NIST Standard Reference Database 4

NIST Thermophysical Properties of Hydrocarbon Mixtures Database (SUPERTRAPP)

Version 3.1

Users' Guide

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and Standard Reference Data

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CONTENTS

Chapter 1: INTRODUCTION

NIST SUPERTRAPP is an interactive computer database for the *prediction* of thermodynamic and transport properties of fluid mixtures. It can be used for pure fluids or for mixtures of up to 20 components. The components are selected from a database of 201 components, mostly hydrocarbons. It also can be used for petroleum fractions that are characterized by an average boiling point and an API gravity. 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, Cp, Cp/Cv, sound speed, Joule-Thomson coefficient) and transport properties (viscosity and thermal conductivity). The database also has many on-line help messages available. The database is very powerful yet easy to use.

NIST SUPERTRAPP features allow users to:

- perform bubble point pressure and temperature calculations;
- perform dew point pressure and temperature calculations;
- perform a variety of calculations on flashes: (T,P), (T,D), (T,S), (P,H), (T,H), and (P,S);
- obtain properties of pure components along the saturation boundary;
- compute tables of properties;
- change units;
- learn (and remember) a new component not in the current database;
- enter data from the keyboard or from data files; and
- save results in a file.

1.2 Uncertainties in Calculated Properties

Our objective in selecting property models for use in SUPERTRAPP is to implement the most accurate models currently available. The user should be aware that the uncertainties in these models vary considerably depending on the fluid, property, and thermodynamic state. It is thus impossible to give a simple, global statement of uncertainties. Even for the most-studied fluids with equations of state based on accurate, wide-ranging data, uncertainties are complicated functions of the temperature and pressure. The interested user is referred to the original literature sources discussing the development of the model. (References to the literature are in Chapter 6.)

The user is further cautioned that, by the very nature of a calculational database, property data are often displayed with more digits than can be justified based on the accuracy of the property models or the uncertainties in the experimental data to which the models were fitted.

Chapter 2: GETTING STARTED

2.1 System requirements

SUPERTRAPP runs in a DOS window under MS Windows 95, 98, 2000, NT, XP or ME. The package requires 430 kilobytes of available RAM and a hard disk drive with 1.5 megabytes of available space.

A math coprocessor is required. A printer is required to run the PRINT command.

2.2 Database files

The database is supplied on diskette, and contains the following files:

1. STPHELP
2. STPLIB2
3. STRAPP.EXE
4. LF90.EER
5. EXMPL1.TXT
6. EXMPL2.TXT
7. README.TXT
8. COPYRGHT.TXT
9. DEFAULTS

Also included are FORTRAN source code subroutines for computing properties, sample driver programs, and sample output.

1. STPV2A.FOR
2. STPV2B.FOR
3. SAMPLE1.FOR, SAMPLE1.OUT
4. SAMPLE2.FOR, SAMPLE2.OUT
5. SAMPLE3.FOR, SAMPLE3.OUT
6. SAMPLE4.FOR, SAMPLE4.OUT
7. SAMPLEP.FOR, SAMPLEP.OUT

8. WRITLIB2.FOR
9. PORTLIB
10. LIBFILE
11.README2.TXT

If any files are missing, please contact the Standard Reference Data Program at (301) 975-2208 or at our website at http://www.nist.gov/srd.

2.3 Installation

Put the CD-ROM in the CD-ROM drive (D or E). In Windows 3.1 or later or Windows NT, select File from the Program Manager's Menu Bar followed by Run from the File menu. In Windows 95, click the Start button and select Run. In the Command line: box, type

D:\SETUP (or E:\SETUP)

and press **ENTER**. Follow the remainder of the Installation instructions. A NIST SUPERTRAPP 3.1 Program Group is created at the end of installation.

NOTE: Because SUPERTRAPP allows changing the database file (STPLIB2) permanently, keeping a backup copy of the original release of STPLIB2 is strongly recommended.

NOTE: In some Windows applications the MS-DOS window may remain open after the program is terminated. To close the window, click the Close button in the upper right corner of the window when the statement "Program Terminated – Exiting NIST4" appears.

Chapter 3: RUNNING SUPERTRAPP

After installing SUPERTRAPP, you can run it by clicking [Start]-[Programs]-[NIST]-[SUPERTRAPP]. There are a few general comments about SUPERTRAPP to keep in mind. First of all, the program is case-insensitive so that either upper or lower case input is allowed. Also, there are many questions for which a YES or NO response is called for. The default answer is whichever appears first after the question-for example, (N,Y) indicates that NO is the default, while (Y,N) indicates that YES is the default. Pressing **ENTER** is equivalent to the default answer. Y or N is also acceptable. Typing a question mark (?) will generally cause a context-appropriate help message to appear.

To start program execution, press **ENTER**.

The database program proceeds by displaying a set of questions, which are

answered by keyboard entry. The first is whether to use the defaults (for units, model, etc.). If the answer is No, the program asks whether the compositions are to be inputted as mole fractions. An **ENTER**, N, or No response means the compositions are inputted as moles, and the program computes the mole fractions. Should you choose to input in mole fraction mode, the program checks that the sum of the mole fractions is unity. The next question is whether to receive input from a previously prepared file. For more information about file input, see the command OPEN described in Chapter 4.

The following questions concern output to a file. You may want to save the results in a file and/or see the results on the screen. To save results in a file, answer YES to this question. See command OPEN in Chapter 4 for more details. The next questions deal with units. SUPERTRAPP starts up with a default set of units (K, bar, liter, kJ, mole, m, s, μpoise, mW). To change any or all of these units, answer YES to this question. Details on changing units are covered in Chapter 4 under the UNITS command.

The program asks for the number of components in the mixture. Enter the appropriate number of species from 1 to 20. A zero causes the program to stop. After the number of components is entered, the program asks for the names of the components. SUPERTRAPP has a built-in library of 196 components, which are listed in Appendix B. To see the library list on screen, enter a ? in response to a prompt for a component name. Be careful to type in the component name, or its synonym, exactly as it appears on the screen or in Appendix B, or the program does not recognize the name. (When this happens, you are given an opportunity to view the component name list and correct the spelling. For a petroleum fraction, enter any of the reserved names (petroleum #1, petroleum #2, petroleum #3 or their synonyms pet1, pet2 and pet3). You are then asked to enter an average boiling point and API gravity. The API gravity is given in degrees API, and is defined as API=(141.5/sp60) - 131.5, where sp60 is the specific gravity of the fluid with respect to water at 60°F. If the component is still not in the database, you then have the option of adding it. If the program does not recognize the name of the component, it asks you a series of questions to allow you to enter the component as a new fluid. For details on this procedure, see Chapter 5.1. After the components have been input, you are asked to enter the composition (unless there is only one component). (Note: although water is present in the component list, calculations for pure water or for mixtures of more than 5 mole percent water are not permitted.)

Finally, you reach at the main "command line," which is:

> Enter command or, if you wish to do a flash calculation,
> enter T(K) and P(bar) separated by a comma.

At this point, you can either do a flash calculation by entering the temperature

and pressure of interest, or enter any of the commands that SUPERTRAPP supports, including the option of changing any pure component property values stored in the library. For details on this step, see the command MODIFY in Chapter 4 (4.16).

Chapter 4: COMMAND OPTIONS

From the command line, any of the following commands can be entered:

TECHNICAL COMMANDS

BUBP	Bubble point pressure calculation
BUBT	Bubble point temperature calculation
DEWT	Dew point temperature calculation
FEED	Change the composition
FLTP	Isothermal flash (default command)
FLTD	T,D flash
FLTS	T,S (isentropic) flash
FLPH	P,H (isenthalpic) flash
FLPS	P,S flash
FLTH	T,H flash
KIJ	Change extended corresponding states (EXCST) interaction parameters
KIJV	Change the vapor-liquid equilibrium (VLE) interaction parameters
MASSIN	Toggle mass/mole input mode
MODEL	Change equation of state model
MODIFY	Change pure component property data
NORMAL	Toggle the composition mode
SATF	Pure component saturation properties
SLATE	Change the components in the mixture
TABLE	Generate a table
UNITS	Change the current units

CONTROL COMMANDS

CLOSE	Close the output file
EDIT	Edit the feed composition
OPEN	Open a new input or output file
RESET	Restart SUPERTRAPP
STOP	Terminate the program

SYSTEM COMMANDS

DIR	List the directory that is associated with a pathname
PRINT	Print file on printer
SYSTEM	Execute a DOS system command
TYPE	List a file on terminal

OTHER COMMANDS

LIB Create portable library file

For on-line help, type the name of the command followed by a question mark, for example, UNITS?. Additional information on the available commands is given in the following sections.

TECHNICAL COMMANDS

4.1 BUBP

A bubble point pressure calculation computes the vapor (bubble) composition and pressure using known values of the liquid composition (in equilibrium with the vapor) and the temperature. To perform the calculation, enter "BUBP" mode at the command line, and then enter the temperature at the point of interest. Enter a new command or an "X" to leave the BUBP mode. A sample BUBP screen is given below (Fig. 1). BUBP can be used for pure components or mixtures. Tables of bubble points can be generated using the TABLE command, (see section 4.20).

2-Phase Bubble Point results at T = 200.000 K and P = 0.116754 MPa

--Component---	--Feed---	--Liquid--	--Vapor---	---Phi----	--K--
propane	0.500000	0.500000	0.927125E-01	0.870237E-01	.19E+00
ethane	0.500000	0.500000	0.907287	0.879587	.18E+01
Molar Basis					
	1.00000	1.00000	0.000000	Feed Fraction	
	37.0823	37.0823	31.3695	Molar Mass	
	0.451373E-02	0.451373E-02	0.965358	Comp. Factor, Z	
	0.576826	0.576826	0.228156E-02	D, kg/liter	
	-3159.78	-3159.78	-2917.66	H, kJ/kg	
	4.05164	4.05164	6.83080	S, kJ/kg.K	
	2.31336	2.31336	1.49442	Cp, kJ/kg.K	
		1.62313	1.26284	Cp/Cv	
		1308.11	249.601	Sound Speed, m/s	
		-0.441795	36.0524	JT, K/MPa	
		204.504	6.23615	Visc., uPa.s	
		153.487	11.9750	Th. Cond.,mW/m.K	

(VLE=PRS, PROPS=EXCST)

Figure 1. Sample bubble point pressure calculation.

This sample BUBP result shows the type of information provided by the calculation. The mole fractions of the components in the phases are given, along with the "Kvalue", which is the ratio of the vapor phase composition of a component to the liquid phase composition of that component. The relative quantities of the phases present are also given in the line labeled “Feed Fraction.” For the example shown, because it is a bubble point calculation, only a minute bubble of vapor is present, and the vapor fraction is essentially zero.

The molecular weights of the phases and feed are also given. Equilibrium

properties (compressibility factor (defined as Z=PV/RT), density (D), enthalpy (H), entropy (S), Cp, Cp/Cv, sound speed and Joule-Thomson coefficient), as well as transport properties (viscosity, thermal conductivity) are calculated. The final entry shows which model was used in the calculations. The phase equilibria (VLE) are always calculated using the PRS option, while the properties can be found using either the PRS or EXCST models. For more information on the models used, see the MODEL command, (see section 4.15).

4.2 DEWP

A dew point pressure calculation finds the liquid (dew) composition and pressure using known values of the vapor composition (in equilibrium with the liquid) and the temperature. To perform the calculation, enter "DEWP" mode at the command line, and then enter the temperature. To leave DEWP, enter any other valid command. An "X" returns program control to the main command line. DEWP can be used for pure components or mixtures. Tables of dew points can be generated using the TABLE command. The output from a DEWP calculation is very similar to that for a BUBP calculation. The mole fractions of the components in the phases are given, along with the "Kvalue". The relative quantities of the phases present are also given in the line labeled “Feed Fraction.” For a dew point calculation, only a minute drop of liquid is present.

4.3 BUBT

A bubble point temperature calculation computes the vapor (bubble) composition and temperature using known values of the liquid composition and the pressure. To perform the calculation, enter "BUBT" mode at the command line, and then enter the pressure at the point of interest. Enter a new command or an "X" to leave the BUBT mode. BUBT can be used for pure components or mixtures. Tables of bubble points can be generated using the TABLE command. The type of information provided by the BUBT

calculation is the same as for BUBP. The difference is that for BUBP, the temperature is a known input, while for BUBT the pressure is a known input.

4.4 DEWT

A dew point temperature calculation computes the dew (liquid) composition and temperature using known values of the vapor composition and the pressure. To perform the calculation, enter "DEWT" mode at the command line, and then enter the pressure at the point of interest. Enter a new command or an "X" to leave the DEWT mode. DEWT can be used for pure components or mixtures. Tables of dew points can be generated using the TABLE command. The type of information provided by the DEWT calculation is the

same as for DEWP. The difference is that for DEWP, the temperature is a known input, while for DEWT the pressure is a known input.

4.5 FEED

The FEED command enables changing the concentrations of the components in the mixture. If you enter FEED, the program prompts for the new concentration of each component.

4.6 FLTP

An isothermal flash calculation finds the quantities and compositions of the vapor and liquid phases in equilibrium at a given pressure, temperature and overall composition. The isothermal flash is the default command at the command line in SUPERTRAPP. Simply enter the temperature and pressure (separated by a comma) at the point of interest. If another command has been performed, to return to a flash calculation, type the command "FLTP". A sample FLTP screen is shown below (Fig. 2). The program is designed to operate within the range 10-1000 K and 0-3000 bar. Points outside this range are ignored.

2-Phase Flash results at T = 265.000 K and P = 1.00000 MPa

-Component----	---Feed---	--Liquid--	--Vapor---	---Phi----	--K--
propane	0.500000	0.554896	0.242160	0.190756	.44E+00
ethane	0.500000	0.445104	0.757840	0.677790	.17E+01
Molar Basis					
	1.00000	0.824466	0.175534	Feed Fraction	
	37.0823	37.8523	33.4657	Molar Mass	
	0.176969	0.345867E-01	0.845725	Comp. Factor, Z	
	0.951033E-01	0.496718	0.179596E-01	D, kg/liter	
	-2940.09	-2974.52	-2757.17	H, kJ/kg	
	4.96122	4.68395	6.43422	S, kJ/kg.K	
	2.59044	2.70354	1.98959	Cp, kJ/kg.K	
		1.71037	1.33695	Cp/Cv	
		849.828	247.259	Sound Speed, m/s	
		-0.119548	19.7208	JT, K/MPa	
		104.723	8.13051	Visc., uPa.s	
		114.109	19.3834	Th. Cond.,mW/m.K	

(VLE=PRS,PROPS=EXCST)

Figure 2. Sample results from a isothermal flash calculation.

The mole fractions of the components in the phases present are given, along with the "Kvalue", which is the ratio of the vapor phase molar composition of a component over the liquid phase molar composition of that component. The relative quantities of the phases present are also given in the line labeled “Feed Fraction”. For the example shown, if there is one mole of feed, the flash calculation predicts 0.824466 moles of liquid and 0.175534 moles of vapor. In addition, the molecular weights of the phases and feed are given. The sample result shows a case where two phases result from the flash calculation. (It also is possible to obtain only one phase from a flash calculation). SUPERTRAPP labels the phases present and gives properties of the phases, calculated with

the currently active model (EXCST or PRS), as noted on the output. (To change the model, see the command MODEL). The phase equilibrium is always done with the PRS model. Equilibrium properties as well as transport properties are displayed in the output.

4.7 FLTD

A T,D flash calculation determines the quantities and compositions of the vapor and liquid phases in equilibrium at a given temperature, density and overall composition. At the command line, enter FLTD to obtain a T,D flash. Next, enter the temperature and density (separated by a comma) at the point of interest. Output from FLTD looks very similar to FLTP.

4.8 FLTS

A T,S flash calculation determines the quantities and compositions of the vapor and liquid phases in equilibrium at a given temperature, entropy and overall composition. At the command line, enter FLTS to obtain a T,S flash. Next, enter the temperature and entropy (separated by a comma) at the point of interest. Output from FLTS looks very similar to FLTP.

4.9 FLPH

A P,H flash calculation determines the quantities and compositions of the vapor and liquid phases in equilibrium at a given pressure, enthalpy and overall composition. At the command line, enter FLPH to obtain a P,H flash. Next, enter the pressure and enthalpy (separated by a comma) at the point of interest. Output from FLPH looks very similar to FLTP.

4.10 FLPS

A P,S flash calculation determines the quantities and compositions of the vapor and liquid phases in equilibrium at a given pressure, entropy and overall composition. At the command line, enter FLPS to obtain a P,S flash. Next, enter the pressure and entropy (separated by a comma) at the point of interest. Output from FLPS looks very similar to FLTP.

4.11 FLTH

A T,H flash calculation determines the quantities and compositions of the vapor and liquid phases in equilibrium at a given temperature, enthalpy and overall composition. At the command line, enter FLTH to obtain a T,H flash. Next, enter the temperature and enthalpy (separated by a comma) at the point of interest. Output from FLTH looks very similar to FLTP.

4.12 KIJ

The KIJ command allows changing or viewing the interaction parameters for the binary pairs in the mixture when using the EXCST model. The parameters can be used to fine-tune the model to a particular point or set of data. In general, the model predictions are sensitive to these parameters, so care should be taken when adjusting them. When you enter KIJ, you are shown the current values of kij and lij for each of the possible binary combinations of the mixture components and prompted for new values. The kij parameter is used in computing the "f", or energy-related shape factor, while the lij parameter is used in computing the "h" or size-related shape factor for the mixture. If you do not use this command, a default set of values is assumed. To view kij and lij, but not change them, press **ENTER** after invoking KIJ. When you change these parameters, the changes are NOT stored permanently in the database, so it is necessary to re-enter the changes each time a new SLATE command is invoked, or upon start-up.

4.13 KIJV

KIJV allows changing or viewing the PRS interaction parameters without changing the EXCST parameters. The phase equilibrium tends to be very sensitive to the KIJV interaction parameters, so care should be used when adjusting them. Upon invoking the KIJV command, you are shown the current value and prompted for a new value for the binary interaction parameter for each possible binary pair in the mixture. The program starts up with default values of Peng-Robinson binary interaction parameters, which are found using a generalized procedure based on the general type or family that a species belongs to. To view the kijv but not change them, press **ENTER** after invoking KIJV. When you change these parameters, the changes are NOT stored permanently in the database, so it is necessary to re-enter the changes each time a new SLATE command is invoked, or upon start-up.

4.14 MASSIN

This command toggles between input on a mass or mole basis.

4.15 MODEL

SUPERTRAPP calculates phase compositions with the Peng-Robinson equation of state (EOS) and offers a choice of the Peng-Robinson (PRS) or the NIST extended corresponding states model (EXCST) for the calculation of phase properties. The MODEL command allows changing the model used for

bulk phase property calculation. Enter PRS for the Peng- Robinson EOS, or EXCST for the NIST extended corresponding states model. The default mode is to compute phase properties using the EXCST model, and vapor-liquid equilibria (VLE) with the Peng-Robinson model. The models used are identified in the output display.

4.16 MODIFY

This command allows changing pure component property data. It also can be used simply to view data for a given component. (Note: you have the option to change data values — permanently or just temporarily. We STRONGLY recommend that, before changing anything, you have a backup copy of the database file STPLIB2.) You are first shown the current values of pure component property values. Next, you are asked which component to modify, and which property to modify. The options for modification are:

Cp	ideal gas heat capacity	Sh	shape factors (see 4.15.8)
H0	enthalpy reference state	Tb	normal boiling point
Hf	heat of fusion	Tc	critical temperature
LJ	Lennard-Jones parameters	Tt	triple point temperature
Mw	molecular mass	Vc	critical volume
Pc	critical pressure	w	acentric factor
S0	entropy reference state		

In addition, if you want to change units at this step, type “Units” or “Un.” You can alter more than one component by entering the name of each component. After finishing the modifications, press **ENTER** to exit the loop. You are asked if you want the modifications to be permanent. If the answer is YES, the modifications are written to the random access file that contains the database and essentially become permanent. If the answer is NO, the modifications are lost when you change the component slate. This allows performing calculations with your modifications until changing the component slate and then being able to return to the original settings. More detailed information on the MODIFY options is given in sections 4.16.1 - 4.16.9.

4.16.1 Cp

SUPERTRAPP uses ideal gas heat capacities in the computation of enthalpy, entropy, thermal conductivity, Cp, Cp/Cv, w, and JT. There are built-in values that may be changed and overwritten by entering Cp data at this step. You are asked to enter data (up to 20 points) as (T, ideal gas Cp) pairs. When entering values, bear in mind that it is best to input the ideal gas heat capacities over as wide a temperature range as possible.

4.16.2 S0,H0

You can change the reference value for entropy or enthalpy. This is useful when trying to compare results with another program or tabular data. The usual value for reference state enthalpy is the heat of formation of the ideal gas at 298.15 K. For entropy, the usual reference state value is the entropy of the ideal gas at 298.15 K and one atmosphere. However, a zero or any other value can be inputted since it is just a reference point value and has no effect on changes in enthalpy or entropy. The program interprets your entry as the value of the ideal gas at 298.15 K and one atmosphere.

4.16.3 Tc,Pc,Vc

The critical properties of the component can be changed with these commands.

4.16.4 Mw

The molecular mass can be changed using this option.

4.16.5 Tb

The normal boiling point (the temperature at which the species boils at a pressure of one atmosphere) can be changed with this command.

4.16.6 Tt,Hf

These commands allow changing the triple point temperature or the heat of fusion of a component. This information is not essential to the operation of the program; it is used only in an ideal solid solubility calculation to check for the presence of solids.

4.16.7 w

The Pitzer acentric factor can be changed with this option. This factor is defined in terms of the reduced vapor pressure of a pure species evaluated at a reduced temperature ($T_r = T/T_c$) of 0.7 and is given by

$$\tilde{w} \; -1.0 - \log_{10}(P_r^{sat})T_{r=0.7}$$

4.16.8 Sh

When SUPERTRAPP performs extended corresponding states calculations (the EXCST model), it uses quantities called shape factors. The current implementation uses vapor pressure and saturated liquid density information to

generate the shape factors for equilibrium thermodynamic properties. It uses information on saturated liquid viscosities and thermal conductivities to develop a kind of mass shape factor used in transport calculations. To change these quantities, invoke the Sh option. You are asked if you have vapor pressure data, then saturated liquid density data, then saturated liquid viscosity and thermal conductivity data. You can enter data for any or all of these quantities (with a maximum of 20 points).

4.16.9 Lennard-Jones Parameters

During the estimation of low density transport properties, SUPERTRAPP can often improve the accuracy of the predictions by using Lennard-Jones potential parameters. Some components have built-in values for these parameters. Others have no values available, and a default method is used in the computations. You can change the values of the Lennard-Jones collision diameter parameter (usually called "sigma") and the Lennard-Jones energy well depth parameter ("epsilon/k") by invoking the LJ option.

4.17 NORMAL

You have the option of always entering a feed composition whose mole fractions sum to unity or having the program normalize the input feed composition. NORMAL enables switching back and forth between the mole fraction input and the molar input modes. The prompt shows which mode is in use when entering a composition.

4.18 SATF

SATF allows the calculation of saturation thermodynamic properties for the pure components in the mixture. The saturated vapor and liquid densities, the saturation pressure, the heat of vaporization and the fugacity coefficient (f/P) are displayed (but not thermal conductivity or viscosity). (If this information is desired, run the DEWP, BUBP, DEWT, BUBT or TABLE options using a pure fluid to get saturation values). The model used for property calculation is also shown. To perform the calculation, enter "SATF" at the command line. Terminate SATF by pressing **ENTER** or entering "X".

4.19 SLATE

The SLATE command enables changing the components in the mixture. You are asked for the number of components, and then the names of the components. If you enter a question mark (?) at the "name the component" prompt, the current component library can be listed. The component names and synonyms supplied in SUPERTRAPP are given in Appendix B. For a petroleum fraction, enter one of the reserved names for petroleum fractions

(PETROLEUM #1, PETROLEUM #2 or PETROLEUM #3) or synonyms (PET1, PET2 or PET3).You are then asked to supply an average boiling point and API gravity. If the component name is not in the database, you may enter it as a new component. For details on the entry of a new component, see Chapter 5.

4.20 TABLE

The TABLE generates tables for selected combinations of independent and output variables. The choices of independent variables are: T, P, D, H, and S. Also available is a "SAT" option that provides results along the vapor-liquid saturation boundary and is valid for both pure fluids and mixtures. You are asked to input the minimum, maximum and increment values for the independent variables chosen for the table. Up to seven output variables can be selected. For a pure fluid, the choices are: T, P, D, Z, H, S, viscosity, thermal conductivity, sound speed, MW, C_p, C_v, and Joule-Thomson coefficient. For mixtures, there are additional choices available: equilibrium phase compositions, Kvalues (defined as y_i/x_i where y_i is the mole fraction of i in the vapor phase, and x_i is the mole fraction of i in the liquid phase), and the feed fraction in each resulting phase. The feed fraction shows how the feed is "split" between the phases.

4.21 UNITS

It is possible to select from various input/output unit combinations in SUPERTRAPP. This command brings up a menu-driven unit selection routine. The current units and the unit options are shown on the menu, as shown below. To change a specific unit, enter the new unit. For example, to change the pressure to megapascals enter "MPA". To select one of four "default" sets of units, enter a number between 1 and 4. To exit, enter an "X". For example, to enter several units on one line and exit, type,

MPA,CAL,X

This selects pressures in MPa, energies in calories and exits the Units subroutines. To see the menu again, press **ENTER**.

CONTROL COMMANDS

4.22 CLOSE

The CLOSE command closes the current output file. Combinations of OPEN and CLOSE commands enable saving results in different files. (Only one output file may be open at a time.)

4.23 EDIT

The EDIT option allows changing the feed composition of a single component selectively, leaving the others unchanged. This option is

particularly useful for the case where you are entering mole fractions and have made a typing mistake that causes the overall composition not to sum to unity. To leave the edit loop, press **ENTER** or enter "X". A sample edit loop is shown below. Note that either the full component name or its synonym can be entered (See Appendix B for synonyms).

4.24 OPEN

This command allows you to open a new file. You are asked whether an input or output file is desired.

i. **output files**

   Output files can be created to save the results of calculations to a file for later use. It is also possible to see the results of the calculations simultaneously on the terminal. Output continues to go to the output file until a CLOSE or RESET command is issued. The output file can be reviewed during the session by using the TYPE or PRINT commands.

ii. **input files**

   Input files can be used instead of keyboard data entry. For an input file, the program reads taking data from that file until an end-of-file or $END is encountered. Two sample data files are shown below (Fig. 3), and are included on the distribution diskettes.

example file 1 (EXMPL1.TXT)

```
COMP 1     N-BUTANE
COMP 2     METHANE
COMP 3     ETHANE
FEED 1          0.5000 FEED
FEED 2          0.2000 PRS
FEED 3          0.2000  KIJV
FLTP       3001.0       FLTP
$END
```

example file 2 (EXMPL2.TXT)

```
COMP01     C2
COMP02     C10
FEED  1              0.5000
2     0.5000

1  2    0.95
        300                1.0
FLTP        350            2.5
EXCST
KIJ    1  2          0.95
LIJ    1  2          0.95
FLTP        300           1.0
FLTP        350           2.5
$END
```

Figure 3. Sample data input file.

The first entries in a data file must be COMP statements, which identify the components in the mixture. The names must be selected from the database, and the name or a synonym (C4 for n-butane) can be used. They must be input in the format COMP##bbbbNAME where ## is a number from 1 to 20, bbbb represents four blank spaces, and then the name. A complete list of the components and their synonyms is given in Appendix B. Note that either upper or lower case can be used. After the COMP statements, the FEED statement is used to input each component in mole or mole fractions (depending on what is chosen when the program was started, or when a NORMAL command is invoked). Default mode is to input feed as moles. The next line can be any of the commands: BUBP, DEWP, BUBT, DEWT, FLTP, FLTD, FLPH, FLTS along with the appropriate input variables. You can also change the calculation model (PRS or EXCST), or specify interaction parameters using KIJV, KIJ and/or LIJ.

In the first example file, FLTP asks for a flash calculation at T=300 K and P=1.0 bar. The current default units as specified in the DEFAULTS file are used. (After entering the data filename, you are asked whether to change the units). In the second example, the model is changed from the default model (which is EXCST) to the Peng-Robinson (PRS). The model used in the calculations is identified in the output and remains the same until another PRS or EXCST is

encountered, as shown in the example. For more information on the

models, see the MODEL command. The second example file shows changing the interaction parameter for the 1-2 pair (c2-c10 in this example) from the default value to 0.95. If the mixture contains more than two components, specify the pair for which you want to change the interaction parameter. For example, to change the butane-ethane VLE interaction parameter in the first example to 0.97, include the line:

KIJV 1 3 0.97

in the data file. The EXCST interaction parameters can also be changed by using KIJ and LIJ commands as shown in the second example. For further details, see instructions for the KIJ and KIJV commands. The last entry in a data file must be a $END statement. At the end of data file operations, the program resumes interactive mode.

iii. filenames

The name of an input or output file can be any legitimate MS/PC DOS filename including device (or drive):filename.extension. Pathnames are not currently supported. examples:

A:DATA.INP
INPUTD.FIL
STPDAT.DAT

NOTE: If problems are encountered with this command, it may be necessary to increase the FILES= statement in your CONFIG.SYS file.

4.25 RESET

RESET starts SUPERTRAPP over from the beginning. (Only the changes explicitly committed to the database remain after RESET.)

4.26 STOP

This command terminates the program and returns to the system prompt.

SYSTEM COMMANDS

4.27 DIR

DIR lists the contents of any directory or subdirectory. After entering the DIR command, you are prompted for the path. Pressing **ENTER** in response to the prompt produces the contents of the current directory. NOTE: If you encounter problems with this command, you may have to increase your FILES= statement in the CONFIG.SYS file.

4.28 PRINT

PRINT lists a file on the printer [PRN] device. Any ASCII file can be printed. If the current output file is to be printed, it is closed and then reopened to flush the buffer. If a file other than the output file is requested, the current output file (if any) remains unchanged.

4.29 SYSTEM

SYSTEM executes an MS/DOS command from within SUPERTRAPP. After entering "SYSTEM", you are prompted for the system command. The total command length must be shorter than 77 characters. For example, if you enter the phrase >CURRENT.DIR DIR C:\DOS, the directory of C:\DOS is placed in the file CURRENT.DIR, which can then be manipulated by SUPERTRAPP or by invoking an editor with the system command.

4.30 TYPE

TYPE lists a file on the screen. Any ASCII file can be typed. If you request the current output file to be typed, it is closed and then reopened to flush the buffer. If you request that a file other than the output file be typed, the current output file (if any) remains unchanged.

OTHER COMMANDS

4.31 LIB

The LIB command is used to create a sequential ASCII library file called PORTLIB. This file contains component constants and parameters for all fluids in the library. It is used to install SUPERTRAPP on non-IBM compatible machines. For more information, see Appendix C, "Use of the Source Code Subroutines". Also see the sample driver routines

(SAMPLE1.FOR, etc.) and the file README2, located on the distribution diskette.

Chapter 5: ADVANCED FEATURES

5.1 Entry of a new component

SUPERTRAPP has an extensive database with 196 components. Advanced users, however, may wish to add new components to the database. (We stress

however, that the program is designed primarily for nonpolar hydrocarbons, and we do not recommend the addition of highly polar or associating substances.) The absolute minimum information required for a new component is the critical temperature, pressure and volume, the molecular weight, and the normal boiling point. The program accepts other information to improve the accuracy of the predictions. Useful information includes the Pitzer acentric factor, ideal gas heat capacities, saturated liquid densities, vapor pressures, saturated liquid viscosity and thermal conductivity, the heat of fusion and the triple point temperature. In addition, a reference value for enthalpy and entropy must be specified.

To enter a new component, first enter the SLATE command. When prompted for the name of the component, enter the new component name. If the program cannot match the name with those in the database, a listing of the components currently in the database is shown. Next, the program asks if the entry is misspelled and gives a chance to correct it. It next asks if you want to enter component parameters for the component. If the answer is YES, you are first prompted for a synonym for the component and then asked to identify the family that best describes the new component. This information is used in a generalized method to determine the Peng-Robinson binary interaction parameters.

If the fluid is not a petroleum fraction, the next series of questions prompts for the molecular weight, the critical pressure, the critical volume and the critical temperature. You must input a value for these quantities. At any time, to change the units, type "UNITS" to enter the units selection menu. After the unit change, you are returned to the previous place in the program. If you change your mind and want to exit the new component entry mode, type an "X".

The next question asks if you have a value for the Pitzer acentric factor. If you do, answer "YES" and then enter the value. Pressing **ENTER** is interpreted as a NO. If you do not provide a value, the program calculates one based on available vapor pressure information and the definition of the acentric factor.

The next question asks for the normal boiling point of the substance. This is essential information, and a value must be inputted.

If the fluid is a petroleum fraction, the program will ask for an average boiling point and API gravity. It will then estimate the properties Tc, Pc, Vc, w, Mw.

Two more questions follow asking for reference values for enthalpy and entropy. The usual value for the reference state enthalpy is the heat of formation of the ideal gas at 298.15 K. For entropy, the usual reference state value is the entropy of the ideal gas entropy or enthalpy at 298.15 K and one atmosphere pressure in Pa. However, a zero or any other value may be inputted, because it is just a reference point value and has no effect on changes in enthalpy or entropy. The program interprets your entry as the value

of the ideal gas at 298.15 K and one atmosphere.

The next two questions ask if the triple point temperature and heat of fusion are known. This information is not essential to the operation of the program; it is used only in an ideal solid solubility calculation to check for the presence of solids.

After these questions, you are then asked if you have ideal gas heat capacities. If so, the program asks how many there are. Up to twenty points may be inputted. The program has a built-in fitting routine, which fits the data to a function. To change the units before entering, type "UNITS". Otherwise, enter the ideal gas heat capacity data as (T, Cp) pairs. The program prints what you have entered and gives you a chance to edit the data before the fit is performed. The ideal gas heat capacities are used in the computation of thermal properties such as enthalpy and entropy as well as thermal conductivity. If you have no values, default values are assumed. If you have values, bear in mind that it is best to input the ideal gas heat capacities over as wide a temperature range as possible. For example, if you are interested in computations at 600 K, be sure to input ideal gas heat capacities valid up to 600 K; otherwise the results for enthalpy, entropy and thermal conductivity may be in error.

The last four quantities requested, vapor pressures, saturated liquid densities, saturated liquid viscosities and thermal conductivities, are used in the computation of "shape factors". The vapor pressure and saturated liquid density are used in calculating shape factors for the equilibrium thermodynamic properties. The transport data are used in calculating a mass shape factor used in transport predictions. SUPERTRAPP takes the user-supplied data and fits them to various correlations. You can input up to twenty points for each property. After the data are inputted, there is an option for editing data before the fitting procedure begins. It is best to supply data over as wide a temperature range as possible. The units can be changed before data entry begins by typing "UNITS". The program does not keep each datum in the database, only the results of the fitting process so that if, in the future, more or better data become available, this step must be repeated using the MODIFY command with the option Sh for SHape factors. If no data are available, a generalized procedure is used by default.

Note: It is easy to add a component, and to change parameters for a component, but once saved permanently in the database, it is not possible to remove a component.

Chapter 6: REFERENCES

This manual is meant to be a users' guide, and not a detailed description of the various methods used in the program. The following publications are useful references on the various technical procedures used in the NIST SUPERTRAPP program.

1. Transport Property Prediction

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2. Corresponding States Method

Cullick, A.S, and Ely, J.F., Densities of Vinyl Chloride from 5 to 65°C and Saturation Pressure, J. Chem. Eng. Data **27**, 276-281 (1982).

Fisher, G. D. and Leland, T. W. The corresponding states principle using shape factors, I&EC Fund., **9**, 537-544 (1970).

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3. Binary Interaction Parameters

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4. Peng-Robinson Equation of State

Peng, D.Y. and Robinson, D.B., A New Two-Constant Equation of State, I&EC Fund., **15**, 59-64 (1976).

Appendix A
NOMENCLATURE

I. List of Commands

BUBP	Bubble point pressure calculation
BUBT	Bubble point temperature calculation
CLOSE	Close the output file
DEWP	Dew point pressure calculation
DEWT	Dew point temperature calculation
DIR	Obtain the directory that is associated with a pathname
EDIT	Edit the feed composition
FEED	Change the composition
FLTP	Isothermal flash (default command)
FLTD	T,D flash
FLTS	T,S (isentropic) flash
FLPH	P,H (isenthalpic) flash
FLPS	P,S flash
FLTH	T,H flash
KIJ	Change EXCST interaction parameters
KIJV	Change the VLE interaction parameters
LIB	Create portable library file
MASSIN	Toggle mass/mole input mode
MODEL	Change equation of state model
MODIFY	Change pure component data
NORMAL	Toggle the composition mode
OPEN	Open a new input or output file
PRINT	Print file on printer
RESET	Restart SUPERTRAPP
SATF	Compute pure component saturation properties
SLATE	Change the components in the mixture
STOP	Terminate the program
SYSTEM	Execute a system command
TABLE	Generate a table
TYPE	List a file on terminal
UNITS	Change the current units

II. List of Abbreviations and Terms

°API	defined by °API =141.5/sp60 -131.5
Comp. Factor	compressibility factor, PV/RT
Cp	specific heat capacity at constant pressure
Cp/Cv	ratio of heat capacity at constant pressure to heat capacity at constant volume
D	density
Dc	critical density
Dsat,L	saturated liquid density
Dsat,V	saturated vapor density
EXCST	NIST extended corresponding states model
f/P	fugacity coefficient divided by pressure
H	enthalpy
H0	enthalpy reference state
Hf	heat of fusion
Hvap	heat of vaporization
JT	Joule-Thomson coefficient
Kvalue	ratio of vapor phase composition of a component to the liquid phase composition of that component
LJ	Lennard-Jones potential function
Mw	molecular mass
P	pressure
Pc	critical pressure
Phi	fugacity coefficient of component divided by pressure
PRS	Peng-Robinson equation of state model
Psat	saturation pressure
S	entropy
S0	entropy reference state
Sh	shape factors
Sp60	specific gravity=density of material at 60□F/density of liquid water at 60□F
T	temperature
Tb	normal boiling point temperature
Therm. Cond.	thermal conductivity
Tc	critical temperature
Tt	triple point temperature
μP	micropoise (displayed on screen as μP)
V	volume
Vc	critical volume
Visc.	viscosity
VLE	vapor-liquid equilibrium
w	Pitzer's acentric factor
Z	compressibility factor, PV/RT

Appendix B

SUPERTRAPP LIBRARY LIST

NAME	SYNONYM	FORMULA
METHANE	C1	CH4
ETHANE	C2	C2H6
PROPANE	C3	C3H8
ISOBUTANE	IC4	C4H10
N-BUTANE	C4	C4H10
NEOPENTANE	22DMC3	C5H12
ISOPENTANE	IC5	C5H12
N-PENTANE	C5	C5H12
2,2-DIMETHYLBUTANE	22DMB	C6H14
2,3-DIMETHYLBUTANE	23DMB	C6H14
3-METHYLPENTANE	3MP	C6H14
2-METHYLPENTANE	IC6	C6H14
N-HEXANE	C6	C6H14
2,2,3-TRIMETHYLBUTANE	223TMB	C7H16
3,3-DIMETHYLPENTANE	33DMP	C7H16
2,4-DIMETHYLPENTANE	24DMP	C7H16
2,3-DIMETHYLPENTANE	23DMP	C7H16
2,2-DIMETHYLPENTANE	22DMP	C7H16
3-ETHYLPENTANE	3EP	C7H16
3-METHYLHEXANE	3MHEX	C7H16
2-METHYLHEXANE	2MH	C7H16
N-HEPTANE	C7	C7H16
2,2,3,3-TETRAMETHYLBUTANE	2233TMB	C8H18
2,3,4-TRIMETHYLPENTANE	234TMP	C8H18
2,3,3-TRIMETHYLPENTANE	233TMP	C8H18
2,2,4-TRIMETHYLPENTANE	224TMP	C8H18
2,2,3-TRIMETHYLPENTANE	223TMP	C8H18
3-METHYL-3-ETHYLPENTANE	3M3EP	C8H18
2-METHYL-3-ETHYLPENTANE	2M3EP	C8H18
3,4-DIMETHYLHEXANE	34DMH	C8H18
3,3-DIMETHYLHEXANE	33DMH	C8H18
2,5-DIMETHYLHEXANE	25DMH	C8H18
2,4-DIMETHYLHEXANE	24DMH	C8H18
2,3-DIMETHYLHEXANE	23DMH	C8H18
2,2-DIMETHYLHEXANE	22DMH	C8H18
3-ETHYLHEXANE	3EH	C8H18

NAME	SYNONYM	FORMULA
4-METHYLHEPTANE	4MC7	C8H18
3-METHYLHEPTANE	3MC7	C8H18
2-METHYLHEPTANE	2MC7	C8H18
N-OCTANE	C8	C8H18
2,3,3,4-TETRAMETHYLPENTANE	2334TMP	C9H20
2,2,4,4-TETRAMETHYLPENTANE	2244TMP	C9H20
2,2,3,4-TETRAMETHYLPENTANE	2234TMP	C9H20
2,2,3,3-TETRAMETHYLPENTANE	2233TMP	C9H20
2,2,5-TRIMETHYLHEXANE	225TMH	C9H20
2,2-DIMETHYLHEPTANE	22DMC7	C9H20
2-METHYLOCTANE	2MC8	C9H20
N-NONANE	C9	C9H20
2,2,5,5-TETRAMETHYLHEXANE	2255TMH	C10H22
2,2,3,3-TETRAMETHYLHEXANE	2233TMH	C10H22
3,3,5-TRIMETHYLHEPTANE	335TMC7	C10H22
N-DECANE	C10	C10H22
N-UNDECANE	C11	C11H24
N-DODECANE	C12	C12H26
N-TRIDECANE	C13	C13H28
N-TETRADECANE	C14	C14H30
N-PENTADECANE	C15	C15H32
N-HEXADECANE	C16	C16H34
N-HEPTADECANE	C17	C17H36
N-OCTADECANE	C18	C18H38
N-NONADECANE	C19	C19H40
N-EICOSANE	C20	C20H42
N-HENEICOSANE	C21	C21H44
N-DOCOSANE	C22	C22H46
N-TRICOSANE	C23	C23H48
N-TETRACOSANE	C24	C24H50
N-TRIACONTANE	C30	C30H62
N-HEXATRIACONTANE	C36	C36H74
N-DOTETRACONTANE	C42	C42H86
N-OCTATETRACONTANE	C48	C48H98
ETHYLENE	ETHENE	C2H4
PROPYLENE	PROPENE	C3H6
2-METHYLPROPENE	IC3-	C4H8
CIS-2-BUTENE	C-2C4-	C4H8
TRANS-2-BUTENE	T-2C4-	C4H8
1-BUTENE	C4-	C4H8
2-METHYL-2-BUTENE	2M2C4-	C5H10
2-METHYL-1-BUTENE	2M1C4-	C5H10

NAME	SYNONYM	FORMULA
3-METHYL-1-BUTENE	3M1C4-	C5H10
CIS-2-PENTENE	C2C5-	C5H10
TRANS-2-PENTENE	T2C5-	C5H10
1-PENTENE	C5-	C5H10
1-HEXENE	C6-	C6H12
1-HEPTENE	C7-	C7H14
1-OCTENE	C8-	C8H16
1-NONENE	C9-	C9H18
1-DECENE	C10-	C10H20
PROPADIENE	12C3=	C3H4
1,3-BUTADIENE	13C4=	C4H6
1,2-BUTADIENE	12C4=	C4H6
CYCLOPROPANE	CC3	C3H6
CYCLOPENTANE	CC5	C5H10
METHYLCYCLOPENTANE	MCC5	C6H12
ETHYLCYCLOPENTANE	ECC5	C7H14
CYCLOHEXANE	CC6	C6H12
METHYLCYCLOHEXANE	MCC6	C7H14
ETHYLCYCLOHEXANE	ECC6	C8H16
BENZENE	BNZ	C6H6
TOLUENE	TOL	C7H8
ETHYLBENZENE	EB	C8H10
ORTHO-XYLENE	OXYL	C8H10
META-XYLENE	MXYL	C8H10
PARA-XYLENE	PXYL	C8H10
PROPYLBENZENE	C3BNZ	C9H12
ISOPROPYLBENZENE	CUMENE	C9H12
BUTYLBENZENE	C4BNZ	C10H14
ISOBUTYLBENZENE	IC4BNZ	C10H14
T-BUTYLBENZENE	TBBNZ	C10H14
NAPHTHALENE	NAPH	C10H8
1-METHYLNAPHTHALENE	1MNAPH	C11H10
2-METHYLNAPHTHALENE	2MNAPH	C11H10
BIPHENYL	BIPHEN	C12H10
HYDROGEN	H2	H2
NITROGEN	N2	N2
OXYGEN	O2	O2
WATER	H2O	HOH
CARBON MONOXIDE	CO	CO
CARBON DIOXIDE	CO2	OCO
SULPHUR DIOXIDE	SO2	OSO
HYDROGEN SULFIDE	H2S	HSH

NAME	SYNONYM	FORMULA
1,1-DIMETHYLCYCLOPENTANE	11DIMECYP	C7H14
TRANS-1,3-DIMETHYLCYCLOPENTANE	TRANS13DIM	C7H14
TRANS-1,2-DIMETHYLCYCLOPENTANE	TRANS12DIM	C7H14
1-TRANS,3-DIMETHYLCYCLOHEXANE	1TR3DMCH	C8H16
TRANS-1,2-CIS-4-TRIMETHYLCYCLOPENTANE	TR12C4TMCP	C8H16
TRANS-1,2-CIS,3-TRIMETHYLCYCLOPENTANE	TR12C3TMCP	C8H16
1-CIS,2-TRANS,4-TRIMETHYLCYCLOPENTANE	1C2T4TMCP	C8H16
1-TRANS,4-DIMETHYLCYCLOHEXANE	1TR4DMCH	C8H16
1,1-DIMETHYLCYCLOHEXANE	11DMCH	C8H16
1-CIS,3-DIMETHYLCYCLOHEXANE	1C3DMCH	C8H16
1-METHYL,TRANS-3-ETHYLCYCLOPENTANE	1MTR3ECP	C8H16
1-METHYL,TRANS-2-ETHYLCYCLOPENTANE	1MTR2ECP	C8H16
1-METHYL,CIS,3-ETHYLCYCLOPENTANE	1MC3ECP	C8H16
1-METHYL-1-ETHYLCYCLOPENTANE	1M1ECP	C8H16
1-CIS-2,CIS-3-TRIMETHYLCYCLOPENTANE	1C2C3TMCP	C8H16
ISOPROPYLCYCLOPENTANE	IPCP	C8H16
CIS-1,2-DIMETHYLCYCLOHEXANE	C12DMCH	C8H16
N-PROPYLCYCLOPENTANE	PRCYPN	C8H16
1,1,3-TRIMETHYLCYCLOPENTANE	113TMCP	C8H16
P-ETHYLTOLUENE	PARA ETOL	C9H12
1,3,5-TRIMETHYLBENZENE	MESITYLENE	C9H12
O-ETHYLTOLUENE	ORTHOETOL	C9H12
1,2,4-TRIMETHYLBENZENE	124TMBNZ	C9H12
1,1,4-TRIMETHYLCYCLOHEXANE	114TMCH	C9H18
1-CIS,3-CIS-5-TRIMETHYLCYCLOHEXANE	1C3C5TMCH	C9H18
1-CIS,2-TRANS,4-TRIMETHYLCYCLOHEXANE	1C2T4TMCH	C9H18
1,1,2-TRIMETHYLCYCLOHEXANE	112TMCH	C9H18
1-CIS,2-CIS,4-TRIMETHYLCYCLOHEXANE	1C2C4TMCH	C9H18

NAME	SYNONYM	FORMULA
ISOBUTYLCYCLOPENTANE	IBCP	C9H18
2,3,5-TRIMETHYLHEXANE	235TMH	C9H20
4-METHYLOCTANE	4MO	C9H20
2,4-DIMETHYLHEPTANE	24DMC7	C9H20
2,5-DIMETHYLHEPTANE	25DMC7	C9H20
3,5-DIMETHYLHEPTANE	35DMC7	C9H20
3,3-DIMETHYLHEPTANE	33DMC7	C9H20
2,3-DIMETHYLHEPTANE	23DMC7	C9H20
3,4-DIMETHYLHEPTANE	34DMC7	C9H20
1-METHYL-3-ISOPROPYLBENZENE	1M3IPBNZ	C10H14
1-METHYL-2-ISOPROPYLBENZENE	1M2IPBNZ	C10H14
1-METHYL-3-PROPYLBENZENE	1M3PBNZ	C10H14
1-METHYL-4-PROPYLBENZENE	1M4PBNZ	C10H14
1,2-DIETHYLBENZENE	12DEBNZ	C10H14
1,4-DIETHYLBENZENE	14DEBNZ	C10H14
1-METHYL-2-PROPYLBENZENE	1M2PBNZ	C10H14
1,4-DIMETHYL-2-ETHYLBENZENE	14DM2EBNZ	C10H14
1,2-DIMETHYL-4-ETHYLBENZENE	12DM4EBNZ	C10H14
SEC-BUTYLBENZENE	SBBNZ	C10H14
1,3-DIMETHYL-2-ETHYLBENZENE	13DM2EBNZ	C10H14
1,2-DIMETHYL-3-ETHYLBENZENE	12DM3EBNZ	C10H14
1,2,4,5-TETRAMETHYLBENZENE	1245TMBNZ	C10H14
ISOBUTYLCYCLOHEXANE	IBCHEX	C10H20
N-BUTYLCYCLOHEXANE	NBCHEX	C10H20
2,2-DIMETHYLOCTANE	22DMO	C10H22
3,6-DIMETHYLOCTANE	36DMO	C10H22
3,3-DIMETHYLOCTANE	33DMO	C10H22
2,3-DIMETHYLOCTANE	23DMO	C10H22
2-METHYLNONANE	2MN	C10H22
3-METHYLNONANE	3MN	C10H22
2-METHYLBUTYLBENZENE	2MBBNZ	C11H16
1-TERT-BUTYL-2-METHYLBENZENE	1TB2MBNZ	C11H16
N-PENTYLBENZENE	NPBNZ	C11H16
1-TERT-BUTYL-3,5-DIMETHYLBENZENE	1TB35DMBNZ	C12H18
1,3,5-TRIETHYLBENZENE	135TEBNZ	C12H18
1,2,4-TRIETHYLBENZENE	124TEBNZ	C12H18
N-HEXYLBENZENE	NHBNZ	C12H18
1-METHYL,TRANS-2-(4-METHYLPENTYL)CYCLOPENTANE	1MTR24MPCP	C12H24
3-METHYLOCTANE	3MO	C9H20
ARGON	AR	Ar

NAME	SYNONYM	FORMULA
M-ETHYLTOLUENE	METHTOL	C9H12
CIS-1,3-DIMETHYLCYCLOPENTANE	C13DMCP	C7H14
CYCLOPENTADIENE	CYCLOPD	C5H6
CIS-DECALIN	C-DECL	C10H18
TRANS-DECALIN	T-DECL	C10H18
ACETYLENE	ETHYNE	C2H2
SILANE	SIH4	H4Si
CIS-1,4-DIMETHYLCYCLOHEXANE	CIS14DMH	C8H16
CARBONYL SULFIDE	CS	COS
SULFURHEXAFLUORIDE	SF6	SF6

** Water is included so that you may calculate properties of a hydrocarbon mixture with water as an impurity of no more than 5 mole percent. The program is not designed to do pure water calculations, nor is it intended to do aqueous solutions.

Appendix C

USE OF SOURCE CODE SUBROUTINES

The NIST Thermophysical Properties of Hydrocarbon Mixtures Database (SUPERTRAPP) is an interactive database for the prediction of the thermodynamic properties of hydrocarbon mixtures. For users who want to link the properties subroutines with their own codes, we also provide the source code for the properties routines along with some sample drivers.

FORTRAN SOURCE CODE

All source code is written in ANSI Standard FORTRAN 77. The following files are included:

STPV2A.FOR	Supertrapp source code subroutines
STPV2B.FOR	Supertrapp source code subroutines
SAMPLE1.FOR	Driver to illustrate sample (T,P), (T,S) and (P,H) flashes.
SAMPLE2.FOR	Driver to illustrate sample density and transport properties calculation.
SAMPLE3.FOR	Driver to illustrate pure component saturation properties.
SAMPLE4.FOR	Driver to illustrate changing the interaction parameters.
SAMPLEP.FOR	Driver to illustrate calculations with a user-defined petroleum fraction, not present in the database.
WRITLIB2.FOR	Reads PORTLIB to create LIBFILE database
PORTLIB	ASCII file to generate LIBFILE, given on distribution diskette, or can be generated by using the “LIB” command described in Section 4.31.
LIBFILE	Direct access FOTRAN file containing pure component parameters. Must be present for source code routines to work. This file must be created by the User’s
FORTRAN	compiler by running WRITLIB2.
README2.TXT	Provides a description of Supertrapp source code subroutines and their argument lists.

We also include the output files obtained from running the sample drivers, SAMPLE1.OUT, SAMPLE2.OUT, SAMPLE3.OUT, SAMPLE4.OUT and SAMPLEP.OUT.

MODIFICATION OF THE COMPONENT LIBRARY FOR USERS OF THE SOURCE CODE

This section is intended for users who wish to add a new component or change existing component parameters. The PC version of the database is required to modify the component library.

The parameters for an existing component in the database can be modified or a new component added using the full PC version of NIST SUPERTRAPP and the MODIFY command, discussed in 4.16. After the desired changes have been made, invoke the "LIB" command. This creates a file called "PORTLIB" containing all the necessary constants and parameters for the fluids in the database.

On your computer, load the "PORTLIB" file. Then compile and run the "WRITLIB2.FOR" program, which reads "PORTLIB" and creates "LIBFILE", the input library for running the SUPERTRAPP source code on your own platform.

The library file STPLIB2 works only with the SUPERTRAPP executable code on the distribution disk states that you must create LIBFILE with your own compiler in order to be able to use the source code.

Appendix D

CONTACTS

If you have comments or questions about the database, the Standard Reference Data Program would like to hear from you. Also, if you should have any problems with the diskettes or installation, please let us know by contacting:

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