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Densities and Viscosities of Binary Mixtures of 1-Chlorobutane with Butanol Isomers at Several Temperatures

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Densities and viscosities of 1-chlorobutane + 1-butanol, + 2-methyl-1-propanol, + 2-butanol, or + 2-methyl-2-propanol were measured at several temperatures between 288.15 K and 318.15 K. At each temperature, the experimental viscosity data were correlated by means of the McAllister biparametric equation. By using our previous thermodynamic measurements (VLE, H^E), we have tested the Wei and Rowley nonparametric model at T = 298.15 K, obtaining average absolute deviations that are comparable to those calculated for the biparametric model.

Introduction

Although considerable progress has been achieved in the description of alkanol + alkane mixtures, the corresponding progress in mixtures of alkanol + a second polar component whose molecules may compete with alcohol molecules for hydrogen bond formation is rather limited. In recent publications, we presented equilibrium thermodynamic properties[1,2] for mixtures of (1-chlorobutane + butanol isomers). In this paper, we report viscosity data for these systems at four temperatures between 288.15 K and 318.15 K as well as density data at three temperatures. Excess molar volumes, at 298.15 K, for mixtures of 1-chlorobutane + 1-butanol or 2-methyl-2-propanol have been published previously,[3] as well as for mixtures of 1-chlorobutane + 2-methyl-1-propanol or 2-butanol.[2] Data are in agreement with other authors' measurements found in the literature[4,5] at 298.15 K and 313.15 K.

Experimental Section

1-Chlorobutane (mole fraction >0.995), 1-butanol (mole fraction >0.998), 2-methyl-1-propanol (mole fraction >0.995), 2-butanol (mole fraction >0.990), and 2-methyl-2-propanol (mole fraction >0.995) were Aldrich products. All of the chemicals had low water content, were supplied with an analysis certificate, and were used without further purification.

Table 1. Density ρ and Dynamic Viscosity η of the Pure Compounds

		ρ/g·cm^{-3}		η/mPa·s	
compound	T/K	exptl	lit	exptl	lit
1-chlorobutane	288.15	0.891 87	0.8909^{a}	0.477	0.469^{b}
	298.15	0.880 18	0.8804^{c}	0.429	0.427^{b}
	303.15	0.875 19	0.8750^{c}	0.409	0.405^{b}
	308.15	0.869 64	0.8694^{a}	0.390	
	313.15	0.863 94	0.8639^{c}	0.372	
	318.15	0.858 31	0.8581^{a}	0.354	
1-butanol	288.15	0.813 42	0.8134^{d}	3.346	3.3790^{c}
	298.15	0.805 40	0.8060^{e}	2.560	2.5710^{f}
	308.15	0.798 14	0.7983^{d}	1.991	2.000^{f}
	318.15	0.790 19	0.7907^{d}	1.569	1.5786^{f}
2-methyl-1-propanol	288.15	0.805 47	0.8055^{d}	4.805	4.6556^{f}
	298.15	0.797 37	0.7978^{e}	3.435	3.3330^{f}
	308.15	0.790 10	0.7897^{d}	2.508	2.445^{f}
	318.15	0.781 99	0.7818^{d}	1.870	1.834^{f}
2-butanol	288.15	0.810 72	0.8111^{d}	4.509	4.444^{f}
	298.15	0.801 82	0.8026^{e}	3.035	2.998^{f}
	308.15	0.794 07	0.7939^{d}	2.111	2.1019^{f}
	318.15	0.785 15	0.7854^{d}	1.523	1.525^{f}
2-methyl-2-propanol	298.15	0.779 96	0.7812^{e}	4.433	4.438^{f}
	303.15	0.775 30	0.7757^{e}	3.355	3.390^{f}
	308.15	0.770 19	0.7703^{d}	2.611	2.644^{f}
	313.15	0.764 83	0.7649^{e}	2.074	2.1037^{f}
	318.15	0.759 52	0.7594^{d}	1.685	1.705^{f}

^{a} Interpolated from ref 7. ^{b} From ref 8. ^{c} From ref 7. ^{d} Interpolated from ref 9. ^{e} From ref 9. ^{f} From ref 10.

Ubbelohde viscometers (Schott) with relatively long flow times (60 s to 600 s, with water) were used to minimize the kinetic energy corrections. At least three readings of the flow time with variations not exceeding ±0.1 s were taken for each solution. The viscosities were calculated from the average flow time, t, by means of the equation

$$\nu = At - \frac{B}{t} \tag{1}$$

where ν is the kinematic viscosity. A and B are viscometer constants that were determined by using values from Marsh[6] for the water viscosity together with the corresponding flow times measured in this study. The viscometer was held in a water bath whose temperature was controlled to within ±10 mK. Three different viscometers were used during the course of this investigation. The masses of both components were determined by weighing, and the uncertainties in the mole fractions are estimated to be less than 0.0003. Flow-time measurements were performed with an electrical stopwatch to ±0.01 s. The uncertainty in the kinematic viscosity measurements is estimated to be $\pm 2 \times 10^{-9}$ m^2·s^{-1}.

Excess molar volumes were calculated from density measurements made with a densimeter (Anton Paar DMA 60/DMA 602). The uncertainty for V^E is 0.002 cm^3·mol^{-1}.

Results

Table 1 presents density and dynamic viscosity data of the pure compounds, which are compared with values

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Table 2. Experimental Densites ρ and Excess Molar Volumes V^{E} at Several Temperatures

x_2	ρ / g·cm^{-3}	V^{E} / cm^3·mol^{-1}	x_2	ρ / g·cm^{-3}	V^{E} / cm^3·mol^{-1}	x_2	ρ / g·cm^{-3}	V^{E} / cm^3·mol^{-1}
			1-Chlorobutane (1) + 1-Butanol (2)					
			T = 288.15 K					
0.0620	0.886 96	0.059	0.3967	0.862 58	0.048	0.6747	0.841 19	−0.019
0.1027	0.883 98	0.072	0.4541	0.858 30	0.034	0.7342	0.836 40	−0.033
0.1383	0.881 38	0.080	0.4822	0.856 17	0.028	0.7698	0.833 49	−0.040
0.2032	0.876 67	0.084	0.5076	0.854 25	0.020	0.8509	0.826 62	−0.043
0.2597	0.872 57	0.080	0.5466	0.851 25	0.012	0.9022	0.822 13	−0.037
0.2859	0.870 67	0.076	0.5818	0.848 53	0.002	0.9582	0.817 04	−0.018
0.3764	0.864 06	0.056	0.6332	0.844 49	−0.009			
			T = 308.15 K					
0.1056	0.861 88	0.132	0.3908	0.842 67	0.158	0.6908	0.821 85	0.063
0.1979	0.855 62	0.164	0.4964	0.835 50	0.129	0.7917	0.814 48	0.026
0.2842	0.849 82	0.172	0.5913	0.828 95	0.095	0.9003	0.806 19	0.000
			T = 318.15 K					
0.0612	0.853 78	0.111	0.3836	0.832 82	0.193	0.7868	0.806 09	0.035
0.0913	0.851 66	0.149	0.4858	0.826 26	0.162	0.8906	0.798 56	0.008
0.1849	0.845 48	0.201	0.5859	0.819 71	0.125			
0.2759	0.839 66	0.211	0.6868	0.812 99	0.076			
			1-Chlorobutane (1) + 2-Methyl-1-propanol (2)					
			T = 288.15 K					
0.0369	0.888 52	0.050	0.4421	0.855 33	0.089	0.7517	0.828 80	−0.002
0.0769	0.885 16	0.079	0.5564	0.845 76	0.057	0.7555	0.828 45	−0.002
0.1526	0.878 94	0.109	0.5739	0.844 30	0.049	0.7567	0.828 35	−0.003
0.2287	0.872 74	0.121	0.6250	0.839 91	0.035	0.8490	0.819 90	−0.016
0.2853	0.868 15	0.119	0.6843	0.834 73	0.020	0.9196	0.813 20	−0.015
0.3791	0.860 52	0.103	0.7309	0.830 64	0.005	0.9806	0.807 26	−0.007
			T = 308.15 K					
0.1006	0.861 12	0.169	0.3894	0.838 94	0.251	0.6914	0.815 70	0.137
0.1959	0.853 68	0.231	0.4895	0.831 33	0.227	0.7941	0.807 44	0.088
0.2770	0.847 47	0.254	0.5863	0.823 90	0.189	0.8989	0.798 78	0.038
			T = 318.15 K					
0.0905	0.850 62	0.196	0.3772	0.829 29	0.311	0.6819	0.806 85	0.197
0.1869	0.843 28	0.277	0.4806	0.821 73	0.290	0.7816	0.799 34	0.129
0.2712	0.837 05	0.306	0.5812	0.814 29	0.256	0.8896	0.791 03	0.048
			1-Chlorobutane (1) + 2-Butanol (2)					
			T = 288.15 K					
0.0500	0.887 10	0.129	0.4058	0.858 45	0.326	0.6634	0.838 14	0.240
0.1177	0.881 38	0.219	0.4104	0.858 09	0.326	0.7388	0.832 24	0.180
0.1435	0.879 24	0.246	0.4986	0.851 12	0.315	0.7984	0.827 45	0.137
0.1962	0.874 99	0.283	0.5241	0.849 12	0.307	0.8286	0.824 99	−1.326
0.2227	0.872 88	0.296	0.5527	0.846 87	0.296	0.8840	0.820 50	−0.980
0.3400	0.863 63	0.325	0.6114	0.842 23	0.272	0.9367	0.816 07	−0.579
			T = 308.15 K					
0.1007	0.860 49	0.291	0.3881	0.838 47	0.503	0.6927	0.816 37	0.370
0.1941	0.853 08	0.410	0.4876	0.831 15	0.495	0.7950	0.808 99	0.269
0.2775	0.846 72	0.471	0.5897	0.823 73	0.453	0.8963	0.801 67	0.146
			T = 318.15 K					
0.0864	0.850 35	0.299	0.3820	0.828 00	0.576	0.6823	0.806 95	0.443
0.1906	0.842 10	0.466	0.4862	0.820 61	0.565	0.7865	0.799 78	0.330
0.2732	0.835 88	0.540	0.5852	0.813 65	0.523	0.8928	0.792 59	0.171
			1-Chlorobutane (1) + 2-Methyl-2-propanol (2)					
			T = 303.15 K					
0.0924	0.864 09	0.325	0.3800	0.834 23	0.653	0.6749	0.804 89	0.630
0.1915	0.853 49	0.497	0.4810	0.824 02	0.689	0.7778	0.795 09	0.515
0.2758	0.844 75	0.592	0.5729	0.814 91	0.679	0.8938	0.784 46	0.300
			T = 308.15 K					
0.0969	0.857 96	0.357	0.3839	0.828 23	0.693	0.6849	0.798 55	0.648
0.1912	0.847 87	0.527	0.4811	0.818 50	0.721	0.7881	0.788 78	0.527
0.2786	0.838 90	0.620	0.5844	0.808 35	0.702	0.8957	0.779 05	0.313
			T = 313.15 K					
0.0930	0.852 60	0.365	0.3778	0.823 11	0.715	0.6796	0.793 58	0.657
0.1869	0.842 51	0.546	0.4841	0.812 56	0.739	0.7766	0.784 47	0.541
0.2685	0.834 13	0.639	0.5777	0.803 43	0.718	0.8972	0.773 57	0.305
			T = 318.15 K					
0.0918	0.847 04	0.380	0.3797	0.817 22	0.750	0.6780	0.788 38	0.661
0.1839	0.837 08	0.571	0.4809	0.807 29	0.764	0.7833	0.778 42	0.545
0.2674	0.828 47	0.677	0.5799	0.797 62	0.747	0.8905	0.768 84	0.324

Table 3. Absolute Viscosities η and Viscosity Deviations $\Delta\eta$ for {1-Chlorobutane (1) + Butanol Isomers (2)} at Different Temperatures

	$T = 288.15$ K		$T = 298.15$ K		$T = 308.15$ K		$T = 318.15$ K	
x_2	η / mPa·s	$\Delta\eta$ / mPa·s	η / mPa·s	$\Delta\eta$ / mPa·s	η / mPa·s	$\Delta\eta$ / mPa·s	η / mPa·s	$\Delta\eta$ / mPa·s
1-Chlorobutane (1) + 1-Butanol (2)								
0.0949	0.509	−0.241	0.452	−0.179	0.407	−0.134	0.367	−0.102
0.1964	0.570	−0.470	0.504	−0.343	0.448	−0.256	0.401	−0.191
0.2961	0.655	−0.671	0.570	−0.489	0.501	−0.363	0.444	−0.269
0.3949	0.774	−0.836	0.661	−0.609	0.576	−0.446	0.503	−0.331
0.4941	0.940	−0.954	0.788	−0.694	0.670	−0.510	0.577	−0.377
0.5915	1.175	−0.999	0.955	−0.735	0.797	−0.539	0.674	−0.398
0.6954	1.503	−0.969	1.204	−0.707	0.984	−0.519	0.816	−0.383
0.7940	1.934	−0.821	1.525	−0.596	1.226	−0.434	0.993	−0.326
0.8920	2.529	−0.507	1.955	−0.375	1.547	−0.271	1.238	−0.200
1-Chlorobutane (1) + 2-Methyl-1-propanol (2)								
0.1003	0.511	−0.401	0.454	−0.276	0.408	−0.194	0.369	−0.137
0.1993	0.568	−0.772	0.499	−0.529	0.445	−0.367	0.397	−0.259
0.2979	0.654	−1.113	0.567	−0.758	0.497	−0.523	0.440	−0.365
0.3954	0.784	−1.405	0.663	−0.955	0.574	−0.654	0.498	−0.455
0.4960	0.948	−1.676	0.787	−1.132	0.663	−0.777	0.567	−0.539
0.5936	1.198	−1.848	0.970	−1.243	0.801	−0.846	0.682	−0.572
0.6894	1.570	−1.891	1.230	−1.272	0.986	−0.864	0.808	−0.591
0.7923	2.196	−1.710	1.669	−1.142	1.295	−0.772	1.025	−0.530
0.8912	3.098	−1.237	2.284	−0.824	1.724	−0.554	1.330	−0.374
1-Chlorobutane (1) + 2-Butanol (2)								
0.0965	0.496	−0.370	0.444	−0.237	0.399	−0.157	0.362	−0.105
0.1973	0.542	−0.731	0.478	−0.465	0.426	−0.303	0.382	−0.202
0.2962	0.601	−1.071	0.524	−0.677	0.462	−0.437	0.410	−0.290
0.3934	0.688	−1.376	0.587	−0.867	0.510	−0.556	0.450	−0.364
0.4917	0.805	−1.655	0.675	−1.035	0.577	−0.658	0.498	−0.431
0.5923	0.995	−1.870	0.811	−1.162	0.676	−0.733	0.571	−0.476
0.6919	1.286	−1.981	1.011	−1.221	0.818	−0.762	0.676	−0.486
0.7931	1.764	−1.911	1.334	−1.161	1.034	−0.721	0.825	−0.456
0.8933	2.648	−1.431	1.901	−0.856	1.419	−0.508	1.072	−0.326

	$T = 298.15$ K		$T = 303.15$ K		$T = 308.15$ K		$T = 313.15$ K		$T = 318.15$ K	
x_2	η / mPa·s	$\Delta\eta$ / mPa·s	η / mPa·s	$\Delta\eta$ / mPa·s	η / mPa·s	$\Delta\eta$ / mPa·s	η / mPa·s	$\Delta\eta$ / mPa·s	η / mPa·s	$\Delta\eta$ / mPa·s
1-Chlorobutane (1) + 2-Methyl-2-propanol (2)										
0.0966	0.442	−0.373	0.419	−0.275	0.397	−0.207	0.378	−0.159	0.359	−0.124
0.2000	0.476	−0.754	0.449	−0.549	0.423	−0.411	0.400	−0.313	0.380	−0.241
0.2904	0.517	−1.074	0.486	−0.779	0.456	−0.579	0.428	−0.438	0.404	−0.337
0.3901	0.577	−1.414	0.537	−1.021	0.502	−0.754	0.468	−0.568	0.439	−0.435
0.4897	0.662	−1.728	0.611	−1.241	0.565	−0.912	0.525	−0.681	0.488	−0.518
0.5956	0.799	−2.015	0.727	−1.438	0.664	−1.049	0.608	−0.778	0.560	−0.587
0.6919	1.000	−2.200	0.892	−1.555	0.801	−1.125	0.724	−0.826	0.658	−0.617
0.8008	1.425	−2.211	1.232	−1.536	1.081	−1.087	0.947	−0.788	0.841	−0.580
0.8889	2.112	−1.876	1.752	−1.276	1.474	−0.890	1.255	−0.630	1.083	−0.455

found in the literature. Excess molar volumes, dynamic viscosity, and viscosity deviations were calculated according to the following equations

$$V^{E} = x_1M_1\left(\frac{1}{\rho} - \frac{1}{\rho_1}\right) + x_2M_2\left(\frac{1}{\rho} - \frac{1}{\rho_2}\right) \qquad (2)$$

$$\eta = \nu\rho \qquad (3)$$

$$\Delta\eta = \eta - (x_1\eta_1 + x_2\eta_2) \qquad (4)$$

where ρ and η are the density and the viscosity of the mixture, x is the mole fraction, M is the molar mass, and subscripts 1 and 2 indicate 1-chlorobutane and alcohol, respectively.

Tables 2 and 3 show the density and viscosity measurements at several temperatures together with excess molar volumes and viscosity deviations, which were fitted to a polynomial

$$Q = x_1x_2\sum_{i=0}^{m}A_i(x_1 - x_2)^i \qquad (5)$$

where Q denotes V^{E} or $\Delta\eta$. Table 4 lists the A_i coefficients together with the standard deviation, which is defined by

$$s(Q) = \left[\frac{\sum(Q_{\text{exptl}} - Q_{\text{calcd}})^2}{N - m}\right] \qquad (6)$$

where N is the number of experimental points and m is the number of parameters in the corresponding analytical equation. In Figures 1 and 2, the excess molar volume and the viscosity deviation are plotted at $T = 318.15$ K.

Discussion

For all systems, both V^{E} and $\Delta\eta$ increase with increasing temperature, and for mixtures containing 2-methyl-2-

Table 4. Coefficients A_i and Standard Deviations $s(V^E)$ and $s(\Delta\eta)$ for Equation 5

	V^E/cm^3·mol^{-1}					$\Delta\eta$/mPa·s				
T/K	A_0	A_1	A_2	A_3	$s(V^E)$	A_0	A_1	A_2	A_3	$s(\Delta\eta)$
1-Chlorobutane (1) + 1-Butanol (2)										
288.15	0.096	0.515	0.165	0.357	0.003	−3.835	1.738	−0.421	−0.218	0.007
298.15						−2.799	1.286	−0.329	−0.199	0.002
308.15	0.505	0.600	0.279	0.422	0.003	−2.055	0.940	−0.241	−0.227	0.002
318.15	0.619	0.729	0.373	0.517	0.004	−1.519	0.691	−0.215	−0.169	0.003
1-Chlorobutane (1) + 2-Methyl-1-propanol (2)										
288.15	0.284	0.572	0.181	0.311	0.003	−6.703	4.333	−2.923	1.427	0.014
298.15						−4.531	2.844	−1.920	0.911	0.010
308.15	0.882	0.670	0.345	0.337	0.004	−3.099	1.891	−1.279	0.555	0.007
318.15	1.136	0.591	0.335	0.859	0.004	−2.133	1.225	−0.887	0.429	0.005
1-Chlorobutane (1) + 2-Butanol (2)										
288.15	1.245	0.489	0.226	0.823	0.004	−6.634	4.901	−4.598	3.076	0.017
298.15						−4.156	2.944	−2.610	1.648	0.009
308.15	1.947	0.565	0.562	0.697	0.008	−2.650	1.808	−1.468	0.735	0.004
318.15	2.237	0.589	0.675	0.878	0.006	−1.725	1.087	−0.911	0.520	0.004
1-Chlorobutane (1) + 2-Methyl-2-propanol (2)										
298.15						−6.898	5.603	−7.149	6.033	0.046
303.15	2.738	−0.133	1.072	0.814	0.006	−4.968	3.921	−4.660	3.692	0.028
308.15	2.858	−0.090	1.207	0.768	0.008	−3.659	2.784	−3.090	2.299	0.018
313.15	2.930	0.045	1.207	0.817	0.008	−2.738	2.001	−2.095	1.446	0.011
318.15	3.039	0.209	1.253	0.717	0.009	−2.086	1.464	−1.473	0.914	0.007

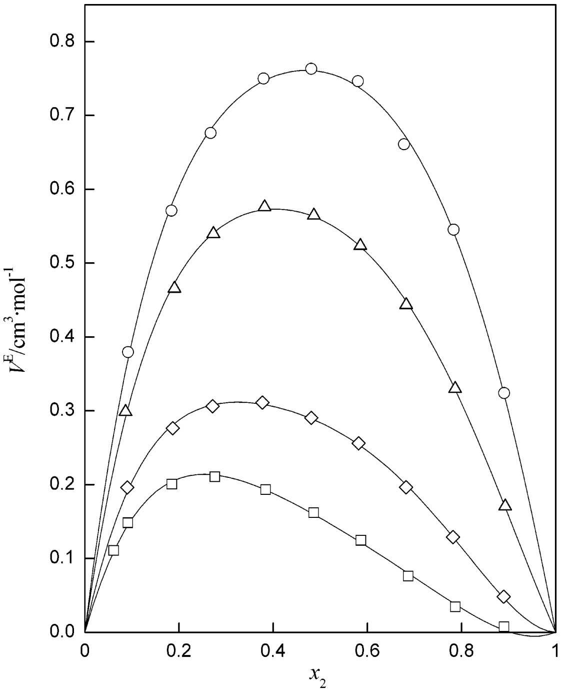

Figure 1. Excess molar volume at T = 318.15 K for □, {x_1 1-chlorobutane + x_2 1-butanol}; ◇, {x_1 1-chlorobutane + x_2 2-methyl-1-propanol}; △, {x_1 1-chlorobutane + x_2 2-butanol}; ○, {x_1 1-chlorobutane + x_2 2-methyl-2-propanol}; and —, from analytical equations.

propanol, we observe the lowest variation in V^E and the highest variation in $\Delta\eta$. At T = 318.15 K, Figures 1 and 2 show the experimental data for the four mixtures (1-chlorobutane + butanol isomers). V^E increases with the branching around the OH group, and for $\Delta\eta$, the more negative values are observed in mixtures containing 2-methyl-2-propanol.

Many semitheoretical and empirical equations have been used to fit the isothermal viscosity data of mixtures. These equations can be distinguished as predictive or correlative and have been reviewed and discussed extensively by Mehrotra et al.[11] We have selected the McAllister two-parameter equation[12] based on Eyring's equation, which takes into account interactions of both like and unlike molecules by a 2D three-body model. The McAllister equation is given by

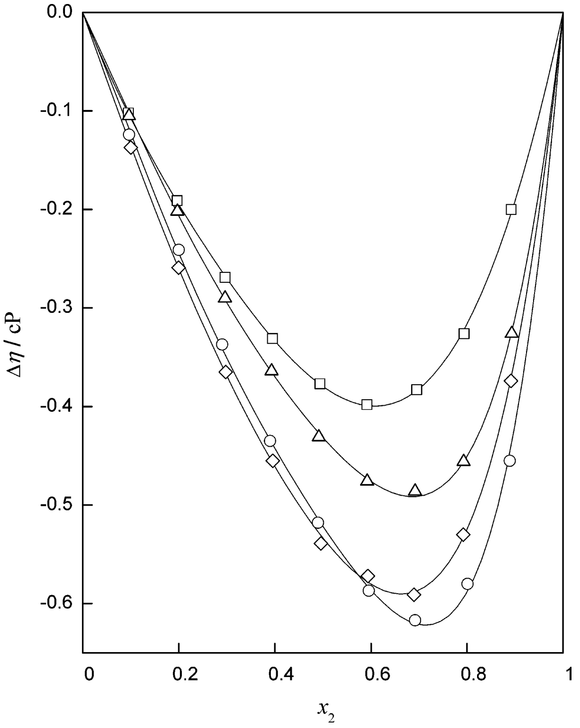

Figure 2. Viscosity deviation at T = 318.15 K for □, {x_1 1-chlorobutane + x_2 1-butanol}; ◇, {x_1 1-chlorobutane + x_2 2-methyl-1-propanol}; △, {x_1 1-chlorobutane + x_2 2-butanol}; ○, {x_1 1-chlorobutane + x_2 2-methyl-2-propanol}; —, from analytical equations.

$$\ln \nu = x_1^{\,3} \ln \nu_1 + 2x_1^{\,2}x_2 \ln \nu_{12} + 2x_1x_2^{\,2} \ln \nu_{21} + x_2^{\,3} \ln \nu_2 - \ln\left(x_1 + x_2\frac{M_2}{M_1}\right) + 3x_1^{\,2}x_2 \ln\left(\frac{2 + \{M_2\}/\{M_1\}}{3}\right) + 3x_1x_2^{\,2} \ln\left(\frac{1 + \{2M_2/M_1\}}{3}\right) + x_2^{\,3} \ln\left(\frac{M_2}{M_1}\right) \qquad (7)$$

Table 5. Mixed Kinematic Viscosity Parameters and Average Absolute Deviations (AAD) of Experimental and Calculated Kinematic Viscosities (10^{-6} m^2·s^{-1}) at Several Temperatures

	1-chlorobutane (1) +							
	1-butanol (2)		2-methyl-1-propanol (2)		2-butanol (2)		2-methyl-2-propanol (2)	
T/K	ν_{12}	ν_{21}	ν_{12}	ν_{21}	ν_{12}	ν_{21}	ν_{12}	ν_{21}
288.15	0.648	1.616	0.673	1.406	0.677	0.908		
298.15	0.583	1.285	0.600	1.131	0.601	0.770	0.690	0.541
303.15							0.633	0.545
308.15	0.527	1.059	0.544	0.928	0.536	0.676	0.580	0.547
313.15							0.537	0.542
318.15	0.481	0.884	0.493	0.787	0.486	0.594	0.502	0.532
AAD/%	0.41		0.56		0.92		2.17	

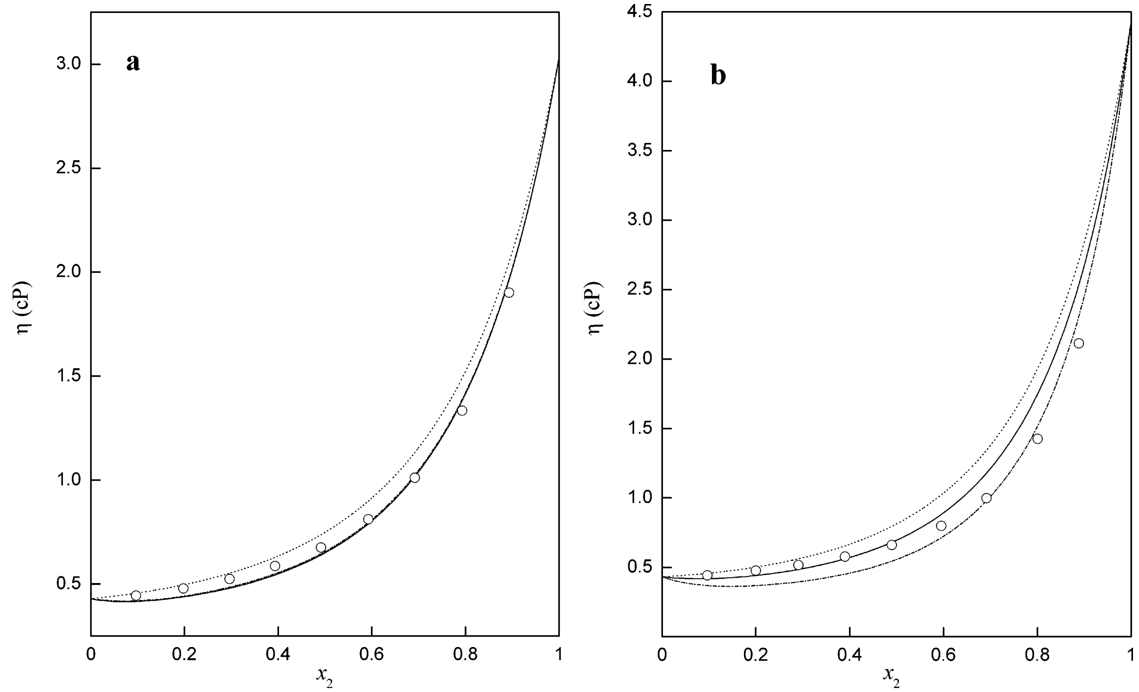

Figure 3. Dynamic viscosity at T = 298.15 K for (a) {x_1 1-chlorobutane + x_2 2-butanol} and (b) {x_1 1-chlorobutane + x_2 2-methyl-2-propanol}. ○, Experimental, from the NRTL model: ···, with σ = 0.00; —, with σ = 0.25 (predictive), – · – · –, with σ (fitted).

i = 1 for 1-chlorobutane and 2 for alcohol, ν is the kinematic viscosity of the pure compounds, x is the mole fraction, M is the molar mass, and ν_{12} and ν_{21} are fitting parameters that denote viscosity contributions for 112 and 221 interactions, respectively, and have been calculated for each temperature by a least-squares method. For each system at several temperatures, the mixed viscosity parameters are collected in Table 5 together with the average absolute deviations (AAD) that are defined by

$$\mathrm{AAD} = \left[\frac{100}{N}\sum\left|\ln \nu_{\mathrm{exptl}} - \ln \nu_{\mathrm{calcd}}\right|\right] \tag{8}$$

where N is the number of experimental points.

Wei and Rowley[13,14] proposed a local composition model for the multicomponent nonelectrolyte liquid mixture viscosity, which requires only binary equilibrium thermodynamic information (H^E, G^E) in addition to pure-component data. No mixture viscosities and no adjustable parameters are required. The basic equations of the model are given by

$$\eta = \frac{\exp(\xi)}{V} \tag{9}$$

$$\xi = \sum_i \phi_i \xi_i^0 + \sum_i \phi_i \left[\frac{\sum_j \phi_j G_{ji}(\xi_{ji} - \xi_j^0)}{\sum_l \phi_l G_{li}}\right] - \frac{\sigma H^E}{RT} \tag{10}$$

$$\xi_{ji} = \xi_{ij} = \frac{\sum_i (\phi_i^* \phi_{ii}^* \xi_i^0)}{\sum_j (\phi_j^* \phi_{jj}^*)} \tag{11}$$

where for an i, j ($i \neq j$) pair of interactions

$$G_{ji} = \exp\left(-\frac{\alpha A_{ji}}{RT}\right) \tag{12}$$

$$\phi_j^* = (1 + \Gamma_{ji})^{-1} \qquad \phi_{ii}^* = \left(1 + \frac{\phi_j^* G_{ji}}{\phi_i^*}\right)^{-1} \tag{13}$$

$$\Gamma_{ji} = \left(\frac{V_i}{V_j}\right)\left(\frac{G_{ij}}{G_{ji}}\right)^{1/2} \exp\left[\frac{\xi_i^0 - \xi_j^0}{2}\right] \tag{14}$$

The * symbol stands for the volume fraction at specific

Table 6. Standard Deviations $s(\eta)$ for Experimental and Calculated Dynamic Viscosity η (mPa·s) According to the Wei and Rowley Model at $T = 298.15$ K for $\sigma = 0.00$, $\sigma = 0.25$, and σ (Fitted)

system	σ	$s(\eta)$	σ	$s(\eta)$	σ	$s(\eta)$
1-chlorobutane (1) + 1-butanol (2)	0.00	0.099	0.25	0.140	−0.39	0.060
1-chlorobutane (1) + 2-methyl-1-propanol (2)	0.00	0.039	0.25	0.103	−0.12	0.020
1-chlorobutane (1) + 2-butanol (2)	0.00	0.083	0.25	0.037	0.23	0.036
1-chlorobutane (1) + 2-methyl-2-propanol (2)	0.00	0.272	0.25	0.173	0.60	0.109

composition defined by eq 12, and ξ_i^0 denotes the pure-component i value

$$\xi_i^0 = \ln(\eta_i V_i) \tag{15}$$

The same notation as in the original paper is used. α, A_{ij}, and A_{ji} stand for the binary NRTL parameters. In this work, these parameters have been calculated from our vapor pressure data, and H^E values have been taken from our experimental results.[1−3] If the σ factor in eq 10 is taken to be 0.25, as in the original paper, then the validity of the model as a nonparametric predictive method is then tested. In Table 6, standard deviations $s(\eta)$, defined by eq 6, at 298.15 K for three σ values [$\sigma = 0.00$ (no H^E contribution), $\sigma = 0.25$ (predictive), and σ (fitted)] are collected, and the corresponding dynamic viscosity is plotted in Figure 3 for 2-butanol and 2-methyl-2-propanol, the best and the worst standard deviation for $\sigma = 0.25$, respectively. We can conclude that in all systems η is well described by the predictive model ($\sigma = 0.25$). The agreement with the experimental results is comparable to that obtained with σ (fitted) (monoparametric) or with the McAllister biparametric equation. Previous studies of mixtures of butanol isomers with butanone or butanenitrile yield similar agreement between experimental and calculated results.[15,16] By taking into account the complicated interactions in these mixtures, we can conclude that the NRTL model (predictive) gives an adequate representation of these systems.

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