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# Dynamic Viscosities of 2-Pentanol with Alkanes (Octane, Decane, and Dodecane) at Three Temperatures $T$ = (293.15, 298.15, and 303.15) K. New UNIFAC−VISCO Interaction Parameters

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In this work, the dynamic viscosities, densities, and speed of sound for the binary mixtures, 2-pentanol with several alkanes (octane, decane, and dodecane), at $T$ = (293.15, 298.15, 303.15) K have been measured over the whole composition range and atmospheric pressure along with the properties of the pure components. Excess molar volumes, isentropic compresibility, deviations in isentropic compressibility, and viscosity for the binary systems at the above-mentioned temperatures were calculated and fitted to Redlich−Kister equation to determine the fitting parameters and the root-mean-square deviations. The UNIQUAC equation was used to correlate the experimental data. Predictions of the dynamic viscosities of these binary mixtures from UNIFAC−VISCO and ASOG−VISCO methods have been made. The interaction parameters within secondary alcohols with alkanes ($OH_s/CH_2$, $OH_s/CH_3$) have been determined for their application in the predictive UNIFAC−VISCO method.

## 1. Introduction

Among the physical properties of fluids needed to optimize the industrial process design, viscosity is one of the most important. In chemical industry, viscosity is necessary for hydraulic calculations, fluid transport through pipes and pore surfaces, and in many mass and energy transfers. As an extension of our work concerning dynamic viscosity of binary systems with alcohols,[1−4] in this paper, we report experimental dynamic viscosity, density, and speed of sound data of the binary systems 2-pentanol with octane, decane, or dodecane at $T$ = (293.15, 298.15, 303.15) K. The results were used to calculate excess molar volumes, isentropic compresibility, deviations in isentropic compresibility, and viscosity over the entire mole fraction range for the mixtures. The UNIFAC−VISCO[5,6] and ASOG−VISCO[7] methods have been applied to compare the difference between predicted and experimental dynamic viscosities.

To improve the results of the prediction of the UNIFAC−VISCO method, the interaction parameter $CH_2$ and $CH_3$ groups proposed by Chevalier et al.[5] have been recalculated using bibliography data. As the interaction parameters ($OH_s/CH_2$, $OH_s/CH_3$) had not been determined, we have used both our experimental and recent bibliography data to calculate them.

## 2. Experimental Section

***Chemicals.*** The pure components were supplied by Fluka, except for 2-pentanol, which was supplied by Merck. The components were degassed ultrasonically and dried over Type 4Å molecular sieves, which were supplied by Aldrich, and kept in inert argon with a maximum content in water of 2 × $10^{-6}$ by mass fraction. The maximum water contents of the liquids were using a Metrohm 737 KF coulometer. Their mass fraction purities were >98 mass % for 2-pentanol, 99.5 mass % for octane, and >99 mass % for decane and dodecane.

**Table 1. Comparison of Density, $\rho$, and Viscosity, $\eta$, with Literature Data for Pure Components at $T$ = 303.15 K**

| | $\rho$/(g·cm$^{-3}$) | | $10^3\,\eta$/(Pa·s) | |
|---|---|---|---|---|
| component | exp | lit | exp | lit |
| 2-pentanol | 0.80090 | 0.8010[a] | 2.774 | 2.77[a] |
| octane | 0.69449 | 0.6945[b] | 0.478 | 0.478[b] |
| decane | 0.72233 | 0.7224[c] | 0.787 | 0.786[d] |
| dodecane | 0.74127 | 0.7415[b] | 1.219 | 1.218[c] |

[a] Riggio et al.[8] [b] Aminabhavi et al.[9] [c] Trenzado et al.[10] [d] Aminabhavi et al.[11]

***Apparatus and Procedure.*** Samples were prepared by mass using a Mettler AX-205 Delta Range balance with a precision of ±$10^{-5}$ g, covering the whole composition range of the mixture.

Kinematic viscosities were determined using an automatic viscosimeter Lauda PVS1 with two Ubbelhode capillary microviscosimeters of 0.4 × $10^{-3}$ m and 0.53 × $10^{-3}$ m diameter. Gravity fall is the principle of measurement on which this viscosimeter is based. The capillary is maintained in a D20KP LAUDA thermostat with a resolution of 0.01 K. The capillaries are calibrated and credited by the company. The uncertainty of the capillary diameter is ±0.005 mm. To verify the calibration, the viscosity of the pure liquids were compared with data recently published (Table 1). The uncertainty for the viscosimeter is ±0.001 mPa·s. The equipment has a control unit PVS1 (Processor Viscosity System) that is a PC-controlled instrument for the precise measurement of fall time, using standardized glass capillaries, with an accuracy of 0.01 s.

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**Table 2. Density, $\rho$, Speed of Sound, $u$, Dynamic Viscosity, $\eta$, Excess Molar Volumes, $V^E$, Isentropic Compressibilities, $\kappa_s$, Deviations in Isentropic Compressibilities, $\Delta\kappa_s$, and Viscosity Deviations, $\Delta\eta$, of 2-Pentanol(1) + Octane(2)**

| $x$ | $\rho$/(g·cm$^{-3}$) | $u$/(m·s$^{-1}$) | $\eta$/(mPa·s) | $V^E$/(cm$^3$·mol$^{-1}$) | $\kappa_s$/(TPa$^{-1}$) | $\Delta\kappa_s$/(TPa$^{-1}$) | $\Delta\eta$/(mPa·s) |
|---|---|---|---|---|---|---|---|
| | | | $T$ = 293.15 K | | | | |
| 0.0000 | 0.70257 | 1193 | 0.538 | 0 | 999 | 0 | 0 |
| 0.0509 | 0.70558 | 1190 | 0.548 | 0.156 | 1000 | 11 | −0.166 |
| 0.1050 | 0.70915 | 1189 | 0.566 | 0.261 | 997 | 20 | −0.336 |
| 0.1853 | 0.71498 | 1188 | 0.598 | 0.357 | 991 | 30 | −0.582 |
| 0.2976 | 0.72378 | 1188 | 0.658 | 0.474 | 979 | 42 | −0.911 |
| 0.3968 | 0.73240 | 1189 | 0.732 | 0.528 | 965 | 49 | −1.180 |
| 0.4953 | 0.74191 | 1192 | 0.841 | 0.533 | 948 | 52 | −1.412 |
| 0.5965 | 0.75273 | 1198 | 1.008 | 0.489 | 926 | 51 | −1.596 |
| 0.6993 | 0.76497 | 1207 | 1.296 | 0.401 | 898 | 44 | −1.664 |
| 0.7971 | 0.77792 | 1218 | 1.727 | 0.279 | 866 | 33 | −1.571 |
| 0.8997 | 0.79282 | 1233 | 2.531 | 0.148 | 829 | 18 | −1.122 |
| 0.9509 | 0.80083 | 1242 | 3.190 | 0.083 | 810 | 9 | −0.641 |
| 1.0000 | 0.80904 | 1250 | 4.001 | 0 | 791 | 0 | 0 |
| | | | $T$ = 298.15 K | | | | |
| 0.0000 | 0.69854 | 1173 | 0.506 | 0 | 1041 | 0 | 0 |
| 0.0509 | 0.70148 | 1170 | 0.517 | 0.174 | 1042 | 12 | −0.130 |
| 0.1050 | 0.70503 | 1169 | 0.530 | 0.283 | 1039 | 21 | −0.267 |
| 0.1853 | 0.71084 | 1168 | 0.560 | 0.383 | 1032 | 32 | −0.459 |
| 0.2976 | 0.71963 | 1168 | 0.613 | 0.501 | 1019 | 45 | −0.717 |
| 0.3968 | 0.72824 | 1169 | 0.678 | 0.558 | 1004 | 52 | −0.926 |
| 0.4953 | 0.73773 | 1172 | 0.770 | 0.563 | 986 | 56 | −1.107 |
| 0.5965 | 0.74853 | 1178 | 0.915 | 0.521 | 963 | 55 | −1.242 |
| 0.6993 | 0.76076 | 1187 | 1.147 | 0.431 | 933 | 48 | −1.294 |
| 0.7971 | 0.77374 | 1199 | 1.495 | 0.304 | 900 | 36 | −1.217 |
| 0.8997 | 0.78869 | 1214 | 2.133 | 0.163 | 860 | 19 | −0.862 |
| 0.9509 | 0.79675 | 1223 | 2.635 | 0.090 | 839 | 10 | −0.502 |
| 1.0000 | 0.80501 | 1232 | 3.273 | 0 | 818 | 0 | 0 |
| | | | $T$ = 303.15 K | | | | |
| 0.0000 | 0.69449 | 1152 | 0.478 | 0 | 1085 | 0 | 0 |
| 0.0509 | 0.69735 | 1149 | 0.486 | 0.193 | 1086 | 13 | −0.109 |
| 0.1050 | 0.70087 | 1148 | 0.498 | 0.310 | 1083 | 23 | −0.221 |
| 0.1853 | 0.70665 | 1147 | 0.525 | 0.414 | 1075 | 34 | −0.379 |
| 0.2976 | 0.71543 | 1147 | 0.572 | 0.531 | 1062 | 48 | −0.589 |
| 0.3968 | 0.72403 | 1149 | 0.629 | 0.589 | 1046 | 55 | −0.760 |
| 0.4953 | 0.73350 | 1153 | 0.709 | 0.594 | 1026 | 59 | −0.906 |
| 0.5965 | 0.74429 | 1158 | 0.826 | 0.552 | 1002 | 58 | −1.021 |
| 0.6993 | 0.75650 | 1167 | 1.022 | 0.463 | 970 | 51 | −1.062 |
| 0.7971 | 0.76948 | 1179 | 1.307 | 0.330 | 935 | 39 | −1.001 |
| 0.8997 | 0.78449 | 1195 | 1.821 | 0.177 | 892 | 21 | −0.723 |
| 0.9509 | 0.79259 | 1204 | 2.215 | 0.098 | 870 | 11 | −0.446 |
| 1.0000 | 0.80090 | 1214 | 2.708 | 0 | 848 | 0 | 0 |

**Table 3. Density, $\rho$, Speed of Sound, $u$, Dynamic Viscosity, $\eta$, Excess Molar Volumes, $V^E$, Isentropic Compressibilities, $\kappa_s$, Deviations in Isentropic Compressibilities, $\Delta\kappa_s$, and Viscosity Deviations, $\Delta\eta$, of 2-Pentanol(1) + Decane(2)**

| $x$ | $\rho$/(g·cm$^{-3}$) | $u$/(m·s$^{-1}$) | $\eta$/(mPa·s) | $V^E$/(cm$^3$·mol$^{-1}$) | $\kappa_s$/(TPa$^{-1}$) | $\Delta\kappa_s$/(TPa$^{-1}$) | $\Delta\eta$/(mPa·s) |
|---|---|---|---|---|---|---|---|
| | | | $T$ = 293.15 K | | | | |
| 0.0000 | 0.72989 | 1254 | 0.911 | 0 | 871 | 0 | 0 |
| 0.0487 | 0.73162 | 1251 | 0.914 | 0.123 | 874 | 7 | −0.147 |
| 0.0987 | 0.73341 | 1248 | 0.912 | 0.265 | 875 | 12 | −0.304 |
| 0.2043 | 0.73814 | 1243 | 0.956 | 0.403 | 876 | 22 | −0.586 |
| 0.2996 | 0.74288 | 1239 | 0.989 | 0.518 | 876 | 30 | −0.847 |
| 0.4006 | 0.74867 | 1236 | 1.084 | 0.588 | 875 | 36 | −1.064 |
| 0.5017 | 0.75531 | 1233 | 1.149 | 0.619 | 871 | 40 | −1.312 |
| 0.6002 | 0.76288 | 1232 | 1.300 | 0.585 | 863 | 41 | −1.465 |
| 0.6985 | 0.77167 | 1233 | 1.531 | 0.502 | 852 | 37 | −1.538 |
| 0.7992 | 0.78240 | 1237 | 1.914 | 0.338 | 836 | 29 | −1.466 |
| 0.8996 | 0.79455 | 1242 | 2.626 | 0.195 | 815 | 17 | −1.064 |
| 0.9500 | 0.80150 | 1246 | 3.205 | 0.103 | 803 | 8 | −0.642 |
| 1.0000 | 0.80904 | 1250 | 4.001 | 0 | 791 | 0 | 0 |
| | | | $T$ = 298.15 K | | | | |
| 0.0000 | 0.72612 | 1235 | 0.845 | 0 | 903 | 0 | 0 |
| 0.0487 | 0.72776 | 1231 | 0.845 | 0.144 | 907 | 8 | −0.118 |
| 0.0987 | 0.72953 | 1228 | 0.844 | 0.293 | 908 | 13 | −0.241 |
| 0.2043 | 0.73423 | 1223 | 0.882 | 0.434 | 910 | 24 | −0.459 |
| 0.2996 | 0.73894 | 1220 | 0.909 | 0.55 | 910 | 32 | −0.664 |
| 0.4006 | 0.74470 | 1216 | 0.990 | 0.622 | 908 | 38 | −0.828 |
| 0.5017 | 0.75130 | 1214 | 1.044 | 0.654 | 904 | 43 | −1.019 |
| 0.6002 | 0.75883 | 1213 | 1.166 | 0.622 | 896 | 44 | −1.136 |
| 0.6985 | 0.76758 | 1214 | 1.352 | 0.538 | 884 | 40 | −1.188 |
| 0.7992 | 0.77829 | 1217 | 1.646 | 0.367 | 867 | 32 | −1.139 |
| 0.8996 | 0.79046 | 1223 | 2.214 | 0.212 | 845 | 18 | −0.815 |
| 0.9500 | 0.79743 | 1228 | 2.651 | 0.113 | 832 | 9 | −0.501 |
| 1.0000 | 0.80501 | 1232 | 3.273 | 0 | 818 | 0 | 0 |
| | | | $T$ = 303.15 K | | | | |
| 0.0000 | 0.72233 | 1215 | 0.787 | 0 | 938 | 0 | 0 |
| 0.0487 | 0.72389 | 1211 | 0.779 | 0.165 | 942 | 9 | −0.105 |
| 0.0987 | 0.72562 | 1209 | 0.782 | 0.310 | 943 | 14 | −0.201 |
| 0.2043 | 0.73028 | 1204 | 0.810 | 0.468 | 945 | 26 | −0.383 |
| 0.2996 | 0.73496 | 1200 | 0.842 | 0.586 | 945 | 34 | −0.540 |
| 0.4006 | 0.74069 | 1197 | 0.883 | 0.658 | 943 | 41 | −0.700 |
| 0.5017 | 0.74725 | 1194 | 0.952 | 0.689 | 938 | 46 | −0.832 |
| 0.6002 | 0.75473 | 1193 | 1.053 | 0.659 | 930 | 47 | −0.927 |
| 0.6985 | 0.76344 | 1194 | 1.201 | 0.574 | 918 | 43 | −0.974 |
| 0.7992 | 0.77412 | 1198 | 1.439 | 0.397 | 900 | 34 | −0.936 |
| 0.8996 | 0.78630 | 1204 | 1.888 | 0.230 | 877 | 20 | −0.687 |
| 0.9500 | 0.79328 | 1209 | 2.244 | 0.123 | 862 | 10 | −0.431 |
| 1.0000 | 0.80090 | 1214 | 2.708 | 0 | 848 | 0 | 0 |

The kinematic viscosity, $\nu$, is determined from the following relationship

$$\nu = k(t - y) \tag{1}$$

where $y$ is the Hagenbach correction, $t$ is the flow time, and $k$ is the Ubbelhode capillary microviscosimeter constant, which is supplied by the company. The dynamic viscosity is determined from

$$\eta = \nu\rho \tag{2}$$

where $\eta$ is the dynamic viscosity, $\nu$ is the kinematic viscosity, and $\rho$ is the density. The densities and the speeds of sound of the pure liquids and mixtures were measured using an Anton Paar DSA-5000 digital vibrating tube densimeter. Uncertainty in density measurement is $\pm 2 \times 10^{-6}$ g·cm$^{-3}$ and for the speed of sound is $\pm 0.1$ m·s$^{-1}$.

## 3. Results and Discussion

Dynamic viscosity, density, speed of sound, excess molar volume, isentropic compressibility (determined by means of the Laplace equation, $k_s = \rho^{-1}u^{-2}$), and deviation in isentropic compressibility for the systems 2-pentanol with octane, decane, or dodecane at 293.15, 298.15, and 303.15 K and atmospheric pressure are reported in Tables 2−4. The excess molar volumes, the deviations in isentropic compressibility, and viscosity deviations are calculated by the following equations

$$V^E = \sum_{i=1}^{N} x_i M_i(\rho^{-1} - \rho_i^{-1}) \tag{3}$$

$$\Delta\kappa_s = \kappa_s - \sum_{i=1}^{N} x_i \kappa_{s,i} \tag{4}$$

$$\Delta\eta = \eta - \sum_{i}^{N} x_i \eta_i \tag{5}$$

where $\rho$ and $\rho_i$ are the density of the mixture and the density of the pure components, respectively, $\kappa_s$ is the isentropic compressibility of the mixture, $\kappa_{s,i}$ is the isentropic compressibility of the pure components, $x_i$ represents the mole fraction of the pure component, and $\eta$ and $\eta_i$ are the dynamic viscosity of the mixture and the pure component, respectively.

The binary deviations at several temperatures were fitted to a Redlich−Kister-type[12] equation

$$\Delta Q_{ij} = x_i x_j \sum_{p=0}^{M} B_p (x_i - x_j)^p \tag{6}$$

where $\Delta Q_{ij}$ is the excess property, $x$ is the mole fraction,

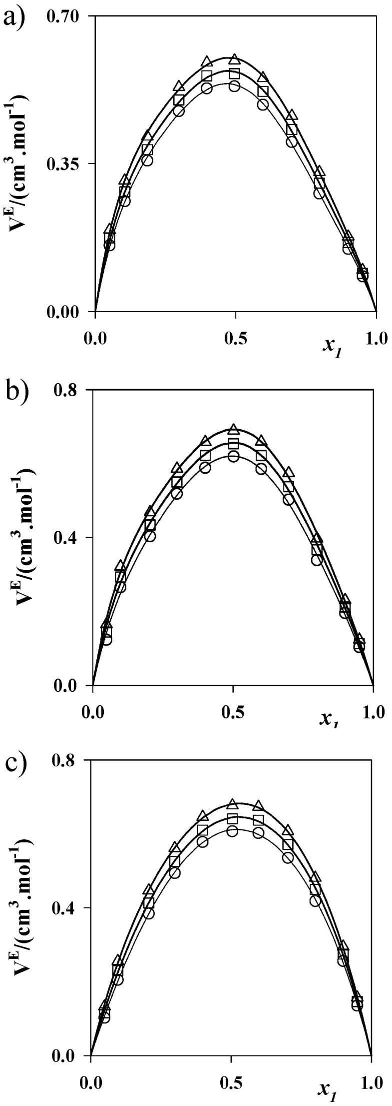

**Figure 1.** Excess molar volume, $V^E$, from the Redlich−Kister equation plotted against mole fraction at ○, $T = 293.15$ K; □, $T = 298.15$ K; △, $T = 313.15$ K for the binary mixtures: a, 2-pentanol(1) + octane(2); b, 2-pentanol(1) + decane(2); c, 2-pentanol(1) + dodecane(2).

**Table 4. Density, $\rho$, Speed of Sound, $u$, Dynamic Viscosity, $\eta$, Excess Molar Volumes, $V^E$, Isentropic Compressibilities, $\kappa_s$, Deviations in Isentropic Compressibilities, $\Delta\kappa_s$, and Viscosity Deviations, $\Delta\eta$, of 2-Pentanol(1) + Dodecane(2)**

| $x$ | $\rho$/ ($g \cdot cm^{-3}$) | $u$/ ($m \cdot s^{-1}$) | $\eta$/ (mPa·s) | $V^E$/ ($cm^3 \cdot mol^{-1}$) | $\kappa_s$/ ($TPa^{-1}$) | $\Delta\kappa_s$/ ($TPa^{-1}$) | $\Delta\eta$/ (mPa·s) |
|---|---|---|---|---|---|---|---|
| | | | $T = 293.15$ K | | | | |
| 0.0000 | 0.74854 | 1297 | 1.454 | 0 | 794 | 0 | 0 |
| 0.0490 | 0.74965 | 1294 | 1.443 | 0.102 | 796 | 3 | −0.136 |
| 0.0965 | 0.75077 | 1291 | 1.441 | 0.205 | 799 | 6 | −0.258 |
| 0.2065 | 0.75381 | 1284 | 1.438 | 0.384 | 805 | 12 | −0.542 |
| 0.2993 | 0.75686 | 1278 | 1.465 | 0.494 | 809 | 16 | −0.751 |
| 0.3986 | 0.76067 | 1271 | 1.499 | 0.578 | 813 | 21 | −0.970 |
| 0.5046 | 0.76560 | 1265 | 1.563 | 0.607 | 817 | 24 | −1.176 |
| 0.5974 | 0.77070 | 1260 | 1.667 | 0.602 | 818 | 26 | −1.308 |
| 0.7026 | 0.77776 | 1255 | 1.865 | 0.535 | 816 | 24 | −1.378 |
| 0.8001 | 0.78582 | 1253 | 2.205 | 0.418 | 811 | 20 | −1.287 |
| 0.8994 | 0.79590 | 1251 | 2.786 | 0.256 | 803 | 12 | −0.959 |
| 0.9497 | 0.80207 | 1251 | 3.267 | 0.135 | 797 | 6 | −0.606 |
| 1.0000 | 0.80904 | 1250 | 4.001 | 0 | 791 | 0 | 0 |
| | | | $T = 298.15$ K | | | | |
| 0.0000 | 0.74490 | 1278 | 1.327 | 0 | 822 | 0 | 0 |
| 0.0490 | 0.74596 | 1275 | 1.316 | 0.116 | 825 | 3 | −0.106 |
| 0.0965 | 0.74703 | 1271 | 1.312 | 0.230 | 828 | 6 | −0.203 |
| 0.2065 | 0.75005 | 1265 | 1.307 | 0.413 | 834 | 13 | −0.422 |
| 0.2993 | 0.75306 | 1259 | 1.330 | 0.525 | 838 | 17 | −0.579 |
| 0.3986 | 0.75684 | 1252 | 1.355 | 0.61 | 843 | 22 | −0.748 |
| 0.5046 | 0.76171 | 1246 | 1.406 | 0.641 | 846 | 26 | −0.903 |
| 0.5974 | 0.76677 | 1241 | 1.487 | 0.637 | 847 | 27 | −1.002 |
| 0.7026 | 0.77376 | 1236 | 1.635 | 0.571 | 846 | 26 | −1.059 |
| 0.8001 | 0.78177 | 1233 | 1.900 | 0.450 | 841 | 22 | −0.984 |
| 0.8994 | 0.79184 | 1232 | 2.347 | 0.275 | 832 | 13 | −0.730 |
| 0.9497 | 0.79802 | 1232 | 2.717 | 0.146 | 826 | 7 | −0.458 |
| 1.0000 | 0.80500 | 1232 | 3.273 | 0 | 818 | 0 | 0 |
| | | | $T = 303.15$ K | | | | |
| 0.0000 | 0.74127 | 1259 | 1.219 | 0 | 851 | 0 | 0 |
| 0.0490 | 0.74226 | 1256 | 1.206 | 0.133 | 854 | 3 | −0.089 |
| 0.0965 | 0.74330 | 1252 | 1.201 | 0.256 | 858 | 7 | −0.168 |
| 0.2065 | 0.74625 | 1245 | 1.194 | 0.447 | 864 | 14 | −0.346 |
| 0.2993 | 0.74923 | 1240 | 1.211 | 0.561 | 869 | 19 | −0.473 |
| 0.3986 | 0.75297 | 1233 | 1.231 | 0.646 | 873 | 23 | −0.608 |
| 0.5046 | 0.75779 | 1227 | 1.270 | 0.677 | 877 | 28 | −0.733 |
| 0.5974 | 0.76279 | 1222 | 1.338 | 0.673 | 878 | 29 | −0.810 |
| 0.7026 | 0.76972 | 1217 | 1.447 | 0.607 | 877 | 28 | −0.864 |
| 0.8001 | 0.77766 | 1214 | 1.652 | 0.481 | 872 | 24 | −0.811 |
| 0.8994 | 0.78771 | 1213 | 1.998 | 0.295 | 863 | 15 | −0.620 |
| 0.9497 | 0.79389 | 1213 | 2.284 | 0.157 | 856 | 8 | −0.412 |
| 1.0000 | 0.80090 | 1 | 0.792 | 0 | 848 | 0 | 0 |

$B_p$ is the fitting parameter, and $M$ is the degree of the polynomic expansion, which was optimized using the F test.[13] The fitting parameters are given in Table 5 together with the root-mean-square deviations. These are calculated from the values of the experimental and calculated property and the number of experimental data are represented by $z_{exp}$, $z_{calc}$, and $n_{dat}$, respectively

$$\sigma = \{\{\sum_{i}^{n_{dat}} (z_{exp} - z_{calc})^2\}/\{n_{dat}\}\}^{1/2} \qquad (7)$$

Figures 1, 2, and 3 show the fitted curves for the excess molar volume and deviations in isentropic compressibility and viscosity values for binary mixtures of 2-pentanol with octane, decane, and dodecane at $T = (293.15, 298.15, 303.15)$ K. In Figure 1, the excess molar volumes are positive over the entire composition range, with a maximum at equimolar composition for the three systems. In Figure 2, the behavior for the deviations in isentropic compressibility is similar to that for excess molar volumes with positive values observed over the entire composition range. These figures show maxima at 0.6 mole fraction, approximately, except 2-pentanol with octane, where the maximum lies at equimolar composition. For viscosity deviations (Figure 3), the sign is negative for all the binary systems, and the minima lie at 0.7 mole fraction approximately.

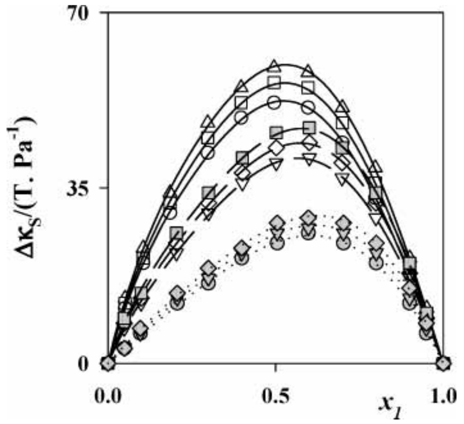

**Figure 2.** Deviations in isentropic compressibility, $\Delta\kappa_s$, from the Redlich−Kister equation plotted against mole fraction for the binary mixtures 2-pentanol(1) + octane(2) at ○, $T = 293.15$ K; □, $T = 298.15$ K; △, $T = 313.15$ K; 2-pentanol(1) + decane(2) at ▽, $T = 293.15$ K; ◇, $T = 298.15$ K; ■, $T = 313.15$ K; 2-pentanol(1) + dodecane(2) at ●, $T = 293.15$ K; ▼, $T = 298.15$ K; ◆, $T = 313.15$ K.

**Table 5. Fitting Parameters and Root-Mean-Square Deviation, $\sigma$, for Binary Mixtures at $T$ = (273.15, 298.15, 303.15) K**

2-Pentanol (1) + Octane (2)

| | $B_0$ | $B_1$ | $B_2$ | $B_3$ | $B_4$ | $\sigma$ |
|---|---|---|---|---|---|---|
| $T$ = 293.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.1443 | −0.3629 | −0.7496 | −0.5236 | 1.3797 | 0.004 |
| $\Delta\kappa_S/(TPa^{-1})$ | 208.86 | 24.02 | −33.53 | −54.97 | 40.87 | 0.17 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −5.6876 | −4.1425 | −2.7914 | −2.0889 | −1.1456 | 0.005 |
| $T$ = 298.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.2677 | −0.3155 | −0.6854 | −0.6867 | 1.4853 | 0.004 |
| $\Delta\kappa_S/(TPa^{-1})$ | 222.89 | 27.86 | −28.12 | −58.00 | 38.27 | 0.16 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −4.4514 | −3.1557 | −2.0799 | −1.6250 | −0.9588 | 0.002 |
| $T$ = 303.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.3950 | −0.2839 | −0.5840 | −0.8678 | 1.5844 | 0.005 |
| $\Delta\kappa_S/(TPa^{-1})$ | 237.30 | 31.14 | −21.20 | −62.91 | 34.45 | 0.18 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −3.6612 | −2.5195 | −1.4845 | −1.6584 | −1.4693 | 0.005 |

2-Pentanol(1) + Decane(2)

| | $B_0$ | $B_1$ | $B_2$ | $B_3$ | $B_4$ | $\sigma$ |
|---|---|---|---|---|---|---|
| $T$ = 293.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.4798 | −0.0501 | −0.7287 | −0.5978 | 1.0523 | 0.009 |
| $\Delta\kappa_S/(TPa^{-1})$ | 160.15 | 50.58 | −13.17 | −36.55 | 21.82 | 0.15 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −5.1884 | −3.8450 | −2.7753 | −2.2106 | −1.4906 | 0.008 |
| $T$ = 298.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.6232 | 0.0023 | −0.6516 | −0.7948 | 1.2062 | 0.009 |
| $\Delta\kappa_S/(TPa^{-1})$ | 171.38 | 57.60 | −6.50 | −43.38 | 23.56 | 0.17 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −4.0280 | −2.9527 | −2.1721 | −1.6679 | −1.1407 | 0.007 |
| $T$ = 303.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.7686 | 0.0297 | −0.5328 | −0.9571 | 1.3112 | 0.008 |
| $\Delta\kappa_S/(TPa^{-1})$ | 182.40 | 62.91 | 2.44 | −46.21 | 20.41 | 0.18 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −3.3205 | −2.2966 | −1.5621 | −1.7119 | −1.5733 | 0.003 |

2-Pentanol (1) + Dodecane (2)

| | $B_0$ | $B_1$ | $B_2$ | $B_3$ | $B_4$ | $\sigma$ |
|---|---|---|---|---|---|---|
| $T$ = 293.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.4424 | 0.2097 | 0.0986 | 0.1326 | 0.1015 | 0.003 |
| $\Delta\kappa_S/(TPa^{-1})$ | 96.47 | 49.08 | −0.50 | −11.43 | 3.75 | 0.10 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −4.6806 | −3.2661 | −1.9985 | −2.3620 | −2.1345 | 0.009 |
| $T$ = 298.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.5752 | 0.2653 | 0.2517 | −0.0056 | 0.1199 | 0.003 |
| $\Delta\kappa_S/(TPa^{-1})$ | 103.01 | 56.02 | 9.93 | −13.88 | −0.72 | 0.13 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −3.5923 | −2.4976 | −1.6175 | −1.7111 | −1.4742 | 0.007 |
| $T$ = 303.15 K | | | | | | |
| $V^E/(cm^3 \cdot mol^{-1})$ | 2.7207 | 0.2808 | 0.3926 | −0.0985 | 0.1801 | 0.003 |
| $\Delta\kappa_S/(TPa^{-1})$ | 109.45 | 60.65 | 20.21 | −12.46 | −5.93 | 0.14 |
| $10^3\ \Delta\eta/(Pa \cdot s)$ | −2.9188 | −1.9335 | −1.2152 | −1.8627 | −1.8528 | 0.009 |

**Table 6. UNIQUAC Parameters and Root-Mean-Square Deviations, $\sigma$**

| systems | $\tau_{12}/(J \cdot mol^{-1})$ | $\tau_{21}/(J \cdot mol^{-1})$ | $\sigma$ |
|---|---|---|---|
| 2-pentanol + octane | −323.977 | 455.028 | 0.436 |
| 2-pentanol + decane | −614.978 | 551.024 | 0.411 |
| 2-pentanol + dodecane | −487.827 | 452.374 | 0.570 |

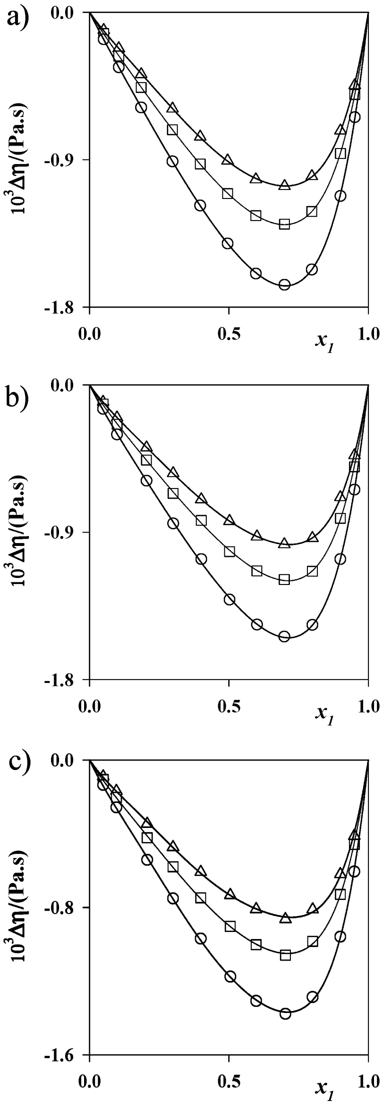

**Figure 3.** Dynamic viscosity, $\eta$, from the Redlich−Kister equation plotted against mole fraction at T = 293.15 K (○), T = 298.15 K (□) and T = 313.15 K (△), for the binary mixtures: a)2-pentanol-(1)+octane(2), b) 2-pentanol(1)+decane(2) and c) 2-pentanol-(1)+dodecane(2).

## 4. Correlation and Prediction

The UNIQUAC[14] equation is used for calculating of the excess molar free energy of activation for flow, $\Delta G^{*E}$, which is related to the viscosity by

$$\ln(\nu M) = \sum_i x_i \ln(\nu_i M_i) + \Delta G^{*E}/RT \qquad (8)$$

The correlation has been performed with experimental data using the UNIQUAC equation for minimizing the following

**Table 7. Experimental Data Used for Calculating New Interaction Parameters**

| binary systems | range $T$/K | no. data points | interaction parameters |
|---|---|---|---|
| pentane with hexane, heptane, octane, nonane, decane, hexadecane[a] | 298.15 | 54 | $CH_2/CH_3$ |
| hexane with heptane, octane, decane[b] | 293.15 | 27 | |
| heptane with octane, decane[b] | 293.15 | 18 | |
| octane with decane[a] | 293.15 | 9 | |
| 3-methylpentane with decane, hexadecane[c] | 298.15 | 14 | |
| 2-methylpentane with hexadecane[c] | 298.15 | 7 | |
| 2,2-dimethylpentane with decane, hexadecane[c] | 298.15 | 14 | |
| 2,2-dimethylhexane with decane, hexadecane[b,c] | 298.15 | 14 | |
| 2-propanol with octane, decane, dodecane[d] | 293.15−303.15 | 117 | $CH_2/OH_S$ and $CH_3/OH_S$ |
| 2-butanol with octane, decane, dodecane[e] | 293.15−303.15 | 117 | |
| 2-pentanol with octane, decane, dodecane[f] | 293.15−303.15 | 117 | |

[a] Aucejo et al.[16] [b] Cooper et al.[17] [c] Aucejo et al.[18] [d] Gonzalez et al.[3] [e] Gonzalez et al.[4] [f] In this paper.

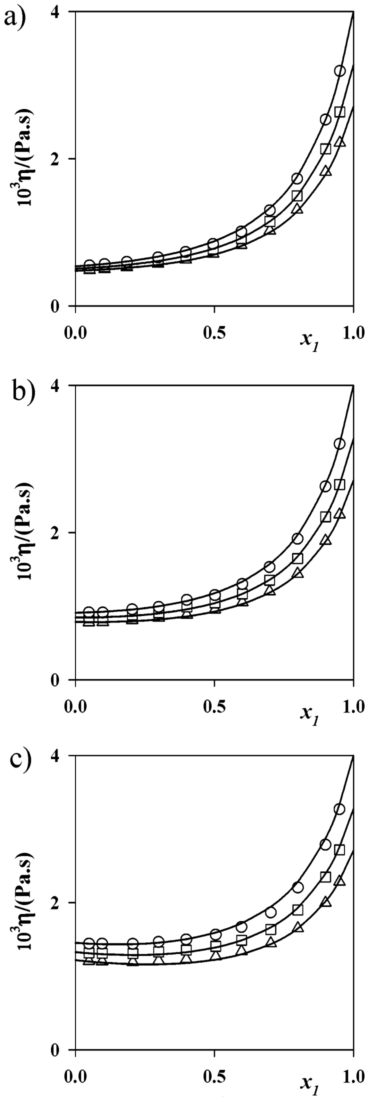

**Figure 4.** Viscosity deviations, $\Delta\eta$, from the UNIQUAC equation plotted against mole fraction at ○, $T$ = 293.15 K; □, $T$ = 298.15 K; △, $T$ = 313.15 K for the binary mixtures: a, 2-pentanol(1) + octane(2); b, 2-pentanol(1) + decane(2); c, 2-pentanol(1) + dodecane(2).

**Table 8. UNIFAC−VISCO Interaction New Parameters**

| $\alpha_{mn}$ | −CH2− | CH3− | $-OH_s-$ |
|---|---|---|---|
| −CH2− | 0 | 194.26 | 1270.60 |
| CH3− | −872.51 | 0 | 4802.35 |
| $-OH_s-$ | 6478.42 | −263.12 | 0 |

objective function (OF)

$$\mathrm{OF} = \sum \left| \frac{\{G^{*E}_{\mathrm{calc}}\}/\{RT\} - \{G^{*E}_{\mathrm{exp}}\}/\{RT\}}{G^{*E}_{\mathrm{exp}}/RT} \right| \qquad (9)$$

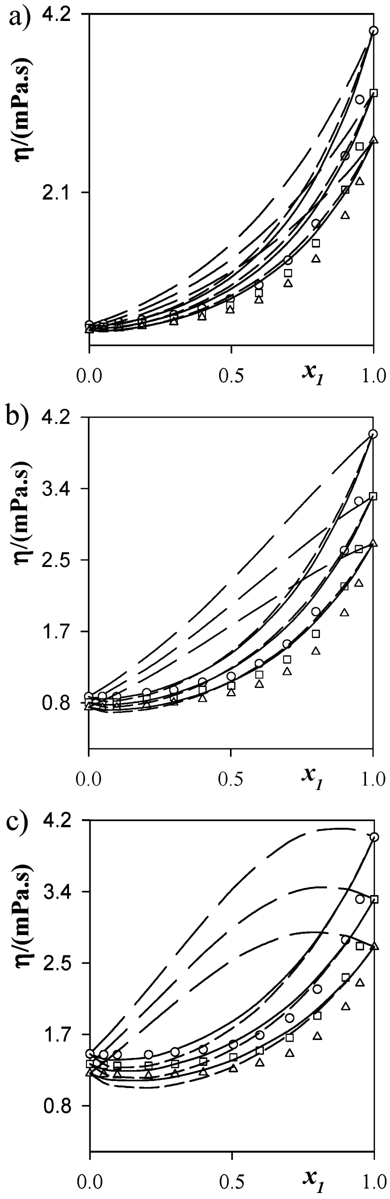

**Figure 5.** Predicted values of dynamic viscosities, $\eta$, from the UNIFAC−VISCO using Chevalier parameters (long-dashed line), UNIFAC−VISCO using new parameters (solid line), and ASOG−VISCO (dashed line) methods plotted against mole fraction at ○, $T$ = 293.15 K (experimental data); □, $T$ = 298.15 K (experimental data); △, $T$ = 303.15 K (experimental data) for the binary mixtures: a, 2-pentanol(1) + octane(2); b, 2-pentanol(1) + decane(2); c, 2-pentanol(1) + dodecane(2).

where $G^{*E}_{\mathrm{calc}}$ is the excess molar free energy calculated and $G^{*E}_{\mathrm{exp}}$ is the excess molar free energy experimental. The fitting parameters ($\tau_{12}$,$\tau_{21}$) together with the root-mean-square deviations ($\sigma$) are reported in Table 6.

**Table 9. Root-Mean-Square Deviation, $\sigma$, of Dynamic Viscosity Resulting by the Prediction Using UNIFAC−VISCO (New Parameters), UNIFAC−VISCO (Chevalier Parameters) and ASOG−VISCO Methods for the Binary Mixtures (2-Pentanol + Alkane) at Several Temperatures**

| systems | $T$/K | $\sigma$ UNIFAC−VISCO (new parameters) | $\sigma$ UNIFAC−VISCO (Chevalier parameters) | $\sigma$ ASOG−VISCO |
|---|---|---|---|---|
| 2-pentanol (1) + octane (2) | 293.15 | 18.2 | 45.8 | 22.0 |
| | 298.15 | 15.3 | 41.9 | 18.6 |
| | 303.15 | 13.0 | 38.6 | 15.9 |
| 2-pentanol (1) + decane (2) | 293.15 | 15.9 | 59.2 | 18.0 |
| | 298.15 | 13.5 | 55.0 | 15.1 |
| | 303.15 | 11.3 | 51.7 | 12.8 |
| 2-pentanol (1) + dodecane (2) | 293.15 | 13.5 | 70.4 | 13.6 |
| | 298.15 | 11.1 | 65.8 | 11.6 |
| | 303.15 | 9.5 | 61.9 | 10.3 |

Figure 4 shows the viscosity correlated by the UNIQUAC equation. It can be seen that this equation fitted fairly well the experimental data at several temperatures.

Predictions using the UNIFAC−VISCO and ASOG−VISCO methods have been determined. These predictive methods have been applied to compare the difference between predicted and experimental dynamic viscosities.

The new parameters of the UNIFAC−VISCO method corresponding to secondary alcohols with alkanes have been calculated. These parameters have been determined from experimental values of dynamic viscosities applying the Nelder and Mead[15] equation for minimizing the following OF

$$\mathrm{OF} = \frac{1}{N}\sum_{i=1}^{N}\frac{|\eta_{i,\mathrm{exp}} - \eta_{i,\mathrm{calc}}|}{\eta_{i,\mathrm{exp}}} \tag{10}$$

where $N$ is the number of experimental data and $\eta_{i,\mathrm{exp}}$ and $\eta_{i,\mathrm{calc}}$ are the experimental and calculated dynamic viscosities, respectively.

The results of the prediction of these systems is not good when we use the interaction parameters of the Chevalier's UNIFAC−VISCO method. Then, to improve the results of the prediction of the UNIFAC−VISCO method for the systems secondary alcohols−alkanes, we first have recalculated the interaction parameter within $CH_2$ and $CH_3$ groups. Table 7 shows the experimental data used for calculating new interaction parameters pointing out the corresponding binary systems employed.

The interaction parameters ($\alpha_{mn}$) are summarized in Table 8. The predictions applying UNIFAC−VISCO using new parameters were compared with the predictions applying UNIFAC−VISCO using Chevalier parameters and ASOG−VISCO methods.

Table 9 shows root-mean-square deviations of dynamic viscosity ($\sigma$) resulting by the prediction using UNIFAC−VISCO with Chevalier parameters, UNIFAC−VISCO with the new and review parameters, and ASOG−VISCO methods for the binary mixtures 2-pentanol with alkanes at $T$ = (293.15, 298.15, 303.15) K.

Figure 5 shows graphically the experimental dynamic viscosities and the predicted values by applying the UNIFAC−VISCO using Chevalier parameters, UNIFAC−VISCO using new parameters, and ASOG-VISCO for the binary mixtures 2-pentanol(1) + octane(2), 2-pentanol(1) + decane(2), and 2-pentanol(1) + dodecane(2) at $T$ = (293.15, 298.15, 303.15) K.

## 5. Conclusions

The correlation of the experimental data had been determined using the UNIQUAC equation. Very good results have been obtained with this equation.

The interaction parameters between $CH_2/CH_3$ were recalculated, and with the experimental data, the interaction parameters of $CH_2/OH_s$ and $CH_3/OH_s$ were determined.

Prediction of the dynamic viscosities of these mixture from UNIFAC−VISCO using new parameters, UNIFAC−VISCO using Chevalier parameters, and ASOG−VISCO methods have been determined. The UNIFAC−VISCO using new parameters and ASOG−VISCO methods predict in a similar way the behavior of these mixtures.

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