Densities and Viscosities for Mixtures of Pentyl Acetate and Hexyl Acetate with Normal Alkanols at 298.15 K

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Densities and viscosities of the binary systems of pentyl and hexyl acetates with *n*-alkanols (ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, and 1-octanol) have been measured at 298.15 K and atmospheric pressure, over the whole composition range. The excess volumes and change in viscosity have been obtained from the density and dynamic viscosity results. For all systems, the excess volumes are positive as the length of the hydrocarbon chain of the alkanol increases. The results of the viscosity−composition are discussed in the light of various viscosity equations suggested by Tamara and Kurata, Hind et al., McAllister, and Heric and Brewer.

Introduction

Recently, there has been increasing interest in the physical properties of several binary systems of aliphatic esters with normal alkanols (Acevedo et al., 1990; Ortega et al., 1985, 1986). In this contribution we report the densities and viscosities for mixtures of pentyl and hexyl acetates with *n*-alkanols (ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, and 1-octanol) at 298.15 K and atmospheric pressure. The results of excess molar volumes (V^E) were correlated by using a polynomial expression. The viscosities were correlated by the models of Tamara and Kurata (1952), Hind et al. (1960), and McAllister (1960). The last method has been used to determine the interaction parameters (ν_{ij}) from the kinematic viscosity results.

Experimental Section

Material. Pentyl and hexyl acetates were obtained from Aldrich (purity >99.5 mol %). The *n*-alkanols were provided by Merck (purity >99.8 mol %). All the chemicals were used without further purifications.

Density (ρ) measurements of the pure components and binary mixtures, over the complete composition range, were carried out using a Kyoto electronic vibrating tube densimeter (model DA 110) with a temperature sensor keeping the temperature within ±0.001 K. The apparatus was calibrated several times with deionized double-distilled and degassed water, benzene, and dry air at atmospheric pressure. The precision of the density measurements was within ±0.001%.

The mixtures were prepared by weight in 2 cm^3 vials using a Mettler analytical balance (model A 160) with an accuracy of ±0.01 mg using a procedure described previously (Ortega et al., 1985). The mole fraction accuracy is estimated to be ±0.01%.

Viscosity (η) measurements of both components and their mixtures were determined by using an Ubbelohde viscometer which was calibrated with doubly distilled water and benzene as described by Singh et al. (1995). The accuracy was estimated to be ±0.05%. The density and viscosity values and those from literature for all the pure compounds are listed in Table 1. Thus our results obtained are in good agreement with those listed in the literature.

Results and Discussion

The density and viscosity for (x)esters + (1 − x)*n*-alkanol mixtures at 298.15 K are reported in Table 2. The density values were used to derive the V^E values from the following equation:

$$V^E/\mathrm{cm}^3\cdot\mathrm{mol}^{-1} = x_1M_1(\rho_m^{-1} - \rho_1^{-1}) + x_2M_2(\rho_m^{-1} - \rho_2^{-1}) \quad (1)$$

where x_i, ρ_i, and M_i are the mole fraction, density, and relative mole mass of pure components respectively, with $i = 1$ for the esters and $i = 2$ for the *n*-alkanols, and ρ_m is the density of the mixture at given composition x.

The excess volumes, V^E, were fitted by the least squares method of the Redlich−Kister (1948) equation:

$$V^E/\mathrm{cm}^3\cdot\mathrm{mol}^{-1} = x(1-x)\sum_{i=0}^{n} A_j(2x-1)^j \quad (2)$$

where A_j are parameters and n is the number of polynomial coefficients ascertained from the variation of the standard error of estimate (σ) with n,

$$\sigma(V^E) = [\sum(V^E_{calc} - V^E_{exp})^2/(N-n)]^{0.5} \quad (3)$$

where N is the number of measurements. The values of A_j and $\sigma(V^E)$ are given in Table 3.

Table 1. Densities and Viscosities for the Pure Components at 298.15 K

	ρ/g cm^{-3}		η/mPa·S	
substance	exp	lit.	exp	lit.
pentyl acetate	0.870 73	0.870 70[a]	0.865	0.862[a]
hexyl acetate	0.868 42	0.868 10[a]	1.107	1.245[a] (15 °C)
				0.968[a] (30 °C)
ethanol	0.785 29	0.785 34[b]	1.086	1.085[b]
n-propanol	0.799 82	0.799 60[c]	1.894	1.898[c]
n-butanol	0.805 81	0.805 80[a]	2.512	2.509[c]
		0.805 70[c]		
n-pentanol	0.810 84	0.810 80[a]	3.318	3.347[a]
				3.310[g]
n-hexanol	0.815 25	0.815 30[a]	4.595	4.592[a]
		0.815 80[d]		4.590[h]
n-heptanol	0.818 87	0.818 70[e]	4.836	6.350[a] (20 °C)
				3.321[a] (30 °C)
n-octanol	0.822 14	0.822 09[f]	6.130	6.125[a]
		0.821 50[e]		

[a] Riddick et al. (1986). [b] El-Banna and Ramadan (1995). [c] Aminabhavi and Gopalakrishna (1995). [d] Kim and Lee (1994). [e] Yu and Tasi (1994). [f] Ortega et al. (1985). [g] Manick (1968). [h] Singh et al. (1990).

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Table 2. Densities (ρ) and Viscosities (η) for (x)Esters + (1 − x)*n*-Alkanols at 298.15 K

x	ρ/g cm^{-3}	η/mPa·s	x	ρ/g cm^{-3}	η/mPa·s	x	ρ/g cm^{-3}	η/mPa·s
			(x)$CH_3COOC_5H_{11}$ + (1 − x)C_2H_5OH					
	±0.001%	±0.05%		±0.001%	±0.05%		±0.001%	±0.05%
0.026 94	0.790 60	1.046	0.341 42	0.833 04	0.989	0.733 12	0.854 98	0.894
0.069 37	0.798 46	1.065	0.422 41	0.839 50	0.968	0.802 45	0.862 61	0.883
0.115 43	0.805 89	1.052	0.503 43	0.845 55	0.946	0.884 13	0.866 16	0.871
0.191 21	0.816 40	1.030	0.583 71	0.850 91	0.926	0.944 78	0.868 60	0.869
0.263 31	0.824 60	1.010	0.652 44	0.854 98	0.909			
			(x)$CH_3COOC_5H_{11}$ + (1 − x)C_3H_7OH					
0.033 21	0.803 89	1.856	0.388 14	0.837 57	1.467	0.750 33	0.859 50	1.085
0.093 54	0.811 11	1.790	0.430 35	0.840 56	1.422	0.826 15	0.863 15	1.017
0.153 72	0.817 50	1.724	0.522 34	0.846 65	1.322	0.900 46	0.866 53	0.948
0.235 61	0.825 24	1.623	0.609 83	0.851 96	1.230	0.964 32	0.869 23	0.893
0.311 20	0.831 69	1.552	0.687 41	0.856 24	1.149			
			(x)$CH_3COOC_5H_{11}$ + (1 − x)C_4H_9OH					
0.035 32	0.808 93	2.449	0.300 54	0.830 61	1.992	0.633 42	0.851 93	1.426
0.089 76	0.813 90	2.355	0.381 03	0.836 21	1.853	0.721 05	0.856 70	1.283
0.127 84	0.817 19	2.289	0.431 22	0.839 48	1.767	0.817 46	0.861 61	1.139
0.175 53	0.821 05	2.207	0.492 04	0.843 30	1.665	0.920 14	0.866 69	0.978
0.223 41	0.824 83	2.124	0.566 71	0.847 85	1.537			
			(x)$CH_3COOC_5H_{11}$ + (1 − x)$C_5H_{11}OH$					
0.042 16	0.813 77	3.208	0.301 36	0.831 13	2.549	0.664 31	0.852 65	1.641
0.093 12	0.817 35	3.078	0.363 44	0.835 02	2.393	0.734 12	0.856 49	1.471
0.142 45	0.820 71	2.953	0.415 10	0.838 12	2.262	0.822 45	0.861 17	1.265
0.190 17	0.823 88	2.832	0.501 03	0.843 15	2.047	0.912 36	0.866 00	1.060
0.259 86	0.828 50	2.654	0.587 62	0.848 23	1.832			
			(x)$CH_3COOC_5H_{11}$ + (1 − x)$C_6H_{13}OH$					
	±0.001%	±0.05%		±0.001%	±0.05%		±0.001%	±0.05%
0.043 03	0.817 61	4.427	0.276 34	0.830 65	3.537	0.693 12	0.853 57	1.958
0.072 42	0.819 37	4.313	0.355 14	0.835 08	3.233	0.770 43	0.857 45	1.656
0.100 41	0.820 87	4.206	0.422 63	0.838 65	2.978	0.855 21	0.862 59	1.373
0.177 35	0.825 23	3.911	0.511 46	0.843 43	2.642	0.944 33	0.867 68	1.057
0.224 11	0.827 91	3.733	0.603 24	0.848 52	2.295			
			(x)$CH_3COOC_5H_{11}$ + (1 − x)$C_7H_{15}OH$					
0.066 41	0.821 72	4.560	0.400 22	0.837 70	3.203	0.755 02	0.856 35	1.785
0.122 01	0.824 36	4.333	0.460 14	0.840 63	2.970	0.832 12	0.860 37	1.490
0.194 53	0.827 72	4.036	0.533 45	0.844 32	2.666	0.882 11	0.863 36	1.300
0.269 94	0.831 27	3.730	0.591 92	0.847 44	2.432	0.955 42	0.867 02	1.026
0.332 51	0.834 44	3.476	0.672 34	0.851 78	2.115			
			(x)$CH_3COOC_5H_{11}$ + (1 − x)$C_8H_{17}OH$					
0.044 13	0.823 74	5.885	0.366 34	0.836 79	4.155	0.766 73	0.856 49	2.028
0.102 45	0.825 94	5.510	0.424 11	0.839 33	3.847	0.838 64	0.860 48	1.669
0.149 93	0.827 79	5.313	0.512 21	0.843 29	3.379	0.900 41	0.864 26	1.353
0.221 07	0.830 71	4.932	0.609 93	0.848 07	2.861	0.964 12	0.868 18	1.032
0.290 14	0.833 49	4.562	0.698 72	0.852 76	2.391			
			(x)$CH_3COOC_6H_{13}$ + (1 − x)C_2H_5OH					
0.062 17	0.798 09	1.083	0.340 05	0.833 62	1.075	0.711 44	0.857 33	1.079
0.104 28	0.805 42	1.081	0.412 43	0.839 57	1.073	0.803 43	0.861 30	1.086
0.174 51	0.815 60	1.080	0.488 32	0.844 98	1.067	0.876 10	0.864 10	1.094
0.223 60	0.821 77	1.079	0.566 30	0.849 82	1.072	0.944 12	0.866 51	1.100
0.284 11	0.828 30	1.077	0.633 56	0.853 51	1.073			
			(x)$CH_3COOC_6H_{13}$ + (1 − x)C_3H_7OH					
	±0.001%	±0.05%		±0.001%	±0.05%		±0.001%	±0.05%
0.055 31	0.807 31	1.845	0.383 10	0.838 17	1.569	0.778 14	0.859 07	1.259
0.098 76	0.812 67	1.808	0.455 22	0.842 83	1.508	0.834 22	0.861 96	1.220
0.166 43	0.820 19	1.750	0.530 03	0.847 23	1.447	0.904 10	0.864 38	1.180
0.224 52	0.825 61	1.702	0.620 24	0.852 18	1.375	0.964 51	0.868 12	1.102
0.307 11	0.832 54	1.632	0.711 53	0.856 74	1.306			
			(x)$CH_3COOC_6H_{13}$ + (1 − x)C_4H_9OH					
0.046 41	0.810 56	2.441	0.310 12	0.832 59	2.052	0.737 62	0.856 87	1.445
0.097 66	0.815 53	2.363	0.402 34	0.838 61	1.918	0.822 41	0.861 05	1.331
0.153 20	0.820 53	2.282	0.487 16	0.842 59	1.795	0.897 42	0.864 14	1.233
0.199 24	0.824 24	2.214	0.563 62	0.847 90	1.686	0.955 36	0.866 61	1.157
0.254 33	0.828 57	2.133	0.641 15	0.852 13	1.576			
			(x)$CH_3COOC_6H_{13}$ + (1 − x)$C_5H_{11}OH$					
0.054 96	0.815 22	3.188	0.414 25	0.839 01	2.370	0.762 87	0.857 30	1.599
0.104 32	0.819 00	3.073	0.491 74	0.843 31	2.196	0.836 45	0.860 78	1.441
0.187 63	0.825 01	2.883	0.567 32	0.847 35	2.026	0.894 11	0.863 50	1.318
0.254 10	0.829 41	2.732	0.620 03	0.850 14	1.909	0.960 24	0.866 53	1.179
0.327 73	0.833 95	2.565	0.694 14	0.853 91	1.748			
			(x)$CH_3COOC_6H_{13}$ + (1 − x)$C_6H_{13}OH$					
0.057 41	0.818 81	4.384	0.404 50	0.838 66	3.149	0.773 24	0.857 35	1.863
0.101 23	0.821 57	4.227	0.486 37	0.842 88	2.860	0.822 45	0.859 78	1.696
0.177 46	0.826 05	3.951	0.553 21	0.846 25	2.624	0.901 01	0.863 59	1.428
0.245 43	0.830 00	3.712	0.627 02	0.850 03	2.365	0.966 74	0.866 61	1.210
0.311 02	0.833 68	3.480	0.707 11	0.854 06	2.091			
			(x)$CH_3COOC_6H_{13}$ + (1 − x)$C_7H_{15}OH$					
	±0.001%	±0.05%		±0.001%	±0.05%		±0.001%	±0.05%
0.070 14	0.822 38	4.559	0.396 05	0.838 42	3.321	0.741 33	0.855 23	2.032
0.143 21	0.826 12	4.279	0.467 17	0.841 82	3.053	0.804 66	0.858 39	1.800
0.202 34	0.828 89	4.054	0.524 53	0.844 56	2.837	0.887 19	0.862 46	1.499
0.271 53	0.832 49	3.792	0.591 15	0.847 73	2.586	0.950 12	0.865 63	1.272
0.338 11	0.835 68	3.550	0.671 02	0.851 72	2.290			

Table 2. (Continued)

x	ρ/g cm^{-3}	η/mPa·s	x	ρ/g cm^{-3}	η/mPa·s	x	ρ/g cm^{-3}	η/mPa·s
			$(x)CH_3COOC_6H_{13} + (1-x)C_8H_{17}OH$					
0.059 02	0.824 59	5.818	0.392 25	0.838 92	4.117	0.721 03	0.853 97	2.468
0.113 15	0.827 01	5.540	0.456 73	0.841 67	3.790	0.804 22	0.858 06	2.051
0.192 42	0.830 37	5.134	0.523 66	0.844 57	3.452	0.873 31	0.861 62	1.711
0.256 33	0.833 04	4.808	0.590 24	0.847 66	3.115	0.954 33	0.865 70	1.314
0.311 46	0.835 44	4.528	0.661 35	0.851 04	2.760			

Table 3. Coefficients A_j and Standard Error $\sigma(V^E)$ of Eq 3 for (x)Esters + $(1-x)$*n*-Alkanols at 298.15 K[a]

alkanol	A_0	A_1	A_2	A_3	$\sigma(V^E)$/ cm^3·mol^{-1}
	$(x)CH_3COOC_5H_{11} + (1-x)C_nH_{2n+1}OH$				
ethanol	0.6291	0.0581	−0.0639	−0.0732	0.0058
1-propanol	0.9316	0.0755	−0.0382	−0.0142	0.0056
1-butanol	1.2040	0.0498	0.1530	−0.2093	0.0140
1-pentanol	1.4192	−0.0874	0.2097	−0.0609	0.0091
1-hexanol	1.6771	−0.4566	−0.0826	0.4219	0.0199
1-heptanol	1.8534	−0.0126	0.7080	−1.2759	0.0435
1-octanol	2.1428	−0.4653	0.1972	−0.0900	0.0130
	$(x)CH_3COOC_6H_{13} + (1-x)C_nH_{2n+1}OH$				
ethanol	0.5109	0.0212	0.0410	−0.1715	0.0028
1-propanol	−0.8567	−0.0458	−0.0992	0.3241	0.0322
1-butanol	1.0316	−0.3439	−0.3898	0.3151	0.0134
1-pentanol	1.1981	−0.4520	−0.1337	−0.0599	0.0080
1-hexanol	1.3393	−0.4153	−0.0317	0.0976	0.0137
1-heptanol	1.5056	−0.4855	0.0516	−0.1129	0.0156
1-octanol	1.7057	−0.5785	−0.1138	−0.0706	0.0175

[a] $n = 2, 3, ..., 8$.

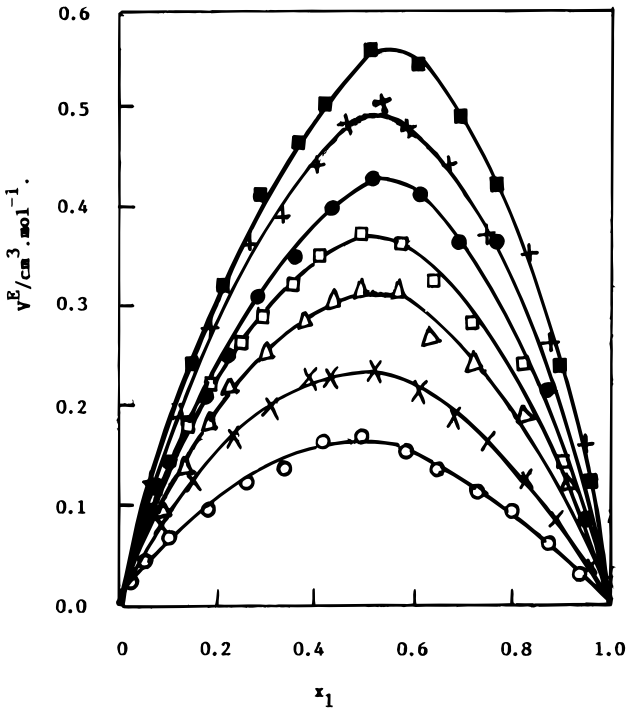

Figure 1. Excess molar volumes, V^E, at 298.15 K of the $(x)CH_3COOC_5H_{11} + (1-x)C_nH_{2n+1}OH$ system ($n = 2, 3, ..., 8$): (○) C_2H_5OH; (×) C_3H_7OH; (△) C_4H_9OH; (□) $C_5H_{11}OH$; (●) $C_6H_{13}OH$; (+) $C_7H_{15}OH$; (■) $C_8H_{17}OH$.

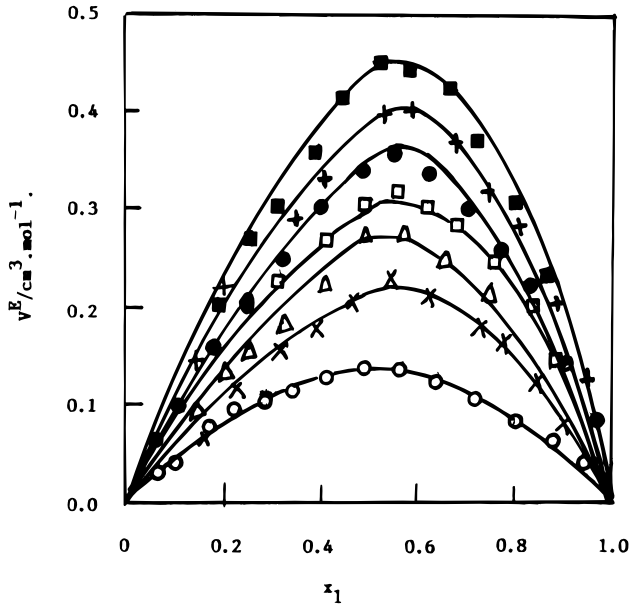

Figure 2. Excess molar volumes, V^E, at 298.15 K of the $(x)CH_3COOC_6H_{13} + (1-x)C_nH_{2n+1}OH$ system: (○) C_2H_5OH; (×) C_3H_7OH; (△) C_4H_9OH; (□) $C_5H_{11}OH$; (●) $C_6H_{13}OH$; (+) $C_7H_{15}OH$; (■) $C_8H_{17}OH$.

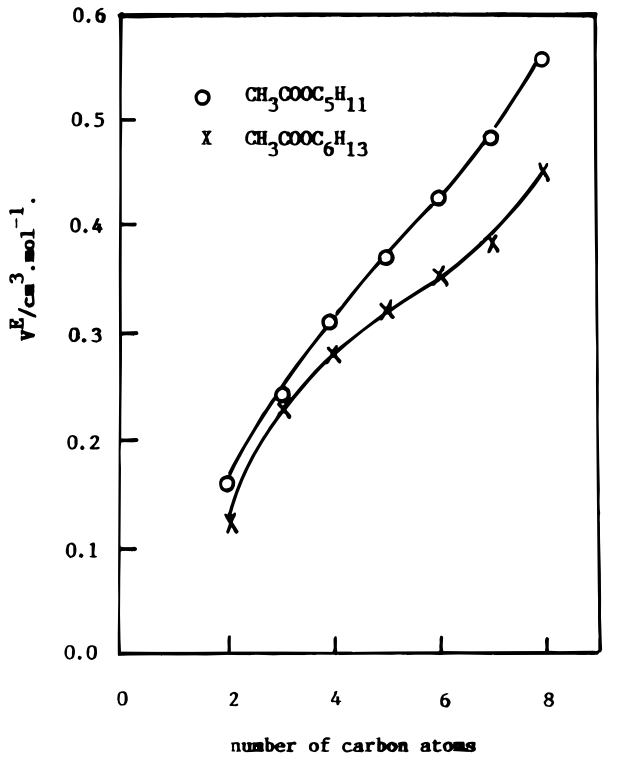

Figure 3. Equimolar V^E values, obtained from the Redlich−Kister equation, as V^E ($x = 0.5$) vs the number of carbon atoms in the alkanol molecule at 298.15 K.

The excess volumes (Figures 1 and 2) are positive and increase. For each ester, the values of V^E increase with increasing length of the hydrocarbon chain of the alkanol (Figure 3) in the sequence: 1-octanol > 1-heptanol > 1-hexanol > 1-pentanol > 1-butanol > 1-propanol > ethanol. The V^E values for pentyl acetate mixtures are more positive than those of the corresponding mixtures of hexyl acetate with the same *n*-alkanols.

Table 4. Values of the Parameters T_{12}, H_{12}, (ν_{12}, ν_{21}), and (a, b, c) of Eqs 4−7

alkanol	T_{12}	H_{12}	ν_{12}	ν_{21}	a	b	c
			$(x)CH_3COOC_5H_{11} + (1-x)C_nH_{2n+1}OH$				
ethanol	0.9052	0.8966	0.5086	1.3027	−0.1667	−0.0029	−0.6210
1-propanol	1.2552	1.2458	0.8313	1.9553	−0.3618	−0.0040	−0.0865
1-butanol	1.8243	1.5633	1.1899	2.4406	−0.3981	−0.0400	−0.0618
1-pentanol	2.2103	1.9646	1.7300	3.0514	−0.4493	−0.0563	−0.0600
1-hexanol	2.8045	2.5854	2.7236	3.9831	−0.5330	−0.0906	−0.0744
1-heptanol	3.0510	3.1781	4.6917	4.9250	−0.5982	−0.1874	−0.1630
1-octanol	3.6533	3.1781	4.6917	4.9250	−0.5982	−0.1879	−0.1630
			$(x)CH_3COOC_6H_{13} + (1-x)C_nH_{2n+1}OH$				
ethanol	1.1004	1.0457	0.5654	1.4348	−0.1013	−0.0030	−0.0185
1-propanol	1.4022	1.3510	0.8757	2.0672	−0.2841	−0.0052	−0.0912
1-butanol	1.7571	1.6674	1.2049	2.5427	−0.3563	−0.0090	−0.1270
1-pentanol	2.4523	2.0145	1.6845	3.1671	−0.3950	−0.0239	−0.1866
1-hexanol	4.0700	2.6564	2.5471	4.1163	−0.4746	−0.0311	−0.1982
1-heptanol	5.8570	2.7592	2.9304	4.2734	−0.5012	−0.0570	−0.2144
1-octanol	6.4211	3.3647	4.1322	5.1643	−0.5813	−0.0870	−0.2626

Various viscosity models for the binary mixtures have been proposed:

Tamara and Kurata (1952)

$$\eta_m = x_1\Phi_1\eta_1 + x_2\Phi_2\eta_2 + 2(x_1x_2\Phi_1\Phi_2)^{0.5}T_{12} \qquad (4)$$

Hind et al. (1960)

$$\eta_m = x_1^2\eta_1 + x_2^2\eta_2 + 2x_1x_2H_{12} \qquad (5)$$

where η_m, η_1, and η_2 are the viscosities of the mixtures and pure components, respectively, Φ_1 and Φ_2 are the volume fractions, and T_{12} and H_{12} values are the new interaction parameters. T_{12} and H_{12} values are found to be positive for all mixtures and are similar in magnitude (Table 4).

The McAllister (1960) correlation is based on a model proposed by Glasstone et al. (1941) which considers that interaction occurs between three bodies:

$$\ln \nu = x_1^3 \ln \nu_1 + x_2^3 \ln \nu_2 + x_1^3 \ln M_1 + x_2^3 \ln M_2 - \ln(x_1M_1 + x_2M_2) + 3x_1^3x_2 \ln(2M_1 + M_2/3) + 3x_1x_2^2 \ln(M_1 + 2M_2/3) + 3x_1^3x_2 \ln \nu_{12} + 3x_1x_2^2 \ln \nu_{21} \qquad (6)$$

where ν is the kinematic viscosity (η/ρ) and ν_{12} and ν_{21} are interaction parameters and found to be positive (Table 4).

Heric and Brewer (1967) suggested the equation

$$\nu = x_1\nu_1 + x_2\nu_2 + x_1x_2[a + b\,(x_1 - x_2) + c\,(x_1 + x_2)^2] \qquad (7)$$

for the kinematic viscosity of binary mixtures. The values of parameters a, b, and c were found to be negative for all the mixtures (Table 4).

Literature Cited

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