

# NBS TECHNICAL NOTE 1039

U.S. DEPARTMENT OF COMMERCE /National Bureau of Standards

## A Computer Program for the Prediction of Viscosity and Thermal Conductivity in Hydrocarbon Mixtures

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A COMPUTER PROGRAM FOR THE PREDICTION OF VISCOSITY AND  
THERMAL CONDUCTIVITY IN HYDROCARBON MIXTURES

by

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A model for the prediction of the density, viscosity and thermal conductivity of non-polar fluid mixtures over the entire range of pVT states is presented. The model is based on the extended corresponding states model and covers molecular weight ranges including C<sub>20</sub>. Only pure component equilibrium data such as the critical constants are required as input to the calculation procedure--no transport data are required. Extensive comparisons with experimental data for pure fluids and binary mixtures are presented. The average percentage deviation for both the viscosity and thermal conductivity was observed to be less than 8 percent. A computer program (TRAPP) which performs the calculations reported in this manuscript is described and listed in the Appendices.

Key words: Computer program; density; extended corresponding states; fluid mixtures; thermal conductivity; viscosity.

## 1. INTRODUCTION

Engineering design requires transport properties for heat exchangers, compressors, pumps and for example, pipelines. Owing to the complexity of transport phenomena in general, accurate methods for the prediction of these properties have not advanced to a level comparable to equilibrium properties. In fact, most engineering calculations of transport properties are based on empirical correlations which are generally limited to narrow ranges of pressure and temperature and very frequently to pure fluids. These methods have been reviewed by Reid, et al. [1].

The purpose of this manuscript is to present a reliable, self-consistent method for predicting the density, viscosity and thermal conductivity of pure non-polar fluids and their mixtures. The method is applicable to a wide variety of chemical types, to thermodynamic states ranging from the dilute gas to compressed liquid and, in principle, the number of mixture components is unrestricted.

The procedure is an extension of a method [2,3] which was proposed to estimate the transport properties of natural gas and similar mixtures and is based on the corresponding states principle and the conformal, one-fluid concept. It is predictive and requires only the critical parameters, Pitzer's acentric factor and the component ideal gas heat capacity as input. No mixture properties or transport data are required. The basic idea is relatively straightforward. It is assumed that the configurational properties of a single phase mixture can be equated to those of a hypothetical pure fluid. The properties of this hypothetical pure fluid are then evaluated via corresponding states with respect to a given reference fluid.

The theoretical foundation of the approach is well defined for a conformal system in equilibrium [4]. It is less well understood for a nonconformal system (i.e., a system in which the mixture components do not interact with the same intermolecular potential, e.g., polyatomic molecules) and for a system in nonequilibrium. The assumptions involved in the latter example have, however, been a topic of recent discussion [5,6]. Nevertheless, we have found by experience that the method gave very good agreement -- typically less than ten percent uncertainty -- for the transport properties of liquefied natural gas (LNG) like fluids (i.e., polyatomic nonpolar species). Further, even though the procedure in our earlier work was optimized for the  $C_1$  to  $C_5$  hydrocarbons and common inorganics, it gave acceptable results -- typically ten to forty percent uncertainty -- for a diverse number of more complex pure components and their mixtures. These results for fluids which were well beyond the intended scope of the original model, encouraged us to explore a systematic extension of the method to more complex systems.

In this manuscript we briefly report the details of the model and results of the method for the viscosity and thermal conductivity of pure paraffins, alkenes, aromatics and cycloalkanes in the  $C_1$  to  $C_{20}$  molecular weight range and their mixtures. Carbon dioxide is included in the comparisons as an example of a common inorganic.

## 2. THE ONE-FLUID MODEL AND EQUATIONS

In our procedure, the viscosity ( $\eta$ ) of a mixture at density,  $\rho$ , and temperature,  $T$ , and composition  $\{x\}$  is equated to the viscosity of a hypothetical pure fluid, i.e.,  $\eta_{\text{mix}}(\rho, T) = \eta_x(\rho, T)$ . Then, via the corresponding states argument

$$\eta_x(\rho, T) = \eta_o(\rho_o, T_o) F_\eta \quad (1)$$

where

$$F_\eta = \left( \frac{M_x^\eta}{M_o^\eta} \right)^{1/2} f_{x,o}^{1/2} h_{x,o}^{-2/3} \quad (2)$$

where the subscript x refers to the fluid of interest, pure fluid or mixture, and o refers to the reference fluid. M is the molecular weight and  $T_o$  and  $\rho_o$  are defined by the ratios

$$T_o = T/f_{x,o} \text{ and } \rho_o = \rho h_{x,o} \quad (3)$$

where  $f_{x,o}$  and  $h_{x,o}$  are, in general, functions of the critical parameters and acentric factor. In the special case of two parameter corresponding states between two pure fluids  $\alpha$  and o, they reduce to the well known ratios of critical constants:

$$f_{\alpha,o} = T_\alpha^C/T_o^C \text{ and } h_{\alpha,o} = V_\alpha^C/V_o^C \equiv \rho_o^C/\rho_\alpha^C \quad (4)$$

where V is the volume and the superscript c indicates a critical value.

Note for the special case of two parameter corresponding states for which  $Z_\alpha^C = Z_o^C$ , the factor  $F_\eta$  can be written in terms of the common viscosity reducing parameter  $\zeta_\alpha$ , viz

$$\zeta_\alpha = T_\alpha^C^{1/6} / M_\alpha^{1/2} \rho_\alpha^C^{2/3} \quad (5)$$

so

$$F_\eta = \zeta_o / \zeta_\alpha \quad (6)$$

where p is the pressure.

The thermal conductivity ( $\lambda$ ) of a mixture or pure fluid must be divided into two contributions -- one arising from the transfer of energy from purely collisional or translational effects,  $\lambda'$ , and the other from the transfer of energy through the internal degrees of freedom,  $\lambda''$ . In our model, the translational contribution to the thermal conductivity is equated to that of a hypothetical pure fluid, i.e.,  $\lambda'_{mix}(\rho, T) = \lambda'_x(\rho, T)$ , then, via the corresponding states argument

$$\lambda'_x(\rho, T) = \lambda'_0(\rho_0, T_0) F_\lambda \quad (7)$$

where

$$F_\lambda = \left( \frac{M_0}{M_x} \right)^{1/2} f_{x,0}^{1/2} h_{x,0}^{-2/3} \quad (8)$$

The internal contribution is calculated via the mixing rule

$$\lambda''_{mix}(\rho, T) = \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} \lambda''_{\alpha\beta}(\rho, T) \quad (9)$$

where

$$\lambda''_{\alpha\beta}(\rho, T) = 2\lambda''_{\alpha}(0, T) \lambda''_{\beta}(0, T) / [\lambda''_{\alpha}(0, T) + \lambda''_{\beta}(0, T)] \quad (10)$$

Generally speaking, the density dependence of the internal contribution is not known on sound theoretical grounds. We assume, therefore, that the contribution for each component is the same as it would be in the dilute gas state {hence the designation (0, T)} which we calculate from a Bromley [1] type formula, viz

$$\lambda''_{\alpha}(0, T) = f_{int} \left[ C_{p\alpha}^0(T) - \frac{5R}{2} \right] \eta_{\alpha}^0(T) / M_{\alpha} \quad (11)$$

where  $C_{p\alpha}^0$  is the ideal gas heat capacity of component  $\alpha$ ,  $\eta_{\alpha}^0$  is the dilute gas viscosity which is evaluated via eq (1) using  $T_0 = T/f_{\alpha,0}$  where  $f_{\alpha,0}$  is the reducing ratio for the component in the mixture,  $R$  is the gas constant and  $f_{int} = 1.32$ . We have then our working equation for the thermal conductivity of a mixture or pure fluid

$$\lambda_{mix}(\rho, T) = \lambda'_0(\rho_0, T_0) F_\lambda + \lambda''_{mix}(\rho, T) \quad (12)$$

## 2.1 Extended Corresponding States

The range of applicability of corresponding states in general can be broadened considerably by introducing the extended corresponding states model [7,8]. In this model, the two parameter corresponding states formalism is maintained except that the equivalent substance reducing ratios become, using the special case of the pure fluid as an example

$$f_{\alpha,0} = (T_{\alpha}^C / T_0^C) \theta_{\alpha,0} (T_{\alpha}^*, V_{\alpha}^*, \omega_{\alpha}) \quad (13)$$



and

$$h_{\alpha,0} = (V_{\alpha}^C/V_0^C) \phi_{\alpha,0} (T_{\alpha}^*, V_{\alpha}^*, \omega_{\alpha}) \quad (14)$$

where  $\theta_{\alpha,0}$  and  $\phi_{\alpha,0}$  are the so-called shape factors [9,10] which are functions of the acentric factor  $\omega$  and of the reduced variables  $T_{\alpha}^*$  and  $V_{\alpha}^*$  where the superscript "\*" indicates reduction by the critical point value.

In principle, the shape factors can be determined exactly for any pure fluid with respect to a reference fluid by simultaneous solution of the conformal solution equations [8]. By performing this solution one could ensure that the pure fluid  $\alpha$  maps exactly with the reference fluid on a pVT surface via the shape factors. However, it is much more convenient to have some generalized analytical relationship for  $\theta$  and  $\phi$ . Leach and Leland [9,10] have obtained such relationships for the pure normal paraffins  $C_1 - C_{15}$  with essentially a methane reference fluid. Their results are generalized as follows

$$\theta_{\alpha,0}(T_{\alpha}, V_{\alpha}, \omega_{\alpha}) = 1 + (\omega_{\alpha} - \omega_0) F(T_{\alpha}^+, V_{\alpha}^+) \quad (15)$$

$$\phi_{\alpha,0}(T_{\alpha}, V_{\alpha}, \omega_{\alpha}) = [1 + (\omega_{\alpha} - \omega_0) G(T_{\alpha}^+, V_{\alpha}^+)] Z_0^C/Z_{\alpha}^C \quad (16)$$

$$F(T_{\alpha}, V_{\alpha}) = a_1 + b_1 \ln T_{\alpha}^+ + (c_1 + d_1/T_{\alpha}^+)(V_{\alpha}^+ - 0.5) \quad (17)$$

$$G(T_{\alpha}, V_{\alpha}) = a_2(V_{\alpha}^+ + b_2) + c_2(V_{\alpha}^+ + d_2) \ln T_{\alpha}^+ \quad (18)$$

$$T_{\alpha}^+ = \min \left\{ 2, \max \left\{ T_{\alpha}, 0.5 \right\} \right\} \quad (19)$$

$$V_{\alpha}^+ = \min \left\{ 2, \max \left\{ V_{\alpha}, 0.5 \right\} \right\} \quad (20)$$

## 2.2 Mixing Rules and Assumptions

There are two basic assumptions of the theory: (1) A pure fluid and a reference fluid obey the two parameter classical corresponding states formalism and, for a mixture, that all interactions in the mixture follow this principle; (2) The mixture can be represented by a hypothetical pure fluid which implies mixing rules exist to evaluate the reducing ratios. Clearly, it has been assumed

that the introduction of extended corresponding states allows these assumptions to be upheld.

As we pointed out in the introduction, the assumptions have been discussed for a system in equilibrium but have received less attention for a system in nonequilibrium, especially for polyatomic molecules. It is at once apparent that the one-fluid concept is formally weak for transport since the transport properties can contain contributions unique to the mixture -- the diffusion coefficient, for example. There is also the difficulty in formulating a consistent mass mixing rule which is unnecessary for the equilibrium properties but is required for eqs (2) and (8). These problems have been recently discussed and the interested reader is referred to references [6] and [11] for details. The mixing rules which are used in the model may be summarized as follows:

$$f_{x,0} = h_{x,0}^{-1} \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} f_{\alpha\beta,0} h_{\alpha\beta,0} \quad (21)$$

$$h_{x,0} = \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} h_{\alpha\beta} \quad (22)$$

$$M_x^{\eta} = \left( \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} h_{\alpha\beta,0}^{4/3} f_{\alpha\beta,0}^{1/2} M_{\alpha\beta}^{1/2} \right)^2 f_{x,0}^{-1} h_{x,0}^{-8/3} \quad (23)$$

and

$$M_x^{\lambda} = \left( \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} M_{\alpha\beta}^{-1/2} f_{\alpha\beta,0}^{1/2} h_{\alpha\beta,0}^{4/3} \right)^{-2} f_{x,0} h_{x,0}^{8/3} \quad (24)$$

The combining rules are needed finally and these were selected to be

$$f_{\alpha\beta,0} = (f_{\alpha,0} f_{\beta,0})^{1/2} (1 - k_{\alpha\beta}) \quad (25)$$

$$h_{\alpha\beta,0} = \frac{1}{8} (h_{\alpha,0}^{1/3} + h_{\beta,0}^{1/3})^3 (1 - \ell_{\alpha\beta}) \quad (26)$$

and

$$M_{\alpha\beta} = 2 M_{\alpha} M_{\beta} / (M_{\alpha} + M_{\beta}) \quad (27)$$

where  $k_{\alpha\beta}$  and  $\ell_{\alpha\beta}$  are correction factors or binary interaction parameters with values close to zero. Although it is well known that thermodynamic calculations (especially phase equilibria) can be sensitive to their numerical value, this

does not appear to be true for the viscosity or thermal conductivity, hence they were set equal to zero for the results reported here.

### 3. SUMMARY OF THE CALCULATION PROCEDURE

A summary of the calculation procedure to evaluate a viscosity or thermal conductivity is as follows. Input parameters are the critical temperature, volume, and pressure, the acentric factor and the ideal gas heat capacity and molecular weight of each component of the mixture of interest. These parameters for the reference fluid are required with an equation of state and some functional form for the viscosity and thermal conductivity for this reference fluid.

Typical experimental input would be the pressure, temperature and mixture composition. The density of the fluid or mixture is obtained by finding the equivalent pressure of the reference substance via the ratio  $p_0 = p_x h_{x,0} / f_{x,0}$  from the corresponding pressure in the mixture,  $p_x$ . Initially, the shape factors in eqs (13) and (14) are set to unity. Given  $p_0 = p(\rho_0, T_0)$ , the density  $\rho_0$  follows. Thus, a first guess of the density is that obtained using eqs (3) and (4). Repeated iterations using eqs (13) and (14) give the final density. Having, therefore, final values of  $\rho$ ,  $f_{x,0}$  and  $h_{x,0}$ , one can evaluate  $F_\eta$  and  $F_\lambda$  of eqs (2) and (11),  $\rho_0$  and  $T_0$  and hence  $\eta_0(\rho_0, T_0)$ ,  $\lambda'_0(\rho_0, T_0)$  and  $\lambda''(\rho, T)$ , thereby obtaining values for  $\eta_x(\rho, T)$  and  $\lambda_x(\rho, T)$ .

### 4. THE REFERENCE FLUID: EXTENDED EQUATIONS FOR METHANE

The procedure outlined in the previous section does not in principle place restrictions on the choice of the reference fluid and, especially, the reference fluid does not have to be a component of the mixture. Nonetheless, common sense suggests that the reference fluid should be similar to the systems of interest. Methane was chosen for the earlier work because we were concerned mainly with the properties of LNG and the light hydrocarbons. Since the object of this work is to study the heavy and aromatic hydrocarbons in particular, it would seem appropriate to select a fluid such as hexane or decane, or say benzene. Unfortunately, at this time, methane is the only fluid which has sufficient reliable data correlated over a wide range of experimental conditions for the equation of state, the viscosity and the thermal conductivity. Methane was, therefore, selected as the reference for this work. One can anticipate problems -- for example, lack of conformality between methane and the mixtures, effects of internal degrees of freedom, of hindered rotation, and so on.



In practice, a more obvious difficulty occurs: methane freezes at a reduced temperature of 0.48 which is well above the reduced temperatures commonly encountered for the liquid states of fluids as simple as propane. This is demonstrated in fig. (1a) where we plot the saturated liquid density for methane and n-decane in terms of  $T^*$  and  $\rho^*$ . One sees that the range of states of n-decane is simply not covered by those of methane. Similarly, for the viscosity as is shown in fig. (1b) in which  $\eta(\rho, T)\zeta$  is plotted versus  $\rho^*$ , where  $\zeta$  was defined by eq (5). Again the data for liquid methane terminate due to freezing well before the freezing point of decane is reached. Similar problems are encountered for the thermal conductivity.

In order to overcome these problems, the methane pVT, shape factor, viscosity and thermal conductivity correlations (surfaces) were extended to 40 K. The details of the methods used in performing these extensions may be found in references [13] and [14]. Summarizing the results, the pVT surface is given by a 32 term BWR type equation [12] whose functional form and coefficients are given in table 1. Table 2 lists the shape factor correlation parameters with the functional form being given by eqs (15-20) except that the restriction given in eq (19) is removed. The reference fluid viscosity is given by the equation

$$\eta_0(\rho_0, T_0) = \eta_0^{(1)}(T_0) + \eta_0^{(2)}(T_0)\rho_0 + \Delta\eta_0(\rho_0, T_0)X_\eta \quad (28)$$

where  $X_\eta$  is a correction factor for non-correspondence in the viscosity given by

$$X_\eta = \left[ \left\{ 1 - \psi \frac{T_x}{f_{x,0}} \left( \frac{\partial f_{x,0}}{\partial T_x} \right)_{V_x} \right\} \frac{Z_x^C}{Z_0^C} \right]^{1/2} \quad (29)$$

where for a mixture  $Z_x^C = \sum x_\alpha Z_\alpha^C$  and  $\psi = 1.5$ . This expression has a basis in the Enskog theory in that the density dependence of the viscosity is strongly dependent on the derivative  $(dp/dT)_V$ . The detailed functional forms and coefficients for eq (28) are given in table 3. Finally, the translational reference fluid thermal conductivity is given by

$$\lambda_0'(\rho_0, T_0) = [\lambda_0^{(1)'}(T_0) + \lambda_0^{(2)}(T_0)\rho_0 + \Delta\lambda_0(\rho_0, T_0)] X_\lambda \quad (30)$$

where

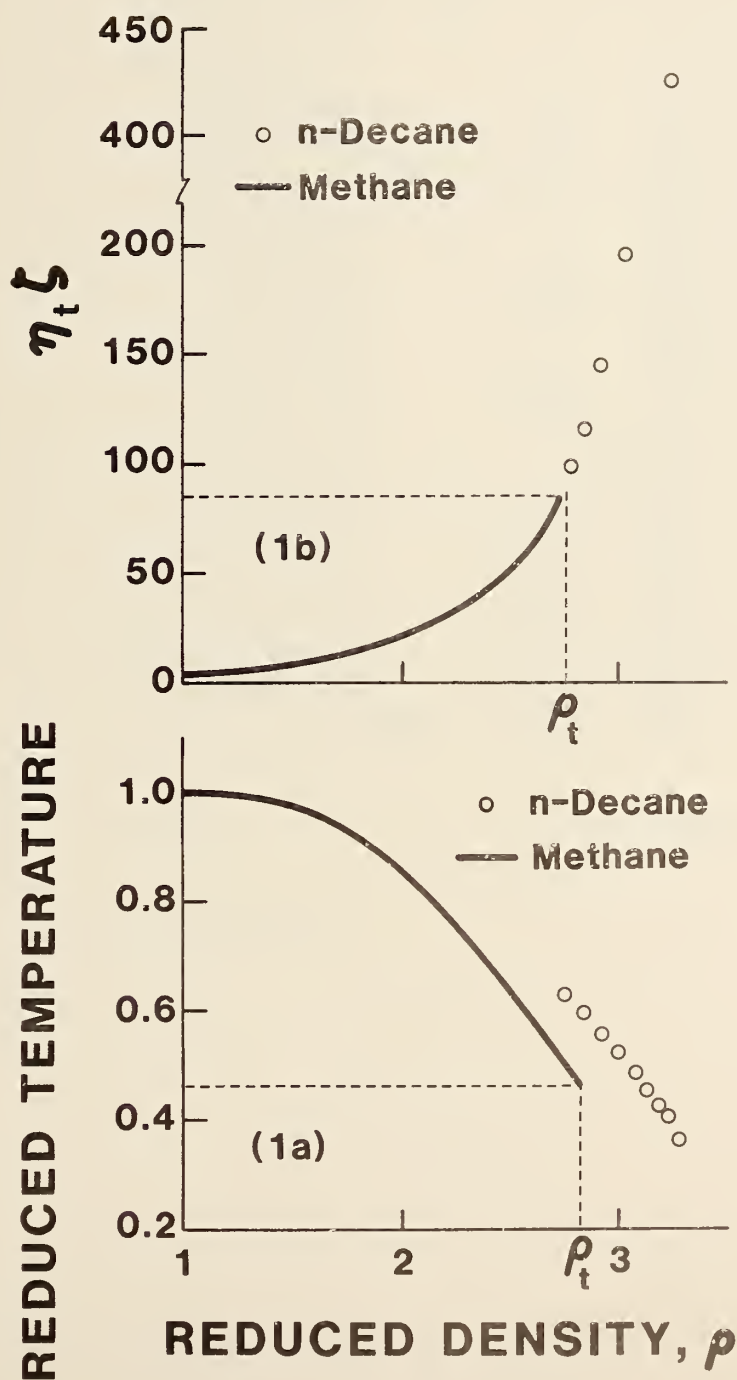


Figure 1. (a) Comparison of reduced density of methane and n-decane as a function of reduced temperature. (b) Comparison of scaled viscosity of methane and n-decane as a function of reduced density.

Table 1. Reference Fluid Equation of State  
(p, atm; ρ, mol/L; T, kelvin)

$$p = \sum_{n=1}^9 a_n(T) \rho^n + \sum_{n=10}^{15} a_n(T) \rho^{2n-17} e^{-\gamma \rho^2}$$

$$\begin{aligned} a_1 &= RT \\ a_2 &= N_1 T + N_2 T^{1/2} + N_3 + N_4/T + N_5/T^2 \\ a_3 &= N_6 T + N_7 + N_8/T + N_9/T^2 \\ a_4 &= N_{10} T + N_{11} + N_{12}/T \\ a_5 &= N_{13} \\ a_6 &= N_{14}/T + N_{15}/T^2 \\ a_7 &= N_{16}/T \\ a_8 &= N_{17}/T + N_{18}/T^2 \\ a_9 &= N_{19}/T^2 \\ a_{10} &= N_{20}/T^2 + N_{21}/T^3 \\ a_{11} &= N_{22}/T^2 + N_{23}/T^4 \\ a_{12} &= N_{24}/T^2 + N_{25}/T^3 \\ a_{13} &= N_{26}/T^2 + N_{27}/T^4 \\ a_{14} &= N_{28}/T^2 + N_{29}/T^3 \\ a_{15} &= N_{30}/T^2 + N_{31}/T^3 + N_{32}/T^4 \end{aligned}$$

Table 1. Reference Fluid Equation of State (Continued)

$i/N_i$		$i/N_i$	
1	- 1.184347314485E-2	17	1.071143181503E-5
2	7.540377272657E-1	18	- 9.290851745353E-3
3	- 1.225769717554E+1	19	1.610140169312E-4
4	6.260681393432E+2	20	3.469830970789E+4
5	- 3.490654409121E+4	21	- 1.370878559048E+6
6	5.301046385532E-4	22	1.790105676252E+2
7	- 2.875764479978E-1	23	1.615880743238E+6
8	5.011947936427E+1	24	6.265306650288E-1
9	- 2.821562800903E+4	25	1.820173769533E+1
10	- 2.064957753744E+5	26	1.449888505811E-3
11	1.285951844828E-2	27	- 3.159999123798E+1
12	- 1.106266656726E+0	28	- 5.290335668451E-6
13	+ 3.060813353408E-4	29	1.694350244152E-3
14	- 3.174982181302E-3	30	8.612049038886E-9
15	5.191608004779E+0	31	- 2.598235689063E-6
16	- 3.074944210271E-4	32	3.153374374912E-5

$$\gamma = 0.0096$$

$$R = 0.08205616$$

$$1 \text{ atm} = 0.101325 \text{ MPa}$$

Table 2. Coefficients for Shape Factor Correlations

Coefficients [eq 16]		Coefficients [eq 17]	
$a_1$	= 0.090569	$a_2$	= 0.394901
$b_1$	= -0.862762	$b_2$	= -1.023545
$c_1$	= 0.316636	$c_2$	= -0.932813
$d_1$	= -0.465684	$d_2$	= -0.754639

Table 3. Reference Fluid Viscosity Correlation

$$\eta(\rho, T) = \eta^{(1)}(T) + \eta^{(2)}(T)\rho + \Delta\eta(\rho, T)$$

where

$$\eta^{(1)} = \sum_{n=1}^9 c_n T^{(n-4)/3}$$

$$\eta^{(2)} = b_1 + b_2 [b_3 - \ln(T/b_4)]^2$$

$$\Delta\eta = \exp \left[ a_1 + a_2/T \right] \left\{ \exp \left[ (a_3 + a_4/T^{3/2}) \rho^{0.1} \right. \right. \\ \left. \left. + (\rho/\rho_c - 1) \rho^{0.5} (a_5 + a_6/T + a_7/T^2) \right] - 1.0 \right\}$$

i	$a_i$	$b_i$	$c_i$
1	-1.0239160427E+1	1.6969859271E+0	2.907741307E+6
2	1.7422822961E+2	-1.3337234608E-1	-3.312874033E+6
3	1.7460545674E+1	1.4	1.608101838E+6
4	-2.8476328289E+3	1.68E+2	-4.331904871E+5
5	1.3368502192E-1		7.062481330E+4
6	1.4207239767E+2		-7.116620750E+3
7	5.0020669720E+3		4.325174400E+2
8			-1.445911210E+1
9			2.037119479E-1

(T, kelvin;  $\rho$ , g/cm<sup>3</sup>,  $\rho_c = 0.1628$ )

$$x_{\lambda} = \left[ \left\{ 1 - \frac{T_x}{f_{x,0}} \left( \frac{\partial f_{x,0}}{\partial T_x} \right)_{V_x} \right\} \frac{Z_0^C}{Z_x^C} \right]^{3/2} \quad (31)$$

The detailed functional forms and coefficients for eq (30) are listed in table 4.

## 5. RESULTS FOR PURE FLUIDS

Having the reference fluid correlations for methane, it was straightforward to calculate the transport properties of any pure species via eqs (1) and (12). A considerable data base was assembled to provide a thorough test of the procedure. The data and references used in this comparison are available upon request. The data were evaluated as far as possible for accuracy and internal consistency. One should point out that in general the data situation is not too satisfactory for transport properties in that the more recent experimental techniques have not been applied to many organic liquids other than methane, and recently to ethane and propane. A realistic guess as to the accuracy of the data is 5-15 percent and probably much worse for the very heavy species.

The results are summarized in tables 5 and 6 and in figs. (2-5). The tables show the average absolute percent deviation, AAD, and the average percentage error, BIAS. The overall deviations between experiment and the calculations are very satisfactory. The viscosity results become somewhat worse, and negative, as the freezing point of the fluid is approached. It is not clear why this should be the case, but one can say that there is a good chance that the viscosity becomes non-Newtonian in this region and that pre-freezing nucleation effects are important. One also observes that the viscosity results are markedly worse for highly branched alkanes and for the cycloalkanes. We attribute this to a failure of the corresponding states model to represent adequately the effect of the molecular structure on the transport coefficient. In spite of these limitations, the overall results are excellent, especially considering the limited input ( $T_C$ ,  $p_C$ ,  $V_C$ ,  $M$ ,  $\omega$ , and  $C_p^0$ ) needed to make the predictions. In fact, the thermal conductivity results are in better agreement with experiment than the estimated error for this property.

## 6. RESULTS FOR MIXTURES

The main objective of this work was to develop a procedure to predict the transport properties of mixtures: there is a real need for such a procedure, yet



Table 4. Reference Fluid Translational Thermal Conductivity Correlation

$$\lambda'(\rho, T) = \lambda^{(1)'}(T) + \lambda^{(2)}(T)\rho + \Delta\lambda(\rho, T)$$

$$\lambda^{(1)'}(T) = \frac{15R}{4M} \eta^{(1)}(T)$$

$$\lambda^{(2)}(T) = b_1 + b[b_3 - \ln(T/b_4)]^2$$

$$\Delta\lambda = \exp \left[ a_1 + a_2/T \right] \left\{ \exp \left[ (a_3 + a_4/T^{3/2}) \rho^{0.1} + (\rho/\rho_c - 1) \rho^{0.5} (a_5 + a_6/T + a_7/T^2) \right] - 1.0 \right\}$$

<u>i</u>	<u>a<sub>i</sub></u>	<u>b<sub>i</sub></u>
1	-7.1977082270E+0	-0.252762920E+0
2	8.5678222640E+1	0.334328590E+0
3	1.2471834689E+1	1.12
4	-9.8462522975E+2	0.1680E+3
5	3.5946850007E-1	
6	6.9798412538E+1	
7	-8.7288332851E+2	

(T, kelvin;  $\rho$ , g/cm<sup>3</sup>;  $\rho_c = 0.1628$ )

Table 5. Summary of Calculated Results for Pure Fluid Viscosity  
(AAD = Average Absolute Percent Deviation;  
BIAS = Percentage Bias)

Fluid	N	AAD	BIAS
Methane	76	3.03	- 2.89
Ethane	48	12.31	9.99
Propane	146	6.56	- 5.10
n-Butane	200	3.39	- 2.80
i-Butane	68	11.49	-11.39
n-Pentane	195	4.15	- 1.49
neo-Pentane	75	32.83	-32.83
n-Hexane	66	3.30	2.16
i-Hexane	12	3.09	- 3.09
n-Heptane	78	6.31	3.45
n-Octane	52	6.22	4.30
n-Nonane	46	2.89	1.54
n-Decane	107	3.25	- 1.56
n-Undecane	19	3.47	1.29
n-Dodecane	41	5.12	1.19
n-Tridecane	58	4.69	- 1.12
n-Tetradecane	53	5.04	- 2.97
n-Pentadecane	18	5.37	- 2.23
n-Hexadecane	39	5.33	2.08
n-Heptadecane	15	6.11	3.56
n-Octadecane	28	9.66	5.89
n-Eicosane	16	6.37	3.89
Ethylene	10	2.02	- 0.61
Propylene	13	9.72	3.18
3-Methyl-1-butene	8	5.53	- 5.53
1-Hexene	27	17.19	17.19
Cyclohexane	48	49.25	-49.25
Methylcyclohexane	14	30.69	-30.69
Ethylcyclohexane	17	30.81	-30.81
Cyclopentane	10	29.20	-29.20
Benzene	82	8.39	- 8.33

Table 5. (Continued)

<u>Fluid</u>	<u>N</u>	<u>AAD</u>	<u>BIAS</u>
Toluene	47	4.13	3.17
m-Xylene	16	20.35	20.35
Propylbenzene	5	8.16	8.16
Butylbenzene	5	12.12	12.12
Carbon Dioxide	111	4.75	- 4.53
Overall	1869	8.42	- 4.10

Table 6. Summary of Calculated Results for Pure Fluid Thermal Conductivity

(AAD = Average Absolute Percent Deviation;

BIAS = Percentage Bias)

Fluid	N	AAD	BIAS
Ethane	15	5.44	5.06
Propane	188	5.12	4.99
n-Butane	32	6.41	6.41
Isobutane	4	12.49	-12.49
n-Pentane	35	5.24	5.24
n-Hexane	10	1.88	-1.31
Isohexane	3	.91	-.91
3-Methylpentane	3	2.56	-2.56
2,2-Dimethylbutane	3	1.03	-1.03
2,3-Dimethylbutane	4	1.42	.95
n-Heptane	84	8.15	-8.13
2,4-Dimethylpentane	3	1.69	1.69
2,2,3-Trimethylbutane	1	4.40	4.40
n-Octane	15	5.37	-5.37
3-Methylheptane	1	1.71	1.71
2,2,4-Trimethylpentane	5	2.30	2.23
n-Nonane	15	6.13	-6.13
2,2,5-Trimethylhexane	4	3.68	.31
n-Decane	44	3.41	-1.54
n-Undecane	8	12.19	-12.19
n-Dodecane	3	6.67	-6.67
n-Tridecane	9	6.90	-6.90
n-Tetradecane	50	1.78	-1.76
n-Pentadecane	51	1.62	-.92
n-Hexadecane	49	.96	.40
n-Heptadecane	38	2.79	-2.19
n-Octadecane	34	3.44	-2.52
n-Nonadecane	8	7.12	-4.42
n-Eicosane	33	1.87	1.75
Cyclopentane	4	1.57	-1.57

Table 6. (Continued)

Fluid	N	AAD	BIAS
Methylcyclopentane	3	.16	.13
Cyclohexane	4	1.80	-.58
Methylcyclohexane	10	5.39	5.39
Ethylene	75	8.53	-8.51
Propylene	42	9.96	-9.96
2-Methylpropene	3	5.27	5.27
1-Hexene	64	4.67	-2.43
1-Heptene	67	9.55	-9.55
Benzene	18	2.88	-1.71
Toluene	67	6.81	6.42
Ethylbenzene	8	4.67	4.67
ortho-Xylene	9	10.64	10.64
meta-Xylene	7	8.69	8.69
para-Xylene	66	6.24	5.72
Propylbenzene	5	2.32	1.04
Cumene	8	3.58	3.58
Butylbenzene	7	3.15	3.15
Biphenyl	14	14.76	-14.76
Carbon Dioxide	22	6.67	6.67
Overall Results	1255	5.06	- 0.67

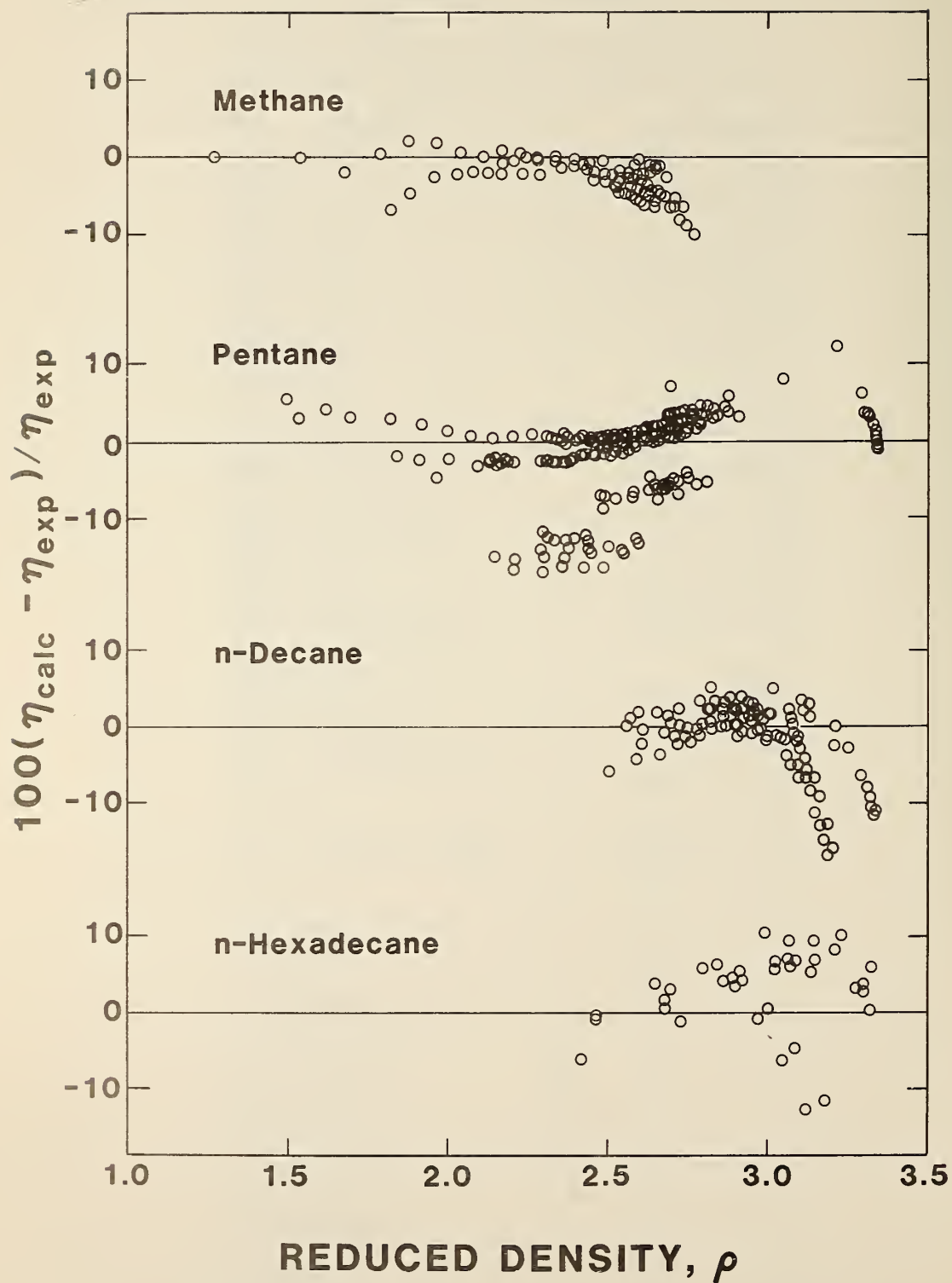


Figure 2. Comparison of calculated and experimental viscosity of methane, pentane, decane and hexadecane as a function of reduced density.

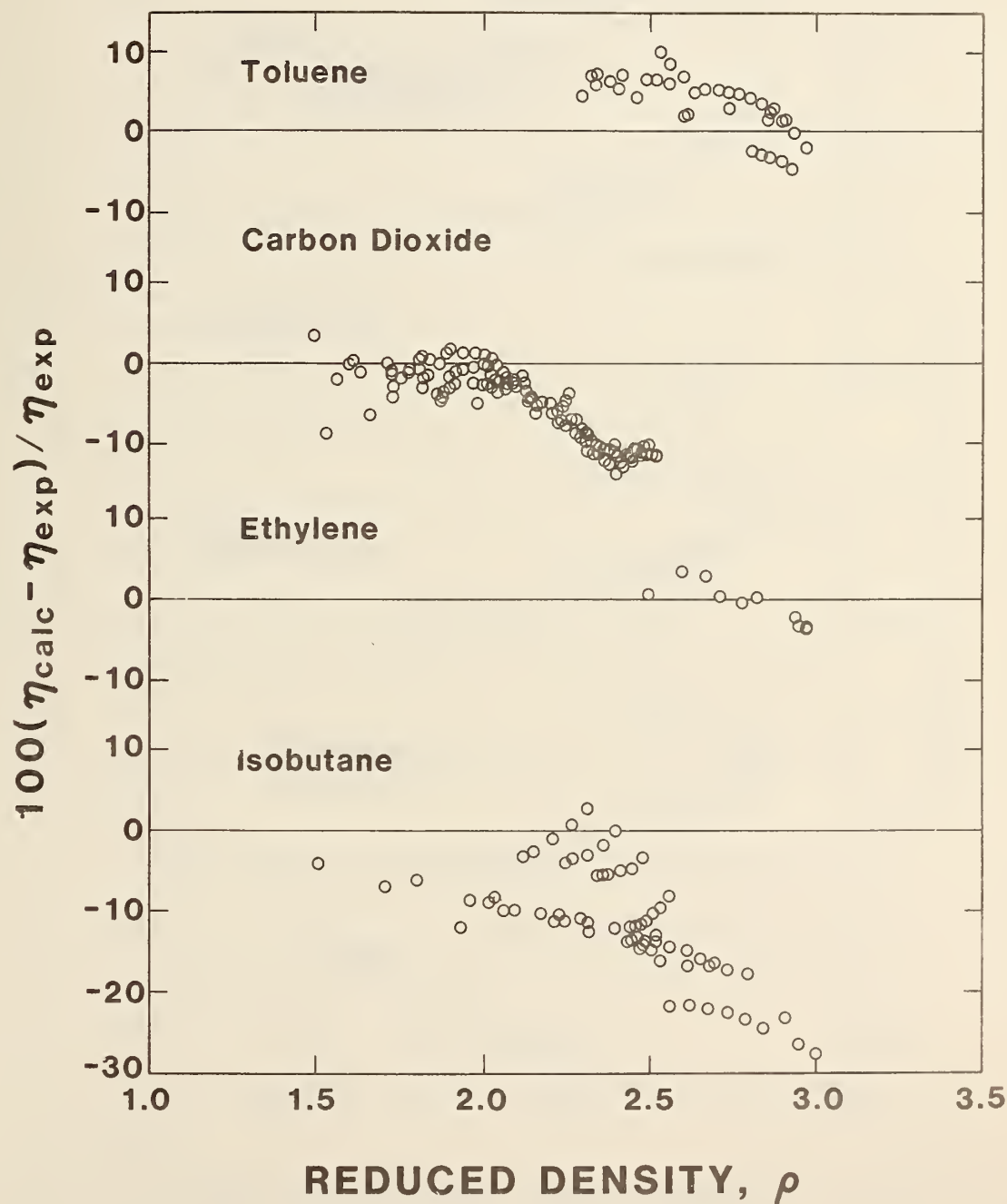


Figure 3. Comparison of calculated and experimental viscosity for toluene, carbon dioxide, ethylene and isobutane.



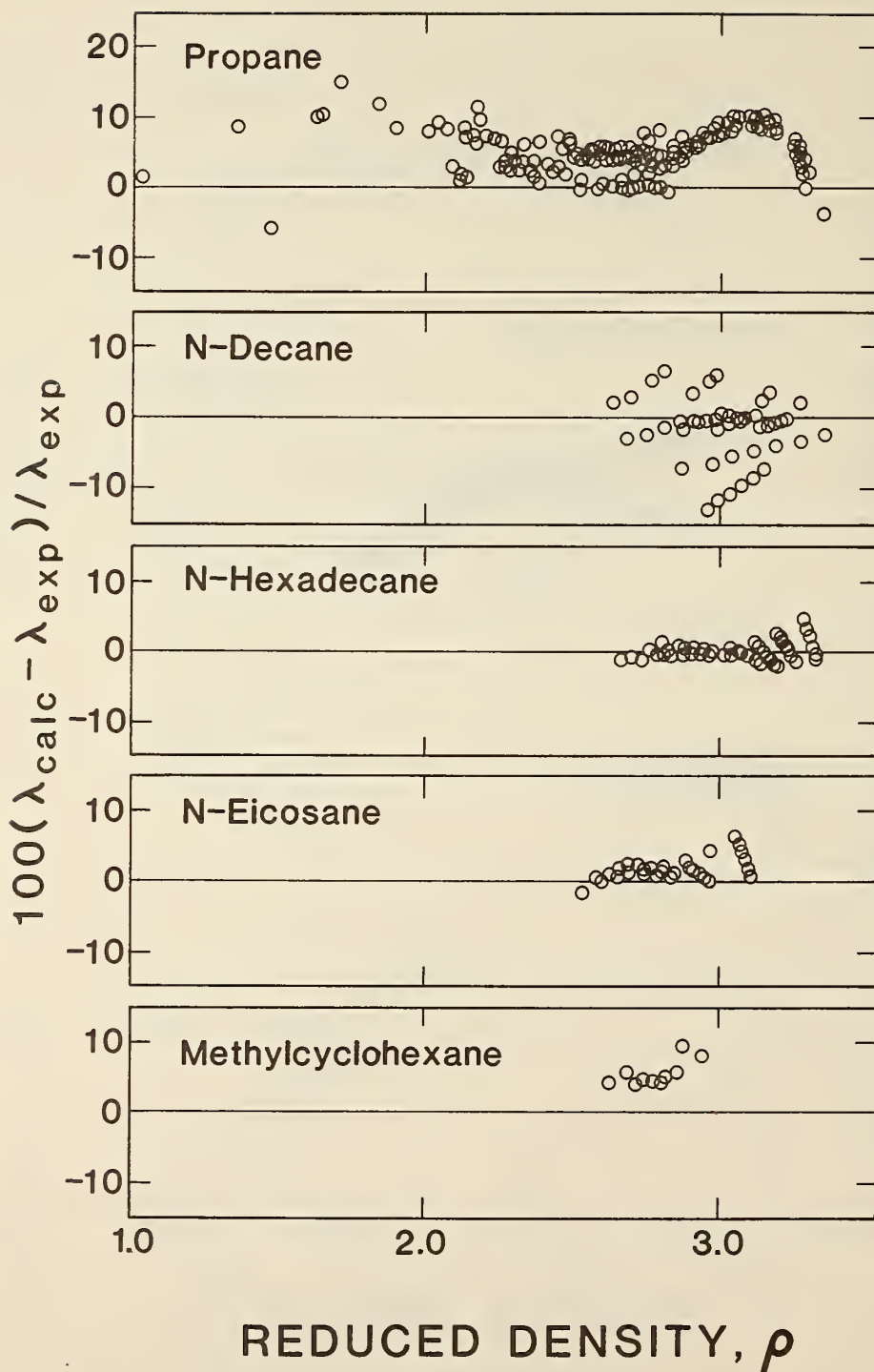


Figure 4. Comparison of calculated and experimental thermal conductivity for propane, decane, hexadecane, eicosane and methylcyclohexane.

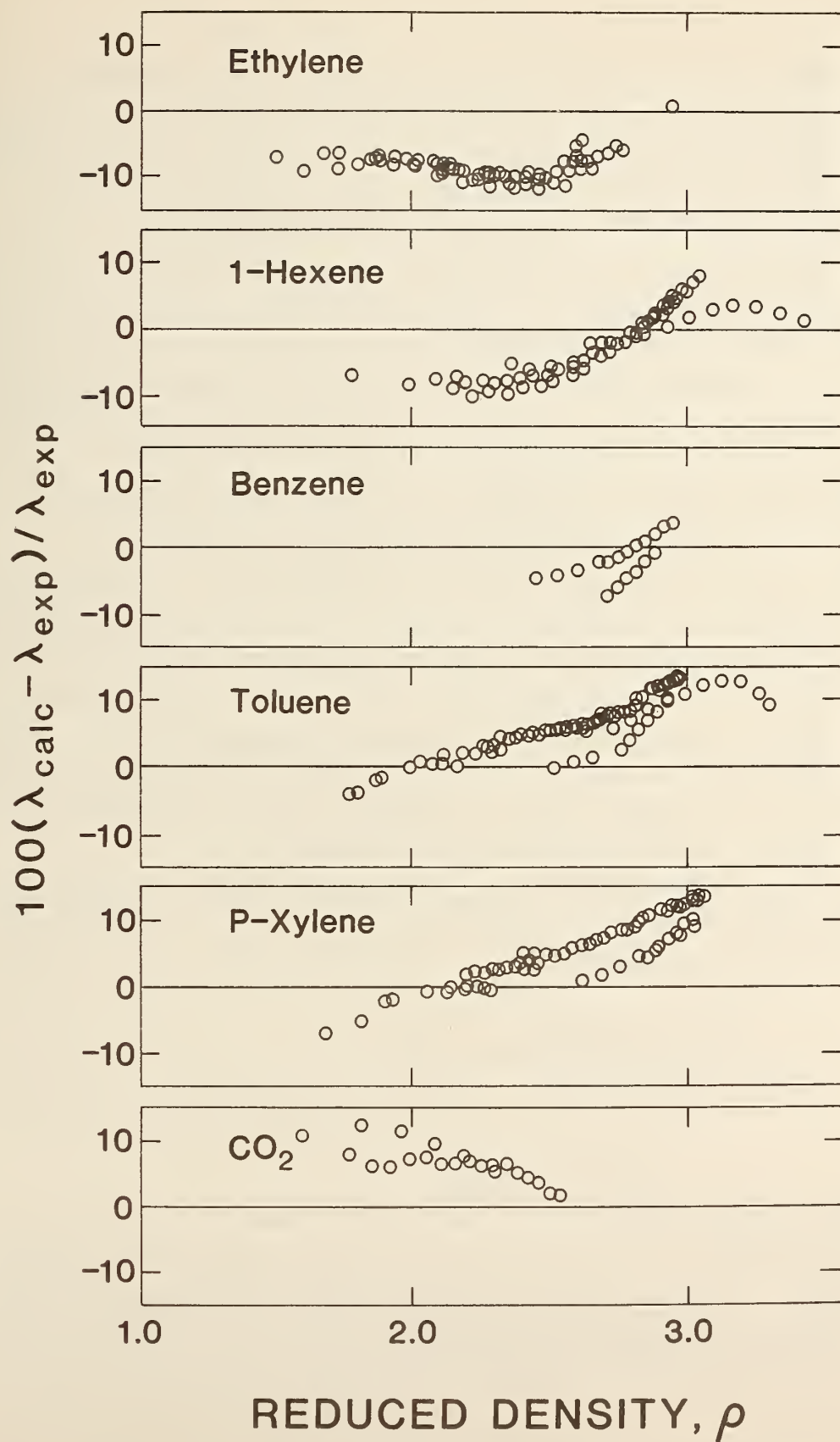


Figure 5. Comparison of calculated and experimental thermal conductivity for ethylene, 1-hexene, benzene, toluene, p-xylene and carbon dioxide.

none exists which does not require in some way transport data of the pure components. Our method, however, avoids this and the mixture evaluations are no more complicated than those for the pure components, given the mixing and combining rules, eqs (21-27). It is also worth remarking that the procedure also gives the mixture density automatically.

One further refinement was considered for the mixture viscosity. We introduced a  $\chi_\eta$  factor in eq (29) to account for the lack of correspondence between the reference fluid and a pure fluid of interest. For mixtures, however,  $\chi_\eta$  will act as a correction not only for lack of correspondence between the reference fluid and hypothetical pure fluid, but should also account for the basic lack of conformality in the mixture. It turns out that although most of the mixtures studied cannot be conformal, the procedure works reasonably well with  $\chi_\eta \approx 1.0$ . Our results for the mixture viscosity (but not thermal conductivity) did show, however, a systematic disagreement with experiment in one special case, namely when the components of the mixture differed substantially in effective size, e.g., in the values of the critical volume. In particular, initial calculations for the methane/decane mixture viscosity showed large deviations at high densities as the mole fraction of methane increased. In effect, the contribution of methane to the mixture viscosity was negligible until its mole fraction approached 0.9 and the procedure tended to overestimate it. For this system the critical volume ratio is approximately 6.

Since a methane/decane type mixture is relatively common, we attempted to account for the size effect empirically in the present model. The correction factor  $\chi_\eta$  was modified to become

$$\chi_\eta = \left[ \left\{ 1 - \psi \frac{T_x}{f_{x,0}} \left( \frac{\partial f_{x,0}}{\partial T_x} \right)_{V_x} \right\} \frac{Z_x^C}{Z_0^C} \right]^{1/2} \frac{a + b\bar{R}}{1 + c\bar{R}} \quad (32)$$

where

$$\bar{R}^{-1} = \sum_{\alpha} x_{\alpha} (V_{\alpha}^C / V_{\min}^C)^{1/3} \quad (33)$$

and  $a = 0.16129$ ,  $b = -4.51613$ , and  $c = -5.35484$ .  $V_{\min}^C$  is the critical volume of the smallest component in the mixture.

It should be noted that for most mixtures, results from eq (32) are very close to those from eq (29) and in fact  $\chi_\eta$  is often very close to unity. No further corrections were made for the mixture thermal conductivity.

Tables 7 and 8 list the mixtures, number of points considered and the AAD and BIAS between experiment and our procedure. Figures (6-8) are typical of the deviations observed. In general the results are excellent with an average absolute deviation of approximately seven percent for both transport properties. An assessment of the method should, however, bear in mind that the data situation for mixtures is very poor and that an assignment of 5-20 percent on the accuracy of the mixture data is reasonable.

## 7. CONCLUSIONS

We have presented a predictive procedure to estimate the viscosity and thermal conductivity of nonpolar pure fluids and mixtures over the entire range of fluid states, from the dilute gas to the dense liquid. Extensive comparisons with data have shown that the transport properties of a wide variety of pure fluids and mixtures are predicted to within an absolute percent deviation of about seven percent. Not shown in this paper are comparisons for the density, which is also predicted and for the dilute gas properties. In general the density is predicted to better than one percent and the dilute gas transport properties are predicted to within five to ten percent.

The basis of the method is the one fluid corresponding states concept with the extended corresponding states approach included. The method is predictive and requires only the common characterization parameters of the pures as input. The number of components of a mixture which can be considered is, in principle, unrestricted.

The application of the methodology described herein to polar fluids and to molecules with structures which could cause hindered rotation and steric effects is under current investigation.

## 8. COMPUTER PROGRAM

A computer program for predicting the transport properties and the density of pure fluids and their mixtures has been developed. The program is essentially identical to that used to generate the results reported here. A detailed user's manual has been prepared which describes the program input, output and overall structure and is given in Appendix A. Appendix B lists the program.

Table 7. Summary of Results for Binary Mixture Viscosity

Component 1	Component 2	N	AAD	BIAS
Methane	Propane	134	3.86	- 2.85
	n-Nonane	32	9.56	8.12
	n-Decane	71	10.62	- 5.80
2,3-Dimethylbutane	n-Octane	2	5.04	- 5.04
n-Hexane	2,3-Dimethylbutane	2	5.19	5.19
	n-Tetradecane	10	1.23	0.99
	n-Hexadecane	26	1.84	- 0.58
n-Heptane	n-Dodecane	3	4.32	4.32
	n-Tetradecane	3	2.47	2.47
	n-Hexadecane	3	1.96	- 0.24
	n-Octadecane	2	1.73	0.27
	Methylcyclohexane	24	17.31	-16.51
2,2,3-Trimethylbutane	2,3,3-Trimethylpentane	2	29.93	-29.93
n-Octane	n-Decane	2	3.83	3.83
n-Tetradecane	n-Hexadecane	11	2.73	2.53
Benzene	n-Hexane	15	6.02	- 1.58
	n-Heptane	3	1.58	6.56
	2,2,4-Trimethylpentane	26	11.21	-11.21
	n-Decane	3	5.68	4.00
	n-Dodecane	3	7.04	7.04
	n-Tetradecane	3	3.41	3.27
	n-Hexadecane	3	3.57	2.46
	n-Octadecane	3	2.79	2.79
	n-Heptane	21	6.09	6.09
Toluene	n-Octane	20	10.14	10.14
	2,2,4-Trimethylpentane	28	5.87	- 3.40
Overall Results		455	6.95	- 2.07



Table 8. Summary of Results for Binary Mixture Thermal Conductivity

Component 1	Component 2	N	AAD	BIAS
Methane	n-Butane	15	11.69	11.49
2,3-Dimethylbutane	2,2,4-Trimethylpentane	6	5.15	5.15
n-Heptane	2,2,4-Trimethylpentane	6	1.94	1.71
n-Heptane	1-Hexene	8	7.18	- 7.18
n-Octane	n-Hexane	5	2.09	- 2.09
n-Octane	n-Heptane	6	2.77	- 2.77
n-Octane	2,2,4-Trimethylpentane	9	3.96	- 3.96
n-Octane	1-Hexene	9	7.19	- 7.19
2,2,5-Trimethylhexane	2,2,4-Trimethylpentane	6	4.35	4.35
n-Tetradecane	2,2,4-Trimethylpentane	6	4.43	- 4.43
n-Hexadecane	n-Heptane	2	2.81	- 2.81
n-Heptadecane	n-Octane	6	4.16	- 4.16
Cyclopentane	n-Heptane	6	1.72	1.29
Cyclopentane	Methylcyclohexane	6	5.90	5.90
Methylcyclohexane	2,2,4-Trimethylpentane	6	11.42	-11.42
Benzene	Cyclohexane	4	5.54	5.54
Benzene	Toluene	12	6.79	6.79
Toluene	n-Heptane	5	6.37	6.37
Toluene	2,2,4-Trimethylpentane	6	11.05	11.05
Toluene	Cyclohexane	4	5.26	5.26
Toluene	o-Xylene	6	13.97	13.97
o-Xylene	2,2,4-Trimethylpentane	6	10.65	10.65
n-Heptane	n-Decane	6	8.89	- 8.89
Benzene	n-Heptane	8	2.80	- 1.71
Overall Results		159	6.58	1.73

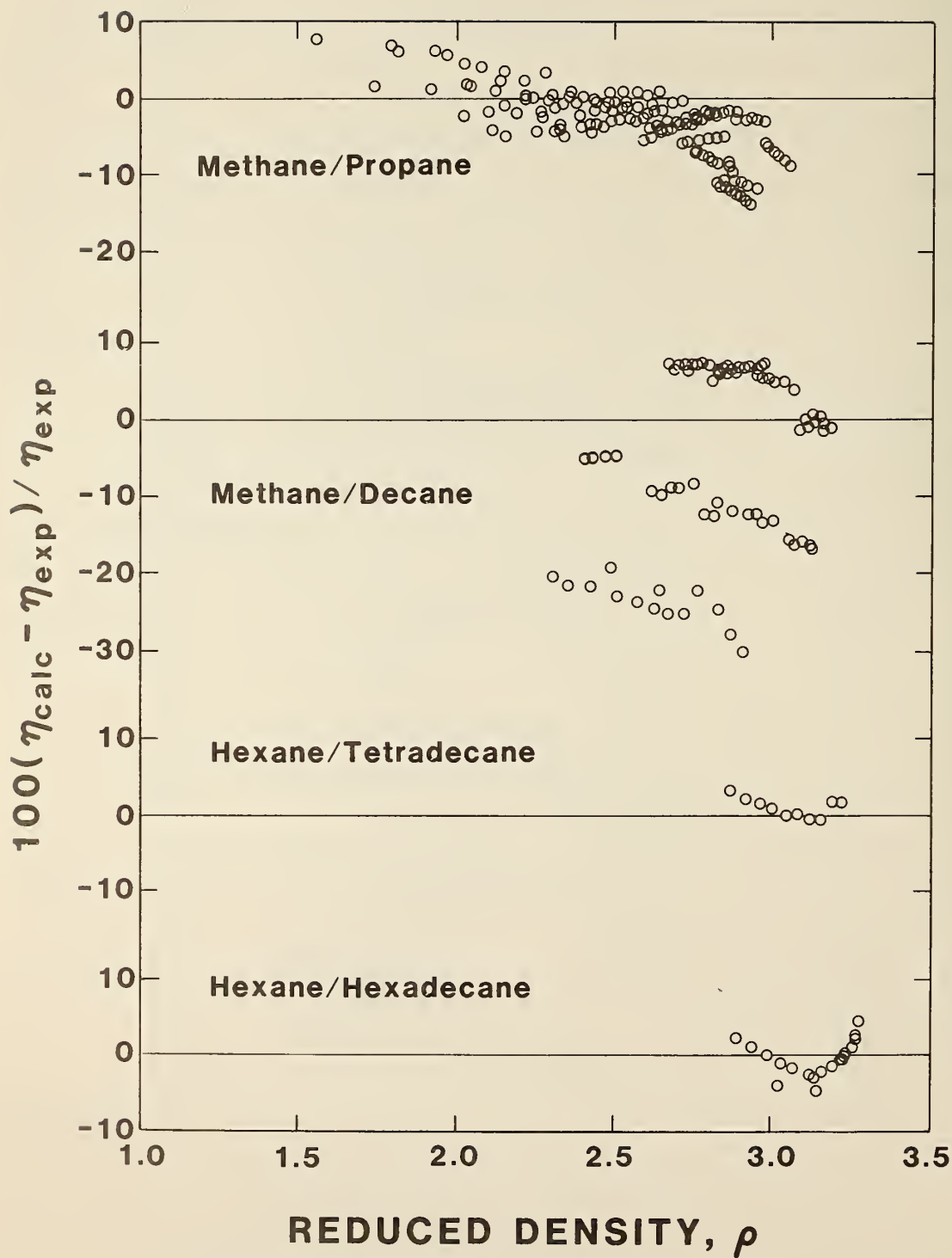


Figure 6. Comparison of calculated and experimental viscosity of selected paraffin binary mixtures as a function of reduced density.



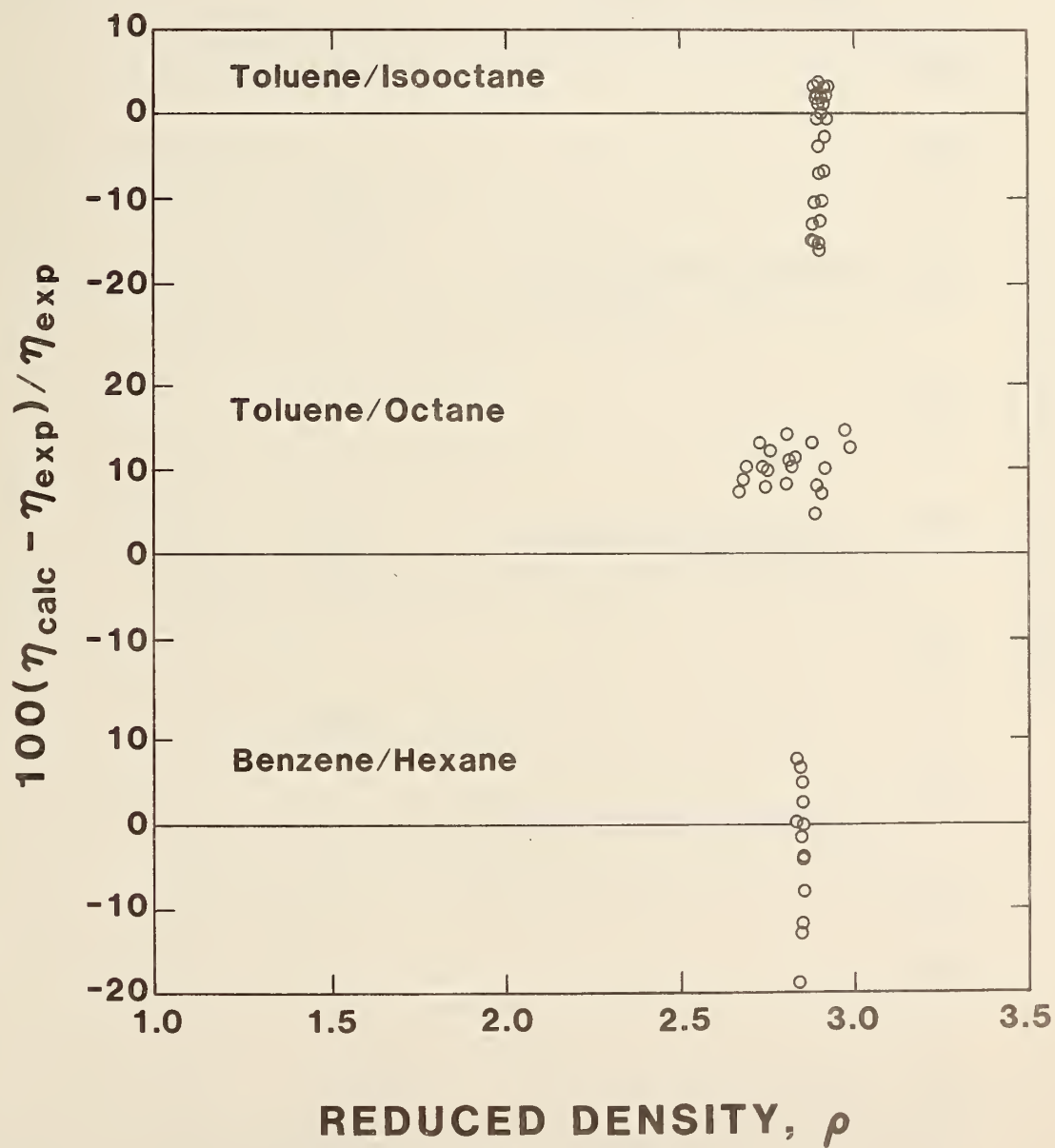


Figure 7. Comparison of calculated and experimental viscosity of selected aromatic/paraffin mixtures.

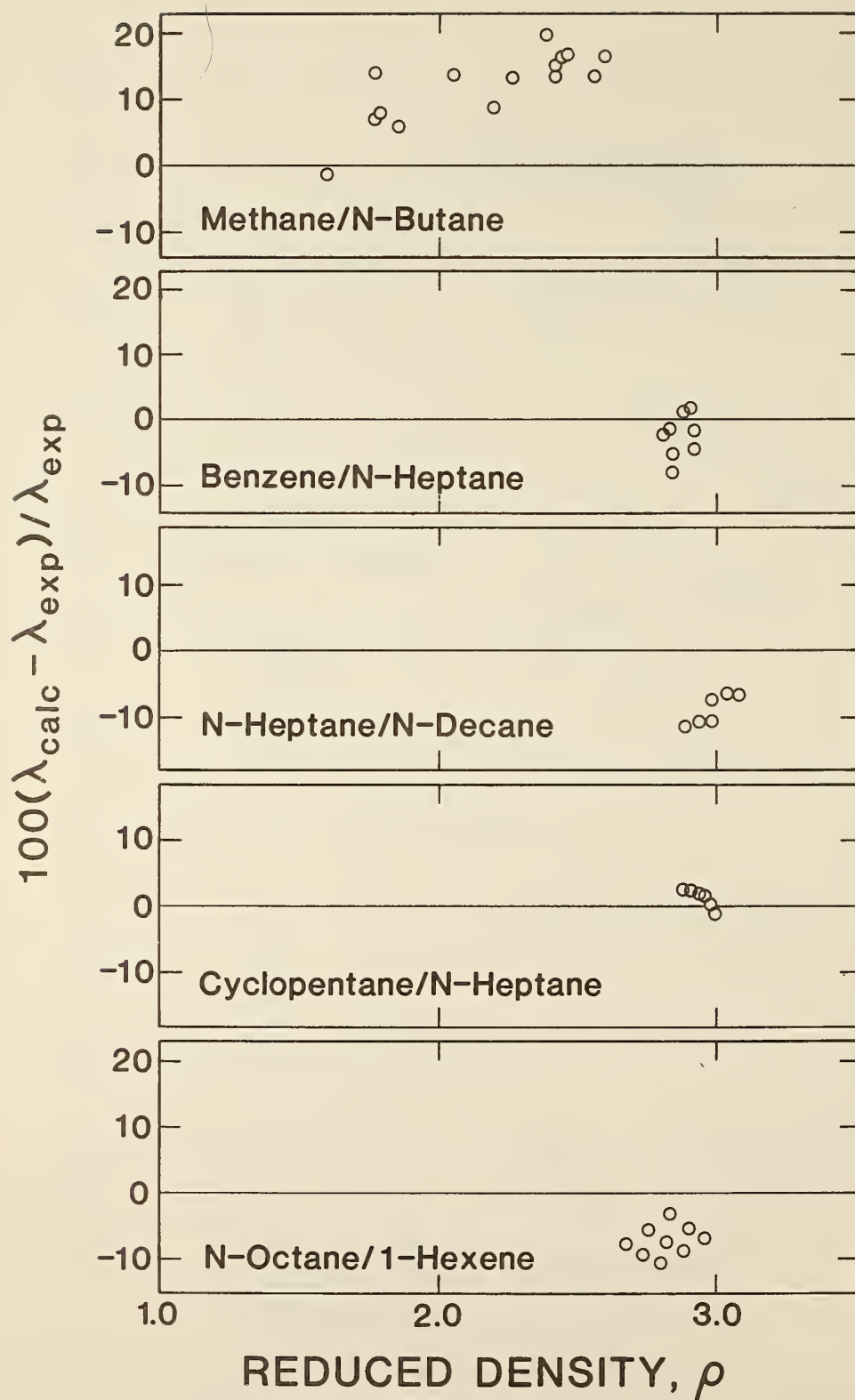


Figure 8. Comparison of calculated and experimental thermal conductivity of selected binary mixtures.

## 9. ACKNOWLEDGMENTS

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## APPENDIX A. TRAPP USER'S GUIDE

The method is applicable to the full range of densities and temperatures, from the dilute gas to dense liquid. The required material constants for each mixture component are the critical parameters,  $T_c$ ,  $p_c$ ,  $V_c$  and Pitzer's acentric factor. The thermal conductivity calculation also requires the ideal gas heat capacity. No transport data for the mixture or components are required. The computer program currently has a built in database for the 61 components. These components and their synonyms are listed in table A1.

### Program Description

The program is modular in construction consisting of a sample driver or main program and a collection of subroutines. Most of the communication between the routines is accomplished via block common with a few parameters being passed in the subroutine calling lists. Figure A1 shows a block diagram of the program communication links. The purpose of these routines are as follows:

TRAPP is the main program which inputs the components, temperature, pressure and compositions. It then makes the appropriate subroutine calls and prints out the calculated density, viscosity and thermal conductivity.

LIB takes the component names from TRAPP and tries to identify them in the component library. After a successful identification, it loads the various material constants in the common block/COMPRP/, initializes the binary interaction constants to zero and returns. If the component is not identified as being in the database, it aborts with an error message. LIB utilizes the block data subroutine LIBSET which loads the common block /LIBDAT/.

DCST takes the input pressure, temperature and composition and calculates the mixture density via the extended corresponding states model. It uses several subroutines to accomplish this calculation which are described below. After the density is calculated it calls the subroutine ECSTX to evaluate the derivatives needed in the viscosity calculation.

RHOF is called by DCST and makes an initial guess at the reference fluid density given the equivalent temperature and pressure.

DO is called by RHOF and performs a Newton-Raphson iteration to calculate the reference fluid density given the temperature and pressure.

PVT0 is called by DO and calculates the reference fluid pressure and its derivative w.r.t. density given the density and temperature.

Table A1. Listing of Components and TRAPP Data Base

<u>Component Name</u>	<u>Synonym</u>	<u>Component Name</u>	<u>Synonym</u>
Methane	C1	2-Methyl-2-Butene	2M2C4-
Ethane	C2	2-Methyl-1-Butene	2M1C4-
Propane	C3	3-Methyl-1-Butene	3M1C4-
Isobutane	IC4	Cis-2-Pentene	C2C5-
n-Butane	C4	Trans-2-Pentene	T2C5-
2,2-Dimethylpropane	22DMPR	1-Pentene	C5-
Isopentane	IC5	1-Hexene	C6-
n-Pentane	C5	1-Heptene	C7-
2,2-Dimethylbutane	22DMB	Propadiene	12C5=
2,3-Dimethylbutane	23DMB	1,3-Butadiene	13C4=
3-Methylpentane	3MP	1,2-Butadiene	12C4=
Isohexane	IC6	Cyclopentane	CC5
n-Hexane	C6	Methylcyclopentane	MCC5
n-Heptane	C7	Ethylcyclopentane	ECC5
n-Octane	C8	Cyclohexane	CC6
n-Nonane	C9	Methylcyclohexane	MCC6
n-Decane	C10	Ethylcyclohexane	ECC6
n-Undecane	C11	Benzene	BNZ
n-Dodecane	C12	Toluene	TOL
n-Tridecane	C13	Ethylbenzene	EB
n-Tetradecane	C14	Ortho-xylene	OXYL
n-Pentadecane	C15	Meta-Xylene	MXYL
n-Hexadecane	C16	Para-Xylene	PXYL
n-Heptadecane	C17	Hydrogen	H2
Ethene	C2-	Nitrogen	N2
Propene	C3-	Oxygen	O2
2-Methylpropene	IC3-	Water	H2O
Cis-2-Butene	C-2C4-	Carbon Monoxide	CO
Trans-2-Butene	T-2C4-	Carbon Dioxide	CO2
1-Butene	C4-	Sulphur Dioxide	SO2
Hydrogen Sulphide	H2S		



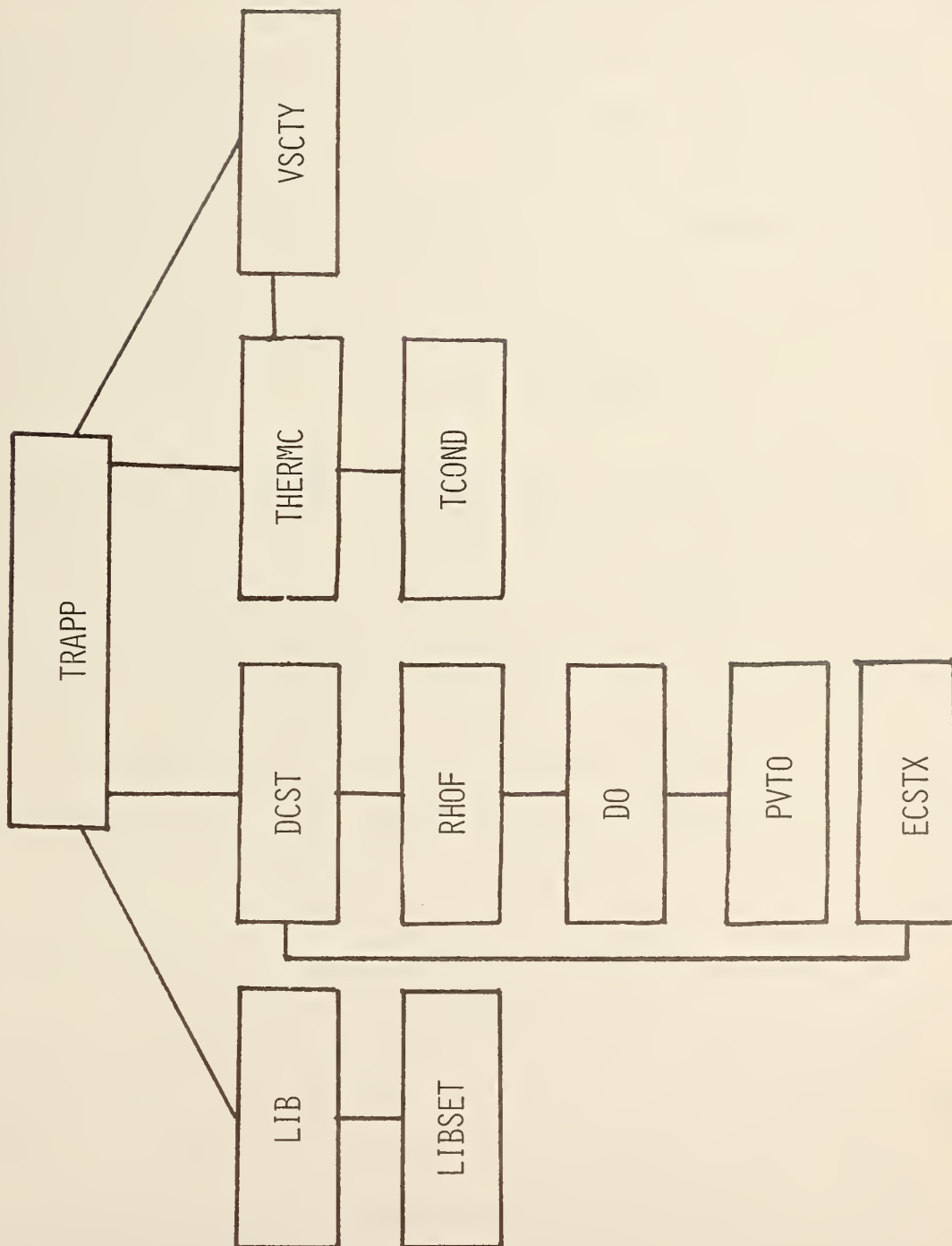


Figure A1. Block diagram of computer program TRAPP.

ECSTX is called by DCST after the density has been calculated. It calculates the appropriate molecular weights for the transport calculations, part of the transport correction factors and the derivatives of the equivalent substance reducing ratios with respect to temperature.

THERMC is called by TRAPP after the density is calculated and evaluates the mixture thermal conductivity. It calculates the contribution to the thermal conductivity from the internal degrees of freedom using the routine VSCTY and ideal gas heat capacity in the text. The routine then calculates the translational contributions to the thermal conductivity using the routine TCOND and combines all the results according to eq (12).

TCOND takes the equivalent temperature and density of the mixture and/or components and calculates the translational contribution to the thermal conductivity via a corresponding states principle. The procedure used is described in the text.

VSCTY is called by TRAPP to evaluate the mixture viscosity via a corresponding states principle. The procedure used is described in the text.

#### Program Input and Output

The program expects input in a specified order and is set up to run in an interactive mode. When the program begins execution it prints a banner and then inquires if the user desires a list of the library components. If the user answers yes as indicated by a "1" followed by a carriage return, the list is displayed. A "0" response indicates a no and the list is skipped. Next the program asks if engineering units are desired. A "0" response indicates that scientific units are desired (K, bar,  $\text{Kg/m}^3$ , Pa•s, and W/m-K) and a "1" response means that engineering units are desired (F, psia,  $\text{lb/ft}^3$ , lb/ft-hr, and BTU/ft-hr- F).

Next, (Step A) the program requests the number of components, the response to which can be 0-20. If 0 is entered, the program stops.

(Step B) A nonzero response causes the program to ask for the component names (7A4 Format), one at a time. If a component name is incorrectly spelled or not in the database, the program aborts with an error message. The synonym may be entered in lieu of the full name.

(Step C) If there is more than one component in the system the program then requests the composition of each component, one component at a time. The compositions may be entered in moles or mole percent. The program automatically

normalizes the compositions to sum to unity, i.e., they are internally converted to mole fraction. If the composition of any component is entered as less than zero, the program assumes that you want to change the mixture components and reverts to step A.

(Step D) The program next requests the temperature and pressure in the units specified previously on one line separated by a comma. If "0,0" is entered the program reverts to step C. For any other response the program then calculates the density, viscosity and thermal conductivity and prints the results of the calculations. The program then reverts to step D. The logical flow of the input/output phases is shown in fig. A2.

#### Sample Input and Output

Tables A2-A4 give typical input/output examples.

#### Cautions

The program assumes that the mixture is single phased. If it is not, the results of the calculations will be meaningless. In addition, if the mixture is single phased but very close to the two-phase boundary it may converge to a liquid solution when the mixture is actually a vapor and vice-versa. If this happens, raise or lower the pressure slightly until you get into the desired phase. Appendix B lists the computer program.

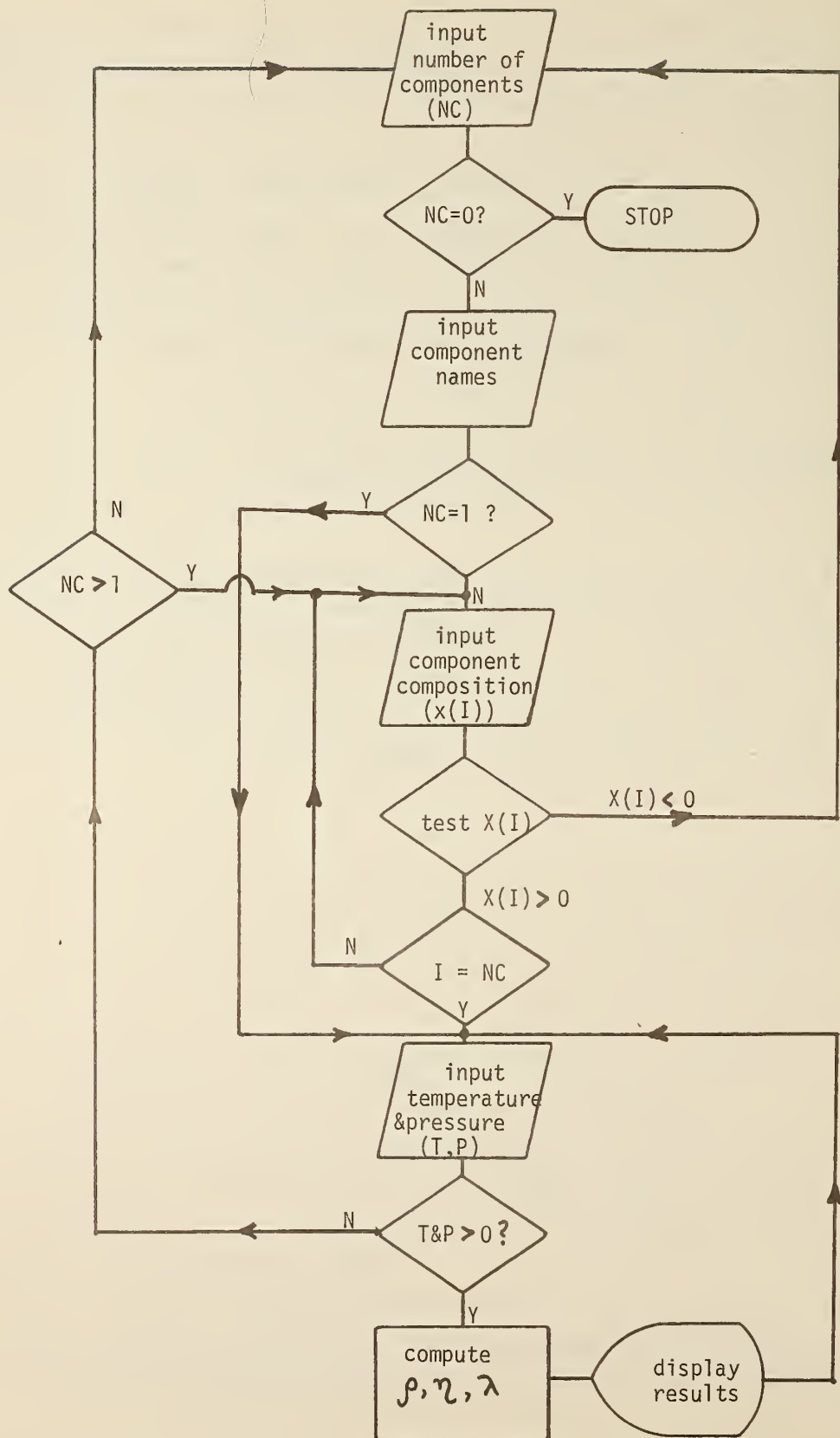


Figure A2. Flow diagram of I/O portion of TRAPP.

Table A2. Sample Input and Output

```

*****
*
*           T R A P P
*
*   TRANSPORT PROPERTIES PREDICTION PROGRAM
*
*           BY
*
*   J. F. ELY  AND  H. J. M. HANLEY
*   U.S. NATIONAL BUREAU OF STANDARDS
*   NATIONAL ENGINEERING LABORATORY
*   THERMOPHYSICAL PROPERTIES DIVISION
*   BOULDER, COLORADO  80303
*
*   (PARTIALLY SPONSORED BY THE OFFICE OF
*   STANDARD REFERENCE DATA)
*
*****

```

DO YOU WANT A LIST OF LIBRARY COMPONENTS(0-NO;1-YES) ? 0

DO YOU WANT ENGINEERING UNITS(0-NO,1-YES)? 0

ENTER NUMBER OF COMPONENTS ? 1

ENTER NAME OF COMPONENT 1 ? METHANE

ENTER T(K) AND P(BAR ) ? 100,1

D= 439.219 KG/M\*\*3 ETA = 1482.3E-7 PA-S TC = .21842 W/M-K

ENTER T(K) AND P(BAR ) ? 120,1

D= 1.654 KG/M\*\*3 ETA = 48.2E-7 PA-S TC = .01471 W/M-K

ENTER T(K) AND P(BAR ) ? 120,5

D= 410.533 KG/M\*\*3 ETA = 971.3E-7 PA-S TC = .17804 W/M-K

ENTER T(K) AND P(BAR ) ? 140,10

D= 377.755 KG/M\*\*3 ETA = 673.5E-7 PA-S TC = .14425 W/M-K

ENTER T(K) AND P(BAR ) ? 190,50

D= 239.837 KG/M\*\*3 ETA = 239.7E-7 PA-S TC = .07190 W/M-K

ENTER T(K) AND P(BAR ) ? 0,0

ENTER NUMBER OF COMPONENTS ? 0

.035 CP SECONDS EXECUTION TIME.



Table A3. Sample Input and Output

```

*****
*
*           T R A P P
*
*   TRANSPORT PROPERTIES PREDICTION PROGRAM
*
*           BY
*
*   J. F. ELY AND H. J. M. HANLEY
*   U.S. NATIONAL BUREAU OF STANDARDS
*   NATIONAL ENGINEERING LABORATORY
*   THERMOPHYSICAL PROPERTIES DIVISION
*   BOULDER, COLORADO 80303
*
*   (PARTIALLY SPONSORED BY THE OFFICE OF
*   STANDARD REFERENCE DATA)
*
*****

```

DO YOU WANT A LIST OF LIBRARY COMPONENTS(0-NO;1-YES) ? 0

DO YOU WANT ENGINEERING UNITS(0-NO;1-YES)? 1

ENTER NUMBER OF COMPONENTS ? 3

ENTER NAME OF COMPONENT 1 ? METHANE

ENTER NAME OF COMPONENT 2 ? PROPANE

ENTER NAME OF COMPONENT 3 ? NITROGEN

ENTER NUMBER OF MOLES OF METHANE ? 3

ENTER NUMBER OF MOLES OF PROPANE ? 1

ENTER NUMBER OF MOLES OF NITROGEN ? 6

ENTER T(F) AND P(PSIA) ? 400,1000

D= 2.8122 LB/FT\*\*3 ETA = .053292 LB/FT-HR TC = .02700 BTU/FT-HR-F

ENTER T(F) AND P(PSIA) ? -100,1000

D= 12.4563 LB/FT\*\*3 ETA = .040324 LB/FT-HR TC = .02040 BTU/FT-HR-F

ENTER T(F) AND P(PSIA) ? -300,1450

D= 44.8939 LB/FT\*\*3 ETA = .553857 LB/FT-HR TC = .11165 BTU/FT-HR-F

ENTER T(F) AND P(PSIA) ? 0,0

ENTER NUMBER OF MOLES OF METHANE ? 7

ENTER NUMBER OF MOLES OF PROPANE ? .5

ENTER NUMBER OF MOLES OF NITROGEN ? 2.5

ENTER T(F) AND P(PSIA) ? 77,14.7

D= .0523 LB/FT\*\*3 ETA = .030090 LB/FT-HR TC = .01912 BTU/FT-HR-F

ENTER T(F) AND P(PSIA) ? 77,3000

D= 12.4219 LB/FT\*\*3 ETA = .051985 LB/FT-HR TC = .03323 BTU/FT-HR-F

ENTER T(F) AND P(PSIA) ? 0,0

ENTER NUMBER OF MOLES OF METHANE ? -1

ENTER NUMBER OF COMPONENTS ? 0

.155 CP SECONDS EXECUTION TIME.



Table A4. Sample Input and Output

```

*****
*
*               T R A P P
*
*   TRANSPORT PROPERTIES PREDICTION PROGRAM
*
*               B Y
*
*   J. F. ELY AND H. J. M. HANLEY
*   U.S. NATIONAL BUREAU OF STANDARDS
*   NATIONAL ENGINEERING LABORATORY
*   THERMOPHYSICAL PROPERTIES DIVISION
*   BOULDER, COLORADO 80303
*
*   (PARTIALLY SPONSORED BY THE OFFICE OF
*   STANDARD REFERENCE DATA)
*
*****

DO YOU WANT A LIST OF LIBRARY COMPONENTS(0-NO;1-YES) ? 0

DO YOU WANT ENGINEERING UNITS(0-NO;1-YES)? 0

ENTER NUMBER OF COMPONENTS ? 6
ENTER NAME OF COMPONENT 1 ? N2
ENTER NAME OF COMPONENT 2 ? CO2
ENTER NAME OF COMPONENT 3 ? C3
ENTER NAME OF COMPONENT 4 ? BNZ
ENTER NAME OF COMPONENT 5 ? H2S
ENTER NAME OF COMPONENT 6 ? ETHENE
ENTER NUMBER OF MOLES OF N2           ? 3
ENTER NUMBER OF MOLES OF CO2          ? 4
ENTER NUMBER OF MOLES OF C3           ? 8
ENTER NUMBER OF MOLES OF BNZ          ? 1
ENTER NUMBER OF MOLES OF H2S          ? 0.4
ENTER NUMBER OF MOLES OF ETHENE       ? 50

ENTER T(K) AND P(BAR ) ? 400,0.01
D= .010 KG/M**3  ETA = 138.6E-7  PA-S  TC = .03563 W/M-K

ENTER T(K) AND P(BAR ) ? 200,100
D= 594.880 KG/M**3  ETA = 1515.8E-7  PA-S  TC = .15493 W/M-K

ENTER T(K) AND P(BAR ) ? 0,0
ENTER NUMBER OF MOLES OF N2           ? -1

ENTER NUMBER OF COMPONENTS ? 2
ENTER NAME OF COMPONENT 1 ? CARBON DIOXIDE
ENTER NAME OF COMPONENT 2 ? C10
ENTER NUMBER OF MOLES OF CARBON DIOXIDE ? 95
ENTER NUMBER OF MOLES OF C10          ? 5

ENTER T(K) AND P(BAR ) ? 273,250
D=1059.534 KG/M**3  ETA = 2158.5E-7  PA-S  TC = .16524 W/M-K

ENTER T(K) AND P(BAR ) ? 0,0
ENTER NUMBER OF MOLES OF CARBON DIOXIDE ? -1

ENTER NUMBER OF COMPONENTS ? 0
.082 CP SECONDS EXECUTION TIME.

```

APPENDIX B. LISTING OF COMPUTER PROGRAM TRAPP

```

C      PROGRAM TRAPP(INPUT,OUTPUT)
C
C      * * * * *
C
C      PURPOSE --- DEMONSTRATION DRIVER FOR EXTENDED CORRESPONDING
C                   STATES ESTIMATION OF VISCOSITY AND THERMAL
C                   CONDUCTIVITY OF HYDROCARBON MIXTURES.
C
C      VERSION G2.3  8/11/80
C
C      CODED BY:  J. F. ELY
C                   NATIONAL BUREAU OF STANDARDS
C                   NATIONAL ENGINEERING LABORATORY
C                   THERMOPHYSICAL PROPERTIES DIVISION
C                   BOULDER, COLORADO  80303
C
C      * * * * *
C      DIMENSION X(20), TA(2), TD(2), PD(2), DM(2), VM(2), TM(2)
C      INTEGER TUNIT(2), PUNIT(2)
C
C      COMMON /COMPRP/ NC, ND, NAME(20,7), DPROPS(20,14), DINC(380)
C
C      COMMON /MIXDAT/ FX, DFXDT, F(20), HX, DHXDT, H(20), CMX, CMXV,
1      CMXT, ZCX, CORV, CORT
C
C      COMMON /LIBDAT/ NLIB, NDUM, PROPS(22,61)
C
C      LOGICAL MIX
C
C      DATA TA, TD, PD, DM, VM, TM / 0.0D0, 459.67D0, 1.0D0, 1.8D0,
1      1.01325D0, 14.69595D0, 1.0D0, 0.06242795D0, 1.0D0, 2.419D-4,
2      1.0D-3, 5.777675D-4 /
C
C      DATA TUNIT, PUNIT / "K", "F", "BAR", "PSIA" /
C
C      PRINT 260
C      PRINT 280
C      READ *, INOT
C      IF(INOT.EQ.0) GO TO 015
C      NC = NLIB / 2
C      PRINT 270
C      DO 010 K=1,NC
010  PRINT 290, (PROPS(J,K),J=1,9), (PROPS(J,K+NC),J=1,9)
      PRINT 290, (PROPS(J,NLIB),J=1,9)
C
C      SEE IF ENGINEERING UNITS ARE DESIRED
015  IU = 1
      PRINT 300
      READ *, INOT
      IF(INOT.EQ.0) GO TO 020
      IU = 2
C
C      INITIALIZE PROGRAM PARAMETERS

```

```

020 X(1) = 1.0
    MIX = .FALSE.
C
C          INPUT THE NUMBER OF COMPONENTS
C          IF IT IS ZERO OR LESS, STOP.
    PRINT 200
    READ *, NC
    IF (NC.LE.0) STOP
    IF(NC.GT.1) MIX = .TRUE.
    DO 040 K=1,NC
    PRINT 210, K
    READ 230, (NAME(K,J),J=1,7)
    CALL LIB(K)
040 CONTINUE
    IF (.NOT.MIX) GO TO 080
C
C          IF A MIXTURE, GET THE COMPOSITION
050 XSUM = 0.0
    DO 060 K=1,NC
    PRINT 220, (NAME(K,J),J=1,4)
    READ *, X(K)
    IF (X(K).LT.0.0) GO TO 020
    XSUM = XSUM + X(K)
060 CONTINUE
    DO 070 K=1, NC
    X(K) = X(K) / XSUM
070 CONTINUE
C
C          INPUT THE TEMPERATURE AND PRESSURE
080 PRINT 240, TUNIT(IU), PUNIT(IU)
    READ *, TIN, PIN
    IF (TIN.NE.0.0 .AND. PIN.NE.0.0) GO TO 100
090 IF(.NOT.MIX) GO TO 020
    GO TO 050
C
C          CONVERT TO K AND ATM FOR CALCULATIONS
100 TK = (TIN + TA(IU)) / TD(IU)
    PATM = PIN / PD(IU)
    CALL DCST(PATM,DX,TK,X)
    ETAX = VM(IU) * VSCTY(DX,TK)
    TCX = TM(IU) * THERMC(DX,TK,X)
    DX = DX * CMX * DM(IU)
    IF (IU.EQ.2) GO TO 110
    PRINT 250, DX, ETAX, TCX
    GO TO 080
110 PRINT 255, DX, ETAX, TCX
    GO TO 080
C
200 FORMAT("/" ENTER NUMBER OF COMPONENTS :K")
210 FORMAT(" ENTER NAME OF COMPONENT",I3," :K")
220 FORMAT(" ENTER NUMBER OF MOLES OF ",4A4," :K")
230 FORMAT(7A4)
240 FORMAT("/" ENTER T(" ,A1," ) AND P(" ,A4," ) :K")
250 FORMAT(" D=" ,F8.3," KG/M**3  ETA =" ,F9.1,"E-7  PA-S  TC =",

```

```

1 F7.5," W/M-K")
255 FORMAT(" D=",F8.4," LB/FT**3  ETA =",F9.6," LB/FT-HR  TC =",
1 F7.5," BTU/FT-HR-F")
260 FORMAT(/6X,48(1H*)/6X,1H*,46X,1H*/6X,1H*,18X,"T R A",
1" P P",19X,1H*/6X,1H*,46X,1H*/6X,  "*"  TRANSPORT P",
2"ROPERTIES PREDICTION PROGRAM  *"/6X,1H*,46X,1H*/
36X,1H*,22X,"BY",22X,1H*/6X,1H*,46X,1H*/6X,1H*,8X,"J. F. ELY  AND
4H. J. M. HANLEY",7X,1H*/6X,1H*,8X,  "U.S. NATIONAL BUREAU OF STA
5NDARDS",5X,1H*/6X,1H*,8X,"NATIONAL ENGINEERING LABORATORY",7X,1H*
6/ 6X,1H*,8X,"THERMOPHYSICAL PROPERTIES DIVISION",4X,1H*/ 6X,1H*
7, 8X,"BOULDER, COLORADO 80303",14X,1H*/ 6X,1H*,46X,1H*/
8 6X,1H*,5X,"(PARTIALLY SPONSORED BY THE OFFICE OF",4X,1H*
9 / 6X,1H*,11X,"STANDARD REFERENCE DATA)", 11X,1H* /
A 6X,1H*,46X,1H*/ 6X,48(1H*)  //)
270 FORMAT(/" COMPONENT NAME",11X,"SYNONYM",7X,"COMPONENT NAME",
1 13X,"SYNONYM")
280 FORMAT(" DO YOU WANT A LIST OF LIBRARY COMPONENTS(0-NO;1-YES) :K")
290 FORMAT(1X,9A4,3X,9A4)
300 FORMAT(/" DO YOU WANT ENGINEERING UNITS(0-NO,1-YES):K")
END

```

SUBROUTINE DCST(PX,DX,TX,X)

\*\*\*\*\*

PURPOSE --- THIS ROUTINE CALCULATES A HYDROCARBON MIXTURE  
DENSITY USING THE SHAPE FACTOR APPROACH TO  
CORRESPONDING STATES.

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VERSION G2.1 - - 1/15/80

\*\*\*\*\*

COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),  
\* CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),  
\* CDT(4), CET(8)  
COMMON /COMPRP/ NC, ND, NAME(20,7), PC(20), DC(20), TC(20),  
\* ZC(20), W(20), CMW(20), TB(20), CPC(20,7),  
\* OMK(190), OML(190)  
COMMON /MIXDAT/ FX, DFXDT, F(20), HX, DHXDT, H(20), CMX, CMXV,  
1 CMXT, ZCX, CORV, CORT  
DIMENSION X(1)  
LOGICAL MASK(20)

DATA TOLERS / 1.0E-5 /

THETAF(TR,VR,WN) = 1. + (WN - WO) \* (CT(1) + CT(2) \* ALOG(TR)  
\* + (CT(3) + CT(4) / TR) \* (VR - 0.5))  
PHIF(TR,VR,WN) = (1.0 + (WN - WO) \* (CP(1) \* (VR + CP(2))  
\* + CP(3) \* (VR + CP(4)) \* ALOG(TR)))

INITIALIZE THE SHAPE FACTORS AND CST PARAMETERS

020 FX = 1.0  
HX = 1.0  
DO 040 N = 1, NC  
MASK(N) = .FALSE.  
IF(X(N).LE.0.0) MASK(N) = .TRUE.  
F(N) = TC(N) / TCO  
H(N) = DCO / DC(N)  
040 CONTINUE

SHAPE FACTOR ITERATION LOOP

DO 200 LOOP = 1, 15

SAVE RESULTS FROM PREVIOUS ITERATION

FXS = FX  
HXS = HX  
HX = 0.0  
FX = 0.0

CALCULATE CST PARAMETERS FOR MIXTURE



```

DO 100 N = 1, NC
IF(MASK(N)) GO TO 100
K = N * (N - 1) / 2
GN = CBRT(H(N))
S2 = 0.0
S3 = 0.0
DO 080 M = 1, N
IF(MASK(M)) GO TO 080
TMP2 = 0.125 * X(M) * (GN + CBRT(H(M)))**3 * OML(K+M)
TMP3 = SQRT(F(N) * F(M)) * TMP2 * OMK(K + M)
S2 = S2 + TMP2
S3 = S3 + TMP3
080 CONTINUE
HX = HX + X(N) * (2.0 * S2 - TMP2)
FX = FX + X(N) * (2.0 * S3 - TMP3)
100 CONTINUE
FX = FX / HX
C          CALCULATE THE EQUIVALENT METHANE DENSITY.
TO = TX / FX
PO = PX * HX / FX
DO = RHOF(PO,TO)
C          RECALCULATE SHAPE FACTORS AND CHECK FOR
C          CONVERGENCE IN FX AND HX
140 DO 160 N = 1, NC
IF(MASK(N)) GO TO 160
TR = AMIN1(2.0,F(N) * TO / TC(N))
VR = AMIN1(2.0,AMAX1(0.5,H(N)*DC(N)/DO))
WN = W(N)
F(N) = TC(N) * THETAF(TR,VR,WN) / TCO
H(N) = DCO * PHIF(TR,VR,WN) * ZCO / (ZC(N) * DC(N))
160 CONTINUE
C          TEST FOR CONVERGENCE
C
IF(ABS(FX / FXS - 1.0).GT.TOLERS) GO TO 200
IF(ABS(HX / HXS - 1.0).GT.TOLERS) GO TO 200
GO TO 220
C          NO CONVERGENCE YET - - TRY AGAIN
200 CONTINUE
C          FAILURE--ISSUE MESSAGE & RETURN
C
210 PRINT 300, TX, PX
C          CONVERGENCE!!!
C
220 DX = DO / HX
CALL ECSTX(PX,DX,TX,X)
RETURN
300 FORMAT("/" /DCST/ FAILED TO CONVERGE AT T="F8.3," AND P="G14.7)
END

```

SUBROUTINE ECSTX(PX,DX,TX,X)

C  
C \* \* \* \* \*  
C

PURPOSE -- THIS ROUTINE EVALUATES VARIOUS SUMS WHICH ARE USED  
TO EVALUATE THE DERIVATIVES OF FX AND HX W.R.T.  
T. IT ASSUMES THAT ECSTD HAS BEEN CALLED TO EVALUATE  
DENSITY, FX AND HX.

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VERSION G2.0 -- 5/20/80

C \* \* \* \* \*  
C

REAL MIJ  
COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),  
\* CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),  
\* CDT(4), CET(8)  
COMMON /COMPRP/ NC, ND, NAME(20,7), PC(20), DC(20), TC(20),  
\* ZC(20), W(20), CMW(20), TB(20), CPC(20,7),  
\* OMK(190), OML(190)  
COMMON /MIXDAT/ FX, DFXDT, F(20), HX, DHXDT, H(20), CMX, CMXV,  
1 CMXT, ZCX, CORV, CORT  
DIMENSION S(5,3), SJ(5), Z(5), X(1)  
EQUIVALENCE (Z(1),FIJ), (Z(2),GIJ), (Z(3),MIJ)  
DATA Z / 5\*0.0 /

C  
C  
C  
C INITIALIZE

ZCX = 0.0  
CMX = 0.0  
CMXV = 0.0  
CMXT = 0.0  
RBAR = 0.0  
DCMAX = 0.0  
DO 015 I = 1, NC  
IF(DC(I).GT.DCMAX) DCMAX = DC(I)  
015 CONTINUE  
DO 020 M=1,3  
DO 020 N=1,5  
020 S(N,M) = 0.0  
C  
DO 120 I = 1,NC  
IF (X(I).LE.0.0) GO TO 120  
K = I \* (I-1) / 2  
GI = CBRT(H(I))  
DO 040 M = 1, 5  
040 SJ(M) = 0.0  
DO 080 J = 1, NC

```

IF (X(J).LE.0.0) GO TO 080
L = K + J
IF (J.GT.I) L = I + J * (J-1) / 2
GIJ = 0.5 * (GI+CBRT(H(J)))
HIJ = GIJ**3 * OML(L)
FIJ = SQRT(F(I)*F(J)) * OMK(L)
RMIJ = CMW(I)*CMW(J)/(CMW(I)+CMW(J))
Z(4) = 1.0 / RMIJ
MIJ = CBRT(HIJ) * SQRT(RMIJ/FIJ)
GIJ = GIJ / GI
TERM = X(J) * HIJ / GIJ
DO 060 M = 1, 5
SJ(M) = SJ(M) + TERM
060 TERM = TERM * Z(M)
080 CONTINUE
THETA = F(I) * TCO / TC(I)
PHI = H(I) * DC(I) / DCO
TR = AMIN1(2.0,F(I) * TX / (FX * TC(I)))
VR = AMIN1(2.0,AMAX1(0.5,H(I)*DC(I)/(HX*DX)))
TEMP = (W(I) - WO) / THETA
Z(1) = 1.0 - TEMP * (CT(2) - CT(4) * (VR-0.5) / TR)
Z(2) = TEMP * (CT(3) + CT(4) / TR) * VR
TEMP = (W(I)-WO) * ZCO / (PHI * ZC(I))
Z(3) = 1.0 - TEMP * (CP(1) + CP(3) * ALOG(TR)) * VR
Z(4) = TEMP * CP(3) * (VR + CP(4))
IF(TR.LT.2.0) GO TO 085
Z(1) = 1.0
Z(4) = 0.0
085 IF (VR.GT.0.5 .AND. VR.LT.2.0) GO TO 090
Z(2) = 0.0
Z(3) = 1.0
090 Z(5) = Z(1) * Z(3) - Z(2) * Z(4)
TERM = HX
DO 100 M = 1, 3
SJ(M) = X(I) * SJ(M) / (Z(5) * TERM)
TERM = FX * HX
DO 100 N = 1, 5
100 S(N,M) = S(N,M) + Z(N) * SJ(M)
CMX = CMX + X(I) * CMW(I)
CMXV = CMXV + X(I) * SJ(4)
CMXT = CMXT + X(I) * SJ(5)
ZCX = ZCX + X(I) * ZC(I)
RBAR = RBAR + X(I) * CBRT(DCMAX/DC(I))
120 CONTINUE
TERM = 1.0 + S(1,1) - S(5,1)
TEMP = S(3,3) + S(4,2)
TRM2 = 1.0 + S(2,3) + S(1,2) - S(5,2)
DFXDT = 1.0 - TERM / (TERM * TEMP - S(4,1) * TRM2)
DHXDT = S(4,1) * (1.0 - DFXDT) / TERM
TERM = FX * HX**(8.0/3.0)
CMXV = 2.0 * CMXV * CMXV / TERM
CMXT = 2.0 * TERM / (CMXT * CMXT)
DFXDT = FX * DFXDT / TX
DHXDT = HX * DHXDT / TX

```

```
RBAR = 1.0/RBAR  
CORV = (0.161290-4.516129*RBAR)/(1.0-5.354839*RBAR)  
RETURN  
END
```

# FUNCTION RHOF(P,T)

PURPOSE --- THIS ROUTINE CALCULATES THE DENSITY IN MOL/L OF A  
FLUID FROM AN EQUATION OF STATE GIVEN THE TEMPERATURE  
T IN KELVIN AND THE PRESSURE P IN ATMOSPHERES.

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BOULDER, COLORADO 80303

VERSION G2.2 -- 1/9/80

COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),  
CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),  
CDT(4), CET(8)

DIMENSION AP(4), BP(3)

DATA AP / 6.3240720088E+00,-6.7447661253E+00,-2.5239605832E+00,  
0.4188447111E+00/

DATA BP / 1.5213153011E+01, 9.2665399400E+00, 1.3551718205E+01/

FIND THE INITIAL DENSITY GUESS. FIRST SEE  
IF THE SYSTEM IS SOLIDLY IN A ONE PHASE REGION.

PS = PCO  
FOP = P / (R \* T)  
IF (T.GT.TCO) GO TO 080

SUB-CRITICAL TEMPERATURE.  
CALCULATE THE VAPOR PRESSURE. IF T > 170 K,  
USE THE CRITICAL REGION FUNCTION. OTHERWISE  
THE FROST-KALKWARF TYPE EQUATION.

TR = T / TCO  
TAU = 1.0 - TR  
IF (T.GT.170.0) GO TO 040  
TMP1 = AP(1) + AP(2) / TR + AP(3)\*ALOG(TR)  
TMP2 = AP(4)/(TR\*TR)  
PRR = 0.100  
DO 020 K = 1, 50  
PR = EXP(TMP1 + TMP2 \* PRR)  
IF (ABS(PR/PRR-1.0).LE.1.0E-6) GO TO 060

020 PRR = PR

040 PR = EXP(BP(1)\*(1.0-1.0/TR) + BP(2)\*TAU + BP(3)\*TAU\*TAU)

```

060 PS = PR * PCO
C
C
C
      IF P % PS, USE A LIQUID DENSITY. OTHERWISE, USE
      IDEAL GAS DENSITY CALCULATED ABOVE.
080 IF (P.GT.PS) FOP = 3.0 * DCO
100 RHOF = DO(P,T,FOP)
    RETURN
    END

```



FUNCTION DO(PO,TO,FOP)  
LOGICAL LIQUID

```

C
C * * * * *
C
C PURPOSE -- THIS ROUTINE CALCULATES THE DENSITY OF A FLUID AT
C             T AND P GIVEN AN INITIAL GUESS IN FOP. ON EXIT,
C             IT RETURNS THE FUGACITY COEFFICIENT IN FOP. IT
C             REQUIRES A ROUTINE "PVTO" WHICH CALCULATES P,
C             DPDD, AND F/P, GIVEN T AND D.
C
C CODED BY : J. F. ELY
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C             NATIONAL ENGINEERING LABORATORY
C             THERMOPHYSICAL PROPERTIES DIVISION
C             BOULDER, COLORADO 80303
C
C VERSION G2.2 -- 1/9/80
C
C * * * * *
C COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),
C *             CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),
C *             CDT(4), CET(8)
C DATA TOLERO, TOLERP / 1.0E-8, 1.0E-8/
C
C             INITIALIZE PARAMETERS
C
C D1=FOP
C NTRY=0
C DMAX=3.2E0*DCO
C
C ESTABLISH BOUNDS AND START NEWTON RAPHSON
020 DLO=0.0
C   DHI=DMAX
C   D=D1
C   DO 100 LAP=1,20
C   CALL PVTO(PX,D,TO,DPDD,FOP)
C
C             IF DPDD IS ZERO OR NEGATIVE, TRY BISECTION
C
C IF(DPDD.LE.1.0E-2) GO TO 120
C DP=PO-PX
C DD=DP/DPDD
C
C SAVE DENSITY FOR POSSIBLE BISECTION
C
C IF (DP) 040,300,060
040 DHI=D
C   GO TO 080
060 DLO=D
C   080 DN=D+DD
C
C KEEP D WITHIN BOUNDS OR GO TO BISECTION
C
C IF (DN.LT.0.0 .OR. DN.GT.DMAX) GO TO 120
C D=DN
C IF(LAP.EQ.1) GO TO 100
C IF(ABS(DP/PO).LE.TOLERP) GO TO 300

```

```

      IF(ABS(DD/D).LE.TOLERD) GO TO 300
100 CONTINUE
C      NEWTON-RAPHSON FAILURE.  TRY BISECTION
120 NTRY=NTRY+1
      IF(NTRY.LT.3) GO TO 130
      PRINT 400, TO, PO
400 FORMAT("/DO/ FAILED TO CONVERGE AT TO=",F8.3," AND PO=",G14.7)
      STOP
130 IF(TO.GT.TCO) GO TO 160
C
C      SUB-CRITICAL.  MAKE SURE THAT WE HAVE THE
C      PROPER BOUNDS ON THE DENSITY.
C
      IF(D1.LT.DCO) GO TO 140
      LIQUID=.TRUE.
      IF(DLO.LE.DCO) DLO=DCO
      IF(DHI.LE.DCO) DHI=DMAX
      GO TO 160
C
140 LIQUID=.FALSE.
      IF(DLO.GE.DCO) DLO=0.0
      IF(DHI.GE.DCO) DHI=DCO
C
C      START THE BISECTION
160 D=0.5EO*(DLO+DHI)
      CALL PVTO(PX,D,TO,DPDD,FOP)
      DP=PX-PO
      IF(DPDD.LT.0.0) GO TO 180
      IF(DP) 200,300,220
180 IF(.NOT.LIQUID) DPDD=-DPDD
      IF(DPDD) 200,240,220
200 DLO=D
      GO TO 240
220 DHI=D
240 IF(ABS(DPDD).LE.TOLERP .AND. ABS(DP).GT.TOLERP) GO TO 260
      IF(ABS(DP/PO) .LE. TOLERP) GO TO 300
      IF(ABS(DLO/DHI-1.0).GT.TOLERD) GO TO 160
C
C      BISECTION FAILED.  WE ARE PROBABLY TRYING ON
C      THE WRONG SIDE OF THE DOME.
260 D1=3.0*DCO
      IF(LIQUID) D1=0.01
      GO TO 020
C      CONVERGENCE ! ! !
300 DO=D
      RETURN
      END

```

SUBROUTINE PVTO(PO,DO,TO,DPDDO,FOP0)

PURPOSE -- THIS ROUTINE CALCULATES THE EQUIVALENT PRESSURE AND  
DERIVATIVE OF PRESSURE WRT DENSITY OF METHANE. THE  
EQUATION USED IS THAT OF STEWART AND JACOBSEN. THE  
DENSITY IS IN G-MOL/LIT AND TEMPERATURE IN KELVIN. IT  
YIELDS THE PRESSURE IN ATMOSPHERES AND RATIO OF THE  
FUGACITY TO THE PRESSURE.

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BOULDER, COLORADO 80303

VERSION G2.1 - - 1/15/80

DIMENSION G(15), B(9), F(6), S(6)

COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),  
CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),  
CDT(4), CET(8)

DATA TLAST, B/ -1.00, 9\*0.0/

DATA F / 1.0, 1.0, 2.0, 6.0, 24.0, 120.0 /

T=TO  
D=DO  
IF(T.EQ.TLAST) GO TO 040  
TLAST=T  
TS=SQRT(T)  
T1=1.0/T  
T2=T1\*T1

G(1)=R\*T  
G(2)=A(1)\*T+A(2)\*TS+A(3)+A(4)\*T1+A(5)\*T2  
G(3)=A(6)\*T+A(7)+A(8)\*T1+A(9)\*T2  
G(4)=A(10)\*T+A(11)+A(12)\*T1  
G(5)=A(13)  
G(6)=A(14)\*T1+A(15)\*T2  
G(7)=A(16)\*T1  
G(8)=A(17)\*T1+A(18)\*T2  
G(9)=A(19)\*T2  
G(10)=T2\*(A(20)+A(21)\*T1)  
G(11)=T2\*(A(22)+A(23)\*T2)  
G(12)=T2\*(A(24)+A(25)\*T1)  
G(13)=T2\*(A(26)+A(27)\*T2)

```

      G(14)=T2*(A(28)+A(29)*T1)
      G(15)=T2*(A(30)+T1*(A(31)+T1*A(32)))
C
      DO 010 J=2,9
010  B(J)=G(J)/(G(1)*FLOAT(J-1))
      DO 030 K=1,6
      S(K)=0.0
      TERM=1.0
      DO 020 J=K,6
      S(K)=S(K)+F(J)*G(J+9)*TERM
020  TERM=TERM/GAMMA
030  S(K)=S(K)/(G(1)*F(K))
C
040  P1=0.0
      D1=0.0
      F1=0.0
      DO 050 J=1,9
      P1=P1*D+G(10-J)
      D1=D1*D+P1
050  F1=F1*D+B(10-J)
C
      DSQ=D*D
      P2=0.0
      D2=0.0
      F2=0.0
      DO 060 J=10,15
      P2=(P2+G(25-J))*DSQ
      D2=D2*DSQ+P2
060  F2=F2*DSQ+S(16-J)
      TERM=EXP(-GAMMA*DSQ)
      P0=D*(P1+P2*TERM)
      IF (P0.EQ.0.0) P0 = 1.0E-20
      Z0=P0/(D*G(1))
      DPDD0=(D1+TERM*(P2+2.0*(D2-DSQ*GAMMA*P2)))
      FOP=F1-(F2*TERM-S(1))/(2.0*GAMMA)+Z0-1.0-ALOG(Z0/P0)
      FOPO=EXP(FOP)/P0
      RETURN
      END

```

FUNCTION VSCTY(DX,TX)

PURPOSE - - THIS ROUTINE CALCULATES THE VISCOSITY OF METHANE  
USING HANLEY'S CORRELATION

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BOULDER, COLORADO 80303

VERSION G2.0 3/12/80

COMMON /MIXDAT/ FX, DFXDT, F(20), HX, DHXDT, H(20), CMX, CMXV,  
CMXT, ZCX, CORV, CORT

COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),  
CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),  
CDT(4), CET(8)

DATA TLAST, PSI / -1.00, 1.5 /  
CALCULATE THE EQUIVALENT DENSITY

DO = 0.001 \* DX \* HX \* CMWO  
TO = TX / FX

CALCULATE THE TEMPERATURE DEPENDENT PART OF THE  
VISCOSITY CORRELATION IF T ISN'T THE SAME AS  
THE LAST CALL TO THIS ROUTINE (USUAL CASE)

IF(TO.EQ.TLAST) GO TO 040

TLAST = TO

TI = 1.0 / TO

ETA1 = CD(1) + CD(2) \* (CD(3) - ALOG(TO / CD(4))) \*\* 2

TRMO = CE(1) + CE(2) \* TI

TRM1 = CE(3) + CE(4) \* TI / SQRT(TO)

TRM2 = CE(5) + TI \* (CE(6) + CE(7) \* TI)

TRMX = EXP(TRMO)

T1 = CBRT(TO)

ETA0 = 0.0

DO 020 J = 1,9

ETA0 = ETA0 + CO(J) \* TI

020 TI = TI \* T1

DENSITY DEPENDENCE IS CALCULATED HERE.

040 R1 = DO \*\* 0.10

R2 = SQRT(DO) \* (DO / CE(8) - 1.0)

ETAX = EXP(TRMO + TRM1 \* R1 + TRM2 \* R2) - TRMX

FETA = SQRT(FX \* CMXV / CMWO) / CBRT(HX \* HX)

CORV = SQRT((1.0 - TO\*PSI\*AMIN1(0.0,DFXDT))\*ZCX/ZCO)\*CORV

VSCTY = (ETA0 + ETA1 \* DO + ETAX \* CORV) \* FETA

RETURN

END

```

C      FUNCTION TCOND(DX,TX)
C      * * * * *
C      PURPOSE - - THIS ROUTINE CALCULATES THE TRANSLATIONAL PORTION
C                  OF THE METHANE THERMAL CONDUCTIVITY USING HANLEY'S
C                  CORRELATIONS
C
C      CODED BY :  J. F. ELY
C                  NATIONAL BUREAU OF STANDARDS
C                  NATIONAL ENGINEERING LABORATORY
C                  THERMOPHYSICAL PROPERTIES DIVISION
C                  BOULDER, COLORADO 80303
C
C      VERSION G2.1  7/12/80
C      * * * * *
C
C      REAL LAMO, LAM1, LAMX
C
C      COMMON /MIXDAT/ FX, DFXDT, F(20), HX, DHXDT, H(20), CMX, CMXV,
1      CMXT, ZCX, CORV, CORT
C
C      COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),
*      CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),
*      CDT(4), CET(8)
C
C      DATA TLAST, CON, PSI / -1.00, 0.19434504, 1.00 /
C
C      CALCULATE THE EQUIVALENT DENSITY
C      DO = 0.001 * DX * HX * CMWO
C      TO = TX / FX
C
C      CALCULATE THE TEMPERATURE DEPENDENT PART OF THE
C      THERMAL CONDUCTIVITY CORRELATION IF T ISN'T THE
C      SAME AS THE LAST CALL TO THIS ROUTINE (USUAL
C      CASE)
C
C      IF(TO.EQ.TLAST) GO TO 040
C      TLAST = TO
C      TI = 1.0 / TO
C      LAM1 = CDT(1) + CDT(2) * (CDT(3) - ALOG(TO / CDT(4))) ** 2
C      TRMO = CET(1) + CET(2) * TI
C      TRM1 = CET(3) + CET(4) * TI / SQRT(TO)
C      TRM2 = CET(5) + TI * (CET(6) + CET(7) * TI)
C      TRMX = EXP(TRMO)
C      T1 = CBRT(TO)
C
C      CALCULATE THE IDEAL GAS TRANSLATIONAL THERMAL
C      CONDUCTIVITY FROM THE EUCKEN FORMULA
C      K = 15 * R * ETAO / (4 * M)
C
C      LAMO = 0.0
C      DO 020 J = 1,9
C      LAMO = LAMO + CO(J) * TI
020  TI = TI * T1
C      LAMO = CON * LAMO
C
C      DENSITY DEPENDENCE IS CALCULATED HERE.

```



```

040 R1 = DO ** 0.10
    R2 = SQRT(DO) * (DO / CET(8) - 1.0)
    LAMX = EXP(TRM0 + TRM1 * R1 + TRM2 * R2) - TRMX
    FLAM = SQRT(FX * CMWO / CMXT) / CBRT(HX * HX)
    CORT = ((1.0 - TO * AMIN1(0.0, PSI*DFXDT)) * ZCO / ZCX) ** 1.5
    TCOND = (LAMO + LAM1 * DO + LAMX) * FLAM * CORT
    RETURN
    END

```

```

C * * * * *
C
C PURPOSE --- THIS ROUTINE CALCULATES THE THERMAL CONDUCTIVITY OF
C A MIXTURE FROM THE EXTENDED CORRESPONDING STATES
C MODEL
C
C CODED BY : J. F. ELY
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C NATIONAL ENGINEERING LABORATORY
C THERMOPHYSICAL PROPERTIES DIVISION
C BOULDER, COLORADO 80303
C
C VERSION G2.1 1/21/81
C * * * * *
C
C COMMON /COMPRP/ NC, ND, NAME(20,7), PC(20), DC(20), TC(20),
C * ZC(20), W(20), CMW(20), TB(20), CPC(20,7),
C * OMK(190), OML(190)
C
C COMMON /MIXDAT/ FX, DFXDT, F(20), HX, DHXDT, H(20), CMX, CMXV,
C 1 CMXT, ZCX, CORV, CORT
C
C DIMENSION TCINT(20), X(20)
C
C FINT = 1.32 * 4.184 / 10.0
C CALCULATE THE TRANSLATIONAL THERMAL
C CONDUCTIVITY OF THE MIXTURE
C TCTMIX = TCOND(DX,TX)
C SAVE THE CST RESULTS
C
C FXS = FX
C HXS = HX
C CMS = CMXV
C CALCULATE THE INTERNAL CONTRIBUTION
C
C TCIMIX = 0.0
C DO 100 J = 1, NC
C FX=F(J)
C HX=H(J)
C CMXV=CMW(J)
C CPO = CPC(J,1)
C TRM = TX
C DO 040 K = 2, 7
C CPO = CPO + TRM * CPC(J,K)
C 040 TRM = TRM * TX
C TCINT(J) = FINT * (CPO - 4.968) * VSCTY(0.0,TX) / CMW(J)
C 100 CONTINUE
C DO 120 I=1,NC
C TRM = 0.0
C DO 110 J=1,I
C TIJ = X(J) * TCINT(J) / (TCINT(I)+TCINT(J))
C TRM = TRM + TIJ

```

```
110 CONTINUE
    TCIMIX = TCIMIX + X(I) * TCINT(I) * (2.0 * TRM - TIJ)
120 CONTINUE
    FX = FXS
    HX = HXS
    CMXV = CMS
    THERMC = TCTMIX + 2.0 * TCIMIX
    RETURN
    END
```

```

      FUNCTION CBRT(X)
C * * * * *
C
C      PURPOSE --- THIS ROUTINE CALCULATES THE CUBE ROOT OF A NUMBER
C
C * * * * *
      SIGN = 1.0
      IF (X.LT.0.0) SIGN = -1.0
      CBRT = SIGN * ABS(X)**(1.0/3.0)
      RETURN
      END

```

```

SUBROUTINE LIB(N)
C * * * * *
C
C   PURPOSE --- THIS ROUTINE TAKES THE COMPONENT NUMBER "N"
C               WHOSE NAME RESIDES IN NOM(N,1-7) AND COMPARES
C               IT WITH NAMES IN THE DATABASE CONTAINED IN /LIBDAT/
C               IF A MATCH IS OBTAINED, THE APPROPRIATE LOCATIONS
C               OF THE COMMON BLOCK /COMPRP/ ARE LOADED WITH THE
C               DATA FROM THE CORRESPONDING COMPONENT IN /LIBDAT/
C
C   CODED BY : J. F. ELY
C               NATIONAL BUREAU OF STANDARDS
C               NATIONAL ENGINEERING LABORATORY
C               THERMOPHYSICAL PROPERTIES DIVISION
C               BOULDER, COLORADO 80303
C
C   VERSION G2.1 - - 8/15/80
C * * * * *
C
C   REAL NOM, CPROPS
C
C   COMMON /COMPRP/ NC, ND, NOM(20,7), P(20,14), OMK(190), OML(190)
C
C   COMMON /LIBDAT/ NLIB, NDUM, CPROPS(22,61)
C
C               READ THROUGH THE LIBRARY TO IDENTIFY
C               THE COMPONENT BY NAME OR SYNONYM.
C
C   DO 040 L = 1, NLIB
C   IF ( NOM(N,1).EQ.CPROPS(8,L) .AND. NOM(N,2).EQ.CPROPS(9,L) )
C * GO TO 030
C   DO 020 K = 1, 7
C   IF (NOM(N,K).NE.CPROPS(K,L)) GO TO 040
C020 CONTINUE
C030 K = L
C   GO TO 120
C040 CONTINUE
C               COMPONENT COULDN'T BE IDENTIFIED.
C
C   PRINT 200, (NOM(N,K),K=1,7)
C   STOP
C
C               COPY DATA FROM LIBRARY TO WORKING
C               COMMON AREA AND CALCULATE ZC
C
C120 L = 9
C   DO 130 M = 1, 14
C   IF(M.EQ.4) GO TO 130
C   L = L + 1
C   P(N,M) = CPROPS(L,K)
C130 CONTINUE
C   P(N,2) = 1000.0 / P(N,2)
C   P(N,4) = P(N,1)/(0.08205616*P(N,2)*P(N,3))
C

```

```

C          DUMMY IN THE INTERACTION CONSTANTS
C
      DO 140 L=1,N
      I=L*(L-1)/2
      DO 140 J=1,L
      K=I+J
      OMK(K)=1.0
      OML(K)=1.0
140  CONTINUE
      RETURN
C
200  FORMAT("/" /LIB/ FAILED TO IDENTIFY THE COMPONENT ",7A4)
      END

```



# BLOCK DATA LIBSET

PURPOSE --- THIS ROUTINES LOADS VARIOUS COMMON BLOCKS WITH  
DATA WHICH DOES NOT CHANGE DURING THE CALCULATIONS

THE ORDER OF THE LIBRARY DATA IS AS FOLLOWS:

XPRPXX(K)	QUANTITY
1-7	COMPONENT NAME
8-9	SYNONYM
10	PC (ATM)
11	VC (CM**3/MOL)
12	TC (KELVIN)
13	ACENTRIC FACTOR
14	MOLECULAR WEIGHT
15	T(NBP) (KELVIN)
16-22	IDEAL HEAT CAPACITY COEFFICIENTS WHERE CPO=SUM(C(J)*T**(J-1)) J=1,7

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BOULDER, COLORADO 80303

VERSION G2.1 - - 8/12/80

COMMON /REFDAT/ R, PCO, DCO, TCO, ZCO, WO, CMWO, GAMMA, A(32),  
CT(4), CP(4), CO(9), CD(4), CE(8), COT(9),  
CDT(4), CET(8)

COMMON /LIBDAT/ NLIB, NDUM, XPRP01(22), XPRP02(22), XPRP03(22),  
XPRP04(22), XPRP05(22), XPRP06(22), XPRP07(22), XPRP08(22),  
XPRP09(22), XPRP10(22), XPRP11(22), XPRP12(22), XPRP13(22),  
XPRP14(22), XPRP15(22), XPRP16(22), XPRP17(22), XPRP18(22),  
XPRP19(22), XPRP20(22), XPRP21(22), XPRP22(22), XPRP23(22),  
XPRP24(22), XPRP25(22), XPRP26(22), XPRP27(22), XPRP28(22),  
XPRP29(22), XPRP30(22), XPRP31(22), XPRP32(22), XPRP33(22),  
XPRP34(22), XPRP35(22), XPRP36(22), XPRP37(22), XPRP38(22),  
XPRP39(22), XPRP40(22), XPRP41(22), XPRP42(22), XPRP43(22),  
XPRP44(22), XPRP45(22), XPRP46(22), XPRP47(22), XPRP48(22),  
XPRP49(22), XPRP50(22), XPRP51(22), XPRP52(22), XPRP53(22),  
XPRP54(22), XPRP55(22), XPRP56(22), XPRP57(22), XPRP58(22),  
XPRP59(22), XPRP60(22), XPRP61(22)

REFERENCE FLUID FIXED POINT DATA  
AND EQUATION OF STATE CONSTANTS

DATA R, TCO, PCO, DCO, ZCO, WO, CMWO/ 0.08205616, 190.555,  
1 45.387, 10.23, 0.283742, 0.01131, 16.043 /

DATA GAMMA / 0.0096 /

DATA A/-1.184347314485E-02, 7.540377272657E-01,-1.225769717554E+01  
\*, 6.260681393432E+02,-3.490654409121E+04, 5.301046385532E-04  
\*, -2.875764479978E-01, 5.011947936427E+01,-2.821562800903E+04  
\*, -2.064957753744E-05, 1.285951844828E-02,-1.106266656726E+00  
\*, 3.060813353408E-04,-3.174982181302E-03, 5.191608004779E+00  
\*, -3.074944210271E-04, 1.071143181503E-05,-9.290851745353E-03  
\*, 1.610140169312E-04, 3.469830970789E+04,-1.370878559048E+06  
\*, 1.790105676252E+02, 1.615880743238E+06, 6.265306650288E-01  
\*, 1.820173769533E+01, 1.449888505811E-03,-3.159999123798E+01  
\*, -5.290335668451E-06, 1.694350244152E-03, 8.612049038886E-09  
\*, -2.598235689063E-06, 3.153374374912E-05/

#### SHAPE FACTOR CORRELATION CONSTANTS

DATA CT / 0.090569,-0.862762, 0.316636,-0.46568 /  
DATA CP / 0.394901,-1.023545,-0.932813,-0.754639 /

#### VISCOSITY CORRELATION CONSTANTS

DATA CO / 0.2907741307E+07,-0.3312874033E+07, 0.1608101838E+07,  
1 -0.4331904871E+06, 0.7062481330E+05,-0.7116620750E+04,  
2 0.4325174400E+03,-0.1445911210E+02, 0.2037119479E+00/

DATA CD / 1.6969859271E+00,-1.3337234608E-01, 1.4000000000E+00,  
1 1.6800000000E+02/

DATA CE /-1.0239160427E+01, 1.7422822961E+02, 1.7460545674E+01,  
1 -2.8476328289E+03, 1.3368502192E-01, 1.4207239767E+02,  
2 5.0020669720E+03, 1.6280000000E-01/

#### THERMAL CONDUCTIVITY CORRELATION CONSTANTS

DATA COT/-0.214762100E+06, 0.219046100E+06,-0.861809700E+05,  
1 0.149609900E+05,-0.473066000E+03,-0.233117800E+03,  
2 0.377843900E+02,-0.232048100E+01, 0.531176400E-01/

DATA CDT/-0.252762920E+00, 0.334328590E+00, 1.120000000E+00,  
1 0.168000000E+03/

DATA CET/-7.1977082270E+00, 8.5678222640E+01, 1.2471834689E+01,  
1 -9.8462522975E+02, 3.5946850007E-01, 6.9798412538E+01,  
2 -8.7288332851E+02, 0.1628000000E+00/

#### LIBRARY COMPONENT DATA

DATA NLIB / 61 /



C

DATA	XPRP10	/ "2,3-",	"DIME",	"THYL",	"BUTA",	"NE "
1	" " " "	"23DM",	"B "	30.861E0,	358.000E0,	
2	499.980E0,	.24700E0,	86.178E0,	331.130E0,		
3	.64690800E+01,	.82804874E-01,	.46561817E-04,	-.45005110E-07,		
4	-.38194312E-10,	-.75539658E-14,	.34978877E-16/			

C

DATA	XPRP11	/ "3-ME",	"THYL",	"PENT",	"ANE "	" "
1	" " " "	"3MP "	" "	30.831E0,	367.000E0,	
2	504.500E0,	.27300E0,	86.178E0,	336.420E0,		
3	.89448557E+01,	.91643076E-01,	-.14514763E-04,	.15734975E-07,		
4	-.29889279E-10,	-.61427879E-18,	.64139897E-17/			

C

DATA	XPRP12	/ "ISOH",	"EXAN",	"E "	" "	" "
1	" " " "	"IC6 "	" "	29.706E0,	367.000E0,	
2	497.500E0,	.27800E0,	86.178E0,	333.410E0,		
3	.71860952E+01,	.75717727E-01,	.10250425E-03,	-.16853579E-06,		
4	-.25632874E-12,	.11153552E-12,	-.48404655E-16/			

C

DATA	XPRP13	/ "N-HE",	"XANE",	" "	" "	" "
1	" " " "	"C6 "	" "	29.884E0,	373.220E0,	
2	507.889E0,	.29777E0,	86.178E0,	341.880E0,		
3	.10736446E+02,	.64479391E-01,	.87557824E-04,	-.11685574E-06,		
4	-.12019797E-11,	.53278033E-13,	-.19076817E-16/			

C

DATA	XPRP14	/ "N-HE",	"PTAN",	"E "	" "	" "
1	" " " "	"C7 "	" "	26.997E0,	431.970E0,	
2	540.140E0,	.34991E0,	100.206E0,	371.580E0,		
3	.15205618E+02,	.22270435E-01,	.36769377E-03,	-.72308061E-06,		
4	.64010192E-09,	-.27923771E-12,	.48332058E-16/			

C

DATA	XPRP15	/ "N-OC",	"TANE",	" "	" "	" "
1	" " " "	"C8 "	" "	24.650E0,	490.000E0,	
2	568.820E0,	.39953E0,	114.232E0,	398.820E0,		
3	.13014803E+02,	.92904278E-01,	.95691535E-04,	-.13010358E-06,		
4	-.18629703E-10,	.77087455E-13,	-.26357422E-16/			

C

DATA	XPRP16	/ "N-NO",	"NANE",	" "	" "	" "
1	" " " "	"C9 "	" "	22.576E0,	548.900E0,	
2	594.561E0,	.44505E0,	128.259E0,	423.970E0,		
3	.18048935E+02,	.40960429E-01,	.42543344E-03,	-.84894194E-06,		
4	.74964999E-09,	-.32490581E-12,	.55750386E-16/			

C

DATA	XPRP17	/ "N-DE",	"CANE",	" "	" "	" "
1	" " " "	"C10 "	" "	20.693E0,	607.530E0,	
2	617.550E0,	.48847E0,	142.287E0,	447.300E0,		
3	.19702209E+02,	.46038560E-01,	.47657798E-03,	-.96332701E-06,		
4	.86409089E-09,	-.38184805E-12,	.67103558E-16/			

C

DATA	XPRP18	/ "N-UN",	"DECA",	"NE "	" "	" "
1	" " " "	"C11 "	" "	19.130E0,	665.000E0,	
2	638.739E0,	.53014E0,	156.314E0,	469.080E0,		
3	.21579239E+02,	.46998191E-01,	.55034064E-03,	-.11325708E-05,		
4	.10434666E-08,	-.47541241E-12,	.86318577E-16/			

C



DATA XPRP19 / "N-DO", "DECA", "NE ", " ", " ", " ",  
 1 " ", " ", " ", "C12 ", " ", " ", 17.828E0, 719.700E0,  
 2 658.250E0, .57083E0, 170.341E0, 489.470E0,  
 3 .17638199E+02, .14817699E+00, .12419743E-03, -.19432137E-06,  
 4 -.56242230E-12, .90481892E-13, -.32622075E-16/

C

DATA XPRP20 / "N-TR", "IDEC", "ANE ", " ", " ", " ",  
 1 " ", " ", " ", "C13 ", " ", " ", 16.610E0, 775.200E0,  
 2 676.150E0, .60960E0, 184.368E0, 508.620E0,  
 3 .28380463E+02, .22925102E-08, .92216274E-03, -.19254228E-05,  
 4 .18610851E-08, -.88915064E-12, .16836658E-15/

C

DATA XPRP21 / "N-TE", "TRAD", "ECAN", "E ", " ", " ",  
 1 " ", " ", " ", "C14 ", " ", " ", 15.525E0, 827.130E0,  
 2 692.950E0, .64416E0, 198.395E0, 526.730E0,  
 3 .25255463E+02, .85908607E-01, .57805430E-03, -.11800856E-05,  
 4 .10398230E-08, -.44714033E-12, .75924416E-16/

C

DATA XPRP22 / "N-PE", "NTAD", "ECAN", "E ", " ", " ",  
 1 " ", " ", " ", "C15 ", " ", " ", 14.459E0, 880.280E0,  
 2 706.750E0, .69180E0, 212.422E0, 543.870E0,  
 3 .22693863E+02, .16252498E+00, .27955425E-03, -.53815627E-06,  
 4 .33992350E-09, -.76462529E-13, -.42904145E-20/

C

DATA XPRP23 / "N-HE", "XADE", "CANE", " ", " ", " ",  
 1 " ", " ", " ", "C16 ", " ", " ", 13.576E0, 930.230E0,  
 2 720.550E0, .73105E0, 226.449E0, 560.010E0,  
 3 .28160385E+02, .10289364E+00, .64807391E-03, -.13426743E-05,  
 4 .12019017E-08, -.52831352E-12, .92412225E-16/

C

DATA XPRP24 / "N-HE", "PTAD", "ECAN", "E ", " ", " ",  
 1 " ", " ", " ", "C17 ", " ", " ", 12.748E0, 977.000E0,  
 2 733.350E0, .76233E0, 240.476E0, 575.200E0,  
 3 .29822159E+02, .10787048E+00, .69939681E-03, -.14565206E-05,  
 4 .13141384E-08, -.58277342E-12, .10288245E-15/

C

DATA XPRP25 / "ETHE", "NE ", " ", " ", " ", " ",  
 1 " ", " ", " ", "C2- ", " ", " ", 49.700E0, 129.000E0,  
 2 282.400E0, .08500E0, 28.054E0, 169.400E0,  
 3 .68128414E+01, .17946490E-04, .75724612E-04, -.11456202E-06,  
 4 .66020561E-10, -.87280118E-14, -.28854092E-17/

C

DATA XPRP26 / "PROP", "ENE ", " ", " ", " ", " ",  
 1 " ", " ", " ", "C3- ", " ", " ", 45.408E0, 181.000E0,  
 2 364.850E0, .14400E0, 42.081E0, 225.460E0,  
 3 .79263134E+01, .35798585E-05, .14916311E-03, -.28064405E-06,  
 4 .24922234E-09, -.11089376E-12, .19695749E-16/

C

DATA XPRP27 / "2-ME", "THYL", "PROP", "ENE ", " ", " ",  
 1 " ", " ", " ", "IC3- ", " ", " ", 39.477E0, 239.000E0,  
 2 417.900E0, .19400E0, 56.108E0, 266.200E0,  
 3 .58687611E+01, .50494597E-01, .18288603E-04, -.40314673E-07,  
 4 -.52767787E-12, .20558363E-13, -.75344261E-17/

C

DATA XPRP28 / "CIS-", "2-BU", "TENE", " " " " "  
 1 " " " " "C-2C", "4- " 41.500E0, 234.000E0,  
 2 435.600E0, .20200E0, 56.108E0, 276.900E0,  
 3 .96192379E+01, .10515795E-07, .17176652E-03, -.25410206E-06,  
 4 .15268957E-09, -.33898932E-13, -.19083062E-22/

C

DATA XPRP29 / "TRAN", "S-2-", "BUTE", "NE " " " "  
 1 " " " " "T-2C", "4- " 40.500E0, 238.000E0,  
 2 428.600E0, .21400E0, 56.108E0, 274.000E0,  
 3 .88738861E+01, .14174777E-01, .16139694E-03, -.32203898E-06,  
 4 .29520414E-09, -.13642628E-12, .25449097E-16/

C

DATA XPRP30 / "1-BU", "TENE", " " " " " "  
 1 " " " " "C4- " " " 39.700E0, 240.000E0,  
 2 419.600E0, .18700E0, 56.108E0, 266.900E0,  
 3 .73262300E+01, .35010204E-01, .57559349E-04, -.74857452E-07,  
 4 .20407881E-11, .30827962E-13, -.11133542E-16/

C

DATA XPRP31 / "2-ME", "THYL", "-2-B", "UTEN", "E " "  
 1 " " " " "2M2C", "4- " 34.000E0, 318.000E0,  
 2 470.000E0, .28500E0, 70.135E0, 311.700E0,  
 3 .96201916E+01, .15760271E-01, .21993817E-03, -.42323440E-06,  
 4 .36676477E-09, -.15714517E-12, .26823430E-16/

C

DATA XPRP32 / "2-ME", "THYL", "-1-B", "UTEN", "E " "  
 1 " " " " "2M1C", "4- " 34.000E0, 318.000E0,  
 2 470.000E0, .28500E0, 70.135E0, 311.700E0,  
 3 .71484098E+01, .54705301E-01, .81847484E-04, -.17371399E-06,  
 4 .11730191E-09, -.28000072E-13, .43375310E-19/

C

DATA XPRP33 / "3-ME", "THYL", "-1-B", "UTEN", "E " "  
 1 " " " " "3M1C", "4- " 34.700E0, 300.000E0,  
 2 450.000E0, .20900E0, 70.135E0, 293.300E0,  
 3 .45379162E+01, .92181863E-01, -.31553563E-04, -.27930456E-07,  
 4 .31632638E-10, -.90871054E-14, .10619723E-20/

C

DATA XPRP34 / "CIS-", "2-PE", "NTEN", "E " " " "  
 1 " " " " "C2C5", "- " 36.000E0, 300.000E0,  
 2 476.000E0, .24000E0, 70.135E0, 310.100E0,  
 3 .10886964E+02, .18074699E-03, .26631192E-03, -.47132444E-06,  
 4 .37648896E-09, -.14593591E-12, .22066633E-16/

C

DATA XPRP35 / "TRAN", "S-2-", "PENT", "ENE " " " "  
 1 " " " " "T2C5", "- " 36.100E0, 300.000E0,  
 2 475.000E0, .23700E0, 70.135E0, 309.500E0,  
 3 .10664039E+02, .73196024E-02, .27286010E-03, -.55874988E-06,  
 4 .53005516E-09, -.25088630E-12, .47520815E-16/

C

DATA XPRP36 / "1-PE", "NTEN", "E " " " " "  
 1 " " " " "C5- " " " 40.000E0, 300.000E0,  
 2 464.700E0, .24500E0, 70.135E0, 303.100E0,  
 3 .11449557E+02, .87397409E-02, .25250466E-03, -.49521402E-06,  
 4 .44436839E-09, -.19770821E-12, .35071268E-16/

C



C

DATA	XPRP37	/ "1-HE",	"XENE",	"	"	"	"	"
1	"	"	"	"	"	"	"	"
2	504.000E0,	.28500E0,	31.300E0,	350.000E0,				
3	.12924405E+02,	.15954369E-01,	.29468316E-03,	-.59197697E-06,				
4	.54032622E-09,	-.24432103E-12,	.43999125E-16/					

C

DATA	XPRP38	/ "1-HE",	"PTEN",	"E	"	"	"	"
1	"	"	"	"	"	"	"	"
2	537.200E0,	.35800E0,	28.000E0,	440.000E0,				
3	.11443281E+02,	.75199352E-01,	.75832570E-04,	-.11000747E-06,				
4	-.18685235E-11,	.51822362E-13,	-.18519920E-16/					

C

DATA	XPRP39	/ "PROP",	"ADIE",	"NE	"	"	"	"
1	"	"	"	"	"	"	"	"
2	393.000E0,	.31300E0,	54.000E0,	162.000E0,				
3	.73395252E+01,	.25859353E-02,	.12880163E-03,	-.26785793E-06,				
4	.25164929E-09,	-.11538423E-12,	.20834873E-16/					

C

DATA	XPRP40	/ "1,3-",	"BUTA",	"DIEN",	"E	"	"	"
1	"	"	"	"	"	"	"	"
2	425.000E0,	.19500E0,	42.700E0,	221.000E0,				
3	.46207895E+01,	.48677440E-01,	.19479788E-04,	-.49883879E-07,				
4	.11138439E-12,	.28137181E-13,	-.10665350E-16/					

C

DATA	XPRP41	/ "1,2-",	"BUTA",	"DIEN",	"E	"	"	"
1	"	"	"	"	"	"	"	"
2	443.700E0,	.25500E0,	44.400E0,	219.000E0,				
3	.61028252E+01,	.46325894E-01,	-.51054392E-07,	-.16761679E-07,				
4	-.11230577E-11,	.79971874E-14,	-.24261265E-17/					

C

DATA	XPRP42	/ "CYCL",	"OPEN",	"TANE",	"	"	"	"
1	"	"	"	"	"	"	"	"
2	511.700E0,	.19600E0,	44.491E0,	260.000E0,				
3	.68700514E+01,	.42027257E-03,	.23024765E-03,	-.28467266E-06,				
4	.91958409E-10,	.34111618E-13,	-.19240855E-16/					

C

DATA	XPRP43	/ "METH",	"YLCY",	"CLOP",	"ENTA",	"NE	"	"
1	"	"	"	"	"	"	"	"
2	532.730E0,	.23100E0,	37.345E0,	319.000E0,				
3	.13644801E+02,	-.74725459E-01,	.69186318E-03,	-.13116369E-05,				
4	.12042006E-08,	-.55158466E-12,	.10065042E-15/					

C

DATA	XPRP44	/ "ETHY",	"LCYC",	"LOPE",	"NTAN",	"E	"	"
1	"	"	"	"	"	"	"	"
2	569.500E0,	.27100E0,	33.526E0,	375.000E0,				
3	.91773872E+01,	.39288596E-01,	.19385635E-03,	-.21636194E-06,				
4	.19215759E-11,	.88362908E-13,	-.31171836E-16/					

C

DATA	XPRP45	/ "CYCL",	"OHEX",	"ANE	"	"	"	"
1	"	"	"	"	"	"	"	"
2	553.500E0,	.21200E0,	40.168E0,	308.000E0,				
3	.70494375E+01,	.80017628E-04,	.33824867E-03,	-.50896443E-06,				
4	.31352284E-09,	-.77854579E-13,	.37046979E-17/					

DATA XPRP46 / "METH", "YLCY", "CLOH", "EXAN", "E", "  
 1 " " " " "MCC6", " " " 34.256E0, 368.000E0,  
 2 572.200E0, .23600E0, 98.190E0, 374.080E0,  
 3 .83217106E+01, -.11802893E-02, .47348840E-03, -.84093213E-06,  
 4 .65936050E-09, -.24415924E-12, .33736263E-16/

C

DATA XPRP47 / "ETHY", "LCYC", "LOHE", "XANE", " " "  
 1 " " " " "ECC6", " " " 29.900E0, 450.000E0,  
 2 609.000E0, .24300E0, 112.216E0, 404.900E0,  
 3 .91781473E+01, .21337048E-02, .57002378E-03, -.11023450E-05,  
 4 .97616516E-09, -.43011162E-12, .76199984E-16/

C

DATA XPRP48 / "BENZ", "ENE", " " " " "  
 1 " " " " "BNZ", " " " 48.340E0, 259.000E0,  
 2 562.160E0, .21200E0, 78.110E0, 353.240E0,  
 3 .36751518E+01, .38030224E-01, .95355250E-04, -.12393250E-06,  
 4 .77250878E-12, .56966582E-13, -.20768997E-16/

C

DATA XPRP49 / "TOLU", "ENE", " " " " "  
 1 " " " " "TOL", " " " 40.503E0, 316.000E0,  
 2 591.790E0, .26300E0, 92.140E0, 383.780E0,  
 3 .75503044E+01, .12938867E-02, .34966311E-03, -.68299765E-06,  
 4 .60172836E-09, -.25926373E-12, .44180039E-16/

C

DATA XPRP50 / "ETHY", "LBEN", "ZENE", " " " " "  
 1 " " " " "EB", " " " 35.529E0, 374.000E0,  
 2 617.200E0, .30200E0, 106.170E0, 409.340E0,  
 3 .94558764E+01, .84744814E-04, .44747164E-03, -.90994589E-06,  
 4 .83863563E-09, -.37872397E-12, .67718502E-16/

C

DATA XPRP51 / "ORTH", "O-XY", "LENE", " " " " "  
 1 " " " " "OXYL", " " " 36.812E0, 369.000E0,  
 2 630.300E0, .31000E0, 106.170E0, 417.580E0,  
 3 .81559858E+01, .36442048E-01, .27996444E-03, -.59909698E-06,  
 4 .55648350E-09, -.25352318E-12, .45943105E-16/

C

DATA XPRP52 / "META", "-XYL", "ENE", " " " " "  
 1 " " " " "MXYL", " " " 34.888E0, 376.000E0,  
 2 617.050E0, .32500E0, 106.170E0, 412.270E0,  
 3 .90353098E+01, .10930140E-01, .38364207E-03, -.78521726E-06,  
 4 .73026082E-09, -.33607092E-12, .61700011E-16/

C

DATA XPRP53 / "PARA", "-XYL", "ENE", " " " " "  
 1 " " " " "PXYL", " " " 34.651E0, 379.000E0,  
 2 616.200E0, .32100E0, 106.170E0, 411.520E0,  
 3 .95711050E+01, .78086095E-02, .38177642E-03, -.76441862E-06,  
 4 .69783379E-09, -.31544447E-12, .56916441E-16/

C

DATA XPRP54 / "HYDR", "OGEN", " " " " " "  
 1 " " " " "H2", " " " 12.760E0, 64.000E0,  
 2 32.980E0, -.21800E0, 2.020E0, 20.280E0,  
 3 .67501459E+01, .38754626E-03, .31844129E-17, -.87429101E-24,  
 4 .18934493E-12, -.95360879E-16, .10839431E-19/

C

DATA XPRP55 / "NITR", "OGEN", " " " " " "  
 1 " " " " "N2 " " " 33.457E0, 89.000E0,  
 2 126.200E0, .03900E0, 28.010E0, 77.350E0,  
 3 .69039288E+01, .10369611E-11, .58071192E-06, .11181148E-08,  
 4 -.10532056E-11, .22631708E-15, -.23281314E-26/

C

DATA XPRP56 / "OXYG", "EN " " " " " "  
 1 " " " " "O2 " " " 49.771E0, 73.000E0,  
 2 154.580E0, .02400E0, 32.000E0, 90.180E0,  
 3 .67519922E+01, .75807436E-03, .24461570E-05, -.25044950E-08,  
 4 .10016526E-11, -.18067817E-15, .12183202E-19/

C

DATA XPRP57 / "WATE", "R " " " " " "  
 1 " " " " "H2O " " " 217.617E0, 56.000E0,  
 2 647.140E0, .32900E0, 18.020E0, 373.150E0,  
 3 .78004847E+01, .36081475E-05, .38989103E-05, -.24559562E-08,  
 4 .67111619E-12, -.87348723E-16, .44003939E-20/

C

DATA XPRP58 / "CARB", "ON M", "ONOX", "IDE " " " "  
 1 " " " " "CO " " " 34.532E0, 93.000E0,  
 2 132.910E0, .05200E0, 28.010E0, 81.650E0,  
 3 .67485971E+01, .74466500E-03, .72321240E-06, -.37141838E-09,  
 4 .31753748E-14, .20581126E-16, -.25343692E-20/

C

DATA XPRP59 / "CARB", "ON D", "IOXI", "DE " " " "  
 1 " " " " "CO2 " " " 72.860E0, 94.430E0,  
 2 304.210E0, .22510E0, 44.010E0, 194.600E0,  
 3 .56366806E+01, .14155747E-01, -.99279448E-05, .38773364E-08,  
 4 -.84820125E-12, .97181323E-16, -.45337256E-20/

C

DATA XPRP60 / "SULP", "HUR " "DIOX", "IDE " " " "  
 1 " " " " "SO2 " " " 77.809E0, 122.000E0,  
 2 430.800E0, .25700E0, 64.060E0, 263.200E0,  
 3 .75942478E+01, .33130160E-02, .19711439E-04, -.35434399E-07,  
 4 .24974158E-10, -.81159935E-14, .10072061E-17/

C

DATA XPRP61 / "HYDR", "OGEN", "SUL", "PHID", "E " "  
 1 " " " " "H2S " " " 88.231E0, 98.000E0,  
 2 373.200E0, .10900E0, 34.080E0, 213.500E0,  
 3 .78297129E+01, .64258499E-10, .48952396E-05, .37981427E-09,  
 4 -.38237442E-11, .20021084E-14, -.31539707E-18/

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## 10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

## 11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

A model for the prediction of the density, viscosity and thermal conductivity of non-polar fluid mixtures over the entire range of pVT states is presented. The model is based on the extended corresponding states model and covers molecular weight ranges including C<sub>20</sub>. Only pure component equilibrium data such as the critical constants are required as input to the calculation procedure--no transport data are required. Extensive comparisons with experimental data for pure fluids and binary mixtures are presented. The average percentage deviation for both the viscosity and thermal conductivity was observed to be less than 8 percent. A computer program (TRAPP) which performs the calculations reported in this manuscript is described and listed in the Appendices.

## 12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

Computer program; density; extended corresponding states; fluid mixtures;  
thermal conductivity; viscosity.

## 13. AVAILABILITY

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