

## **Correlation and Prediction of Dense Fluid Transport Coefficients. VI. *n*-Alcohols**

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A previously described method, based on considerations of hard-sphere theory, is used for the simultaneous correlation of the coefficients of viscosity, self-diffusion, and thermal conductivity for the *n*-alcohols, from methanol to *n*-decanol, in excellent agreement with experiment, over extended temperature and pressure ranges. Generalized correlations are given for the roughness factors and the characteristic volume. The overall average absolute deviations of the experimental viscosity, self-diffusion, and thermal conductivity measurements from those calculated by the correlation are 2.4, 2.6, and 2.0%, respectively. Since the proposed scheme is based on accurate density values, a Tait-type equation was also employed to correlate successfully the density of the *n*-alcohols. The overall average absolute deviation of the experimental density measurements from those calculated by the correlation is  $\pm 0.05\%$ .

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**KEY WORDS:** *n*-alcohols; density; high pressure; self-diffusion; Tait equation; thermal conductivity; viscosity.

### **1. INTRODUCTION**

In a series of recent papers [1–5], a scheme was developed for the simultaneous correlation of viscosity, self-diffusion, and thermal conductivity coefficient data over a wide range of temperatures and pressures, using a consistent set of values for the close-packed volume  $V_0$ . It was shown that the scheme provides a satisfactory correlation of dense fluid *n*-alkane transport coefficient data [1, 4], and consequently, it can be used with confidence to predict transport coefficients for these compounds under other conditions of temperature and pressure. The method has also been

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applied to simple organic molecular liquids [2] and has been extended to *n*-alkane mixtures [3] and aromatic hydrocarbons [5]. It has been demonstrated that this scheme can lead to predictions of transport coefficients for these systems, at pressures up to 600 MPa, with an accuracy of  $\pm 6\%$ .

The scheme is based on the assumption that transport coefficients of real dense fluids, expressed in terms of the reduced volume  $V/V_0$ , are directly proportional to values given by the exact hard-sphere theory [6]. The proportionality factor, described as the roughness factor  $R$ , accounts for molecular roughness and departure from molecular sphericity.

As it has been shown, in this scheme, it is the density of the liquid that is the important parameter, and not the temperature and pressure. To overcome this, a generalized Tait-type equation was employed to correlate successfully the density of *n*-alkanes [7]. This, in conjunction with the aforementioned scheme, allowed the calculation of the transport properties of *n*-alkanes and their mixtures as a function of the temperature and pressure, rather than the density.

In this paper, the general applicability of the scheme is further tested using polar liquids such as the *n*-alcohols from methanol to *n*-decanol. Furthermore, prior to the application of the scheme, accurate experimental density data are employed to develop a Tait equation for the correlation of the density of these alcohols.

## 2. THE DENSITY

The Tait equation is usually expressed in the form

$$\frac{\rho - \rho_0}{\rho_0} = C \log \left[ \frac{B + P}{B + P_0} \right] \quad (1)$$

where  $\rho$  and  $\rho_0$  are the liquid densities at the corresponding pressures,  $P$  and  $P_0$ , and  $B$  and  $C$  are parameters. In most cases  $P_0$  is taken to be equal to the atmospheric pressure (0.101 MPa) and  $\rho_0$  the corresponding atmospheric-pressure density.

Parameter  $C$  has generally been found to be a constant, while parameter  $B$  definitely varies with temperature. In the case of *n*-alkane liquid density [7],  $C$  was found to be a constant equal to 0.2000 and  $B$  a quadratic function of temperature.

Following our previous work [7], the liquid density at atmospheric pressure was correlated as a function of the reduced temperature,  $T_r$  ( $= T/T_c$ ), as [8]

$$\rho_0 = \rho_c \left\{ 1 + \sum_{i=0}^6 a_i (1 - T_r)^{i/3} \right\} \quad (2)$$

Table I. Critical Constants and Coefficients of Eq. (2)

| Alcohol                               | $T_c$<br>(K) | $\rho_c$<br>( $\text{kg} \cdot \text{m}^{-3}$ ) | $a_0$     | $a_1$     | $a_2$     | $a_3$     | $a_4$     | $a_5$    | $a_6$     |
|---------------------------------------|--------------|---|-----------|-----------|-----------|-----------|-----------|----------|-----------|
| $\text{CH}_3\text{OH}$                | 512.60       | 272   | 2.627813  | -4.047421 | 15.83425  | -22.50656 | 10.91597  | 0.304774 | —         |
| $\text{C}_2\text{H}_5\text{OH}$       | 513.88       | 276   | -0.992640 | 38.02867  | -181.1172 | 445.9045  | -588.5184 | 393.9196 | -104.3443 |
| $\text{C}_3\text{H}_7\text{OH}$       | 536.74       | 274   | 0.940534  | 12.94424  | -53.95190 | 113.6388  | -113.8656 | 43.38324 | —         |
| $\text{C}_4\text{H}_9\text{OH}$       | 563.01       | 271   | -3.573785 | 50.24497  | -175.9335 | 308.5883  | -265.6281 | 89.49966 | —         |
| $\text{C}_5\text{H}_{11}\text{OH}$    | 588.11       | 270   | -2.611289 | 42.33751  | -149.6396 | 262.2095  | -223.0897 | 73.78793 | —         |
| $\text{C}_6\text{H}_{13}\text{OH}$    | 610.7        | 268   | -0.155309 | 17.72617  | -57.60072 | 99.90259  | -86.58833 | 29.62810 | —         |
| $\text{C}_7\text{H}_{15}\text{OH}$    | 632.5        | 267   | 1.841512  | 0.656310  | 0.561043  | -0.343507 | —         | —        | —         |
| $\text{C}_8\text{H}_{17}\text{OH}$    | 652.5        | 266   | -3.533725 | 54.85805  | -199.6525 | 345.7972  | -285.0304 | 90.54450 | —         |
| $\text{C}_9\text{H}_{19}\text{OH}$    | 671.5        | 265   | 3.500512  | -6.128173 | 9.354806  | -3.990277 | —         | —        | —         |
| $\text{C}_{10}\text{H}_{21}\text{OH}$ | 689          | 264   | 2.250129  | 3.402373  | -14.54532 | 20.62086  | -8.993219 | —        | —         |

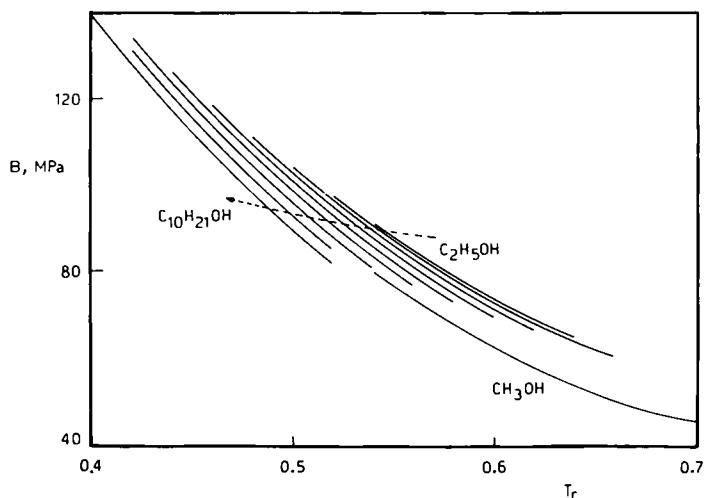


Fig. 1. The dependence of parameter  $B$  on the reduced temperature.

Table II. Comparison of Calculated Density Values with Experimental Values for the Alcohols

| Alcohol                            | First author | Ref. No. | Temp. range (K) | Press. max. (MPa) | No. of data | Av. dev. (%) | Max. dev. (%) |
|------------------------------------|--------------|----------|-----------------|-------------------|-------------|--------------|---------------|
| CH <sub>3</sub> OH                 | Kubota       | 9        | 283–349         | 97                | 29          | 0.06         | 0.14          |
|                                    | Matsuo       | 10       | 298–324         | 100               | 20          | 0.05         | 0.14          |
|                                    | Easteal      | 11       | 278–314         | 60                | 10          | 0.03         | 0.09          |
|                                    | Papaioannou  | 12       | 298             | 72                | 16          | 0.08         | 0.11          |
| C <sub>2</sub> H <sub>5</sub> OH   | Kubota       | 9        | 298–324         | 90                | 21          | 0.08         | 0.20          |
|                                    | Easteal      | 11       | 298             | 94                | 4           | 0.07         | 0.19          |
|                                    | Papaioannou  | 12       | 298             | 72                | 16          | 0.07         | 0.20          |
| C <sub>3</sub> H <sub>7</sub> OH   | Kubota       | 9        | 283–349         | 88                | 24          | 0.09         | 0.19          |
|                                    | Papaioannou  | 12       | 298             | 72                | 16          | 0.07         | 0.11          |
| C <sub>4</sub> H <sub>9</sub> OH   | Kubota       | 9        | 283–349         | 85                | 24          | 0.07         | 0.15          |
|                                    | Papaioannou  | 12       | 298             | 72                | 16          | 0.04         | 0.09          |
| C <sub>5</sub> H <sub>11</sub> OH  | Garg         | 13       | 323–374         | 10                | 60          | 0.02         | 0.09          |
| C <sub>6</sub> H <sub>13</sub> OH  | Matsuo       | 10       | 298–349         | 40                | 27          | 0.03         | 0.09          |
|                                    | Garg         | 13       | 323–374         | 10                | 60          | 0.06         | 0.19          |
| C <sub>7</sub> H <sub>15</sub> OH  | Garg         | 13       | 323–374         | 10                | 60          | 0.03         | 0.11          |
| C <sub>8</sub> H <sub>17</sub> OH  | Matsuo       | 10       | 298–349         | 41                | 26          | 0.07         | 0.10          |
|                                    | Garg         | 13       | 323–374         | 10                | 60          | 0.02         | 0.09          |
| C <sub>9</sub> H <sub>19</sub> OH  | Garg         | 13       | 323–374         | 10                | 60          | 0.05         | 0.13          |
| C <sub>10</sub> H <sub>21</sub> OH | Matsuo       | 10       | 298–349         | 41                | 29          | 0.04         | 0.10          |
| Total                              |              |          |                 |                   | 578         | 0.05         | 0.20          |

where  $\rho_c$  and  $T_c$  represent the critical density and critical temperature of the liquid. The coefficients  $a_i$  and the critical constants are shown in Table I.

Equations (1) and (2) were used to examine the temperature dependence of parameter  $B$ , after it had been found that  $C$  could be, similarly to the situation for the  $n$ -alkanes, taken as a constant equal to 0.2000. The examination of all available experimental density data enabled the best calculation of this dependence in a generalized form, as a function of the reduced temperature,  $T_r$ , and the number of carbon atoms,  $C_n$ , in the alcohol molecule.

The results given for  $B$  in Fig. 1 show a family of curves having the same general reduced-temperature dependence but displaced from one another in a regular manner. The exception is methanol, for which the curve lies significantly lower than that for ethanol, but this is not entirely unexpected since it has frequently been observed that the first member of a series shows anomalous behavior compared with other members of the series. A similar situation was noticed with the  $n$ -alkanes for methane [7].

Parameter  $B$  has been expressed as follows:

$$B = 520.23 - 1240T_r + 827T_r^2 - F$$

where

$$\begin{array}{ll} \text{for methanol} & F = 11.8 \\ \text{for ethanol to } n\text{-decanol} & F = 0.015C_n(1 + 11.5C_n) \end{array} \quad (3)$$

In Table II, the experimental measurements [9–13] considered in this work and the experimental temperature ranges and maximum pressures are shown. In the same table the average percentage deviation and the maximum percentage deviation for every data set in each  $n$ -alcohol are also given. The average absolute percentage deviation of all 578 data points considered is 0.05%, while the maximum absolute percentage deviation is 0.20%. However, it should be pointed out that in the data shown in the table, the maximum pressure of Kubota et al. [9], Matsuo and Makita [10], and Eastal and Woolf [11] had to be restricted to about 100 MPa. Above this pressure, large deviations started to appear, rising with increasing pressure. Furthermore, the investigators were found not to agree well among themselves. Thus, as it was found impossible to produce a generalized correlation that covered the entire pressure range (up to about 400 MPa) with a good uncertainty, it was preferred to restrict the pressure range to 100 MPa.

### 3. THE TRANSPORT PROPERTIES

According to the proposed scheme [1-5], it was found that the reduced coefficients for viscosity  $\eta^*$ , self-diffusion  $D^*$ , and thermal conductivity  $\lambda^*$ , defined as

$$\eta^* = 6.035 \times 10^8 \left[ \frac{1}{MRT} \right]^{1/2} \eta V^{2/3} \quad (4)$$

$$D^* = 5.030 \times 10^8 \left[ \frac{M}{RT} \right]^{1/2} D V^{-1/3} \quad (5)$$

$$\lambda^* = 1.936 \times 10^7 \left[ \frac{M}{RT} \right]^{1/2} \lambda V^{2/3} \quad (6)$$

are functions of the reduced molar volume  $V_r = (V/V_0)$ , where  $V_0$  is a characteristic molar volume of the liquid, weakly dependent on temperature. In the above equations (all quantities in SI units),  $M$  represents the molecular mass and  $R$  the universal gas constant. According to this scheme [1-5] the aforementioned functions were found to be universal for all liquids and equal to

$$\log \left[ \frac{\eta^*}{R_\eta} \right] = \sum_{i=0}^7 a_{\eta i} V_r^{-i} \quad (7)$$

$$\log \left[ \frac{D^*}{R_D} \right] = \sum_{i=0}^5 a_{D i} V_r^{-i} \quad (8)$$

$$\log \left[ \frac{\lambda^*}{R_\lambda} \right] = \sum_{i=0}^4 a_{\lambda i} V_r^{-i} \quad (9)$$

where parameters  $R_\eta$ ,  $R_D$ , and  $R_\lambda$  account for deviations from the behavior of smooth hard spheres [1]. The coefficients  $a_{\eta i}$ ,  $a_{D i}$ , and  $a_{\lambda i}$  are shown in Table III. In the case of pure  $n$ -alkanes [1] and aromatic

Table III. Coefficients of Eqs. (7)-(10)

| $i$ | $a_{\eta i}$ | $a_{D i}$ | $a_{\lambda i}$ | $b_i$    | $d_i$    | $g_i$                    |
|-----|--------------|-----------|-----------------|----------|----------|--------------------------|
| 0   | 1.0945       | 3.33076   | 1.0655          | -28.842  | 486.505  | 34.6986                  |
| 1   | -9.26324     | -31.74261 | -3.538          | -2759.29 | -478.064 | -3.944                   |
| 2   | 71.0385      | 133.0472  | 12.121          | —        | 217.9562 | 0.169911                 |
| 3   | -301.9012    | -285.1914 | -12.469         | —        | -47.901  | $-3.681 \times 10^{-3}$  |
| 4   | 797.6900     | 298.1413  | 4.562           | —        | 4.139    | $3.94017 \times 10^{-5}$ |
| 5   | -1221.9770   | -125.2472 | —               | —        | —        | $-1.6598 \times 10^{-7}$ |
| 6   | 987.5574     | —         | —               | —        | —        | —                        |
| 7   | -319.4636    | —         | —               | —        | —        | —                        |

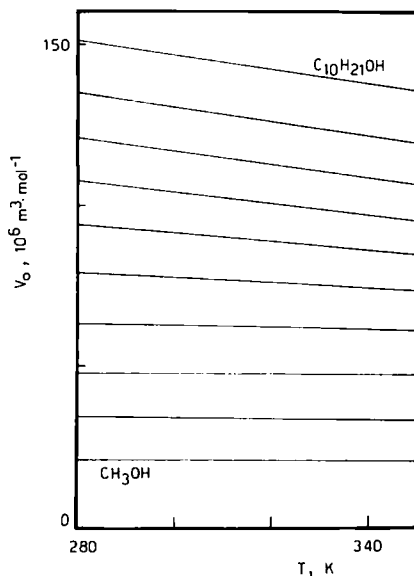


Fig. 2. The dependence of the characteristic molar volume on temperature.

hydrocarbons [5], experimental measurements were used to calculate the temperature dependence of the characteristic molar volumes and the values of parameters  $R$ . Furthermore, in all previous work [1–5] parameters  $R$  were found to be constants, characteristic only of the liquid and the property.

Similarly, in this work experimental measurements of viscosity, self-diffusion, and thermal conductivity coefficients were used to calculate the aforementioned parameters. However, in this case, parameters  $R_\eta$  and  $R_D$  were found to be weak functions of temperature, especially for the first

Table IV. Coefficients of Eq. (11)

| Alcohol                           | $R_\eta$     |                       |                        | $R_D$        |                         |                         |
|-----------------------------------|--------------|-----------------------|------------------------|--------------|-------------------------|-------------------------|
|                                   | $h_0$<br>(-) | $h_1$<br>( $K^{-1}$ ) | $h_2$<br>( $K^{-2}$ )  | $f_0$<br>(-) | $f_1$<br>( $K^{-1}$ )   | $f_2$<br>( $K^{-2}$ )   |
| CH <sub>3</sub> OH                | 41.152       | -0.2175               | $3.057 \times 10^{-4}$ | -2.747       | $1.771 \times 10^{-2}$  | $-2.598 \times 10^{-5}$ |
| C <sub>2</sub> H <sub>5</sub> OH  | 49.74        | -0.2505               | $3.325 \times 10^{-4}$ | -0.255       | $7.150 \times 10^{-4}$  | $2.368 \times 10^{-6}$  |
| C <sub>3</sub> H <sub>7</sub> OH  | 119.69       | -0.6770               | $9.817 \times 10^{-4}$ | -0.360       | $-8.800 \times 10^{-6}$ | $5.965 \times 10^{-6}$  |
| C <sub>4</sub> H <sub>9</sub> OH  | 55.07        | -0.2950               | $4.110 \times 10^{-4}$ |              |                         |                         |
| C <sub>5</sub> H <sub>11</sub> OH | 46.11        | -0.2580               | $3.802 \times 10^{-4}$ |              |                         |                         |

alcohols of the series, while only parameter  $R_\lambda$  was found to be still a constant for a liquid. Thus, these parameters had to be optimized together with the characteristic molar volumes.

The equation obtained for the characteristic molar volume,  $V_0$ , as a function of the absolute temperature,  $T$ , and the number of carbon atoms,  $C_n$ , in the alcohol molecule is

$$V_0 = \sum_{i=0}^1 b_i T^{-i/2} + \sum_{i=0}^4 d_i C_n^{(i+2)/2} + \sum_{i=0}^5 g_i (C_n T)^{(i+1)/2} \quad (10)$$

The coefficients  $b_i$ ,  $d_i$ , and  $g_i$  are shown in Table III, while the values of  $V_0$  for the 10 alcohols as a function of temperature are shown in Fig. 2. For the higher alcohols,  $V_0$  values decrease steadily as the temperature is increased as expected when a hard-sphere model is applied to real molecules for which the repulsive part of the interaction energy curve is

Table V. Values of  $R_n$ ,  $R_D$ , and  $R_\lambda$  at Selected Temperatures

| Alcohol                            | Temperature (K) |          |      |      |      |      |      |      |
|------------------------------------|-----------------|----------|------|------|------|------|------|------|
|                                    | 280             | 290      | 300  | 310  | 320  | 330  | 340  | 350  |
|                                    | $R_n$           |          |      |      |      |      |      |      |
| CH <sub>3</sub> OH                 | 4.22            | 3.79     | 3.42 | 3.10 | 2.86 | 2.67 | 2.54 | 2.48 |
| C <sub>2</sub> H <sub>5</sub> OH   | 5.67            | 5.06     | 4.51 | 4.04 | 3.63 | 3.28 | 3.01 | 2.80 |
| C <sub>3</sub> H <sub>7</sub> OH   | 7.10            | 5.92     | 4.94 | 4.16 | 3.58 | 3.19 | 2.99 |      |
| C <sub>4</sub> H <sub>9</sub> OH   | 4.69            | 4.09     | 3.56 | 3.12 | 2.76 | 2.48 | 2.28 |      |
| C <sub>5</sub> H <sub>11</sub> OH  |                 | 3.26     | 2.93 | 2.67 | 2.48 | 2.37 | 2.34 |      |
| C <sub>6</sub> H <sub>13</sub> OH  |                 | ← 3.00 → |      |      |      |      |      |      |
| C <sub>7</sub> H <sub>15</sub> OH  | ←               | 3.70 →   |      |      |      |      |      |      |
| C <sub>8</sub> H <sub>17</sub> OH  | ←               | 4.54 →   |      |      |      |      |      |      |
| C <sub>9</sub> H <sub>19</sub> OH  | ←               | 4.86 →   |      |      |      |      |      |      |
| C <sub>10</sub> H <sub>21</sub> OH | ←               | 4.01 →   |      |      |      |      |      |      |
|                                    | $R_D$           |          |      |      |      |      |      |      |
| CH <sub>3</sub> OH                 | 0.17            | 0.20     | 0.23 | 0.25 | 0.26 | 0.27 | 0.27 | 0.27 |
| C <sub>2</sub> H <sub>5</sub> OH   | 0.13            | 0.15     | 0.17 | 0.19 | 0.22 | 0.24 | 0.26 | 0.29 |
| C <sub>3</sub> H <sub>7</sub> OH   | 0.11            | 0.14     | 0.17 | 0.21 | 0.25 | 0.29 | 0.33 | 0.37 |
|                                    | $R_\lambda$     |          |      |      |      |      |      |      |
| CH <sub>3</sub> OH                 | ←               |          |      | 1.43 | →    |      |      |      |
| C <sub>2</sub> H <sub>5</sub> OH   | ←               |          |      | 1.42 | →    |      |      |      |
| C <sub>3</sub> H <sub>7</sub> OH   | ←               |          |      | 1.47 | →    |      |      |      |
| C <sub>4</sub> H <sub>9</sub> OH   | ←               |          |      | 1.58 | →    |      |      |      |
| C <sub>5</sub> H <sub>11</sub> OH  | ←               |          |      | 1.74 | →    |      |      |      |
| C <sub>6</sub> H <sub>13</sub> OH  | ←               |          |      | 1.95 | →    |      |      |      |



Table VI. Comparison of Calculated Viscosity Values with Experimental Values for the Alcohols

| Alcohol                            | First author  | Ref. No. | Temp. range (K) | Press. max. (MPa) | No. of data | Dev. 5-8% | Av. dev. (%) | Max. dev. (%) |
|------------------------------------|---------------|----------|-----------------|-------------------|-------------|-----------|--------------|---------------|
| CH <sub>3</sub> OH                 | Isdale        | 14       | 298-324         | 473               | 44          | 3         | 2.9          | 5.9           |
|                                    | Papaioannou   | 12       | 298             | 72                | 16          | —         | 3.3          | 4.2           |
|                                    | Tanaka        | 15       | 283-349         | 69                | 31          | 4         | 3.5          | 8.0           |
|                                    | Assael        | 16       | 295-324         | 28                | 26          | —         | 3.3          | 4.2           |
|                                    | Isakova       | 17       | 293-334         | 25                | 18          | —         | 2.8          | 3.4           |
|                                    | Rauf          | 18       | 288-329         | 0.1               | 5           | —         | 3.5          | 4.5           |
|                                    | Mikhail       | 19       | 298-324         | 0.1               | 5           | —         | 4.0          | 4.8           |
|                                    | Kikuchi       | 20       | 283-324         | 0.1               | 5           | —         | 2.6          | 3.9           |
|                                    | Crabtree      | 21       | 303-319         | 0.1               | 3           | —         | 3.9          | 4.3           |
|                                    | Aminabhavi    | 22       | 298-309         | 0.1               | 3           | —         | 4.7          | 4.8           |
| C <sub>2</sub> H <sub>5</sub> OH   | Tanaka        | 15       | 298-324         | 79                | 16          | 5         | 3.4          | 8.0           |
|                                    | Papaioannou   | 12       | 298             | 72                | 16          | 2         | 2.7          | 6.0           |
|                                    | Assael        | 16       | 298-329         | 28                | 27          | —         | 1.6          | 3.5           |
|                                    | Rauf          | 18       | 288-329         | 0.1               | 5           | —         | 4.3          | 5.0           |
|                                    | Phillips      | 23       | 273-349         | 0.1               | 16          | —         | 2.5          | 5.0           |
|                                    | Kikuchi       | 20       | 288-324         | 0.1               | 8           | —         | 1.8          | 3.1           |
|                                    | Crabtree      | 21       | 303-319         | 0.1               | 3           | —         | 3.9          | 4.7           |
|                                    | Aminabhavi    | 22       | 298-309         | 0.1               | 3           | —         | 3.2          | 3.7           |
|                                    | Tanaka        | 15       | 283-324         | 99                | 33          | 6         | 3.2          | 8.0           |
|                                    | Papaioannou   | 12       | 298             | 72                | 16          | —         | 1.2          | 1.9           |
| C <sub>3</sub> H <sub>7</sub> OH   | Assael        | 16       | 294-329         | 28                | 28          | —         | 1.3          | 3.3           |
|                                    | Rauf          | 18       | 288-329         | 0.1               | 5           | 2         | 5.9          | 8.0           |
|                                    | Paez          | 24       | 293-324         | 0.1               | 5           | —         | 2.6          | 3.6           |
|                                    | Kikuchi       | 20       | 292-334         | 0.1               | 8           | 1         | 1.8          | 6.4           |
|                                    | Crabtree      | 21       | 303-319         | 0.1               | 3           | —         | 3.1          | 3.5           |
|                                    | Aminabhavi    | 22       | 298-309         | 0.1               | 3           | 1         | 5.0          | 5.5           |
|                                    | Mikhail       | 25       | 298-324         | 0.1               | 5           | —         | 2.5          | 2.7           |
|                                    | Papaioannou   | 12       | 298             | 72                | 16          | —         | 1.5          | 2.4           |
|                                    | Assael        | 16       | 293-334         | 29                | 29          | —         | 0.7          | 1.9           |
|                                    | Rauf          | 18       | 288-329         | 0.1               | 5           | —         | 0.7          | 1.5           |
| C <sub>4</sub> H <sub>9</sub> OH   | Aminabhavi    | 22       | 298-309         | 0.1               | 3           | —         | 2.5          | 3.2           |
|                                    | Dakshinamurty | 27       | 303-334         | 0.1               | 4           | —         | 1.5          | 1.9           |
|                                    | Garcia        | 26       | 298-334         | 0.1               | 5           | —         | 2.1          | 3.2           |
| C <sub>5</sub> H <sub>11</sub> OH  | Aminabhavi    | 22       | 298-309         | 0.1               | 3           | —         | 1.3          | 1.6           |
|                                    | Matsuo        | 28       | 298-349         | 40                | 27          | —         | 1.5          | 4.8           |
| C <sub>6</sub> H <sub>13</sub> OH  | Aminabhavi    | 22       | 298-309         | 0.1               | 3           | —         | 2.0          | 3.9           |
|                                    | Singh         | 29       | 303-334         | 0.1               | 4           | —         | 2.6          | 4.9           |
|                                    | Rauf          | 18       | 288-329         | 0.1               | 5           | —         | 2.4          | 3.5           |
| C <sub>7</sub> H <sub>15</sub> OH  | Aminabhavi    | 22       | 298-309         | 0.1               | 3           | —         | 1.5          | 2.9           |
|                                    | Matsuo        | 28       | 298-349         | 41                | 26          | —         | 1.5          | 5.0           |
| C <sub>8</sub> H <sub>17</sub> OH  | Rauf          | 18       | 288-329         | 0.1               | 5           | —         | 2.9          | 3.8           |
|                                    | Rauf          | 18       | 288-329         | 0.1               | 5           | 1         | 2.7          | 5.4           |
| C <sub>9</sub> H <sub>19</sub> OH  | Rauf          | 18       | 288-329         | 0.1               | 5           | —         | 1.5          | 2.4           |
| C <sub>10</sub> H <sub>21</sub> OH | Matsuo        | 28       | 298-349         | 41                | 29          | —         | 1.5          | 2.4           |
|                                    | Rauf          | 18       | 288-329         | 0.1               | 5           | —         | 0.7          | 1.5           |
| Total                              |               |          |                 |                   | 533         | 25        | 2.4          | 8.0           |

soft, and not infinitely steep. For the first few members of the series,  $V_0$  shows remarkably little temperature dependence.

The optimal equations obtained for the  $R$  factors are as follows:

$$\begin{aligned}
 \text{for } \text{CH}_3\text{OH}-\text{C}_5\text{H}_{11}\text{OH} \quad R_\eta &= \sum_{i=0}^2 h_i T^i \\
 \text{for } \text{C}_6\text{H}_{13}\text{OH}-\text{C}_{10}\text{H}_{21}\text{OH} \quad R_\eta &= 38.22 - 16.071C_n + 2.353C_n^2 - 0.1088C_n^3 \\
 \text{for } \text{CH}_3\text{OH}-\text{C}_3\text{H}_7\text{OH} \quad R_D &= \sum_{i=0}^2 f_i T^i \\
 \text{for } \text{CH}_3\text{OH}-\text{C}_6\text{H}_{13}\text{OH} \quad R_\lambda &= 1.493 - 0.09139C_n + 0.02804C_n^2
 \end{aligned} \tag{11}$$

The coefficients  $h_i$  and  $f_i$  are shown in Table IV, while in Table V, values of the three  $R$  parameters for each alcohol at selected temperatures where experimental data exist are shown. It can be seen that  $R_\eta$  and  $R_D$  for the low alcohols of the series are a function of temperature.  $R_\eta$  decreases with a rise in temperature and  $R_D$  decreases as the temperature is increased. This is in keeping with the fact that these lower alcohols are associated liquids due to hydrogen bonding, where the extent of hydrogen bonding falls off as the temperature is raised.  $R_\eta$  and  $R_D$  should therefore exhibit a temperature dependence. It was found previously for the  $n$ -alkane series that  $R_\eta$  increased with an increase in carbon number, a trend that was to be expected. Here a similar pattern is found, with the highest temperature  $R_\eta$  values for butanol and pentanol and the temperature independent values for  $n$ -hexanol to  $n$ -nonanol. The value for  $n$ -decanol is low, but where measurements on only one property are available there is the possibility of different pairs of values for  $R_\eta$  and  $V_0$  fitting the data almost equally well. There is a need for more, accurate data on the transport properties for higher members of this series.

In Tables VI, VII, and VIII a direct comparison of the available

**Table VII.** Comparison of Calculated Diffusion Values with Experimental Values for the Alcohols

| Alcohol                          | First author | Ref. No. | Temp. range (K) | Press. max. (MPa) | No. of data | Dev. 5-9% | Av. dev. (%) | Max. dev. (%) |
|----------------------------------|--------------|----------|-----------------|-------------------|-------------|-----------|--------------|---------------|
| CH <sub>3</sub> OH               | Hurle        | 30       | 278-329         | 386               | 32          | 5         | 3.3          | 8.2           |
| C <sub>2</sub> H <sub>5</sub> OH | Hurle        | 30       | 298             | 266               | 6           | —         | 2.8          | 5.0           |
|                                  | Meckl        | 31       | 287-323         | 150               | 35          | —         | 2.3          | 4.9           |
| C <sub>3</sub> H <sub>7</sub> OH | Meckl        | 31       | 283-323         | 300               | 54          | 6         | 2.4          | 9.0           |
| Total                            |              |          |                 |                   | 127         | 11        | 2.6          | 9.0           |

**Table VIII.** Comparison of Calculated Thermal Conductivity Values with Experimental Values for the Alcohols

| Alcohol                           | First author | Ref. No. | Temp. range (K) | Press. max. (MPa) | No. of data | Dev. 5-7% | Av. dev. (%) | Max. dev. (%) |
|-----------------------------------|--------------|----------|-----------------|-------------------|-------------|-----------|--------------|---------------|
| CH <sub>3</sub> OH                | Wakeham      | 32       | 308             | 40                | 7           | —         | 2.6          | 3.3           |
|                                   | Golubev      | 33       | 293-325         | 40                | 20          | —         | 0.8          | 1.4           |
|                                   | Assael       | 34       | 301-326         | 0.1               | 9           | —         | 1.5          | 2.8           |
|                                   | Takizawa     | 35       | 273-304         | 0.1               | 4           | —         | 1.6          | 2.5           |
| C <sub>2</sub> H <sub>5</sub> OH  | Golubev      | 33       | 296-324         | 40                | 12          | —         | 1.7          | 3.0           |
|                                   | Assael       | 34       | 305-336         | 0.1               | 10          | —         | 2.0          | 4.6           |
|                                   | Takizawa     | 35       | 273-324         | 0.1               | 6           | 1         | 1.8          | 5.5           |
| C <sub>3</sub> H <sub>7</sub> OH  | Assael       | 36       | 300-341         | 0.1               | 10          | —         | 2.5          | 4.2           |
| C <sub>4</sub> H <sub>9</sub> OH  | Assael       | 36       | 301-346         | 0.1               | 9           | —         | 2.4          | 4.5           |
| C <sub>5</sub> H <sub>11</sub> OH | Assael       | 36       | 303-343         | 0.1               | 10          | 2         | 3.2          | 6.7           |
| C <sub>6</sub> H <sub>13</sub> OH | Assael       | 36       | 300-340         | 0.1               | 10          | 2         | 3.3          | 6.7           |
| Total                             |              |          |                 |                   | 107         | 5         | 2.0          | 6.7           |

experimental data for the viscosity, self-diffusion, and thermal conductivity coefficient, respectively, with the values obtained by the scheme described by Eqs. (4)–(11) is presented. In the case of the viscosity experimental measurements, of the 533 data points used, only 25 (4.7%) were found to show deviations larger than 5%. Of the 127 experimental measurements of the self-diffusion coefficient employed, only 11 (8.7%) show deviations larger than 5%, while from the 107 thermal conductivity measurements, only 5 (4.7%) show deviations more than 5%. The overall average absolute deviations of the experimental viscosity, self-diffusion, and thermal conductivity measurements from those calculated by the correlation are 2.4, 2.6, and 2.0% respectively, as also shown in the tables. Considering the fact that in some cases experimental measurements employed included measurements up to 400 MPa pressure, this agreement is considered very satisfactory.

It should finally be noted that for the value of the density, the scheme described in this work was used, except in some cases where the pressure range was above that covered by the scheme. In that particular case the density quoted by the investigator was employed.

#### 4. CONCLUSIONS

Viscosity, self-diffusion, and thermal conductivity coefficient data for the *n*-alcohols up to *n*-decanol have been successfully correlated using a scheme developed for hydrocarbons based on a consideration of the hard-

sphere theory of transport properties. Coupled with a Tait-type generalized correlation for the density of these alcohols, the scheme allows the calculation of the transport properties of the *n*-alcohols as a function of temperature and pressure, with an uncertainty of about  $\pm 5\%$ .

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