Sandia National Laboratories
Waste Isolation Pilot Plant

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

Task Number 1.4.1.2

ERMS # 532900

Date: December 15, 2003

Document Version 1.0

Author:	Joseph Kanney, 6821	Date: 12/15/03
Technical Review:	L. H. Brush Laurence Brush, 6822	Date: 12/15/03
Technical Review:	L. H. Brush for J. S. Stein Joshua S. Stein, 6852	Date: 12/15/03
QA Review:	Mario Chavez Mario Chavez, 6820	Date: 12/15/03
Management Review:	Paul E. Shoemaker Paul E. Shoemaker, Manager 6820	Date: 12/15/03

WIPP:1.4.1.2:PA:QA-L:DPRP1:530218

Information Only

Contents

Table of Contents 2

List of Figures 3

List of Tables 3

1 Introduction 4
- 1.1 Objective 4
- 1.2 Analysis Overview 4

2 Background 4

3 Approach 6

4 Results 6

5 Conclusions 9

References 10

Appendices: 12

A. supertrapp Input and Output Files 12

B. supertrapp Code Verification 28
- B.1 Code Description 29
- B.2 Verification Procedure 30
- B.3 Verification Results and Conclusions 31
- B.4 Input Files, User Interaction, and Output Files for supertrapp Verification 36
- B.4.1 H_2 36
- B.4.2 Carbon Dioxide 41
- B.4.3 CH_4 46
- B.4.4 Natural Gas 51

Information Only

List of Figures

1 Predicted Compressibility (Z) and Viscosity (η) at $T = 300K$. 9

List of Tables

1 Predicted Compressibility and Viscosity of H_2-CO_2 Mixtures at 300K 7
2 Predicted Compressibility and Viscosity of H_2-CH_4 Mixtures at 300K 8
3 Summary of **supertrapp** Verification Tests 30
4 Atomic and Molecular Data Used in **supertrapp** Verification . . 31
5 **supertrapp** Results Compared with Literature Values: H_2 . . . 33
6 **supertrapp** Results Compared with Literature Values: CO_2 . . 33
7 **supertrapp** Results Compared with Literature Values: CH_4 . . 34
8 **supertrapp** Results Compared with Literature Values: Natural Gas Mixture 34

Information Only

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

Information Only

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 boundary (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)
η	=	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 because 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

Information Only

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 Hydrocarbon Mixtures Database (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.

Information Only

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			
χ_{H_2} (-)	Z (-)	Z/Z_{H_2} (-)	η (μPa s)	η/η_{H_2} (-)	Z (-)	Z/Z_{H_2} (-)	η (μPa s)	η/η_{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
χ = mole fraction
Z = compressibility factor
η = viscosity

Information Only

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

	$P = 7$ MPa				$P = 15$ MPa			
χ_{H_2}	Z	Z/Z_{H_2}	η (μPa s)	η/η_{H_2}	Z	Z/Z_{H_2}	η (μPa s)	η/η_{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

χ = mole fraction
Z = compressibility factor
η = viscosity

Information Only

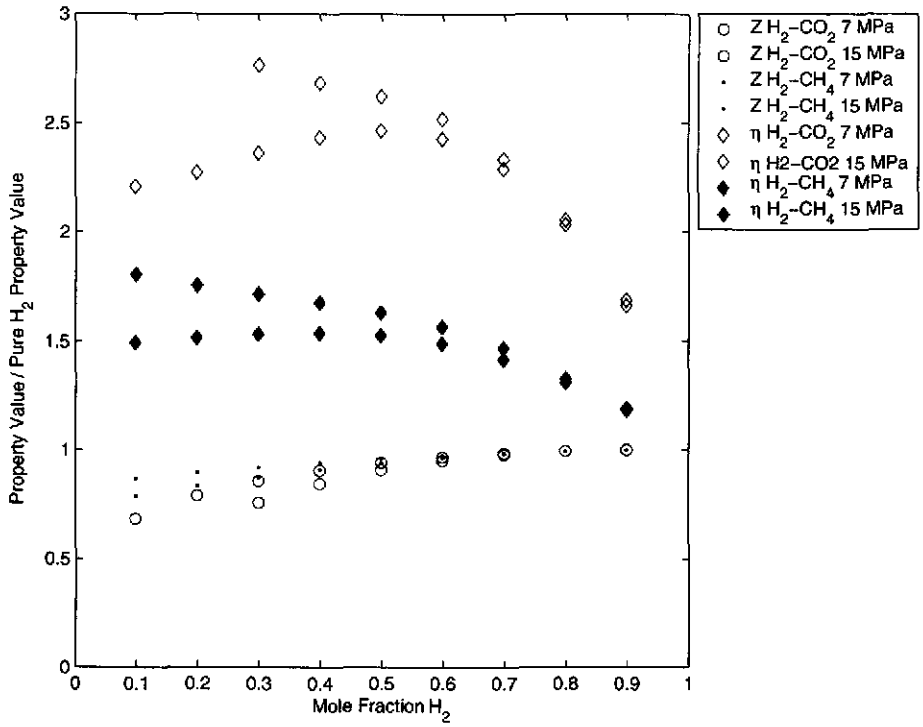

Figure 1: Predicted Compressibility (Z) and Viscosity (η) at $T = 300K$

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.

Information Only

References

[1] J.W. Amyx, D.H. Bass, and R.L. Whiting. *Petroleum Reservoir Engineering.* McGraw-Hill, 1960.

[2] M.J. Assael, N.K. Dalaouti, and V. Vesovic. Viscosity of natural-gas mixtures: Measurements and prediction. *International Journal of Thermophysics*, 22(1):61–71, January 2001.

[3] L. Brush. Test plan for laboratory and modeling studies of repository and radionuclide chemistry for the Waste Isolation Pilot Plant. Sandia Report SAND90-0266, Sandia National Laboratories, Albuquerque, NM, 1990.

[4] M.J. Chaves. *Nuclear Waste Management Procedure NP 9-1: Analyses, Revsion 4.* Sandia National Laboratories, Carlsbad, NM, August 2001.

[5] D.E. Diller and M.J. Ball. Shear viscosity coefficients of compressed gaseous and liquid carbon dioxide at temperatures between 220 and 320 K and at pressures to 30 MPa. *International Journal of Thermophysics*, 6(6):619–629, November 1985.

[6] DOE (U.S. Department of Energy). Title 40 CFR Part 191 Compliance certification application for the Waste Isolation Pilot Plant. Compliance Certification Application DOE/CAO-1996-2184, U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office, Carlsbad, NM, 1996.

[7] EPA (U.S. Environmental Protection Agency). Letter to manager of US DOE Carlsbad Field Office (Inés Triay) from director of US EPA Radiation Protection Division (Frank Marcinowski), October 29 2003.

[8] C. Evers, H.W. Lösch, and W. Wagner. An absolute viscometer-densimeter and measurements of the viscosity of nitrogen, methane, helium, neon, argon, and krypton over a wide range of density and temperature. *International Journal of Thermophysics*, 23(6):1411–1439, November 2002.

[9] C.W. Hansen, L.H. Brush, M.B. Gross, D.D. Hansen, B. Park, J.S. Stein, and T.W. Thompson. Effects of supercompacted waste and heterogeneous waste emplacement on repository performance, Revision 1. Technical report ERMS #532475, Sandia National Laboratories, Carlsbad, NM, October 2003.

[10] M.L. Huber. *NIST Thermophysical Properties of Hydrocarbon Mixtures Database (SUPERTRAPP) Version 3.1 User's Guide.* National Institute of Standards and Technology Standard Reference Data Program, Gaithersburg, MD, February 2003.

[11] L' Air Liquide. *Gas Encyclopaedia.* Elsevier, Amsterdam, 1976.

Information Only

[12] D.R. Lide, editor. *CRC Handbook of Chemistry and Physics.* CRC Press, Cleveland, OH, 84th edition, 2003.

[13] J.D. Schreiber. *WIPP PA User's Manual for BRAGFLO, Version 4.10.* Sandia National Laboratories, Carlsbad, NM, May 1997.

[14] M.R. Telander and R.E. Westerman. Hydrogen generation by metal corrosion in simulated Waste Isolation Pilot Plant environments. Sandia Report SAND96-2538, Sandia National Laboratories, Albuquerque, NM, 1997.

Information Only

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

Information Only

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
```


Information Only

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/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)?
```


Information Only

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>_
```


Information Only

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
                      16.3646      16.3646     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
                                  -0.290723    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
                                   20.3485     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
```


Information Only

```
                                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
                      64.3555      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
                                   394.407     Sound Speed, m/s
                                   1.34026     JT, K/MPa
                                   21.9005     Visc., uPa.s
                                 0.540990E-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
                      79.0956      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
                                   364.460     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
                                   1.63707     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
```


Information Only

```
                    -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
                                   5.91944      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
                                  836.552      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     0.846715
 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
                     79.1568      79.1568      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
```


Information Only

```
                    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     0.698554
 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     0.399519
,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
                                 1.50044     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     1.08578
 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
                                 3.47845     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)
```


Information Only

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
```


Information Only

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                 *
        *                                                         *
        *    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.  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)?
```


Information Only

User Interaction with supertrapp: H_2-CH_4 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>_
```


Information Only

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      2.01588     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
                                  -0.686445    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     -2138.53     H, kJ/kg
                      30.4379      30.4379     S, kJ/kg.K
                      9.42530      9.42530     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     0.756297
 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
```


Information Only

```
                                  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
                                   636.365     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
                                 0.62331BE-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     0.235833
 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
                                 0.569476E-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
```


Information Only

```
                    -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
                                 0.506119E-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
                                  1.96128      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
                                 -0.334229     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, Z
                     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, K/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
```


Information Only

```
                    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
                    16.2118      16.2118     S, kJ/kg.K
                    4.79772      4.79772     Cp, kJ/kg.K
                                 1.41841     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
                                0.736930E-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
                    3.45582      3.45582      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----
```


Information Only

```
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
                  0.891925     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)
```


Information Only

Appendix B: `supertrapp` Code Verification

Information Only

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.

Information Only

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

Information Only

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

where P is the absolute pressure, ρ 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.

Information Only

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
                                   8.98036     Visc., uPa.s
                                   20.9478     Th. Cond.,mW/m.K
 (VLE=PRS,PROPS=EXCST)
```


Information Only

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} (-)	ΔZ (%)	η (μPa ·s)	η_{st} (μPa ·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
η = 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)	ρ (kg/m^3)	Z (-)	Z_{st} (-)	ΔZ (%)	η (μPa ·s)	η_{st} (μPa ·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
η = viscosity
$(\cdot)_{st}$ = supertrapp computed value

Information Only

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)	ρ (kg/m^3)	Z (-)	Z_{st} (-)	ΔZ (%)	η (μPa ·s)	η_{st} (μPa ·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
η = 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)	ρ (kg/m^3)	Z (-)	Z_{st} (-)	ΔZ (%)	η (μPa ·s)	η_{st} (μPa ·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
η = viscosity
$(\cdot)_{st}$ = supertrapp computed value

Information Only

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.

Information Only

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
```


Information Only

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)?
```


Information Only

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>
```


Information Only

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
                      1.13587      1.13587     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
                      1.17706      1.17706     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
                                   1.36849     Cp/Cv
                                   1510.39     Sound Speed, m/s
                                 -0.636380     JT, K/MPa
                                   8.84798     Visc., uPa.s
                                  0.220563     Th. Cond.,W/m.K
```


Information Only

(VLE=PRS,PROPS=EXCST)

Information Only

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
```


Information Only

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)?
```


Information Only

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>_
```


Information Only

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
                       3.35354      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
                                    61.1858     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      44.0095     Molar Mass
                      0.222925     0.222925     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
                                    510.685     Sound Speed, m/s
                                    0.638586    JT, K/MPa
                                    80.8654     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
                       3.25630      3.25630     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      866.590     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
                                    0.496386    JT, K/MPa
```


Information Only

```
                                  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
                                    88.5405     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
                                    590.752     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)
```


Information Only

B.4.3 CH_4

CH_4: supertrapp Input 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
```


Information Only

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)?
```


Information Only

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>_
```


Information Only

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
```


Information Only

```
                                 16.7122      Visc., uPa.s
                               0.588594E-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)
```


Information Only

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       0.0060
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    12.180
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
```


Information Only

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          ,P          ,          ,     ,    >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)?
```


Information Only

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>
```


Information Only

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     0.843567
 ethane              0.840000E-01 0.840000E-01 0.824474E-01
 propane             0.500000E-02 0.500000E-02 0.485893E-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
                     -4059.65     -4059.65     H, kJ/kg
                      10.1859      10.1859     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     0.788206
 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 0.676865E-01
 carbon dioxide      0.660000E-02 0.660000E-02 0.687959E-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
                      8.67865      8.67865     S, kJ/kg.K
                      2.66085      2.66085     Cp, kJ/kg.K
                                   1.51267     Cp/Cv
                                   399.358     Sound Speed, m/s
                                   4.25489     JT, K/MPa
                                   12.9780     Visc., uPa.s
                                  0.413693E-01 Th. Cond.,W/m.K
```


Information Only

```
(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
                                    13.8580     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     0.690828
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 0.445795E-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
                                    17.4062     Visc., uPa.s
                                   0.554743E-01 Th. Cond.,W/m.K
(VLE=PRS,PROPS=EXCST)
```


Information Only