J. Chem. Eng. Data **2009,** *54,* 2527–2531 **2527**

Correlation and Prediction of the Viscosity and Thermal Conductivity of Dense Fluids[†]

Tongfan Sun and Amyn S. Teja*

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0100

A method based on the rough-hard-sphere theory has been extended to the calculation of the viscosity and thermal conductivity of a wide range of compounds including alkanes, 1-alkanols, alkanediols, benzene, toluene, and 11 refrigerants. The method is simple to use and is capable of fitting data within experimental error. Generalized forms of the parameters for homologous series of alkanes, 1-alkanols, alkanediols, and halogentated methanes are presented. The extrapolation capability of the method was evaluated by predicting the viscosities of the higher alkanes and alkanols using parameters obtained from the properties of lower members of the homologous series.

Introduction

Accurate values of liquid viscosity and thermal conductivity are essential for the design of processing equipment. Such values also provide fundamental information on intermolecular forces in liquids. Consequently, many measurements of transport properties have been reported in the literature, although it is unlikely that these measurements include all systems at all conditions of interest. There is therefore a continuing need for reliable methods of prediction of transport properties for process design. Group contribution methods for predicting transport properties (such as those reported in Poling et al.,[1] Przezdziecki and Sridhar,[2] Sastri and Rao,[3] Dutt and Venugopal,[4] and Dutt et al.[5]) have proved to be convenient and useful for many classes of fluids. However, they are not accurate for all fluids, and they cannot generally be used over wide ranges of conditions.[1]

One method that has proved reliable for dense fluid transport properties is that proposed by Assael, Dymond, and co-workers.[6−9] These workers have developed a model based on the rough-hard-sphere theory that is able to correlate viscosity, thermal conductivity, and self-diffusion coefficients of many systems, including *n*-alkanes,[6] 1-alkanols,[7] aromatic hydrocarbons,[8] and refrigerants.[9] However, the predictive capabilities of the method are limited. For example, it has been noted[7] that the viscosity correlation for 1-alkanols (obtained by fitting data for alkanols from methanol to 1-decanol) cannot be extrapolated to 1-dodecanol because negative values of the coupling parameter are obtained in this case. This limits the use of this method to cases where transport property data are available.

In our previous work, we have proposed a modified rough-hard-sphere method to calculate fluid viscosity and thermal conductivity of refrigerants[10] and polar liquids[11] over extended ranges of temperature and pressure. We have shown that our method is simple to use and yields results that are comparable to the Assael et al. method for refrigerants.[10] In the present work, we report further generalizations of our method for dense fluids containing aromatic hydrocarbons, refrigerants, and four homologous series of alkanes, 1-alkanols, halogenated methanes, and alkanediols. In particular, we have investigated the predictive capabilities of the method by calculating transport properties of compounds not used in the correlations. Finally, we present generalizations of the parameters of the method to homologous series of alkanes, 1-alkanols, halogenated methanes, and alkanediols.

Modified Rough-Hard-Sphere Method

The rough-hard-sphere concept was originally proposed by Chandler[12] and extended by Assael and co-workers,[6−9] who expressed the reduced viscosity η^* and thermal conductivity λ^* of fluids as universal functions of the reduced molar volume V_r as follows

$$\log(\eta^*/R_\eta) = 1.0945 - 9.26324V_r^{-1} + 71.0385V_r^{-2} - 301.9012V_r^{-3} + 797.69V_r^{-4} - 1221.977V_r^{-5} + 987.5574V_r^{-6} - 319.4636V_r^{-7} \quad (1)$$

$$\log(\lambda^*/R_\lambda) = 1.0655 - 3.538V_r^{-1} + 12.120V_r^{-2} - 12.469V_r^{-3} + 4.562V_r^{-4} \quad (2)$$

In eqs 1 and 2, R_η and R_λ are parameters that account for deviations of the transport properties of the fluid from those of smooth hard spheres. The parameters reflect the degree of coupling between translational and rotational motions of molecules such that their numerical values are close to unity for nearly spherical molecules and become increasingly different from unity as the molecules become more nonspherical. In practice, however, R_η and R_λ are used to empirically account for deviations from the behavior of smooth hard spheres.

The reduced viscosity, reduced thermal conductivity, and reduced volume are defined as follows

$$\eta^* = 6.035\cdot 10^8(MRT)^{-0.5}\eta V^{2/3} \quad (3)$$

$$\lambda^* = 1.936\cdot 10^7(M/RT)^{0.5}\lambda V^{2/3} \quad (4)$$

$$V_r = V/V_0 \quad (5)$$

where M is the molar mass, R the gas constant, T the temperature,

---

* Corresponding author. E-mail address: amyn.teja@chbe.gatech.edu.

[†] Part of the "William A. Wakeham Festschrift".

10.1021/je900096n CCC: $40.75

Table 1. Comparison of Two Rough-Hard-Sphere Methods for Calculating Viscosities of Refrigerants and Aromatic Liquids[a]

			$10^5\ D_0$	$10^3\ D_1$	this work		Assael method	
system	# data	T/K	$m^3\cdot mol^{-1}$	$m^3\cdot kmol^{-1}$	AAD	MAD	AAD	MAD
R11 ($CFCl_3$)	45	273 to 353	3.7863	0.10426	0.60	1.9	0.90	2.1
R12 (CF_2Cl_2)	44	273 to 343	2.9175	0.10316	1.94	11.9	1.75	5.1
R22 ($CF_2Cl\ H$)	49	273 to 333	2.2104	0.07448	0.91	7.1	1.07	6.7
R32 (CF_2H_2)	56	231 to 323	1.2932	0.06063	1.09	2.5	2.76	15.6
R124 ($C_2F_4Cl\ H$)	163	160 to 370	3.6093	0.11219	3.23	12.1	4.23	41.8
R125 (C_2F_5H)	133	176 to 315	3.2778	0.08435	1.44	10.3	2.49	14.4
R134a ($C_2F_4H_2$)	200	175 to 343	2.9267	0.08613	3.14	17.2	2.86	17.0
R141b ($C_2FCl_2H_3$)	89	190 to 353	3.0851	0.15504	1.87	8.9	1.92	7.4
R152a ($C_2F_2H_4$)	73	243 to 353	1.4490	0.12964	1.24	7.1	1.18	5.0
average					1.72		2.13	
benzene	83	283 to 433	2.7263	0.18147	0.82	6.1		
toluene	160	288 to 393	4.0462	0.16955	1.40	12.3		

[a] AAD = $(100/n)\ \Sigma\ |\Delta\eta/\eta_{exp}|$ and MAD = $\max(100\ |\Delta\eta/\eta_{exp}|)$.

Table 2. Comparison of Two Rough-Hard-Sphere Methods for Calculating Thermal Conductivities of Refrigerants and Aromatic Liquids[a]

				$10^3\ C_1$	this work		Assael method	
system	# data	T/K	C_0	K^{-1}	AAD	MAD	AAD	MAD
R11 ($CFCl_3$)	68	211 to 426	1.5308	0.82760	1.16	6.9	1.47	6.1
R12 (CF_2Cl_2)	50	203 to 334	1.4991	0.97920	1.86	6.7	1.94	28.4
R22 ($CF_2Cl\ H$)	67	223 to 339	1.4796	1.04420	0.85	5.5	2.09	5.6
R32 (CF_2H_2)	65	205 to 323	1.6464	1.86810	2.87	7.6	3.01	8.1
R124 ($C_2F_4Cl\ H$)	73	234 to 353	1.5167	0.41680	1.73	9.9	1.84	6.7
R125 (C_2F_5H)	34	216 to 313	1.6086	2.22210	2.75	8.7	3.56	16.2
R134a ($C_2F_4H_2$)	122	223 to 343	1.5200	2.10390	2.50	9.6	2.40	9.5
R141b ($C_2FCl_2H_3$)	76	248 to 392	1.4755	−0.32110	1.44	8.9	1.64	11.7
R152a ($C_2F_2H_4$)	67	223 to 353	1.4503	2.21780	2.70	10.3	3.19	11.0
average					1.98		2.35	
benzene	81	298 to 360	1.4915	0.17740	0.36	1.0		
toluene	117	273 to 373	1.7376	0.15620	0.38	1.4		

[a] AAD = $(100/n)\ \Sigma\ |\Delta\lambda/\lambda_{exp}|$ and MAD = $\max(100|\Delta\lambda/\lambda_{exp}|)$.

η the viscosity, λ the thermal conductivity, V the molar volume, and V_0 the characteristic volume of the substance. The viscosity and thermal conductivity of the fluid at a given temperature T and pressure p can be calculated using eqs 1 to 5 if R_η, R_λ, and V_0 are known, and a relationship between V, p, and T is available. Assael and co-workers[6−9] expressed these parameters as polynomial functions of temperature for several classes of compounds, although they often required a large number of coefficients (about 20 in the case of n-alkanes and 1-alkanols).

Bleazard and Teja[11] proposed simple expressions for V_0, R_η, and R_λ for polar fluids as follows

$$R_\eta = A_0 \tag{6}$$

$$V_0 = B_0 + B_1/T \tag{7}$$

$$R_\lambda = C_0 + C_1 T \tag{8}$$

The five coefficients A_0, B_0, B_1, C_0, and C_1 of eqs 6 to 8 were obtained by simultaneously fitting viscosity and thermal conductivity data for 58 polar liquids that included diols, disulfides, amines, carboxylic acids, alcohol-ethers, pyridines, ethanolates, and polyethylene glycols. They were able to correlate transport properties of these 58 liquids within experimental error over a wide range of temperatures, T = (293 to 423) K, and found that the parameters exhibited regular trends for series of diols, carboxylic acids, ethanolates, and polyethylene glycols.

Teja et al.[10] determined A_0, B_0, and B_1 by fitting viscosity data for refrigerants and then obtained C_0 and C_1 for these refrigerants by fitting thermal conductivity data. They based their procedure on the observation by Dymond and Awan[13] that R_η, R_λ, and V_0 are not equally significant for correlating viscosities and thermal conductivities. Viscosities were found to be very sensitive to changes in V_0 but less sensitive to changes in R_η, whereas calculated thermal conductivities showed only a slight dependence on V_0. Therefore, they were able to determine V_0 by fitting viscosity data only and used the same value of V_0 to

Table 3. Comparison of Two Generalized Rough-Hard-Sphere Methods for Calculating Viscosities of Refrigerants and Aromatic Liquids

				this work		Assael method	
system	C_n	# data	T/K	AAD	MAD	AAD	MAD
			alkanes				
ethane	2	68	120 to 285	2.43	6.9	2.87	5.2
propane	3	23	150 to 300	3.43	10.9	1.79	5.5
butane	4	55	180 to 310	4.00	7.8	1.72	5.7
pentane	5	8	210 to 330	7.58	15.5	5.35	11.2
hexane	6	56	280 to 373	3.10	12.3	1.69	3.7
heptane	7	42	240 to 370	3.38	8.5	1.74	6.4
octane	8	36	290 to 400	4.50	10.6	3.72	8.6
nonane	9	40	275 to 380	1.25	4.0	2.80	5.0
decane	10	147	270 to 510	4.08	12.3	5.38	12.7
undecane	11	39	270 to 480	1.20	2.5	1.54	3.5
dodecane	12	36	280 to 380	3.98	7.5	3.37	10.6
tridecane	13	12	290 to 480	2.67	3.6	1.15	2.0
tetradecane	14	12	290 to 380	3.10	8.5	4.12	7.1
pentadecane	15	9	300 to 380	2.25	4.8	1.38	1.9
hexadecane	16	37	298 to 520	3.11	14.9	3.99	8.7
average				3.34		2.84	
			1-alkanols				
ethanol	2	72	273 to 348	2.28	9.6	2.91	10.2
1-propanol	3	80	283 to 333	5.37	9.2	2.64	13.8
1-butanol	4	41	293 to 333	2.35	8.2	0.92	4.0
1-pentanol	5	5	298 to 333	5.50	9.5	2.07	3.1
1-hexanol	6	11	298 to 348	3.34	5.4	1.77	4.6
1-heptanol	7	5	288 to 328	2.39	3.5	2.26	3.4
1-octanol	8	16	288 to 348	1.74	3.0	1.87	5.2
1-nonanol	9	5	288 to 328	1.93	2.9	2.59	5.1
1-decanol	10	16	288 to 348	2.27	3.4	1.62	3.3
average				3.02		2.07	

Table 4. Comparison of Two Generalized Rough-Hard-Sphere Methods for Calculating Thermal Conductivities of Refrigerants and Aromatic Liquids

				this work		Assael et al.	
system	C_n	# data	T/K	AAD	MAD	AAD	MAD
			alkanes				
ethane	2	51	120 to 250	3.71	5.1	3.66	6.5
propane	3	70	111 to 299	2.00	6.5	3.00	5.6
butane	4	8	296 to 299	0.99	1.2	2.21	2.6
pentane	5	68	305 to 342	1.18	4.3	2.23	4.2
hexane	6	138	298 to 333	2.03	3.8	2.15	4.3
heptane	7	120	298 to 368	1.12	5.1	1.37	6.4
octane	8	152	283 to 373	0.98	4.3	1.23	5.5
nonane	9	86	308 to 361	0.92	2.8	1.42	2.8
decane	10	20	298 to 373	1.32	2.0	1.63	3.7
undecane	11	79	308 to 373	1.10	4.4	1.72	5.2
dodecane	12	7	298 to 373	1.18	3.4	1.76	3.0
tridecane	13	57	308 to 346	1.19	2.7	2.03	3.7
tetradecane	14	26	284 to 367	2.20	4.7	1.60	3.9
pentadecane	15	4	286 to 362	3.90	4.2	2.96	6.2
hexadecane	16	14	295 to 362	4.20	5.6	2.39	6.5
average				1.87		2.09	
			1-alkanols				
ethanol	2	16	273 to 335	2.19	5.5	1.86	5.2
1-propanol	3	10	300 to 340	4.30	5.9	2.56	4.4
1-butanol	4	9	301 to 345	1.34	2.2	2.49	4.7
1-pentanol	5	11	303 to 344	0.69	1.0	3.57	6.8
1-hexanol	6	10	300 to 339	1.67	3.0	3.27	6.3
average				2.04		2.75	

fit thermal conductivity data. A major advantage of this procedure is that it makes it easier to generalize the parameters to homologous series of substances.

In the present work, we have refitted the data on the 58 polar liquids studied by Bleazard and Teja[11] using the procedure employed by Teja et al.[10] We found that differences between the original fits of Bleazard and Teja and the new fits were extremely small, with maximum deviations between values of transport properties calculated by the two procedures averaging less than 0.1 %. We also confirmed that the viscosity results were not very sensitive to values of R_η.

In the present work, we propose that for refrigerants and aromatic liquids, eqs 6 and 7 be replaced by the following

$$R_\eta = 1 \tag{9}$$

$$V_0 = D_0 + D_1/T^{0.3} \tag{10}$$

This reduces the number of coefficients that must be optimized for these substances to four. Furthermore, we have obtained the coefficients D_0 and D_1 for 9 refrigerants (R11, R12, R22, R32, R124, R125, R134a, R141b, R152a) and 2 aromatic liquids (benzene and toluene) by fitting viscosity data from the references cited in Teja et al.[10] and Assael et al.[8,9] A total of 852 viscosity data were regressed for the refrigerants, and 243 for the two aromatic hydrocarbons. Coefficients C_0 and C_1 (eq 8) for these 11 fluids were then obtained by fitting 622 thermal conductivity data for the refrigerants and 198 thermal conductivity data for the two aromatic hydrocarbons from the references cited in Teja et al.[10] and Assael et al.[9] Pressures ranged from p = (0.1 to 300) MPa for both the viscosity and thermal conductivity data. Tables 1 and 2 list the results of our calculations of viscosities and thermal conductivities for these 11 fluids. Average absolute deviations (AAD %) and maximum absolute deviations (MAD %) between experimental and calculated properties using our method and the method of Assael et al. are listed in the tables. Best fit values of the coefficients are listed in Tables 1 and 2. Note that only four coefficients were obtained by regression in our method, whereas the Assael method needs as many as nine. In general, our method appears to fit the data somewhat better than the Assael method.

Generalized Parameters for Homologous Series

For homologous series, we have generalized the parameters by assuming that R_η, R_λ, and V_0 change smoothly with temperature and number of carbon atoms C_n (or halogen atoms in the case of halogenated methanes). The volume V required in the calculations was obtained using the Tait equation fitted by Assael et al.[14] to alkane and 1-alkanol densities, the Rackett equation fitted by Teja et al.[10] to the densities of halogenated methanes, and by Bleazard and Teja[11] to the densities of alkanediols.

***n*-Alkanes.** Experimental transport property data for 15 alkanes from ethane to *n*-hexadecane were obtained from the references cited in Assael et al.[6] A total of 620 viscosity data and 900 thermal conductivity data over a range of temperatures T = (120 to 520) K and pressures p = (0.1 to 300) MPa were compiled from these references. Tables 3 and 4 list the results of our calculations for the alkanes. Average absolute deviations

Table 5. Viscosities and Thermal Conductivities of Homologous Series of Halogenated Methanes and Alkanediols Using the Generalized Rough-Hard-Sphere Method

		viscosity				thermal conductivity			
system	C_n	# data	T/K	AAD	MAD	# data	T/K	AAD	MAD
				Halogenated Methanes					
R14(CF_4)	0	11	121 to 201	1.43	2.7	11	121 to 201	2.62	7.5
R13($CClF_3$)	1	11	151 to 256	1.98	3.2	11	151 to 256	1.56	3.1
R12(CCl_2F_2)	2	10	205 to 327	1.80	6.4	10	205 to 327	1.43	2.6
R11(CCl_3F)	3	11	235 to 400	1.37	4.4	11	235 to 400	0.94	2.1
R10(CCl_4)	4	11	265 to 480	3.39	6.2	11	273 to 343	1.75	3.4
average				1.99				1.66	
				Alkanediols					
1,3-propanediol	3	10	298 to 420	1.58	6.0	10	297 to 469	2.53	2.8
1,4-butanediol	4	10	298 to 422	1.00	2.9	7	292 to 466	1.29	2.9
1,5-pentanediol	5	10	298 to 433	1.86	4.0	7	296 to 471	3.16	4.0
1,6-hexanediol	6	9	318 to 433	0.70	1.4	7	323 to 470	2.40	2.8
1,8-octanediol	8	8	335 to 432	3.98	10.9	8	338 to 472	0.75	2.4
1,9-nonanediol	9	9	323 to 432	1.00	1.6	7	328 to 465	1.70	2.4
1,10-decanediol	10	7	348 to 433	3.06	3.6	7	352 to 471	2.00	2.9
average				1.88				1.98	

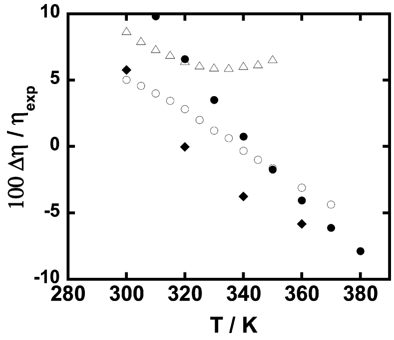

Figure 1. Deviations between experimental and predicted viscosities: ◆, heptadecane; ○, octadecane; Δ, onadecane; and ●, eicosane.

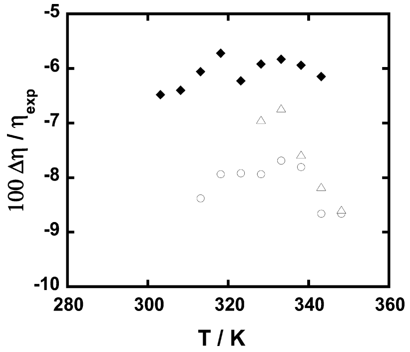

Figure 2. Deviations between experimental and predicted viscosities: ◆, 1-dodecanol; ○, 1-tetradecanol; and Δ, 1-hexadecanol.

(AAD %) and maximum absolute deviations (MAD %) between experimental and calculated viscosities using our method and the method of Assael et al.[6] are given in the tables. In general, both methods show good agreement between calculation and experiment, with the Assael method being slightly better for correlating viscosity and the new model being somewhat better for correlating thermal conductivity. Best fit coefficients for our method are given below

$$R_\eta = 1.0055 + 0.0472C_n \tag{11}$$

$$10^5 V_0 = (0.85501 + 0.39526C_n) + (3.162C_n^{1.17694})/(T/\mathrm{K})^{0.3} \tag{12}$$

$$10^3 R_\lambda = 928.19 + 205.89C_n + (-1.5175 + 0.36567C_n)\{(T/\mathrm{K}) - 273.15\} \tag{13}$$

Note that 10 coefficients have been optimized from alkane data, whereas Assael et al.[6] used 20 coefficients to fit data for the alkanes.

1-Alkanols. The 251 experimental viscosity data for 1-alkanols from ethanol to 1-decanol and 56 thermal conductivity data for 1-alkanols from ethanol to 1-hexanol were compiled from the references cited in Assael et al.[7] The data span a temperature range $T = (273 \text{ to } 348)$ K. Tables 3 and 4 list the AAD % and MAD % between experimental and calculated transport properties using our method and the method of Assael et al. The two methods are able to correlate data equally well for 1-alkanols. Best fit coefficients for our method are given by

$$R_\eta = 3.1 - 0.01{*}\{(T/\mathrm{K}) - 273.15\} \tag{14}$$

$$10^3 V_0 = -1.157927(1 - 1.00825^{C_n}) + (2.86074 + 1.2238C_n/(T/\mathrm{K}) \tag{15}$$

$$10^3 R_\lambda = 818.32 + 131.47C_n + (2.2808 + 0.50291C_n)\{(T/\mathrm{K}) - 273.15\} \tag{16}$$

Note that once again 10 coefficients are used in these correlations, whereas the Assael method requires 20.

Halogenated Methanes. Data for five halogenated methanes, with increasing number of Cl atoms substituting for F atoms, were obtained from the compilation of Rowley et al.[14] The data consisted of saturated liquid densities and transport properties over a temperature range $T = (300 \text{ to } 470)$ K at ambient pressures. The viscosity and thermal conductivity data could be fitted with an AAD of less than 2 % and MAD of less than 8 % using our method, as shown in Table 5. The best fits of the data were obtained using

$$R_\eta = 1 \tag{17}$$

$$10^5 V_0 = (1.93373 + 0.56532C_n) + (6.0640 + 1.7923C_n)/(T/\mathrm{K})^{0.3} \tag{18}$$

$$10^3 R_\lambda = 141.29 + 53.42C_n + (-0.6577 + 0.05308C_n)\{(T/\mathrm{K}) - 273.15\} \tag{19}$$

There are no published studies of halogenated methanes using the Assael et al. method. Therefore no comparisons with the Assael method are shown in Table 5.

Alkanediols. 63 viscosity data and 53 thermal conductivity data were obtained from Bleazard and Teja[11] on seven alkanediols from 1,3-propanediol to 1,10-decanediol. The data covered a temperature range $T = (300 \text{ to } 470)$ K at ambient pressures. The viscosity and thermal conductivity data could be fitted with an AAD of less than 2 % and MAD of less than 10 % using our method, as shown in Table 5. The best fits of R_η, V_0, and R_λ are

$$R_\lambda = 1 + 0.04C_n \tag{20}$$

$$10^5 V_0 = (1.25134 + 0.92663C_n) + (89.04 + 186.823C_n)/(T/\mathrm{K}) \tag{21}$$

$$10^3 R_\lambda = 468.28 + 194.53C_n + (1.9720 + 0.43313C_n)\{(T/\mathrm{K}) - 273.15\} \tag{22}$$

Again, there are no published studies of alkanediols using the Assael et al. method. Therefore no comparisons with this method are shown in Table 5.

Extrapolation Capability of the Method

The extrapolation capability of our method was investigated by calculating the viscosities of the higher alkanes and 1-alkanols that were not included in the regression of the data. The calculations require the volume V for the higher alkanes and 1-alkanols. Since these volumes were not available, we generalized the available volumes of the alkanes at $p = 0.1$ MPa as a function of temperature and carbon number as follows

$$10^6V = (-17.45126 + 22.90472\tau) + (20.86902 - 2.584705\tau + 0.314002\tau^2)\cdot(1 - q^{C_n-1})/(1 - q) \quad (23)$$

$$q = 0.980011 + 0.007527\tau \quad (24)$$

and for the 1-alkanols

$$10^6V = (22.99863 + 6.291717\tau) + (17.46862 - 1.460893\tau + 0.409259\tau^2)\cdot(1 - q^{C_n-1})/(1 - q) \quad (25)$$

$$q = 0.998499 - 0.00002\tau \quad (26)$$

In these equations, $\tau = (T/\mathrm{K})/100$. For alkanes, the volume data were obtained from the Tait equation fits of Assael et al.[15] at temperatures between $T = (300$ and $380)$ K and carbon numbers $C_n = (7$ to $16)$. For 1-alkanols, the volume data were obtained from the Tait equation fits[15] at temperatures $T = (300$ to $360)$ K and carbon numbers $C_n = (2$ to $10)$. The average absolute deviations (AAD %) and maximum average deviations (MAD %) were 0.05 % and 0.24 % for the *n*-alkanes and 0.06 % and 0.28 % for the 1-alkanols, respectively.

Experimental[16] and calculated viscosities of heptadecane, octadecane, nonadecane, and eicosane are plotted in Figure 1. In general, the agreement between calculated and experimental values is reasonable, with AAD of about 5 % and MAD of 10 %. Experimental[17] and calculated viscosities of 1-dodecanol, 1-tetradecanol, and 1-hexadecanol are shown in Figure 2. The AAD between calculated and experimental values was about 7 % and the MAD about 10 %.

The method of Assael et al. works well for the higher alkanes. However, as noted previously, negative values of R_η are obtained when the 1-alkanol correlations are extrapolated to 1-dodecanol, 1-tetradecanol, and 1-hexadecanol.

Summary

The modified rough-hard-sphere model is successful in correlating viscosity and thermal conductivity for a variety of compounds over wide ranges of temperature and pressure. The model is both simple and accurate and requires a small number of coefficients to characterize each compound. The model parameters R_η, R_λ, and V_0 can be generalized for homologous series, which allows extrapolation to higher members of each series. Also, since the parameters are independent of pressure, high-pressure viscosities and thermal conductivities can be predicted successfully using correlations obtained from data at ambient pressures.

Literature Cited

(1) Poling, B. E.; Prausnitz, J. M.; O'Connell, J. *The properties of gases and liquids*, 5th ed.; McGraw Hill: NY, 2001.

(2) Przezdziecki, J. W.; Sridhar, T. Prediction of liquid viscosities. *AIChE J.* **1985**, *31*, 333–335.

(3) Sastri, S. R. S.; Rao, K. K. A new group contribution method for predicting viscosity of organic liquids. *Chem. Eng. J.* **1992**, *50*, 9–26.

(4) Dutt, N. V. K.; Ravikumar, Y. V. L.; Rajiah, A. Prediction of liquid viscosities of phosphorus-containing compounds by Souders' method. *Chem. Eng. J.* **1993**, *51*, 41–44.

(5) Dutt, N. V. K.; Venugopal, D. Prediction of liquid viscosities of fluorinated hydrocarbons by the extended Thomas method. *Chem. Eng. J.* **1990**, *44*, 173–175.

(6) Assael, M. J.; Dymond, J. H.; Papadaki, M.; Patterson, P. M. Correlation and prediction of dense fluid transport coefficients. I. n-Alkanes. *Int. J. Thermophys.* **1992**, *13*, 269–281.

(7) Assael, M. J.; Dymond, J. H.; Polimatidou, S. K. Correlation and prediction of dense fluid transport coefficients. IV. n-Alkanols. *Int. J. Thermophys.* **1994**, *15*, 189–201.

(8) Assael, M. J.; Dymond, J. H.; Polimatidou, S. K. Correlation and prediction of dense fluid transport coefficients. V. Aromatic Hydrocarbons. *Int. J. Thermophys.* **1992**, *13*, 895–905.

(9) Assael, M. J.; Dymond, J. H.; Polimatidou, S. K. Correlation and prediction of dense fluid transport coefficients. *Int. J. Thermophys.* **1995**, *16*, 761–772.

(10) Teja, A. S.; Smith, R. L.; King, R. K.; Sun, T. F. Correlation and Prediction of the Transport Properties of Refrigerants Using Two Modified Rough Hard-Sphere Models. *Int. J. Thermophys.* **1999**, *20*, 149–161.

(11) Bleazard, J. G.; Teja, A. S. Extension of the Rough Hard-Sphere Theory for Transport Properties to Polar Liquids. *Ind. Eng. Chem. Res.* **1996**, *35*, 2453–2459.

(12) Chandler, D. Rough hard sphere theory of the self-diffusion constant for molecular liquids. *J. Chem. Phys.* **1975**, *62*, 1358–1363.

(13) Dymond, J. H.; Awan, M. A. Correlation of high-pressure diffusion and viscosity coefficients for n-alkanes. *Int. J. Thermophys.* **1989**, *10*, 941–951.

(14) Rowley, R. L.; Wilding, W. V.; Oscarson, J. L.; Yang, Y. *Data Compilation of Pure Chemical Properties, Design Institute for Physical Properties*; American Institute of Chemical Engineers: New York, NY, 2008.

(15) Assael, M. J.; Dymond, J. H.; Exadakitilou, D. An improved representation for n-alkane liquid densitities. *Int. J. Thermophys.* **1994**, *15*, 155–164.

(16) Viswanath, D. S.; Natarajan, G. *Data book on the viscosity of liquids*; Hemisphere Pub: New York, 1989.

(17) Matsuo, S.; Makita, T. Viscosities of six 1-alkanols at temperatures in the range 298−348 K and pressures up to 200 MPa. *Int. J. Thermophys.* **1989**, *4*, 833–843.

Received for review January 23, 2009. Accepted March 2, 2009.

JE900096N