

H. J. M. HANLEY

Thermophysical Properties Division
National Engineering Laboratory
National Bureau of Standards
Boulder, Colorado 80303



PREDICTION OF TRANSPORT PROPERTIES: APPLICATION OF BASIC THEORY *

The transport prediction procedure of Ely and Hanley is discussed in this paper as an example of how theory can contribute to practical usable methods required by industry. The procedure is outlined and one particular failure of the original approach is isolated, i.e., that the procedure failed to predict correctly the viscosity of a mixture whose components differ substantially in size. A companion computer simulation molecular dynamic study is discussed, the results of which give insight into the problem of the real system. A correction based on the Enskog theory as introduced and suggested by Ely is proposed. The modified prediction procedure is shown to give excellent results.

* Publication of the National Bureau of Standards (U.S.), not subject to copyright.

This paper is an edited version of the lecture delivered at the Symposium on Transport Properties of Fluids, Lisbon (23-26 March 1982).

1 — INTRODUCTION

In this paper we discuss a procedure to predict the viscosity and thermal conductivity of pure fluids and mixtures. The results, some of which have been published previously [1-3], will be reviewed but our principal aim is to outline the procedure in a particular context; namely as an illustration of the role theory plays to develop a practical predictive method for thermophysical properties required by industry. From the larger viewpoint this is one example of the conflict between theory on the one hand and practical utility on the other.

On a positive note, there is no doubt that very real opportunities exist to combine basic science with realistic innovative engineering practice. Industry sets challenges which theory and experiment will have to meet and which sharpen the focus of current research. In turn, the results of a basic theoretical study, or from a controlled experiment, can suggest a possible industrial application.

As a slight digression, we remark that as much as 80% of the capital and annual operating costs in the major fluid industries — fuel, chemical and energy — come from separation and the processing of feedstocks. These industries are concerned with the conservation and productivity of their technology and with developing methods to handle new feedstocks. Moreover, the operating conditions will often be extreme: high temperatures, high pressures; the fluid could be near melting or freezing or a critical or consolute point, and so on. In short; theory is needed to understand fluid behavior; prediction procedures are needed to estimate the thermophysical properties (and we emphasize prediction as opposed to correlation) because naturally one cannot have data for all possible systems of interest; and of course a data base has to be established. A study of transport phenomena fits into the above scheme. We need a prediction procedure to estimate the viscosity and thermal conductivity of pure fluids and mixtures over a wide range of experimental conditions, and there are interesting and still unresolved problems associated with fluid nonequilibrium behavior in general. The problems range from the most fundamental such as questions on the definition of a system in nonequilibrium or on the form of the Hamiltonian, to the practical understanding and description of flow, multiphase flow, mixing and separation.

The approach we follow at the National Bureau of Standards is biased to the fact that common characteristics describe new feedstocks: most often they are defined mixtures whose species are substantially different (i.e., in size, polarity or chemical nature) or undefined mixtures such as coal liquid fractions, heavy oils or tars. Accordingly, experiments are made with a system which is simple yet represents a class which is relevant, *e.g.*, a mixture such as carbon dioxide and butane is relatively straightforward and accessible to a theoretical and experimental study, yet is a prototype of mixtures which are characterized by containing one species which is both small and of a different chemical nature than the others. Fig. 1 gives another example: it shows a

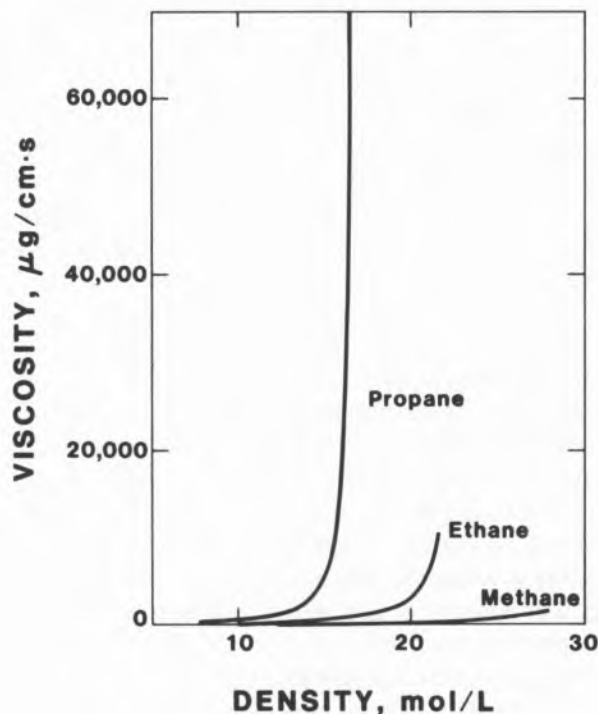


Fig. 1

Plot of the viscosity of methane, ethane and propane versus density

plot of the viscosity of methane, ethane and propane *versus* density. Note that the behavior of propane is quantitatively quite different from the other compounds. In fact the viscosity at high densities approaches that of a very heavy hydrocarbon such as C_{20} . The point to be made is that a theoretical and experimental investigation of propane — which is of interest in itself — will give an insight into the behavior of hydrocarbons such as C_{20} and can be

undertaken with relatively simple theoretical and experimental tools.

No claim is made as to the originality of this plan, but the concept has perhaps not been followed as it might because of the gap between fluid theory and practice, and to a lack of high quality data. But one can argue that the situation has improved. The computer has had a tremendous impact; one can study a fluid via computer simulation, which allows theories to be tested unambiguously and suggests lines for future research; and, of course, the computer has played a major role in data correlation, in numerical integration and differentiation, and as general mathematical tool. On the experimental side, sophisticated electronics are commonplace in measurement, control and data reduction. Laser light scattering, with neutron and X-ray scattering, have led to significant advances in our knowledge of fluid structure and in the measurement of fluid properties.

The organization of this paper is as follows. We outline the procedure which is based on the one-fluid conformal solution concept. A well-defined failure is commented on but we emphasize how a companion computer simulation study with a model mixture gives an insight for systematic improvement. A modification of the procedure is proposed. Finally, tables illustrating how the procedure predicts data are given and we emphasize that a computer package [TRAPP] is available.

2 — ONE-FLUID MODEL

The basis of this report is the technique proposed recently by ELY and HANLEY [1-3] and follows the earlier work of HANLEY [4] and MO and GUBBINS [5] which introduced the one-fluid equilibrium extended corresponding states arguments of LELAND [6] and others to transport phenomena. The basic idea is straightforward, that the configurational properties of a 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.

Since the expressions have been presented and discussed in detail in references [1-3], we only give an outline here. Also we will only discuss the viscosity (η) in any detail; similar equations can be written down for the thermal conductivity (λ).

Table 1

Summary of Viscosity and Thermal Conductivity Predictions for Pure Fluids Compared with Experiment (data sources in references [1-3]) N = Number of points, AAD = Average absolute percent deviations, BIAS = Average percent deviation

Fluid type	Viscosity			Thermal conductivity		
	N	AAD	BIAS	N	AAD	BIAS
<i>n</i> -Paraffins	1301	4.89	- 0.48	721	4.44	0.03
<i>i</i> -Paraffins	155	21.17	-21.17	31	3.44	-1.16
Alkenes	58	11.29	7.85	251	5.77	-7.32
Cycloalkanes	89	40.56	-40.56	21	3.23	2.18
Alkylbenzenes	155	8.45	- 0.69	209	6.62	3.92
Carbon Dioxide	111	4.75	- 4.53	22	6.67	6.67
Overall	1869	8.42	- 4.10	1255	5.06	-0.67

Table 2

Summary of Calculated and Experimental Dense Fluid Binary Mixture Viscosities (see caption to Table 1)

Component 1	Component 2	N	AAD	BIAS
Methane	Propane	134	4.62	- 3.45
	<i>n</i> -Nonane	32	4.12	- 2.61
	<i>n</i> -Decane	71	5.35	- 1.54
2,3-Dimethylbutane	<i>n</i> -Hexane	2	5.31	- 5.31
	<i>n</i> -Octane	2	5.65	- 5.65
<i>n</i> -Hexane	<i>n</i> -Tetradecane	10	1.92	0.54
	<i>n</i> -Hexadecane	26	2.59	- 1.97
<i>n</i> -Heptane	<i>n</i> -Dodecane	3	3.44	3.44
	<i>n</i> -Tetradecane	3	1.82	1.51
	<i>n</i> -Hexadecane	3	2.52	- 1.32
<i>n</i> -Octane	<i>n</i> -Octadecane	2	1.92	- 0.71
	<i>n</i> -Decane	2	3.27	3.27
	<i>n</i> -Hexadecane	11	2.32	2.10
<i>n</i> -Tetradecane	<i>n</i> -Hexane	15	5.74	- 2.28
	<i>n</i> -Heptane	3	5.85	5.85
	2,2,4-Trimethylpentane	26	12.46	-12.46
Benzene	<i>n</i> -Decane	3	5.47	3.46
	<i>n</i> -Dodecane	3	6.47	6.47
	<i>n</i> -Tetradecane	3	3.63	2.55
	<i>n</i> -Hexadecane	3	3.76	1.46
	<i>n</i> -Octadecane	3	2.73	1.97
	<i>n</i> -Heptane	21	5.32	5.32
	<i>n</i> -Octane	20	9.50	9.50
	2,2,4-Trimethylpentane	28	6.62	- 4.37
Overall		429	5.31	- 1.86

Consider the viscosity of a mixture η_{mix} at a density, ρ , temperature, T , and composition $\{x_\alpha\}$ where x_α is the mole fraction of species α with $\alpha = 1, 2, \dots, n$ for an n -component mixture. We assume $\eta_{\text{mix}}(\rho, T, \{x_\alpha\}) \equiv \eta_x(\rho, T)$ where η_x is the viscosity of the hypothetical pure fluid characterized by mole fraction set x . If a reference fluid is denoted

by subscript o we have

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

where

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

Table 3
Summary of Calculated Results for Binary Mixture Thermal Conductivity (see caption to Table 1)

Component 1	Component 2	N	AAD	BIAS
Methane	<i>n</i> -butane	15	12.20	12.09
2,3-dimethylbutane	2,2,4-trimethylpentane	6	4.70	4.70
<i>n</i> -hexane	<i>n</i> -octane	14	6.17	— 6.17
<i>n</i> -heptane	<i>n</i> -octane	6	2.01	— 2.01
	2,2,4-trimethylpentane	6	1.96	1.81
	<i>n</i> -decane	6	8.99	— 8.99
	<i>n</i> -hexadecane	2	3.44	— 3.44
<i>n</i> -octane	2,2,4-trimethylpentane	9	4.97	— 4.97
	<i>n</i> -heptadecane	6	4.77	— 4.66
2,2,4-trimethylpentane	2,2,5-trimethylpentane	6	4.71	— 4.71
	<i>n</i> -tetradecane	6	5.06	— 5.06
1-hexene	<i>n</i> -heptane	279	8.11	— 8.09
	<i>n</i> -octane	279	8.84	— 8.83
Benzene	<i>n</i> -heptane	8	3.55	— 3.39
	Toluene	32	6.15	6.15
	Cyclohexane	4	4.42	4.42
Toluene	<i>n</i> -heptane	5	6.29	6.29
	2,2,4-trimethylpentane	6	10.78	10.78
	<i>o</i> -xylene	6	15.71	15.71
<i>o</i> -xylene	2,2,4-trimethylpentane	6	11.51	11.51
Cyclopentane	<i>n</i> -heptane	6	0.66	0.16
	Methylcyclohexane	6	5.20	5.20
Cyclohexane	Toluene	4	4.12	4.12
Methylcyclohexane	2,2,4-trimethylpentane	6	11.72	—11.72
Overall		167	6.83	1.42

with M the molecular weight and T_o and q_o defined by ratios

$$T_o = T/f_{x,o}; \quad q_o = qh_{x,o} \quad (3)$$

where $f_{x,o}$, $h_{x,o}$ are defined by the mixing rule expressions

$$f_{x,o} = h_{x,o}^{-1} \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} f_{\alpha\beta,o} h_{\alpha\beta,o} \quad (4)$$

$$h_{x,o} = \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} h_{\alpha\beta} \quad (5)$$

with

$$f_{\alpha\beta,o} = (f_{\alpha,o} f_{\beta,o})^{1/2} (1 - k_{\alpha\beta}) \quad (6)$$

$$h_{\alpha\beta,o} = \frac{1}{8} (h_{\alpha,o}^{1/3} + h_{\beta,o}^{1/3})^3 (1 - \ell_{\alpha\beta}) \quad (7)$$

in which $k_{\alpha\beta}$ and $\ell_{\alpha\beta}$ are the usual correction binary interaction coefficients. The mass mixing rule is discussed in reference [10] and can be written as

$$h_{x,o}^{4/3} \sqrt{f_{x,o} M_x} = \sum_{\alpha} \sum_{\beta} x_{\alpha} x_{\beta} h_{\alpha\beta,o}^{4/3} \sqrt{f_{\alpha\beta,o} M_{\alpha\beta}}$$

where $M_{\alpha\beta} = 2M_{\alpha}M_{\beta}/(M_{\alpha} + M_{\beta})$.

Finally we have

$$f_{\alpha,o} = (T_{\alpha}^c/T_o^c) \theta(T^*, V^*, \omega) \quad (8)$$

$$h_{\alpha,o} = (V_{\alpha}^c/V_o^c) \Phi(T^*, V^*, \omega) \quad (9)$$

where superscript c refers to the critical point value and θ and ϕ are shape factors which are functions of the Pitzer acentric factor ω and of reduced (asterisks) temperature and volume (or density, $V = 1/\rho$). We refer to reference [1] for their functional form.

The key point of the extended corresponding states approach is that the format of classical corresponding states is followed. Should the solution be conformal [i.e., that all intermolecular interactions follow the same force law and $\omega_{\alpha} = \omega_o$ (and strictly that $\omega_o = 0$) and that the critical compressibility

factor becomes a universal constant) the ratios (5) and are simply the ratios of the critical constants and equations (4) and (5) are the "Van der Waals one" mixing rules.

Summary of the calculation procedure: A summary of the calculation procedure to evaluate the viscosity from equation (1) is as follows. We have a single phase mixture (or a pure) at a given temperature, pressure and mole fraction. Required as input parameters are the critical temperature, critical pressure, critical volume, acentric factor and molecular weight of each mixture component. We are given an equation of state and functional form for the viscosity of the reference substance. Note the method is thus predictive in that transport data for the mixture or its components are not needed. We also do not require the mixture to be in any particular phase or limit the number of components.

The first step is to evaluate the density. To do this the equivalent pressure (p_o) of the reference substance is evaluated via the ratio $p_o = p_x h_{x,o}/f_{x,o}$. Initially the shape factors of equations (8) and (9) are set to unity. Given $p_o = p(\rho_o, T_o)$, the density ρ_o follows and hence ρ_x is obtained from equation (3). Repeated iterations give a final density $f_{x,o}$ and $h_{x,o}$ and T_o and ρ_o . Hence the viscosity follows from equation (1).

Methane is used as the reference fluid in our work: the equation of state is the BENEDICT-WEBB-RUBIN of reference [7] and the viscosity and thermal conductivity equations are based on the correlation of reference [8]. Further details are given in reference [1].

3 — COMPUTER SIMULATIONS OF FLUIDS UNDER SHEAR: EVALUATION OF THE PROCEDURE

The transport procedure is generally very successful for nonpolar fluids and mixtures and some deviation tables will be given in section 5. There are some failures which were anticipated, *e.g.*, for polar molecules and molecules with pronounced structure such as very branched hydrocarbons. However, others occurred whose origin was not so obvious. In particular, the method did not predict too well the viscosity of mixtures whose species differ substantially in size and/or mass. The methane/decane mixture is an example. Fig. 2 shows the percent deviations for three mixtures and there is clearly

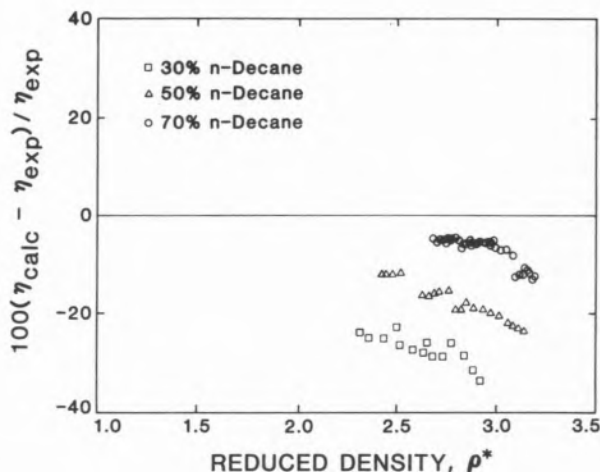


Fig. 2

Deviations between results calculated from equation (1) and experiment for methane/decane mixtures. Data sources listed in reference [13]

a systematic discrepancy at high densities. We stress, however, that this mixture is quite unusual as seen by fig. 3 which gives a plot of the viscosity

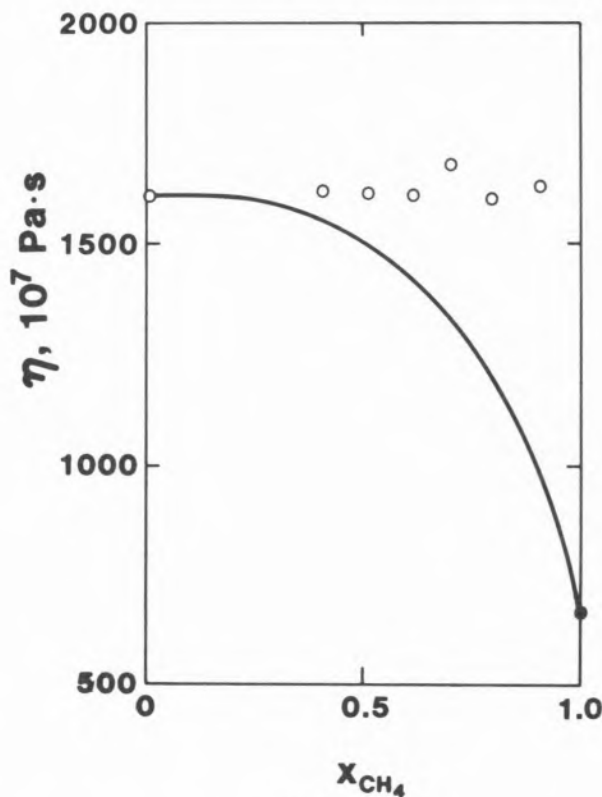


Fig. 3

Plot of the viscosity of a methane/decane mixture at 440 K at a constant density of 2.5 g/cm³. The points are data, the curve is calculated using equation (1)

at the sample temperature of 440 K *versus* methane mole fraction at a *constant density* of about 2 1/2 times critical. The points are data, the curve is the prediction procedure. Note that the mixture viscosity is constant until $x(\text{CH}_4)$ is about 0.9.

Results such as those of fig. 2 suggested that a systematic evaluation of transport properties in mixtures in general, and of the assumptions of our predictive method in particular would be productive. It turned out that this goal dovetailed with an investigation of the nonequilibrium behavior of fluids using the computer simulation technique of nonequilibrium molecular dynamics carried out by EVANS [9], EVANS and HANLEY [10-11] and by HESS and HANLEY [12].

We will outline the simulation method but refer to reference [11] for details. A model system — that is, a system whose particles have a known size, shape and force law — is examined in equilibrium by conventional molecular dynamics. The system is then subjected to an external shear force by constraining the periodic boundaries. Results from this technique are very rich. Of interest here, we can evaluate the pressure tensor and the radial distribution function $g(r)$. Under shear this latter quantity reflects directly the distortion of the microstructure of the system and can be written in the form

$$g(r) = g^s(r) + \sum v_k f_k(r) \quad (10)$$

where g^s is the scalar contribution and v_k are expansion coefficients coupled with functions of r , the vector separation between molecular pairs. The scalar g^s would be the equilibrium radial distribution in equilibrium (g_o^s), the first coefficient v_1 is related to the potential contribution to the shear viscosity and the higher order coefficients are associated with other transport coefficients representing differences in the normal pressure.

The expansion (10) is powerful in that it depicts the microscopic distortion of the structure of a fluid in nonequilibrium and is especially useful in a study of mixtures because one can identify the contributions of a mixture species in the mixture. For the viscosity, for example, we have

$$\eta_{\text{mix}} = \sum x_i x_j \eta(ij) \quad (11)$$

where

$$\eta(ij) = -\frac{2}{15} \pi \rho^2 \int v_1(ij) \phi'(ij) r^3 dr \quad (12)$$

with $v_1(ij)$ the coefficient from equation (10) and $\phi'(ij)$ the derivative of the pair potential for the i - j pair. Note that $\eta(ii)$ is *not* the viscosity of a pure but of species i in the presence of species j .

Simulation of a mixture of soft spheres: In reference [11] we decided to approximate a real binary equimolar mixture of decane and methane by a model mixture of soft spheres of different size and mass. No apologies were made for the obvious gross simplification because it turned out that the behavior of the model seems to represent the real liquid very closely.

The model mixture was characterized by soft spheres with the potentials

$$\phi_{11} = d/r^{12}, \phi_{12} = d/r^{12}, \phi_{22} = 1296 d/r^{12} \quad (13)$$

with species 1 representing the smaller lighter methane and species 2 representing decane. The factor 1296 arises from the ratio $V^c(\text{decane})/V^c(\text{methane}) \approx 6$. Species 2 was given a mass ten times that of species 1. It should be stressed that equation (13) indicates that classical two parameter corresponding states is obeyed for all potential interactions.

The mixture was studied at a reduced state point (density) of $\rho = 0.2667$: this state point corresponds to a pure fluid at a reduced equivalent density of 0.6, which is about three-quarters of the melting density, for an equivalent pure liquid.

We show two results here: (1) the variation of the distribution functions g_o^s and v_1 ; (2) an evaluation of the local or ambient mole fractions x_{ij} as a function of partial separation r where $x_1 = x_2 = 0.5$ in the limit of $r \rightarrow \infty$:

$$x_{ij} = n_{ij}/(n_{ij} + n_{jj}) \quad (14)$$

where n_{ij} is the number of particles of species j around a central particle i , all for a given r .

(1) *Variation of the distribution Functions.* Fig. 4 displays g_o^s and v_1 for a pure fluid at $\rho = 0.6$ *versus* reduced $r[r/d(ij)]$, equation (13)] while fig. 5 shows g and v , scaled approximately, for the i - j contributions of the mixture at an equivalent state point. The basic assumption of

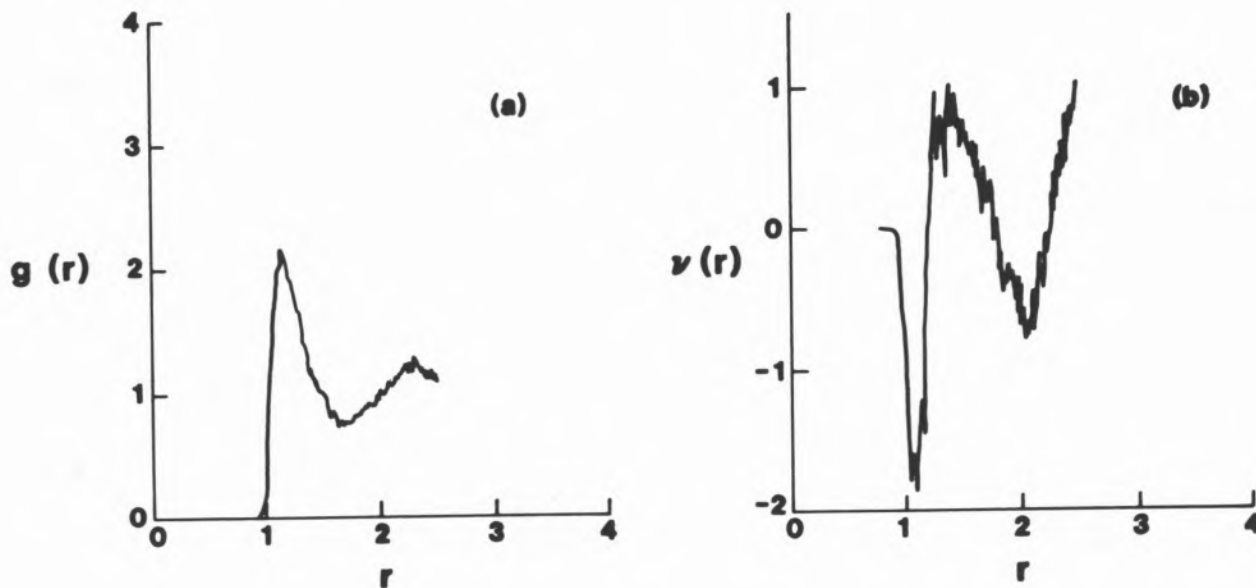


Fig. 4

Plots of $g_o^s(r)$ and $v(r)$ for a pure soft sphere liquid at $\rho = 0.6$

a conformal one fluid model is that the g_{ij} and v_{ij} scale with one another and with a pure. Thus all plots of g should show the same structure, as should the plots of v . This is not the case for this mixture in which it is seen from the figures that the larger species 2 dominates the g_o^s (and also v although it not quite so obvious).

Using these model results as a guide to the behavior of the real fluid, one would thus expect that our transport procedure will fail if the species of a real mixture are substantially different in size and/or mass, as is the case of methane/decane.

(2) *Local or Ambient Mole Fraction.* An alternative way to analyse the variation of $g(r)$ is to consider the local mole fraction of equation (14) since

$$n_{ij}(R) = 4\pi \frac{\rho}{2} \int_0^R r^2 g_{ij}(r) dr \quad (15)$$

Hence given $g_{ij}(r)$, as in fig. 5, we calculate x_{ij} from equation (14), using (15). The results for x_{11} and x_{22} are shown in fig. 6. Although $x_1 = x_2 = 0.5$ overall, the results indicate that $x_{22} \approx 0.85$ and $x_{11} \approx 0.35$ for $r \leq 2.0$.

Since, moreover, the macroscopic properties of a system are largely controlled by intermolecular forces over short r only, effectively we do not have an equimolar mixture at all; rather the mixture is behaving approximately as pure species 2. This line of reasoning gives a facile answer to the apparently

anomalous plot of fig. 3 for the real system. Even though the mole fraction of methane varies, the local or effective mole fraction of decane is close to one until $x(\text{methane}) \approx 0.9$.

4 — SYSTEMATIC CORRECTION TO THE PROCEDURE: ELY'S APPLICATION OF THE ENSKOG THEORY

In this next section we follow the philosophy of the introduction and suggest a correction to the transport procedure based on theory. The flavor is as follows: the computer simulations suggest that size and mass differences are of paramount importance to the properties of a mixture. but such differences are essentially structure or ordering effects and it is known that the structure of a fluid is not too dependent on the details of the pair potentials of the molecules. Consequently, one would hope that a correction to the transport procedure could be based on as simple a model as possible but yet apply to the real system. This idea was suggested by HANLEY in 1976 [4] and considerably expanded and reformulated by ELY recently [13]. The correction introduces the hard sphere ENSKOG model [14] which, although not exact, is a well known systematic transport theory whose assumptions can be justified quantitatively.

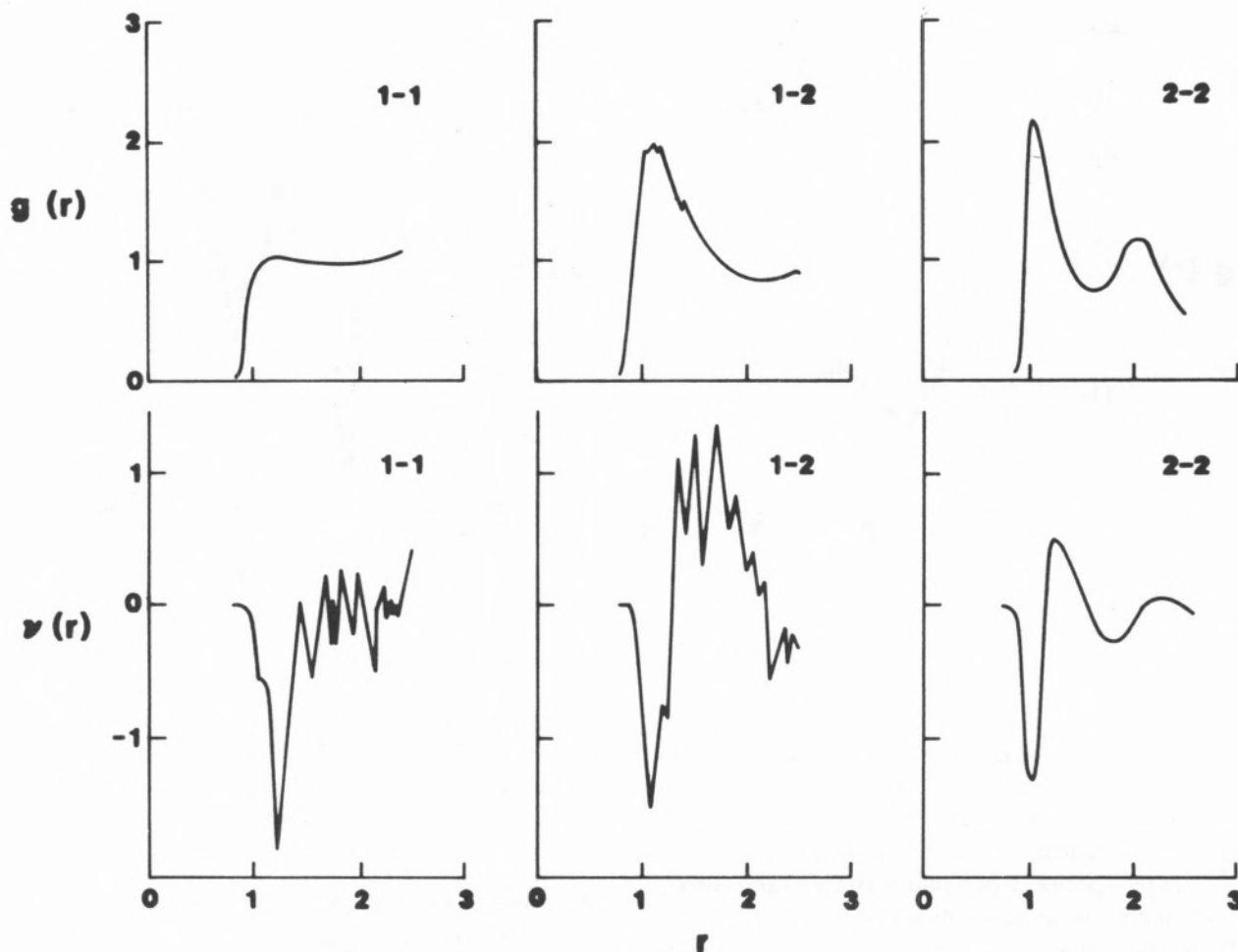


Fig. 5

Plots of $g_{ij}^S(r)$ and $v(r)$ for a mixture of soft spheres for which one species (2) is approximately twice as large and ten times as heavy as species 1. The state point for the mixture is equivalent to a pure at $\rho = 0.6$. Note (a) differences between the plots of fig. 4 and 5 and, (b) that the curves for the i - j interactions do not scale

Let us write

$$\eta_{\text{mix}}^E(\{\rho\sigma_\alpha^3\}, \{x_\alpha\}, \{m_\alpha\}) = \eta_x^E(\rho\sigma_\alpha^3, m_x) + \Delta\eta^E \quad (16)$$

where η_{mix}^E is the exact Enskog viscosity of a mixture of hard spheres each of diameter σ_α and mass m_α for a given density and mole fraction set. The properties of this mixture can be evaluated, but we will not write down the expressions [13,15]. The hypothetical pure η_x^E can also be evaluated given the standard Enskog equation

$$\eta^E = \eta^{\text{HS}}(\rho)b\rho \left[\frac{1}{b\rho\chi} + 0.8 + 0.761 b\rho\chi \right] \quad (17)$$

where

$$\frac{p}{\rho kT} = 1 + b\rho\chi \quad (18)$$

where $b = 2\pi\sigma_\alpha^3/3$ and $\chi = 1 + 0.625b\rho + \dots$ and $\eta^E(o)$ is the dilute gas hard sphere viscosity. We chose mixing a rule for σ_α :

$$\sigma_x^3 = \sum_\alpha \sum_\beta x_\alpha x_\beta \sigma_{\alpha\beta}^3 \quad (19)$$

with

$$\sigma_{\alpha\beta} = \frac{1}{2} [\sigma_\alpha + \sigma_\beta] \quad (20)$$

where σ_α is to be evaluated via equation (18) of reference [13]. The mass mixing rule is

$$\sigma_x^4 \sqrt{m_x} = \sum_\alpha \sum_\beta x_\alpha x_\beta \sigma_{\alpha\beta}^4 \sqrt{m_{\alpha\beta}} \quad (21)$$

where $m_{\alpha\beta} = 2m_\alpha m_\beta / (m_\alpha + m_\beta)$ as before.

We thus can obtain $\Delta\eta^E$ as a function of density and mole fraction for given ratios of $\sigma_\alpha/\sigma_\beta$ and

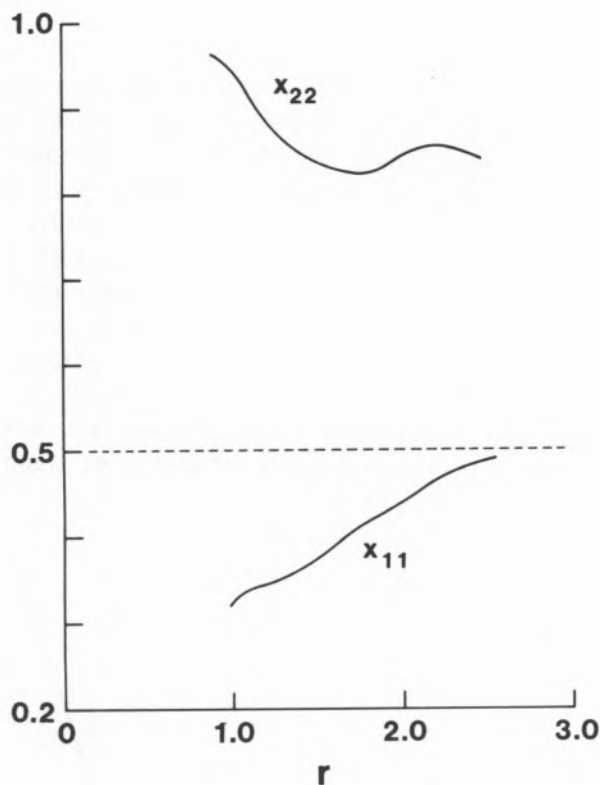


Fig. 6

Plot of the local mole fractions x_{22} and x_{11} defined by equation (14) using the g_o^s values of fig. 5 for the soft sphere mixture. Although the mixture is equimolar, i.e., $x_{22} \rightarrow x_2 = 0.5$ and $x_{11} \rightarrow x_1 = 0.5$ for $r \rightarrow \infty$, it behaves as a mixture in which $x \approx 0.9$

m_α/m_β . And, as remarked, we then assume that $\Delta\eta^E$ is independent of the nature of the mixture, so the original equation (1) becomes

$$\eta_{\text{mix}} = \eta_o(\rho_o, T_o) F_\eta + \Delta\eta^E \quad (22)$$

Equation (22) is now the basic equation for the viscosity procedure and as a first test we predict the viscosity of the methane/decane mixture shown before in fig. 3. The new result using equation (22) is presented as fig. 7 and one sees the substantial improvement.

5 — RESULTS

Detailed results are presented in references [1-3] and in reference [13]. Here we give three tables which summarize them. The computer program which generates the data is known as TRAPP and is available from the Gas Processors Association, 1812 First Place, Tulsa, Oklahoma 74103, USA.

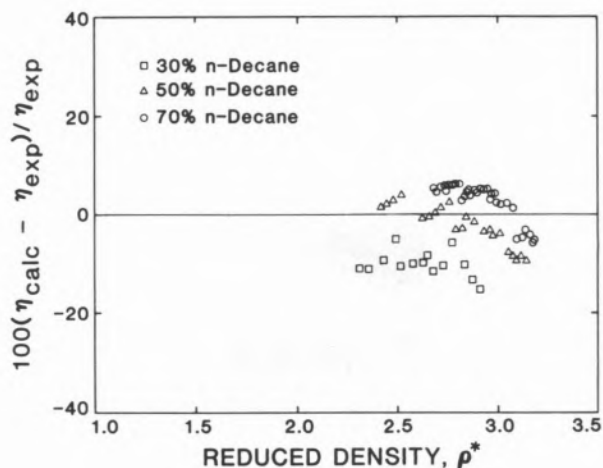


Fig. 7

Deviations between the methane/decane data and the revised equation (22): compare with fig. 2

ACKNOWLEDGEMENTS

We are grateful for discussions with Dr. Ely who provided much material prior to publication. The work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Contract No. DE-A101-76PRO6010 with computer money supplied by the Gas Research Institute.

REFERENCES

- [1] J.F. ELY, H.J.M. HANLEY, *Ind. Eng. Chem. Fund.* **20**, 323 (1981).
- [2] J.F. ELY, H.J.M. HANLEY, *Nat. Bur. Stand. (U.S.)*, Technical Note, No. 1039 (1981).
- [3] J.F. ELY, H.J.M. HANLEY, *Ind. Eng. Chem. Fund.* (in press). [Added in proof: **22**, 90 (1983)].
- [4] H.J.M. HANLEY, *Cryogenics* **16**, 643 (1976).
- [5] K.C. MO, K.E. GUBBINS, *Mol. Phys.* **31**, 825 (1976).
- [6] J.W. LEACH, P.S. CHAPPELEAR, T.W. LELAND, *A.I.Ch.E. J.* **14**, 568 (1968).
- [7] R.D. McCARTY, *Cryogenics* **14**, 276 (1974).
- [8] H.J.M. HANLEY, R.D. McCARTY, W.M. HAYNES, *J. Phys. Chem. Ref. Data* **3**, 979 (1974).
- [9] D.J. EVANS, *J. Stat. Phys.* **20**, 547 (1979).
- [10] D.J. EVANS, H.J.M. HANLEY, *Phys. Rev.* **20A**, 1648 (1979).
- [11] H.J.M. HANLEY, D.J. EVANS, *Int. J. Thermophysics* **2**, 1 (1981).
- [12] S. HESS, H.J.M. HANLEY, *Phys. Rev.* **25A**, 1801 (1982).
- [13] J.F. ELY, *J. Res. Nat. Bur. Stand. (U.S.)*, **86**, 597 (1981).
- [14] H.J.M. HANLEY, R.D. McCARTY, E.G.D. COHEN, *Physica* **60**, 322 (1972).
- [15] M.K. THAM, K.E. GUBBINS, *J. Chem. Phys.* **55**, 268 (1971).

KEY WORDS:

Conformal solution theory; corresponding states; data prediction; Enskog theory; mixtures; non-equilibrium; viscosity.