institute of Standards and Technology (NIST)
Physical and Chemical Properties Division
Boulder, CO

**Vendor**

U.S. Department of Commerce
National Institute of Standards and Technology (NIST)
Standard Reference Data Program
Gaithersburg, MD 20899

**Abstract**

NIST `supertrapp` is an interactive computer program for the prediction of thermodynamic properties of mixtures. It may be used for pure fluids or for mixtures of up to 20 components. NIST `supertrapp` performs phase equilibria calculations and gives the thermophysical properties of all phases and the feed. These results include both equilibrium properties (density, compressibility factor, enthalpy, entropy, specific heats, sound speed, Joule-Thompson coefficient) and transport properties (viscosity and thermal conductivity).

**Usage in this Analysis**

The `supertrapp` code was used to calculate compressibility factors and viscosity for pure $H_2$ gas and for gas mixtures ( $H_2$-$CO_2$ and $H_2$-$CH_4$) over a range of compositions. These calculations were performed at a temperature of 300K and for pressures ranging from 7 to 15 Mpa.

## B.2 Verification Procedure

The NIST supertrapp code was verified using a two-step procedure. First an installation check was performed by comparing the results of two sample calculations run on the target platform (a PC workstation running the Windows XP operating system, Version 5.1.2600) with sample output files provided by the code author. Next, a series of tests were performed to compare values of viscosity and compressibility predicted by supertrapp to values reported in the scientific literature.

### B.2.1 Installation Check

For the installation check, we select a 50/50 by mole mixture of C1/C4 and perform flash calculations at T=300K for P=20 bar and P=1 bar. We compare the results with those obtained by the code author on the her machine.

### B.2.2 Comparison of supertrapp Results with Literature Values

The supertrapp code is used in this analysis to compute compressibility and viscosity for $H_2$-$CO_2$ and $H_2$-$CH_4$ mixtures at 300K over a range of pressures. In order to verify supertrapp for this purpose, supertrapp compressibility and viscosity predictions are compared with values published in the scientific literature for similar temperature and pressures. Since data for $H_2$-$CO_2$ and $H_2$-$CH_4$ mixtures are not readily available, this comparison is performed for pure $H_2$, $CO_2$, and $CH_4$, as well as a natural gas mixture composed of $CH_4$, $C_2H_6$, $C_3H_8$, $N_2$, and $CO_2$. A summary of the cases used for comparison is given in Table 3.

Table 3: Summary of supertrapp Verification Tests

| Name | Composition | Temperature (K) | Pressure (MPa) | Reference |
|---|---|---|---|---|
| Hydrogen | $H_2$ | $\approx$ 298 | $\approx$ 5-20 | [11] |
| Carbon Dioxide | $CO_2$ | 300 | $\approx$ 7-18 | [5] |
| Methane | $CH_4$ | $\approx$ 293 | $\approx$ 4-18 | [8] |
| Natural Gas | $CH_4$, 84.84 mol %; $C_2H_6$, 8.4 mol %; $C_3H_8$, 0.50 mol %; $N_2$, 5.60 mol %; $CO_2$, 0.66 mol % | $\approx$ 294 | $\approx$ 4-14 | [2] |

For $H_2$, we use reported values for both compressibility factor and for viscosity. For the other gases and for the natural gas mixture, we compute the compressibility factor from the reported temperature, pressure, density, and composition according to the following formula

$$Z = \frac{P}{\rho RT} \tag{3}$$

where $P$ is the absolute pressure, $\rho$ is the density, and $R$ is the gas constant for the gas in question. The gas constant for a specific gas can be computed from

$$R = \frac{\mathcal{R}}{mw} \tag{4}$$

where $\mathcal{R}$ is the universal gas constant and $mw$ is the molecular weight. In this analysis, we use $\mathcal{R} = 8314.4 \quad (N \cdot m)/(kg \cdot mole \cdot K)$. The molecular weights for the various gases calculated from their molecular formula and atomic weights obtained from [12] are shown in Table 4 along with the calculated gas constant for each.

Table 4: Atomic and Molecular Data Used in `supertrapp` Verification

| Atomic Data from [12] | | | |
|---|---|---|---|
| Name | Symbol | Atomic Weight | |
| Hydrogen | H | 1.00794 | |
| Carbon | C | 12.0107 | |
| Nitrogen | N | 14.0067 | |
| Oxygen | O | 15.9994 | |
| Computed Molecular Data | | | |
| Name | Composition | Molecular Weight | R $(N \cdot m/kg/K)$ |
| Hydrogen | $H_2$ | 2.01588 | 4124.5 |
| Carbon Dioxide | $CO_2$ | 44.0095 | 188.9 |
| Methane | $CH_4$ | 16.0425 | 518.2709 |
| Natural Gas | $CH_4$, 84.84 mol %; $C_2H_6$, 8.4 mol %; $C_3H_8$, 0.50 mol %; $N_2$, 5.60 mol %; $CO_2$, 0.66 mol % | 18.2159 | 456.4 |

The input files, recorded user interaction with `supertrapp`, and output files for the verification exercises are included in section B.4.

## B.3 Verification Results and Conclusions

### B.3.1 Installation Check Results

The results of the flash calculations were written to the file `chk_01.out` which we compare to the file `sampleca.txt` supplied by the code author. Comparison of the files shows that they contain identical results.

## CHK_01.OUT Listing

```
 2-Phase Flash results at T =  300.000 K and P =  20.0000     bar
-----Component------ ---Feed---   --Liquid--   --Vapor---    ---Phi----   --K--
 methane              0.500000     0.933345E-01 0.834113      0.812336     .89E+01
 n-butane             0.500000     0.906666     0.165887      0.122120     .18E+00
,Molar Basis
                       1.00000     0.451029     0.548971      Feed Fraction
                       37.0823     54.1947      23.0229       Molar Mass
                      0.543842     0.785324E-01 0.926136      Comp. Factor, Z
                      0.646733E-01 0.553336     0.199327E-01  D, g/cm**3
                      -2.95670     -2.60142     -3.64380      H, kJ/g
                       5.46448      4.14421      8.01785      S, J/g.K
                       2.42781      2.52442      2.24096      Cp, J/g.K
                                    1.47193      1.29326      Cp/Cv
                                    856.526      346.364      Sound Speed, m/s
                                   -0.216219E-01 0.631247     JT, K/bar
                                    139.662      10.8666      Visc., uPa.s
                                    108.054      31.2262      Th. Cond.,mW/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  1.00000     bar
-----Component------ ---Feed---   --Vapor---   ---Phi----
 methane              0.500000     0.500000     0.501146
 n-butane             0.500000     0.500000     0.489220
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       37.0823      37.0823     Molar Mass
                      0.990291     0.990291     Comp. Factor, Z
                      0.150126E-02 0.150126E-02 D, g/cm**3
                      -2.70883     -2.70883     H, kJ/g
                       6.85816      6.85816     S, J/g.K
                       1.85481      1.85481     Cp, J/g.K
                                    1.14417     Cp/Cv
                                    274.703     Sound Speed, m/s
                                    1.11512     JT, K/bar
                                    8.98036     Visc., uPa.s
                                    20.9478     Th. Cond.,mW/m.K
 (VLE=PRS,PROPS=EXCST)
```

## Sampleca.txt Listing

```
 2-Phase Flash results at T =  300.000 K and P =  20.0000     bar
-----Component------ ---Feed---   --Liquid--   --Vapor---    ---Phi----   --K--
 methane              0.500000     0.933345E-01 0.834113      0.812336     .89E+01
 n-butane             0.500000     0.906666     0.165887      0.122120     .18E+00
,Molar Basis
                       1.00000     0.451029     0.548971      Feed Fraction
                       37.0823     54.1947      23.0229       Molar Mass
                      0.543842     0.785324E-01 0.926136      Comp. Factor, Z
                      0.646733E-01 0.553336     0.199327E-01  D, g/cm**3
                      -2.95670     -2.60142     -3.64380      H, kJ/g
                       5.46448      4.14421      8.01785      S, J/g.K
                       2.42781      2.52442      2.24096      Cp, J/g.K
                                    1.47193      1.29326      Cp/Cv
                                    856.526      346.364      Sound Speed, m/s
                                   -0.216219E-01 0.631247     JT, K/bar
                                    139.662      10.8666      Visc., uPa.s
                                    108.054      31.2262      Th. Cond.,mW/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  1.00000     bar
-----Component------ ---Feed---   --Vapor---   ---Phi----
 methane              0.500000     0.500000     0.501146
 n-butane             0.500000     0.500000     0.489220
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       37.0823      37.0823     Molar Mass
                      0.990291     0.990291     Comp. Factor, Z
                      0.150126E-02 0.150126E-02 D, g/cm**3
                      -2.70883     -2.70883     H, kJ/g
                       6.85816      6.85816     S, J/g.K
                       1.85481      1.85481     Cp, J/g.K
                                    1.14417     Cp/Cv
                                    274.703     Sound Speed, m/s
                                    1.11512     JT, K/bar
                                    8.96036     Visc., uPa.s
                                    20.9478     Th. Cond.,mW/m.K
 (VLE=PRS,PROPS=EXCST)
```

### B.3.2 Comparison of supertrapp Results with Literature Values

The comparison of `supertrapp` results for compressibility and viscosity of $H_2$ with published values [11] is shown in Table 5. In this case, the literature values are not direct measurements, but rather correlations to based upon experimental data. We note that the `supertrapp` predictions agree with the published values to within 5%. The uncertainty in the literature values was not reported.

Table 5: `supertrapp` Results Compared with Literature Values: $H_2$

| $P$ (MPa) | $Z$ (-) | $Z_{st}$ (-) | $\Delta Z$ (%) | $\eta$ ($\mu$Pa ·s) | $\eta_{st}$ ($\mu$Pa ·s) | $\Delta\eta$ (%) |
|---|---|---|---|---|---|---|
| 3.040 | 1.0182 | 1.0295 | 1.1118 | | | |
| 5.066 | 1.0303 | 1.0484 | 1.7529 | 8.9500 | 8.8480 | -1.1399 |
| 10.133 | 1.0613 | 1.0932 | 3.0095 | 9.0500 | 8.8480 | -2.2323 |
| 15.199 | 1.0929 | 1.1359 | 3.9317 | | | |
| 20.265 | 1.1252 | 1.1770 | 4.6081 | 9.3100 | 8.8480 | -4.9626 |

$Z$ = compressibility factor
$\eta$ = viscosity
$(\cdot)_{st}$ = `supertrapp` computed value

Comparison of `supertrapp` results for compressibility and viscosity of $CO_2$ with published values [5] is shown in Table 6. We note that the `supertrapp` predictions agree with the published values to within 2%. The estimated experimental error in the published values is approximately 2%.

Table 6: `supertrapp` Results Compared with Literature Values: $CO_2$

| $P$ (MPa) | $\rho$ (kg/m$^3$) | $Z$ (-) | $Z_{st}$ (-) | $\Delta Z$ (%) | $\eta$ ($\mu$Pa ·s) | $\eta_{st}$ ($\mu$Pa ·s) | $\Delta\eta$ (%) |
|---|---|---|---|---|---|---|---|
| 7.365 | 728.357 | 0.1784 | 0.1774 | -0.5430 | 61.4000 | 61.1858 | -0.3489 |
| 10.169 | 792.171 | 0.2265 | 0.2229 | -1.5709 | 73.6000 | 73.1707 | -0.5833 |
| 13.060 | 846.259 | 0.2723 | 0.2730 | 0.2441 | 81.9000 | 80.8654 | -1.2632 |
| 14.310 | 859.814 | 0.2937 | 0.2945 | 0.2922 | 83.5000 | 83.6430 | 0.1713 |
| 15.295 | 869.364 | 0.3104 | 0.3114 | 0.3200 | 86.4000 | 85.6799 | -0.8334 |
| 16.773 | 882.346 | 0.3354 | 0.3366 | 0.3606 | 88.5000 | 88.5405 | 0.0458 |
| 17.761 | 890.268 | 0.3520 | 0.3534 | 0.3838 | 92.1000 | 90.3452 | -1.9053 |

$Z$ = compressibility factor
$\eta$ = viscosity
$(\cdot)_{st}$ = `supertrapp` computed value

The comparison of supertrapp results for compressibility and viscosity of $CH_4$ with published values [8] is shown in Table 7. We note that the supertrapp predictions agree with the published values to within 3%. The reported uncertainty in the measured values is ±0.15 to ±0.4% for viscosity and ±0.02 to ±0.05%

Table 7: supertrapp Results Compared with Literature Values: $CH_4$

| $P$ (MPa) | $\rho$ (kg/m$^3$) | $Z$ (-) | $Z_{st}$ (-) | $\Delta Z$ (%) | $\eta$ ($\mu$Pa ·s) | $\eta_{st}$ ($\mu$Pa ·s) | $\Delta\eta$ (%) |
|---|---|---|---|---|---|---|---|
| 4.219 | 30.017 | 0.9251 | 0.9237 | -0.1527 | 11.8070 | 11.9758 | 1.4297 |
| 7.912 | 60.058 | 0.8671 | 0.8680 | 0.1011 | 12.9660 | 13.2580 | 2.2520 |
| 11.298 | 89.924 | 0.8269 | 0.8315 | 0.5506 | 14.4280 | 14.8331 | 2.8077 |
| 11.310 | 90.033 | 0.8268 | 0.8314 | 0.5534 | 14.4420 | 14.8392 | 2.7503 |
| 14.702 | 120.156 | 0.8053 | 0.8117 | 0.7853 | 16.2930 | 16.7122 | 2.5729 |
| 18.351 | 150.057 | 0.8049 | 0.8113 | 0.7977 | 18.5350 | 18.9284 | 2.1225 |

$Z$ = compressibility factor
$\eta$ = viscosity
$(\cdot)_{st}$ = supertrapp computed value

The comparison with literature values for the natural gas mixture is shown in Table 8. We note that the supertrapp predictions agree with the published values to within approximately 3%. The uncertainty of the reported measurements is estimated to be ±1%.

Table 8: supertrapp Results Compared with Literature Values: Natural Gas Mixture

| $T$ (K) | $P$ (MPa) | $\rho$ (kg/m$^3$) | $Z$ (-) | $Z_{st}$ (-) | $\Delta Z$ (%) | $\eta$ ($\mu$Pa ·s) | $\eta_{st}$ ($\mu$Pa ·s) | $\Delta\eta$ (%) |
|---|---|---|---|---|---|---|---|---|
| 293.963 | 0.310 | 2.326 | 0.9933 | 0.9935 | 0.0173 | 11.4400 | 11.5134 | 0.6416 |
| 293.956 | 2.060 | 16.050 | 0.9566 | 0.9569 | 0.0287 | 11.5800 | 11.8013 | 1.9111 |
| 293.949 | 4.030 | 32.760 | 0.9169 | 0.9171 | 0.0293 | 12.0500 | 12.2951 | 2.0340 |
| 293.929 | 6.020 | 51.090 | 0.8783 | 0.8801 | 0.2100 | 12.6500 | 12.9780 | 2.5929 |
| 293.929 | 8.040 | 71.090 | 0.8430 | 0.8473 | 0.5094 | 13.4700 | 13.8560 | 2.8656 |
| 293.924 | 10.080 | 92.140 | 0.8155 | 0.8200 | 0.5543 | 14.4700 | 14.9180 | 3.0961 |
| 293.936 | 12.190 | 114.980 | 0.7902 | 0.7989 | 1.0972 | 15.7700 | 16.1824 | 2.6151 |
| 293.963 | 14.040 | 134.460 | 0.7782 | 0.7873 | 1.1623 | 17.0200 | 17.4062 | 2.2691 |

$Z$ = compressibility factor
$\eta$ = viscosity
$(\cdot)_{st}$ = supertrapp computed value

### B.3.3 Conclusions

The supertrapp predictions of compressibility factor and viscosity agree with the published values to within 5% over a wide range of compositions and pressures. For the application reported in this memo, we are interested in compressibility and viscosity changes with changing gas composition that are 1-2 orders of magnitude larger than this estimated uncertainty in the supertrapp results. Thus we conclude that the use of supertrapp is appropriate for this application.

## B.4 Input Files, User Interaction, and Output Files for supertrapp Verification

### B.4.1 $H_2$

$H_2$: supertrapp Input File (h2.inp)

```
COMP 1    HYDROGEN
FEED 1       1.0000
FLTP      298.15       3.03975
FEED 1       1.0000
FLTP      298.15       5.06625
FEED 1       1.0000
FLTP      298.15      10.1325
FEED 1       1.0000
FLTP      298.15      15.19875
FEED 1       1.0000
FLTP      298.15      20.265
$END
```

## $H_2$: User Interaction with supertrapp (Part 1/2)

```
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.

C:\PROGRA~1\NIST\sprtrap>strapp

        ************************************************************
        *             NIST Standard Reference Database 4           *
        *  NIST THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES  *
        *            Program SUPERTRAPP - Version 3.1              *
        *                                                          *
        *               Based on research sponsored by             *
        *              the NASA Lewis Research Center,             *
        *     the NIST Supercritical Fluid Property Consortium    *
        *              and Standard Reference Data                 *
        *                                                          *
        *                                                          *
        *       Physical and Chemical Properties Division         *
        *                                                          *
        *          Distributed by Standard Reference Data         *
        *     National Institute of Standards and Technology      *
        *              Gaithersburg, MD 20899 USA                  *
        *                                                          *
        *     Copyright 2003 by the U.S. Secretary of Commerce    *
        *        on behalf of the United States of America        *
        *                  All rights reserved.                    *
        ************************************************************

For help in response to any question, enter "?".
For a brief description of SUPERTRAPP, enter "?".
Press enter to continue.

Do you want to use default settings? (Y/N)
(The default settings are whatever you last selected for units and file I/O.)
n

Do you want to input from a file (N/Y)? y
Please enter the name of the input file.  h2.inp
Do you want to output to a file (N/Y)? y
Please enter the output file name.  h2.out
Do you also want output to the terminal (Y/N) ? n

Do you want to change the units (N/Y) ? y



                           **************************
                           SUPERTRAPP 2.00 Property Unit Menu
                           **************************

Property     ************************options************************  current

Temperature<K     ,R        ,C         ,F         ,          ,    ,    >K
Pressure   <atm   ,bar      ,MPa       ,Psig      ,Psia      ,mmHg,kpf)bar
Volume     <liter ,m**3     ,cm**3     ,in**3     ,ft**3     ,    ,    >liter
Energy     <cal   ,J        ,btu       ,kcal      ,kJ        ,    ,    >kJ
Mass       <mol   ,lb-mol   ,kg        ,g         ,lb        ,    ,    >mol
Velocity   <m/s   ,cm/s     ,ft/s      ,in/s      ,          ,    ,    >m/s
Viscosity  <uP    ,cP       ,uPa.s     ,lb/ft.s   ,lb/ft.h,       ,    >uP
Thm. Cond. <W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,      ,    >mW/m.K

default set options

(1)  Scientific  <K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP      ,cal/cm.s.K>
(2)  S.I.        <K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s   ,W/m.K     >
(3)  Engineering <F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s ,btu/ft.h.F>
(4)  Mixed       <K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP      ,mW/m.K    >

Enter the new unit or default option (X to exit)?
```

## $H_2$: User Interaction with supertrapp (Part 2/2)

```
Enter the new unit or default option (X to exit)? 2


                                  ****************************
                                  SUPERTRAPP 2.00 Property Unit Menu
                                  ****************************

Property     **************************options************************  current

Temperature<K      ,R          ,C          ,F          ,          ,      ,    >K
Pressure    <atm   ,bar        ,MPa        ,Psig       ,Psia      ,mmHg,kpf>MPa
Volume      <liter ,m**3       ,cm**3      ,in**3      ,ft**3     ,      ,    >m**3
Energy      <cal   ,J          ,btu        ,kcal       ,kJ        ,      ,    >kJ
Mass        <mol   ,lb-mol     ,kg         ,g          ,lb        ,      ,    >kg
Velocity    <m/s   ,cm/s       ,ft/s       ,in/s       ,          ,      ,    >m/s
Viscosity   <uP    ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,         ,    >uPa.s
Thm. Cond.  <W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,          ,    >W/m.K

default set options

<1>  Scientific  <K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K>
<2>  S.I.        <K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     >
<3>  Engineering <F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F>
<4>  Mixed       <K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    >

Enter the new unit or default option (X to exit)? x


                                  ****************************
                                  SUPERTRAPP 2.00 Property Unit Menu
                                  ****************************

Property     **************************options************************  current

Temperature<K      ,R          ,C          ,F          ,          ,      ,    >K
Pressure    <atm   ,bar        ,MPa        ,Psig       ,Psia      ,mmHg,kpf>MPa
Volume      <liter ,m**3       ,cm**3      ,in**3      ,ft**3     ,      ,    >m**3
Energy      <cal   ,J          ,btu        ,kcal       ,kJ        ,      ,    >kJ
Mass        <mol   ,lb-mol     ,kg         ,g          ,lb        ,      ,    >kg
Velocity    <m/s   ,cm/s       ,ft/s       ,in/s       ,          ,      ,    >m/s
Viscosity   <uP    ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,         ,    >uPa.s
Thm. Cond.  <W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,          ,    >W/m.K

default set options

<1>  Scientific  <K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K>
<2>  S.I.        <K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     >
<3>  Engineering <F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F>
<4>  Mixed       <K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    >
The units have been reset as requested.

Do you want to enter compositions on a mass basis <N/Y>?n

Do you want to input composition as mole fractions
 (If the answer is no, input can be in moles)  <N/Y>?y


End-of-file encountered on input file
returing to interactive input mode
For a list of available options, type ? Otherwise
enter command or, if you wish to do a flash calculation,
enter T(K) and P(MPa) separated by a comma.
quit

 Program Terminated- Exiting NIST4

C:\PROGRA~1\NIST\sprtrap>
```

## $H_2$: supertrapp Output File (H2.OUT)

```
 1-Phase Flash results at T =  298.150 K and P =  3.03975       MPa
-----Component------ ---Feed---  --Vapor---   ---Phi----
 hydrogen              1.00000    1.00000      1.03041
,Molar Basis
                       1.00000    1.00000      Feed Fraction
                       2.01588    2.01588      Molar Mass
                       1.02952    1.02952      Comp. Factor, Z
                       2.40106    2.40106      D, kg/m**3
                       34.3021    34.3021      H, kJ/kg
                       50.9503    50.9503      S, kJ/kg.K
                       15.4739    15.4739      Cp, kJ/kg.K
                                  1.36518      Cp/Cv
                                  1333.39      Sound Speed, m/s
                                 -0.714359     JT, K/MPa
                                  8.84798      Visc., uPa.s
                                  0.201468     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  298.150 K and P =  5.06625       MPa
-----Component------ ---Feed---  --Vapor---   ---Phi----
 hydrogen              1.00000    1.00000      1.05071
,Molar Basis
                       1.00000    1.00000      Feed Fraction
                       2.01588    2.01588      Molar Mass
                       1.04836    1.04836      Comp. Factor, Z
                       3.92987    3.92987      D, kg/m**3
                       56.4423    56.4423      H, kJ/kg
                       48.8372    48.8372      S, kJ/kg.K
                       15.5184    15.5184      Cp, kJ/kg.K
                                  1.36479      Cp/Cv
                                  1356.78      Sound Speed, m/s
                                 -0.698348     JT, K/MPa
                                  8.84798      Visc., uPa.s
                                  0.204044     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  298.150 K and P =  10.1325       MPa
-----Component------ ---Feed---  --Vapor---   ---Phi----
 hydrogen              1.00000    1.00000      1.10177
,Molar Basis
                       1.00000    1.00000      Feed Fraction
                       2.01588    2.01588      Molar Mass
                       1.09324    1.09324      Comp. Factor, Z
                       7.53707    7.53707      D, kg/m**3
                       110.008    110.008      H, kJ/kg
                       45.9623    45.9623      S, kJ/kg.K
                       15.6189    15.6189      Cp, kJ/kg.K
                                  1.36340      Cp/Cv
                                  1411.30      Sound Speed, m/s
                                 -0.664566     JT, K/MPa
                                  8.84798      Visc., uPa.s
                                  0.210019     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  298.150 K and P =  15.1988       MPa
-----Component------ ---Feed---  --Liquid--   ---Phi----
 hydrogen              1.00000    1.00000      1.15355
,Molar Basis
                       1.00000    1.00000      Feed Fraction
                       2.01588    2.01588      Molar Mass
                       1.13567    1.13567      Comp. Factor, Z
                       10.8813    10.8813      D, kg/m**3
                       161.928    161.928      H, kJ/kg
                       44.2748    44.2748      S, kJ/kg.K
                       15.7038    15.7038      Cp, kJ/kg.K
                                  1.36131      Cp/Cv
                                  1461.99      Sound Speed, m/s
                                 -0.645815     JT, K/MPa
                                  8.84798      Visc., uPa.s
                                  0.215478     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  298.150 K and P =  20.2650       MPa
-----Component------ ---Feed---  --Liquid--   ---Phi----
 hydrogen              1.00000    1.00000      1.20635
,Molar Basis
                       1.00000    1.00000      Feed Fraction
                       2.01588    2.01588      Molar Mass
                       1.17705    1.17705      Comp. Factor, Z
                       14.0009    14.0009      D, kg/m**3
                       212.966    212.966      H, kJ/kg
                       43.0748    43.0748      S, kJ/kg.K
                       15.7737    15.7737      Cp, kJ/kg.K
                                  1.35849      Cp/Cv
                                  1510.39      Sound Speed, m/s
                                 -0.635380     JT, K/MPa
                                  8.84798      Visc., uPa.s
                                  0.220563     Th. Cond.,W/m.K
```

(VLE=PRS,PROPS=EXCST)

### B.4.2 Carbon Dioxide

**Carbon Dioxide: Input supertrapp File (co2.inp)**

```
COMP 1     CO2
FEED 1        1.0000
FLTP       300.00       7.3648
FEED 1        1.0000
FLTP       300.00       10.1685
FEED 1        1.0000
FLTP       300.00      13.0598
FEED 1        1.0000
FLTP       300.00      14.3100
FEED 1        1.0000
FLTP       300.00      15.2947
FEED 1        1.0000
FLTP       300.00      16.7726
FEED 1        1.0000
FLTP       300.00      17.7611
FEED 1        1.0000
FLTP       300.00      18.0004
$END
```

## Carbon Dioxide: User Interaction with supertrapp (Part 1/2)

```
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.

C:\PROGRA~1\NIST\sprtrap>strapp

     **************************************************************
     *            NIST Standard Reference Database 4              *
     *   NIST THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES   *
     *            Program SUPERTRAPP - Version 3.1                *
     *                                                            *
     *               Based on research sponsored by               *
     *              the NASA Lewis Research Center,               *
     *    the NIST Supercritical Fluid Property Consortium        *
     *               and Standard Reference Data                  *
     *                                                            *
     *                                                            *
     *        Physical and Chemical Properties Division           *
     *                                                            *
     *          Distributed by Standard Reference Data            *
     *       National Institute of Standards and Technology       *
     *               Gaithersburg, MD 20899 USA                   *
     *                                                            *
     *      Copyright 2003 by the U.S. Secretary of Commerce      *
     *           on behalf of the United States of America        *
     *                    All rights reserved.                    *
     **************************************************************

For help in response to any question, enter "?".
For a brief description of SUPERTRAPP, enter "?".
Press enter to continue.

Do you want to use default settings? (Y/N)
(The default settings are whatever you last selected for units and file I/O.)
n

Do you want to input from a file (N/Y)? y
Please enter the name of the input file.  co2.inp
Do you want to output to a file (N/Y)? y
Please enter the output file name.  co2.out
Do you also want output to the terminal (Y/N) ? n
Do you want to change the units (N/Y) ? y



                            ***************************
                            SUPERTRAPP 2.00 Property Unit Menu
                            ***************************

Property     ***********************options*********************  current

Temperature(K      ,R          ,C          ,F          ,          ,    ,   )K
Pressure   (atm    ,bar        ,MPa        ,Psig       ,Psia      ,mmHg,kpf)bar
Volume     (liter  ,m**3       ,cm**3      ,in**3      ,ft**3     ,    ,   )liter
Energy     (cal    ,J          ,btu        ,kcal       ,kJ        ,    ,   )kJ
Mass       (mol    ,lb-mol     ,kg         ,g          ,lb        ,    ,   )mol
Velocity   (m/s    ,cm/s       ,ft/s       ,in/s       ,          ,    ,   )m/s
Viscosity  (uP     ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h   ,    ,   )uP
Thm. Cond. (W/m.K  ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K     ,    ,   )mW/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal  ,mol  ,cm/s ,uP      ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ   ,kg   ,m/s  ,uPa.s   ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu  ,lb   ,ft/s ,lb/ft.s ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ   ,mol  ,m/s  ,uP      ,mW/m.K    )

Enter the new unit or default option (X to exit)?
```

## Carbon Dioxide: User Interaction with supertrapp (Part 1/2)

```
Enter the new unit or default option (X to exit)? 2


                              ****************************
                              SUPERTRAPP 2.00 Property Unit Menu
                              ****************************

Property     *************************options*************************  current

Temperature(K      ,R         ,C         ,F         ,          ,    ,    )K
Pressure   (atm    ,bar       ,MPa       ,Psig      ,Psia      ,mmHg,kpf )MPa
Volume     (liter  ,m**3      ,cm**3     ,in**3     ,ft**3     ,    ,    )m**3
Energy     (cal    ,J         ,btu       ,kcal      ,kJ        ,    ,    )kJ
Mass       (mol    ,lb-mol    ,kg        ,g         ,lb        ,    ,    )kg
Velocity   (m/s    ,cm/s      ,ft/s      ,in/s      ,          ,    ,    )m/s
Viscosity  (uP     ,cP        ,uPa.s     ,lb/ft.s   ,lb/ft.h,  ,    ,    )uPa.s
Thm. Cond. (W/m.K  ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,  ,    ,    )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )

Enter the new unit or default option (X to exit)? x


                              ****************************
                              SUPERTRAPP 2.00 Property Unit Menu
                              ****************************

Property     *************************options*************************  current

Temperature(K      ,R         ,C         ,F         ,          ,    ,    )K
Pressure   (atm    ,bar       ,MPa       ,Psig      ,Psia      ,mmHg,kpf )MPa
Volume     (liter  ,m**3      ,cm**3     ,in**3     ,ft**3     ,    ,    )m**3
Energy     (cal    ,J         ,btu       ,kcal      ,kJ        ,    ,    )kJ
Mass       (mol    ,lb-mol    ,kg        ,g         ,lb        ,    ,    )kg
Velocity   (m/s    ,cm/s      ,ft/s      ,in/s      ,          ,    ,    )m/s
Viscosity  (uP     ,cP        ,uPa.s     ,lb/ft.s   ,lb/ft.h,  ,    ,    )uPa.s
Thm. Cond. (W/m.K  ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,  ,    ,    )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )
The units have been reset as requested.

Do you want to enter compositions on a mass basis (N/Y)?n

Do you want to input composition as mole fractions
 (If the answer is no, input can be in moles)  (N/Y)?y


End-of-file encountered on input file
returing to interactive input mode
For a list of available options, type ? Otherwise
enter command or, if you wish to do a flash calculation,
enter T(K) and P(MPa) separated by a comma.
quit

 Program Terminated- Exiting NIST4

C:\PROGRA~1\NIST\sprtrap>_
```

## Carbon Dioxide: supertrapp Output File (CO2.OUT)

```
 1-Phase Flash results at T =  300.000 K and P =  7.36480     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide       1.00000      1.00000     0.831333
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       44.0095      44.0095     Molar Mass
                      0.177439     0.177439     Comp. Factor, Z
                       732.336      732.336     D, kg/m**3
                      -9175.03     -9175.03     H, kJ/kg
                       3.35364      3.35354     S, kJ/kg.K
                       4.81529      4.81529     Cp, kJ/kg.K
                                    5.26161     Cp/Cv
                                    341.916     Sound Speed, m/s
                                    1.77429     JT, K/MPa
                                    61.1868     Visc., uPa.s
                                 0.875187E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  10.1685     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide       1.00000      1.00000     0.487448
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       44.0095      44.0096     Molar Mass
                      0.222926     0.222926     Comp. Factor, Z
                       804.815      804.815     D, kg/m**3
                      -9187.99     -9187.99     H, kJ/kg
                       3.29826      3.29826     S, kJ/kg.K
                       2.95518      2.95518     Cp, kJ/kg.K
                                    3.37258     Cp/Cv
                                    445.627     Sound Speed, m/s
                                   0.947964     JT, K/MPa
                                    73.1707     Visc., uPa.s
                                 0.953999E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  13.0598     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide       1.00000      1.00000     0.403720
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       44.0095      44.0095     Molar Mass
                      0.272954     0.272954     Comp. Factor, Z
                       844.197      844.197     D, kg/m**3
                      -9194.08     -9194.08     H, kJ/kg
                       3.26628      3.26628     S, kJ/kg.K
                       2.51262      2.51262     Cp, kJ/kg.K
                                    2.91788     Cp/Cv
                                    510.665     Sound Speed, m/s
                                   0.638586     JT, K/MPa
                                    80.8854     Visc., uPa.s
                                   0.101658     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  14.3100     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide       1.00000      1.00000     0.378126
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       44.0095      44.0095     Molar Mass
                      0.294510     0.294510     Comp. Factor, Z
                       857.308      857.308     D, kg/m**3
                      -9195.91     -9195.91     H, kJ/kg
                       3.25530      3.25530     S, kJ/kg.K
                       2.40342      2.40342     Cp, kJ/kg.K
                                    2.80445     Cp/Cv
                                    533.561     Sound Speed, m/s
                                   0.552209     JT, K/MPa
                                    83.6430     Visc., uPa.s
                                   0.104055     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  15.2947     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide       1.00000      1.00000     0.360984
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       44.0095      44.0095     Molar Mass
                      0.311404     0.311404     Comp. Factor, Z
                       866.590      366.590     D, kg/m**3
                      -9197.13     -9197.13     H, kJ/kg
                       3.24743      3.24743     S, kJ/kg.K
                       2.33441      2.33441     Cp, kJ/kg.K
                                    2.73232     Cp/Cv
                                    550.137     Sound Speed, m/s
                                   0.495386     JT, K/MPa
```

```
                                   85.6799     Visc., uPa.s
                                   0.105847    Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  16.7726     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide        1.00000      1.00000     0.339157
,Molar Basis
                        1.00000      1.00000     Feed Fraction
                        44.0095      44.0095     Molar Mass
                       0.336606     0.336606     Comp. Factor, Z
                        879.177      879.177     D, kg/m**3
                       -9198.68     -9198.68     H, kJ/kg
                        3.23661      3.23661     S, kJ/kg.K
                        2.25013      2.25013     Cp, kJ/kg.K
                                     2.64362     Cp/Cv
                                     573.103     Sound Speed, m/s
                                    0.423587     JT, K/MPa
                                     88.6405     Visc., uPa.s
                                    0.108402     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  17.7611     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide        1.00000      1.00000     0.326670
,Molar Basis
                        1.00000      1.00000     Feed Fraction
                        44.0095      44.0095     Molar Mass
                       0.353354     0.353354     Comp. Factor, Z
                        886.864      886.864     D, kg/m**3
                       -9199.57     -9199.57     H, kJ/kg
                        3.22993      3.22993     S, kJ/kg.K
                        2.20327      2.20327     Cp, kJ/kg.K
                                     2.59394     Cp/Cv
                                     587.402     Sound Speed, m/s
                                    0.382515     JT, K/MPa
                                     90.3452     Visc., uPa.s
                                    0.110033     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  300.000 K and P =  18.0004     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 carbon dioxide        1.00000      1.00000     0.323864
,Molar Basis
                        1.00000      1.00000     Feed Fraction
                        44.0095      44.0095     Molar Mass
                       0.357396     0.357396     Comp. Factor, Z
                        888.649      888.649     D, kg/m**3
                       -9199.77     -9199.77     H, kJ/kg
                        3.22837      3.22837     S, kJ/kg.K
                        2.19285      2.19285     Cp, kJ/kg.K
                                     2.58286     Cp/Cv
                                     590.762     Sound Speed, m/s
                                    0.373263     JT, K/MPa
                                     90.7708     Visc., uPa.s
                                    0.110419     Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)
```

### B.4.3 $CH_4$

**$CH_4$: supertrapp Inpnt File (ch4.inp)**

```
COMP 1     METHANE
FEED 1        1.0000
FLTP       293.15       0.151
FEED 1        1.0000
FLTP       293.15       0.163
FEED 1        1.0000
FLTP       293.15       4.219
FEED 1        1.0000
FLTP       293.15       7.912
FEED 1        1.0000
FLTP       293.15      11.298
FEED 1        1.0000
FLTP       293.15      11.310
FEED 1        1.0000
FLTP       293.15      14.702
FEED 1        1.0000
FLTP       293.15      18.351
$END
```

## $CH_4$: User Interaction with supertrapp (Part 1/2)

```
C:\PROGRA~1\NIST\sprtrap>strapp

          ************************************************************
          *          NIST Standard Reference Database 4              *
          *  NIST THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES  *
          *           Program SUPERTRAPP - Version 3.1               *
          *                                                          *
          *             Based on research sponsored by               *
          *            the NASA Lewis Research Center,               *
          *   the NIST Supercritical Fluid Property Consortium       *
          *              and Standard Reference Data                 *
          *                                                          *
          *                                                          *
          *       Physical and Chemical Properties Division          *
          *                                                          *
          *          Distributed by Standard Reference Data          *
          *       National Institute of Standards and Technology     *
          *              Gaithersburg, MD 20899 USA                  *
          *                                                          *
          *      Copyright 2003 by the U.S. Secretary of Commerce    *
          *          on behalf of the United States of America       *
          *                   All rights reserved.                   *
          ************************************************************

For help in response to any question, enter "?".
For a brief description of SUPERTRAPP, enter "?".
Press enter to continue.

Do you want to use default settings? (Y/N)
(The default settings are whatever you last selected for units and file I/O.)
n

Do you want to input from a file (N/Y)? y
Please enter the name of the input file.  ch4.inp
Do you want to output to a file (N/Y)? y
Please enter the output file name.  ch4.out
Do you also want output to the terminal (Y/N) ? n
Do you want to change the units (N/Y) ? y



                           **************************
                           SUPERTRAPP 2.00 Property Unit Menu
                           **************************

Property      *************************options**********************  current

Temperature(K      ,R          ,C          ,F          ,         ,    ,   )K
Pressure    (atm   ,bar        ,MPa        ,Psig       ,Psia     ,mmHg,kpf)bar
Volume      (liter ,m**3       ,cm**3      ,in**3      ,ft**3    ,    ,   )liter
Energy      (cal   ,J          ,btu        ,kcal       ,kJ       ,    ,   )kJ
Mass        (mol   ,lb-mol     ,kg         ,g          ,lb       ,    ,   )mol
Velocity    (m/s   ,cm/s       ,ft/s       ,in/s       ,         ,    ,   )m/s
Viscosity   (uP    ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h, ,    ,   )uP
Thm. Cond.  (W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,    ,   )mW/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP      ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s   ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP      ,mW/m.K    )

Enter the new unit or default option (X to exit)?
```

$CH_4$: User Interaction with supertrapp (Part 2/2)

```
Enter the new unit or default option (X to exit)? 2


                            ****************************
                            SUPERTRAPP 2.00 Property Unit Menu
                            ****************************

Property     **************************options***********************  current

Temperature(K       ,R         ,C         ,F         ,          ,    ,   )K
Pressure   (atm     ,bar       ,MPa       ,Psig      ,Psia      ,mmHg,kpf)MPa
Volume     (liter   ,m**3      ,cm**3     ,in**3     ,ft**3     ,    ,   )m**3
Energy     (cal     ,J         ,btu       ,kcal      ,kJ        ,    ,   )kJ
Mass       (mol     ,lb-mol    ,kg        ,g         ,lb        ,    ,   )kg
Velocity   (m/s     ,cm/s      ,ft/s      ,in/s      ,          ,    ,   )m/s
Viscosity  (uP      ,cP        ,uPa.s     ,lb/ft.s   ,lb/ft.h,  ,    ,   )uPa.s
Thm. Cond. (W/m.K   ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K    ,    ,   )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )

Enter the new unit or default option (X to exit)? x


                            ****************************
                            SUPERTRAPP 2.00 Property Unit Menu
                            ****************************

Property     **************************options***********************  current

Temperature(K       ,R         ,C         ,F         ,          ,    ,   )K
Pressure   (atm     ,bar       ,MPa       ,Psig      ,Psia      ,mmHg,kpf)MPa
Volume     (liter   ,m**3      ,cm**3     ,in**3     ,ft**3     ,    ,   )m**3
Energy     (cal     ,J         ,btu       ,kcal      ,kJ        ,    ,   )kJ
Mass       (mol     ,lb-mol    ,kg        ,g         ,lb        ,    ,   )kg
Velocity   (m/s     ,cm/s      ,ft/s      ,in/s      ,          ,    ,   )m/s
Viscosity  (uP      ,cP        ,uPa.s     ,lb/ft.s   ,lb/ft.h,  ,    ,   )uPa.s
Thm. Cond. (W/m.K   ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K    ,    ,   )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )
The units have been reset as requested.

Do you want to enter compositions on a mass basis (N/Y)?n

Do you want to input composition as mole fractions
 (If the answer is no, input can be in moles)  (N/Y)?y


End-of-file encountered on input file
returing to interactive input mode
For a list of available options, type ? Otherwise
enter command or, if you wish to do a flash calculation,
enter T(K) and P(MPa) separated by a comma.
quit

 Program Terminated- Exiting NIST4

C:\PROGRA~1\NIST\sprtrap>_
```

## $CH_4$: supertrapp Output File (CH4.OUT)

```
 1-Phase Flash results at T =  293.150 K and P =  4.21900     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 methane              1.00000      1.00000     0.924916
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       16.0425      16.0425     Molar Mass
                      0.923702     0.923702     Comp. Factor, Z
                       30.0629      30.0629     D, kg/m**3
                      -4722.64     -4722.64     H, kJ/kg
                       9.52561      9.52561     S, kJ/kg.K
                       2.60339      2.60339     Cp, kJ/kg.K
                                    1.43199     Cp/Cv
                                    431.926     Sound Speed, m/s
                                    4.20830     JT, K/MPa
                                    11.9758     Visc., uPa.s
                                   0.413464E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.150 K and P =  7.91200     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane              1.00000      1.00000     0.867215
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       16.0425      16.0425     Molar Mass
                      0.867976     0.867976     Comp. Factor, Z
                       59.9973      59.9973     D, kg/m**3
                      -4762.93     -4762.93     H, kJ/kg
                       9.09566      9.09566     S, kJ/kg.K
                       2.94908      2.94908     Cp, kJ/kg.K
                                    1.58517     Cp/Cv
                                    432.305     Sound Speed, m/s
                                    3.64704     JT, K/MPa
                                    13.2580     Visc., uPa.s
                                   0.471741E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.150 K and P =  11.2980     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane              1.00000      1.00000     0.821954
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       16.0425      16.0425     Molar Mass
                      0.831503     0.831503     Comp. Factor, Z
                       89.4316      89.4316     D, kg/m**3
                      -4798.25     -4798.25     H, kJ/kg
                       8.81834      8.81834     S, kJ/kg.K
                       3.28644      3.28644     Cp, kJ/kg.K
                                    1.73300     Cp/Cv
                                    443.216     Sound Speed, m/s
                                    3.04868     JT, K/MPa
                                    14.8331     Visc., uPa.s
                                   0.528919E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.150 K and P =  11.3100     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane              1.00000      1.00000     0.821807
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       16.0425      16.0425     Molar Mass
                      0.831402     0.831402     Comp. Factor, Z
                       89.5375      89.5376     D, kg/m**3
                      -4798.37     -4798.37     H, kJ/kg
                       8.81747      8.81747     S, kJ/kg.K
                       3.28760      3.28760     Cp, kJ/kg.K
                                    1.73350     Cp/Cv
                                    443.274     Sound Speed, m/s
                                    3.04652     JT, K/MPa
                                    14.8392     Visc., uPa.s
                                   0.529126E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.150 K and P =  14.7020     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane              1.00000      1.00000     0.784005
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       16.0425      16.0425     Molar Mass
                      0.811674     0.811674     Comp. Factor, Z
                       119.220      119.220     D, kg/m**3
                      -4830.29     -4830.29     H, kJ/kg
                       8.59707      8.59707     S, kJ/kg.K
                       3.57732      3.57732     Cp, kJ/kg.K
                                    1.85841     Cp/Cv
                                    465.806     Sound Speed, m/s
                                    2.43128     JT, K/MPa
```

```
                                  16.7122     Visc., uPa.s
                                  0.528594E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.150 K and P =  18.3510     MPa
-----Component------ ---Feed---   --Liquid--    ---Phi----
 methane              1.00000      1.00000     0.751617
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       16.0425      16.0425     Molar Mass
                      0.811348     0.811348     Comp. Factor, Z
                       148.870      148.870     D, kg/m**3
                      -4858.52     -4858.52     H, kJ/kg
                       8.40773      8.40773     S, kJ/kg.K
                       3.74398      3.74398     Cp, kJ/kg.K
                                    1.92491     Cp/Cv
                                    503.572     Sound Speed, m/s
                                    1.79561     JT, K/MPa
                                    18.9284     Visc., uPa.s
                                  0.652464E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)
```

### B.4.4 Natural Gas

**Natural Gas: supertrapp Input File (mix.inp)**

```
COMP 1    METHANE
COMP 2    ETHANE
COMP 3    PROPANE
COMP 4    NITROGEN
COMP 5    CO2
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.963      0.310
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.956      2.060
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.949      4.030
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.929      6.020
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.929      8.040
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.924     10.080
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.936     12.190
FEED 1       0.8484
FEED 2       0.0840
FEED 3       0.0050
FEED 4       0.0560
FEED 5       0.0066
FLTP      293.963     14.040
$END
```

## Natural Gas: User Interaction with supertrapp (Part 1/2)

```
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.

C:\PROGRA~1\NIST\sprtrap>strapp

          ***********************************************************
          *          NIST Standard Reference Database 4              *
          *  NIST THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES  *
          *            Program SUPERTRAPP - Version 3.1              *
          *                                                          *
          *               Based on research sponsored by             *
          *              the NASA Lewis Research Center,             *
          *   the NIST Supercritical Fluid Property Consortium       *
          *              and Standard Reference Data                 *
          *                                                          *
          *                                                          *
          *      Physical and Chemical Properties Division           *
          *                                                          *
          *         Distributed by Standard Reference Data           *
          *     National Institute of Standards and Technology       *
          *             Gaithersburg, MD 20899 USA                   *
          *                                                          *
          *     Copyright 2003 by the U.S. Secretary of Commerce     *
          *        on behalf of the United States of America         *
          *                 All rights reserved.                     *
          ***********************************************************

For help in response to any question, enter "?".
For a brief description of SUPERTRAPP, enter "?".
Press enter to continue.

Do you want to use default settings? (Y/N)
(The default settings are whatever you last selected for units and file I/O.)
n

Do you want to input from a file (N/Y)? y
Please enter the name of the input file.  mix.inp
Do you want to output to a file (N/Y)? y
Please enter the output file name.  mix.out
Do you also want output to the terminal (Y/N) ? n

Do you want to change the units (N/Y) ? y



                           ****************************
                           SUPERTRAPP 2.00 Property Unit Menu
                           ****************************


Property       **************************options**************************  current

Temperature(K      ,R          ,C          ,F          ,         ,    ,    )K
Pressure   (atm    ,bar        ,MPa        ,Psig       ,Psia     ,mmHg,kpf)bar
Volume     (liter  ,m**3       ,cm**3      ,in**3      ,ft**3    ,    ,    )liter
Energy     (cal    ,J          ,btu        ,kcal       ,kJ       ,    ,    )kJ
Mass       (mol    ,lb-mol     ,kg         ,g          ,lb       ,    ,    )mol
Velocity   (m/s    ,cm/s       ,ft/s       ,in/s       ,         ,    ,    )m/s
Viscosity  (uP     ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h, ,    ,    )uP
Thm. Cond. (W/m.K  ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,    ,    )mW/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP      ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s   ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP      ,mW/m.K    )

Enter the new unit or default option (X to exit)?
```

## Natural Gas: User Interaction with supertrapp (Part 2/2)

```
Enter the new unit or default option (X to exit)? 2


                              ****************************
                              SUPERTRAPP 2.00 Property Unit Menu
                              ****************************

Property     **************************options***********************  current

Temperature(K      ,R          ,C          ,F          ,          ,     ,    )K
Pressure    (atm   ,bar        ,MPa        ,Psig       ,Psia      ,mmHg,kpf)MPa
Volume      (liter ,m**3       ,cm**3      ,in**3      ,ft**3     ,     ,    )m**3
Energy      (cal   ,J          ,btu        ,kcal       ,kJ        ,     ,    )kJ
Mass        (mol   ,lb-mol     ,kg         ,g          ,lb        ,     ,    )kg
Velocity    (m/s   ,cm/s       ,ft/s       ,in/s       ,          ,     ,    )m/s
Viscosity   (uP    ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,        ,    )uPa.s
Thm. Cond.  (W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,     ,    )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )

Enter the new unit or default option (X to exit)? x


                              ****************************
                              SUPERTRAPP 2.00 Property Unit Menu
                              ****************************

Property     **************************options***********************  current

Temperature(K      ,R          ,C          ,F          ,          ,     ,    )K
Pressure    (atm   ,bar        ,MPa        ,Psig       ,Psia      ,mmHg,kpf)MPa
Volume      (liter ,m**3       ,cm**3      ,in**3      ,ft**3     ,     ,    )m**3
Energy      (cal   ,J          ,btu        ,kcal       ,kJ        ,     ,    )kJ
Mass        (mol   ,lb-mol     ,kg         ,g          ,lb        ,     ,    )kg
Velocity    (m/s   ,cm/s       ,ft/s       ,in/s       ,          ,     ,    )m/s
Viscosity   (uP    ,cP         ,uPa.s      ,lb/ft.s    ,lb/ft.h,        ,    )uPa.s
Thm. Cond.  (W/m.K ,cal/cm.s.K,btu/ft.s.F,btu/ft.h.F,mW/m.K ,     ,    )W/m.K

default set options

(1)  Scientific  (K ,atm   ,liter ,cal   ,mol   ,cm/s  ,uP       ,cal/cm.s.K)
(2)  S.I.        (K ,MPa   ,m**3  ,kJ    ,kg    ,m/s   ,uPa.s    ,W/m.K     )
(3)  Engineering (F ,Psia  ,ft**3 ,btu   ,lb    ,ft/s  ,lb/ft.s  ,btu/ft.h.F)
(4)  Mixed       (K ,bar   ,liter ,kJ    ,mol   ,m/s   ,uP       ,mW/m.K    )
The units have been reset as requested.

Do you want to enter compositions on a mass basis (N/Y)?n

Do you want to input composition as mole fractions
 (If the answer is no, input can be in moles)  (N/Y)?y

End-of-file encountered on input file
returing to interactive input mode
For a list of available options, type ? Otherwise
enter command or, if you wish to do a flash calculation,
enter T(K) and P(MPa) separated by a comma.
quit

 Program Terminated- Exiting NIST4

C:\PROGRA~1\NIST\sprtrap>
```

## Natural Gas: supertrapp Output File (MIX.OUT)

```
 1-Phase Flash results at T =  293.963 K and P = 0.310000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 methane             0.848400     0.848400     0.843667
 ethane              0.840000E-01 0.840000E-01 0.824474E-01
 propane             0.500000E-02 0.500000E-02 0.495893E-02
 nitrogen            0.560000E-01 0.560000E-01 0.561011E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.654242E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.993477     0.993477     Comp. Factor, Z
                       2.32560      2.32560     D, kg/m**3
                      -4069.66     -4069.66     H, kJ/kg
                       10.1869      10.1869     S, kJ/kg.K
                       2.09948      2.09948     Cp, kJ/kg.K
                                    1.29006     Cp/Cv
                                    413.331     Sound Speed, m/s
                                    4.84327     JT, K/MPa
                                    11.5134     Visc., uPa.s
                                   0.328966E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.956 K and P =  2.06000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 methane             0.848400     0.848400     0.816867
 ethane              0.840000E-01 0.840000E-01 0.740861E-01
 propane             0.500000E-02 0.500000E-02 0.412235E-02
 nitrogen            0.560000E-01 0.560000E-01 0.567590E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.622374E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.956880     0.956880     Comp. Factor, Z
                       16.0454      16.0454     D, kg/m**3
                      -4077.80     -4077.80     H, kJ/kg
                       9.27654      9.27654     S, kJ/kg.K
                       2.21784      2.21784     Cp, kJ/kg.K
                                    1.34714     Cp/Cv
                                    406.917     Sound Speed, m/s
                                    4.75231     JT, K/MPa
                                    11.8013     Visc., uPa.s
                                   0.353363E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.949 K and P =  4.03000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 methane             0.848400     0.848400     0.788306
 ethane              0.840000E-01 0.840000E-01 0.655278E-01
 propane             0.500000E-02 0.500000E-02 0.341132E-02
 nitrogen            0.560000E-01 0.560000E-01 0.576865E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.687969E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.917148     0.917148     Comp. Factor, Z
                       32.7504      32.7504     D, kg/m**3
                      -4098.88     -4098.88     H, kJ/kg
                       8.91721      8.91721     S, kJ/kg.K
                       2.37610      2.37610     Cp, kJ/kg.K
                                    1.42364     Cp/Cv
                                    401.683     Sound Speed, m/s
                                    4.56177     JT, K/MPa
                                    12.2951     Visc., uPa.s
                                   0.382510E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.929 K and P =  6.02000     MPa
-----Component------ ---Feed---   --Vapor---   ---Phi----
 methane             0.848400     0.848400     0.761281
 ethane              0.840000E-01 0.840000E-01 0.578354E-01
 propane             0.500000E-02 0.500000E-02 0.281246E-02
 nitrogen            0.560000E-01 0.560000E-01 0.588240E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.555023E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.880141     0.880141     Comp. Factor, Z
                       50.9830      50.9830     D, kg/m**3
                      -4120.57     -4120.57     H, kJ/kg
                       8.67866      8.67865     S, kJ/kg.K
                       2.66085      2.56085     Cp, kJ/kg.K
                                    1.51267     Cp/Cv
                                    399.358     Sound Speed, m/s
                                    4.25469     JT, K/MPa
                                    12.9780     Visc., uPa.s
                                   0.413693E-01 Th. Cond.,W/m.K
```

```
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.929 K and P =  8.04000     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane             0.848400     0.848400     0.735945
 ethane              0.840000E-01 0.840000E-01 0.510192E-01
 propane             0.500000E-02 0.500000E-02 0.231632E-02
 nitrogen            0.560000E-01 0.560000E-01 0.601747E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.523785E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.847296     0.847296     Comp. Factor, Z
                       70.7297      70.7297     D, kg/m**3
                      -4142.48     -4142.48     H, kJ/kg
                       8.49001      8.49001     S, kJ/kg.K
                       2.76789      2.76789     Cp, kJ/kg.K
                                    1.61187     Cp/Cv
                                    400.657     Sound Speed, m/s
                                    3.88713     JT, K/MPa
                                    13.8560     Visc., uPa.s
                                 0.447124E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.924 K and P =  10.0800     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane             0.848400     0.848400     0.712584
 ethane              0.840000E-01 0.840000E-01 0.451068E-01
 propane             0.500000E-02 0.500000E-02 0.191429E-02
 nitrogen            0.560000E-01 0.560000E-01 0.617096E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.494668E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.819976     0.819976     Comp. Factor, Z
                       91.6320      91.6320     D, kg/m**3
                      -4164.11     -4164.11     H, kJ/kg
                       8.33036      8.33036     S, kJ/kg.K
                       2.98669      2.98669     Cp, kJ/kg.K
                                    1.71624     Cp/Cv
                                    406.047     Sound Speed, m/s
                                    3.48170     JT, K/MPa
                                    14.9180     Visc., uPa.s
                                 0.482522E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.936 K and P =  12.1900     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane             0.848400     0.848400     0.690838
 ethane              0.840000E-01 0.840000E-01 0.399618E-01
 propane             0.500000E-02 0.500000E-02 0.158758E-02
 nitrogen            0.560000E-01 0.560000E-01 0.634246E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.467326E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.798897     0.798897     Comp. Factor, Z
                       113.732      113.732     D, kg/m**3
                      -4185.38     -4185.38     H, kJ/kg
                       8.18780      8.18780     S, kJ/kg.K
                       3.20306      3.20306     Cp, kJ/kg.K
                                    1.81898     Cp/Cv
                                    416.485     Sound Speed, m/s
                                    3.04262     JT, K/MPa
                                    16.1824     Visc., uPa.s
                                 0.520589E-01 Th. Cond.,W/m.K
 (VLE=PRS,PROPS=EXCST)

 1-Phase Flash results at T =  293.963 K and P =  14.0400     MPa
-----Component------ ---Feed---   --Liquid--   ---Phi----
 methane             0.848400     0.848400     0.673787
 ethane              0.840000E-01 0.840000E-01 0.362128E-01
 propane             0.500000E-02 0.500000E-02 0.136426E-02
 nitrogen            0.560000E-01 0.560000E-01 0.649665E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.445796E-02
,Molar Basis
                       1.00000      1.00000     Feed Fraction
                       18.2159      18.2159     Molar Mass
                      0.787269     0.787269     Comp. Factor, Z
                       132.915      132.915     D, kg/m**3
                      -4202.58     -4202.58     H, kJ/kg
                       8.07819      8.07819     S, kJ/kg.K
                       3.35958      3.35958     Cp, kJ/kg.K
                                    1.89243     Cp/Cv
                                    430.238     Sound Speed, m/s
                                    2.64723     JT, K/MPa
                                    17.4067     Visc., uPa.s
                                 0.554743E-01 Th. Cond.,W/m.K

 (VLE=PRS,PROPS=EXCST)
```