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Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures

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ABSTRACT: In this work, kinematic viscosities of binary mixtures formed by an alkane (3-methylpentane, 2,2-dimethylbutane, *n*-hexane, and *n*-heptane) and an isomeric chlorobutane (1-chlorobutane, 2-chlorobutane, 1-chloro-2-methylpropane, and 2-chloro-2-methylpropane) have been determined as a function of composition under atmospheric at three temperatures, T = (283.15, 298.15, and 313.15) K and correlated using the McAllister equation. Kinematic viscosities were measured using an Ubbelohde viscometer. Finally, we have used the Asfour method for predicting the dependence of viscosity with composition, and the predictions were compared with the experimental data.

INTRODUCTION

Among the physical properties of fluids needed to design and optimized the industrial processes, viscosity is one of the most important. Viscosity is necessary for an efficient design of chemical industrial processes involving heat and mass transfer phenomena, and it is also an important property in hydraulic calculations for surface facilities, pipeline systems, and flow through porous media. The modeling of the viscosity of liquid mixtures can be performed using both correlative and predictive methods.[1,2] On one hand, correlative models[3−6] require viscosity data to determine interaction parameters that have specific values for each mixture at the working conditions. On the other hand, with the aim to predict the viscosity of liquid mixtures, several models founded on different approaches have been developed; an important group of such methods are based on the absolute reaction theory of Eyring[7] Wu method,[8] UNIFAC-VISCO[9,10] and ASOG-VISCO[11] which combine the Eyring equation with the UNIFAC or ASOG group contribution methods,[12,13] the GC-UNIMOD[14] which uses both, a group contribution viscosity equation and an activity coefficient equation, and finally the Asfour method[15−18] which calculates the McAllister equation parameters using the effective carbon number concept; this number can be obtained taking into account only the kinematic viscosities of the pure compounds.

In this paper, the Asfour method was used to predict kinematic viscosities of the systems studied. These systems were binary mixtures containing alkanes, 3-methylpentane, 2,2-dimethylbutane, *n*-hexane, or *n*-heptane, and isomeric chlorobutanes, 1-chlorobutane, 2-chlorobutane, 1-chloro-2-methylpropane, and 2-chloro-2-methylpropane, at the temperatures of (293.15, 303.15, and 313.15) K under atmospheric pressure over the whole composition range; the obtained results were correlated using the McAllister equation.[3]

A survey of the literature shows that there are only two works involving the viscosimetric study of this kind of mixtures.[19,20]

EXPERIMENTAL SECTION

The liquids used were 1-chlorobutane, 2-chlorobutane, 2-chloro-2-methylpropane, hexane, heptane, 3-methylpentane, and 2,2-dimethylbutane (>0.99 in mass fraction) obtained from Aldrich and 1-chloro-2-methylpropane (>0.99 in mass fraction) provided by Fluka. No additional purification was carried out.

Kinematic viscosities, ν, were determined using an Ubbelohde viscometer with a Schott-Geräte automatic measuring unit model AVS-440. The temperature was kept constant within ± 0.01 K by means of a Schott-Geräte CT 1150/2 thermostat. The viscometer was calibrated with deionized doubly distilled water. The uncertainty of the time flow measurements was ± 0.01 s, and the corresponding uncertainty in the kinematic viscosity was ± $1 \cdot 10^{-4}$ $mm^2 \cdot s^{-1}$. Kinetic energy corrections were applied to the experimental data.

The kinematic viscosity values of the pure components at work temperatures appear together with their corresponding literature values[20−33] at 298.15 K in Table 1.

The mixtures were prepared using a Sartorious semimicro balance CP225-D with a precision of ± 10^{-5} g. The maximum estimated error in the mole fraction is ± $1 \cdot 10^{-4}$.

RESULTS AND DISCUSSION

The kinematic viscosities, ν, for the binary mixtures are given in Table 2 and graphically represented in Figures 1 to 4. The kinematic viscosity data were correlated using the McAllister theory. This theory of liquid mixtures is based on Eyring's theory of absolute reaction rates, and it assumes that for liquid mixtures the free energies of activation for viscous flow are additive on a mole fraction basis and that interactions of like and unlike molecules must be considered.

If the types of interaction considered are only three-bodied, a cubic equation for the viscosity with two parameters is derived:

$$\ln \nu = x_1^3 \ln \nu_1 + 3x_1^2 x_2 \ln \nu_{12} + 3x_1 x_2^2 \ln \nu_{21} + x_2^3 \ln \nu_2 - \ln[x_1 + x_2 M_2/M_1] + 3x_1^2 x_2 \ln[(2 + M_2/M_1)/3] + 3x_1 x_2^2 \ln[(1 + 2M_2/M_1)/3] + x_2^3 \ln[M_2/M_1] \quad (1)$$

where ν refers to the kinematic viscosity of the mixture, ν_1 and ν_2 are the kinematic viscosities of components 1 and 2, M_1 and M_2

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Table 1. Kinematic Viscosities, ν, of the Pure Compounds

	ν (mm^2·s^{-1})			
	T/K = 283.15	T/K = 298.15		T/K = 313.15
compound	exptl	exptl	lit.	exptl
3-methylpentane	0.4928	0.4366	0.4274 to 0.4411[a]	0.3881
2,2-dimethylbutane	0.6234	0.5206	0.5283;[b] 0.5104[c]	0.4579
n-hexane	0.5125	0.4493	0.4458 to 0.4529[d]	0.4039
n-heptane	0.6697	0.5754	0.5702 to 0.584[e]	0.4986
1-chlorobutane	0.5564	0.4785	0.4837;[f] 0.4823[g]	0.4216
2-chlorobutane	0.5237	0.4603		0.4049
1-chloro-2-methylpropane	0.5800	0.4929	0.4940[h]	0.4363
2-chloro-2-methylpropane	0.6992	0.5696		0.4770

[a] Refs 21 to 24. [b] Ref 22. [c] Ref 24. [d] Refs 20 and 24 to 28. [e] Refs 21, 25, 26 and 28 to 31. [f] Ref 20. [g] Ref 32. [h] Ref 33.

Table 2. Experimental Kinematic Viscosities, ν, of the Binary Mixtures: Alkane with Isomeric Chlorobutanes

	ν (mm^2·s^{-1})				ν (mm^2·s^{-1})		
x_1	T/K = 283.15	T/K = 298.15	T/K = 313.15	x_1	T/K = 283.15	T/K = 298.15	T/K = 313.15
	3-Methylpentane (1) + 1-Chlorobutane (2)				3-Methylpentane (1) + 2-Chlorobutane (2)		
0.0518	0.5496	0.4734	0.4175	0.0518	0.5193	0.4574	0.4031
0.0940	0.5448	0.4704	0.4155	0.1010	0.5142	0.4542	0.4004
0.2038	0.5326	0.4622	0.4088	0.2014	0.5066	0.4483	0.3958
0.3040	0.5228	0.4553	0.4036	0.3025	0.4995	0.4431	0.3919
0.4059	0.5143	0.4500	0.3988	0.4027	0.4943	0.4390	0.3885
0.5021	0.5075	0.4453	0.3952	0.4998	0.4906	0.4362	0.3865
0.5999	0.5017	0.4411	0.3921	0.6043	0.4881	0.4345	0.3851
0.7043	0.4970	0.4382	0.3896	0.7008	0.4870	0.4340	0.3844
0.8049	0.4945	0.4365	0.3884	0.8004	0.4874	0.4337	0.3847
0.9038	0.4928	0.4351	0.3879	0.8981	0.4897	0.4344	0.3858
0.9492	0.4928	0.4355	0.3877	0.9481	0.4911	0.4356	0.3868
	3-Methylpentane (1) + 1-Chloro-2-methylpropane (2)				3-Methylpentane (1) + 2-Chloro-2-methylpropane (2)		
0.0522	0.5703	0.4870	0.4322	0.0496	0.6755	0.5548	0.4681
0.1013	0.5618	0.4823	0.4275	0.0995	0.6538	0.5400	0.4576
0.2024	0.5464	0.4717	0.4187	0.2046	0.6148	0.5140	0.4400
0.3032	0.5324	0.4631	0.4113	0.3023	0.5848	0.4937	0.4256
0.4028	0.5212	0.4550	0.4048	0.4050	0.5592	0.4767	0.4140
0.5056	0.5115	0.4484	0.3994	0.5064	0.5394	0.4637	0.4051
0.6040	0.5043	0.4430	0.3951	0.6033	0.5235	0.4536	0.3984
0.7018	0.4988	0.4396	0.3918	0.7038	0.5114	0.4462	0.3933
0.8002	0.4949	0.4370	0.3896	0.8012	0.5026	0.4410	0.3900
0.8980	0.4930	0.4357	0.3881	0.9018	0.4964	0.4377	0.3881
0.9486	0.4927	0.4355	0.3879	0.9514	0.4946	0.4372	0.3880
	2,2-Dimethylbutane (1) + 1-Chlorobutane (2)				2,2-Dimethylbutane (1) + 2-Chlorobutane (2)		
0.0524	0.5594	0.4802	0.4231	0.0448	0.5266	0.4621	0.4070
0.1010	0.5603	0.4809	0.4239	0.0993	0.5300	0.4640	0.4086
0.1995	0.5627	0.4822	0.4253	0.2003	0.5356	0.4679	0.4120
0.3081	0.5663	0.4846	0.4275	0.3010	0.5421	0.4719	0.4157
0.3985	0.5705	0.4867	0.4294	0.3993	0.5494	0.4761	0.4200
0.4990	0.5760	0.4898	0.4322	0.4989	0.5579	0.4815	0.4251
0.5984	0.5822	0.4943	0.4362	0.6039	0.5683	0.4880	0.4309
0.7015	0.5899	0.5000	0.4409	0.7002	0.5793	0.4949	0.4368

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Table 2. Continued

	ν (mm^2·s^{-1})				ν (mm^2·s^{-1})		
x_1	T/K = 283.15	T/K = 298.15	T/K = 313.15	x_1	T/K = 283.15	T/K = 298.15	T/K = 313.15
0.7986	0.5992	0.5063	0.4463	0.8033	0.5935	0.5036	0.4438
0.9002	0.6098	0.5133	0.4520	0.9028	0.6070	0.5122	0.4508
0.9487	0.6160	0.5170	0.4550	0.9518	0.6147	0.5165	0.4546
	2,2-Dimethylbutane (1) + 1-Chloro-2-methylpropane (2)				2,2-Dimethylbutane (1) + 2-Chloro-2-methylpropane (2)		
0.0487	0.5820	0.4940	0.4366	0.0499	0.6937	0.5657	0.4748
0.0994	0.5816	0.4941	0.4365	0.1017	0.6864	0.5592	0.4715
0.1995	0.5814	0.4939	0.4362	0.1983	0.6729	0.5493	0.4664
0.2985	0.5821	0.4939	0.4363	0.3004	0.6600	0.5405	0.4607
0.3993	0.5834	0.4942	0.4366	0.3990	0.6491	0.5333	0.4568
0.5018	0.5866	0.4958	0.4380	0.4989	0.6399	0.5275	0.4538
0.6011	0.5899	0.4986	0.4402	0.6017	0.6320	0.5225	0.4522
0.6985	0.5953	0.5025	0.4439	0.7034	0.6270	0.5200	0.4518
0.7995	0.6024	0.5071	0.4476	0.8000	0.6228	0.5180	0.4519
0.8988	0.6115	0.5130	0.4524	0.8967	0.6221	0.5184	0.4541
0.9479	0.6158	0.5163	0.4542	0.9504	0.6224	0.5190	0.4556
	n-Hexane (1) + 1-Chlorobutane (2)				*n*-Hexane (1) + 2-Chlorobutane (2)		
0.0508	0.5501	0.4740	0.4182	0.0509	0.5186	0.4579	0.4034
0.0992	0.5449	0.4701	0.4169	0.1002	0.5147	0.4548	0.4012
0.1972	0.5351	0.4634	0.4118	0.1802	0.5090	0.4501	0.3980
0.2966	0.5269	0.4577	0.4080	0.3029	0.5025	0.4448	0.3948
0.3976	0.5198	0.4531	0.4048	0.4045	0.4989	0.4420	0.3932
0.5009	0.5145	0.4495	0.4027	0.4991	0.4975	0.4408	0.3926
0.6006	0.5112	0.4467	0.4011	0.5974	0.4968	0.4401	0.3926
0.6982	0.5092	0.4451	0.4005	0.6992	0.4982	0.4406	0.3939
0.7972	0.5082	0.4455	0.4010	0.7996	0.5007	0.4419	0.3961
0.8979	0.5094	0.4464	0.4023	0.8981	0.5055	0.4447	0.3993
0.9472	0.5103	0.4474	0.4027	0.9477	0.5086	0.4465	0.4015
	n-Hexane (1) + 1-Chloro-2-methylpropane (2)				*n*-Hexane (1) + 2-Chloro-2-methylpropane (2)		
0.0512	0.5712	0.4863	0.4320	0.0495	0.6722	0.5527	0.4671
0.0999	0.5631	0.4817	0.4282	0.0989	0.6489	0.5369	0.4565
0.2003	0.5468	0.4711	0.4196	0.2019	0.6091	0.5105	0.4391
0.2993	0.5339	0.4633	0.4128	0.2987	0.5810	0.4916	0.4266
0.4005	0.5239	0.4566	0.4077	0.4043	0.5575	0.4756	0.4162
0.4977	0.5171	0.4517	0.4041	0.4985	0.5415	0.4651	0.4095
0.5980	0.5120	0.4478	0.4017	0.6024	0.5287	0.4571	0.4048
0.6993	0.5089	0.4462	0.4010	0.7017	0.5203	0.4516	0.4019
0.7990	0.5077	0.4455	0.4002	0.7996	0.5151	0.4489	0.4009
0.8967	0.5092	0.4457	0.4006	0.9025	0.5123	0.4478	0.4016
0.9472	0.5103	0.4474	0.4023	0.9498	0.5119	0.4483	0.4023
	n-Heptane (1) + 1-Chlorobutane (2)				*n*-Heptane (1) + 2-Chlorobutane (2)		
0.0508	0.5595	0.4824	0.4248	0.0506	0.5287	0.4649	0.4086
0.1017	0.5632	0.4857	0.4278	0.0989	0.5334	0.4686	0.4121
0.1981	0.5703	0.4927	0.4335	0.2012	0.5440	0.4780	0.4202
0.2989	0.5788	0.5000	0.4396	0.3016	0.5558	0.4876	0.4283
0.4022	0.5882	0.5088	0.4471	0.3997	0.5677	0.4978	0.4370
0.4998	0.5984	0.5177	0.4545	0.4984	0.5812	0.5087	0.4461
0.6008	0.6102	0.5278	0.4624	0.5994	0.5966	0.5206	0.4558
0.6989	0.6229	0.5386	0.4705	0.6994	0.6128	0.5331	0.4652
0.7985	0.6367	0.5501	0.4792	0.7996	0.6304	0.5467	0.4757
0.8980	0.6520	0.5626	0.4882	0.9006	0.6496	0.5609	0.4866
0.9498	0.6608	0.5692	0.4935	0.9503	0.6600	0.5684	0.4927

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Table 2. Continued

	ν (mm^2·s^{-1})				ν (mm^2·s^{-1})		
x_1	T/K = 283.15	T/K = 298.15	T/K = 313.15	x_1	T/K = 283.15	T/K = 298.15	T/K = 313.15
	n-Heptane (1) + 1-Chloro-2-methylpropane (2)				*n*-Heptane (1) + 2-Chloro-2-methylpropane (2)		
0.0507	0.5818	0.4950	0.4381	0.0519	0.6840	0.5603	0.4741
0.0979	0.5817	0.4970	0.4396	0.1021	0.6722	0.5532	0.4711
0.2004	0.5851	0.5015	0.4438	0.2015	0.6546	0.5438	0.4675
0.3008	0.5905	0.5064	0.4483	0.3006	0.6440	0.5389	0.4666
0.3993	0.5970	0.5134	0.4536	0.3997	0.6391	0.5380	0.4679
0.4999	0.6054	0.5215	0.4599	0.5027	0.6376	0.5391	0.4699
0.5973	0.6156	0.5306	0.4663	0.6011	0.6397	0.5434	0.4735
0.6994	0.6268	0.5403	0.4733	0.7014	0.6441	0.5489	0.4780
0.8006	0.6397	0.5516	0.4809	0.8007	0.6504	0.5572	0.4832
0.9002	0.6538	0.5633	0.4894	0.8966	0.6591	0.5652	0.4894
0.9491	0.6615	0.5692	0.4940	0.9518	0.6651	0.5706	0.4944

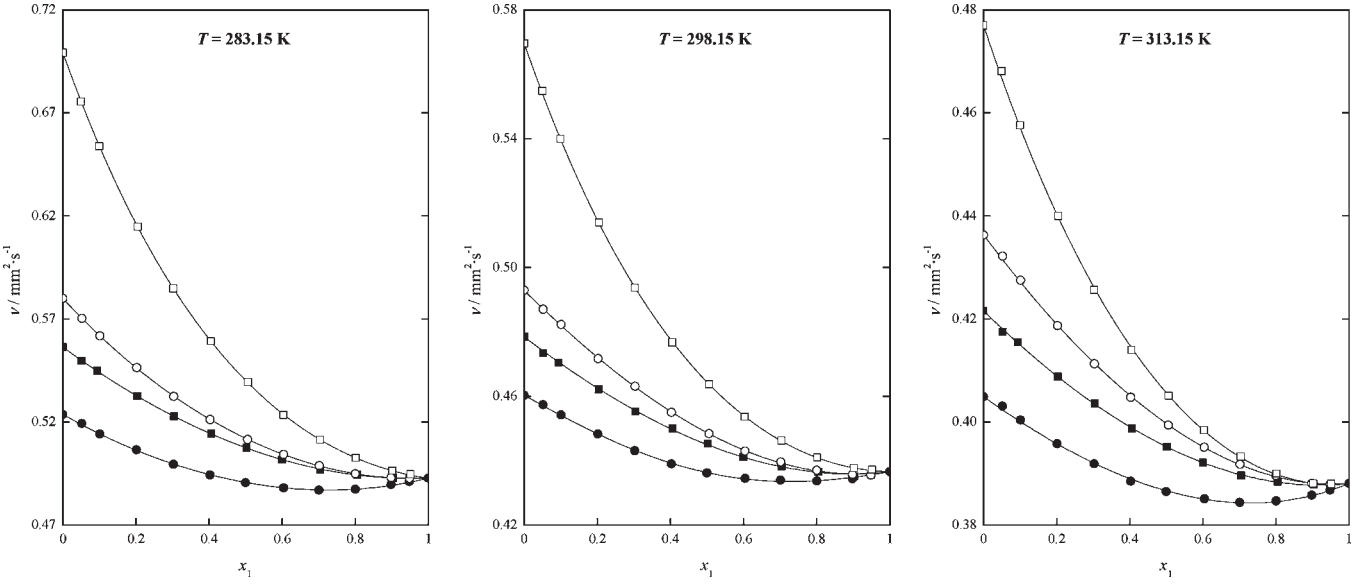

Figure 1. Kinematic viscosities, ν, for 3-methylpentane with isomeric chlorobutane: ■, 1-chlorobutane; ●, 2-chlorobutane; ○, 1-chloro-2-methylpropane; □, 2-chloro-2-methylpropane; —, four-body McAllister equation.

are their corresponding molar masses, and ν_{12} and ν_{21} are adjustable parameters characteristic of the system.

When the size of one component molecule is much greater than the size of the other component molecule the three-body interactions may not always be realistic. So, the four-bodied interaction must be taken into account, and a quartic equation for the viscosity with three parameters is obtained:

$$\begin{aligned}\ln \nu = {} & x_1^4 \ln \nu_1 + 4x_1^3 x_2 \ln \nu_{1112} + 6x_1^2 x_2^2 \ln \nu_{1122} \\ & + 4x_1 x_2^3 \ln \nu_{2221} + x_2^4 \ln \nu_2 - \ln[x_1 + x_2 M_2/M_1] \\ & + 4x_1^3 x_2 \ln[(3 + M_2/M_1)/4] + 6x_1^2 x_2^2 \ln[(1 + M_2/M_1)/2] \\ & + 4x_1 x_2^3 \ln[(1 + 3M_2/M_1)/4] x_2^4 \ln[M_2/M_1] \qquad (2)\end{aligned}$$

where ν_{1112}, ν_{1122}, and ν_{2221} are the adjustable parameters of the equation.

The estimated parameters of the three-body and four-body McAllister equations are shown in Table 3 together with the corresponding average absolute deviations, AAD, between experimental and correlated values:

$$\mathrm{AAD}(\%) = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\nu_{i,\mathrm{exp}} - \nu_{i,\mathrm{cal}}}{\nu_{i,\mathrm{exp}}}\right| \cdot 100 \qquad (3)$$

where N is the number of experimental data.

The AAD values are in all cases less than 0.2 %, so we can conclude that the McAllister equation is able to correlate the kinematic viscosity data with good accuracy, being the four-body McAllister equation results slightly better than those of the three-body McAllister equation.

The shape of the viscosity−composition curve can provide information about the energetic and structural effects occurring in the mixing process;[2] energetic effects are related with the breaking or weakening of interactions in the pure compounds, and the establishment of new ones between the unlike molecules and the structural effects is attributed to differences in size and shape of the chemicals. The viscosity−composition curve for all

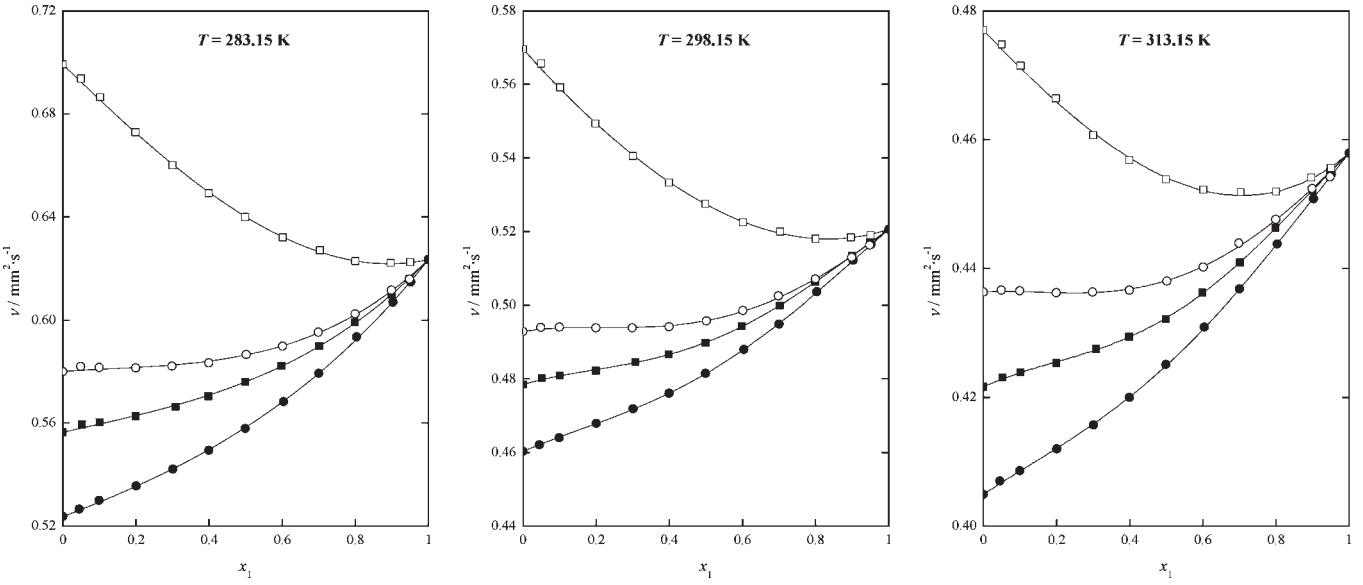

Figure 2. Kinematic viscosities, ν, for 2,2-dimethylbutane with isomeric chlorobutane: ■, 1-chlorobutane; ●, 2-chlorobutane; ○, 1-chloro-2-methylpropane; □, 2-chloro-2-methylpropane; —, four-body McAllister equation.

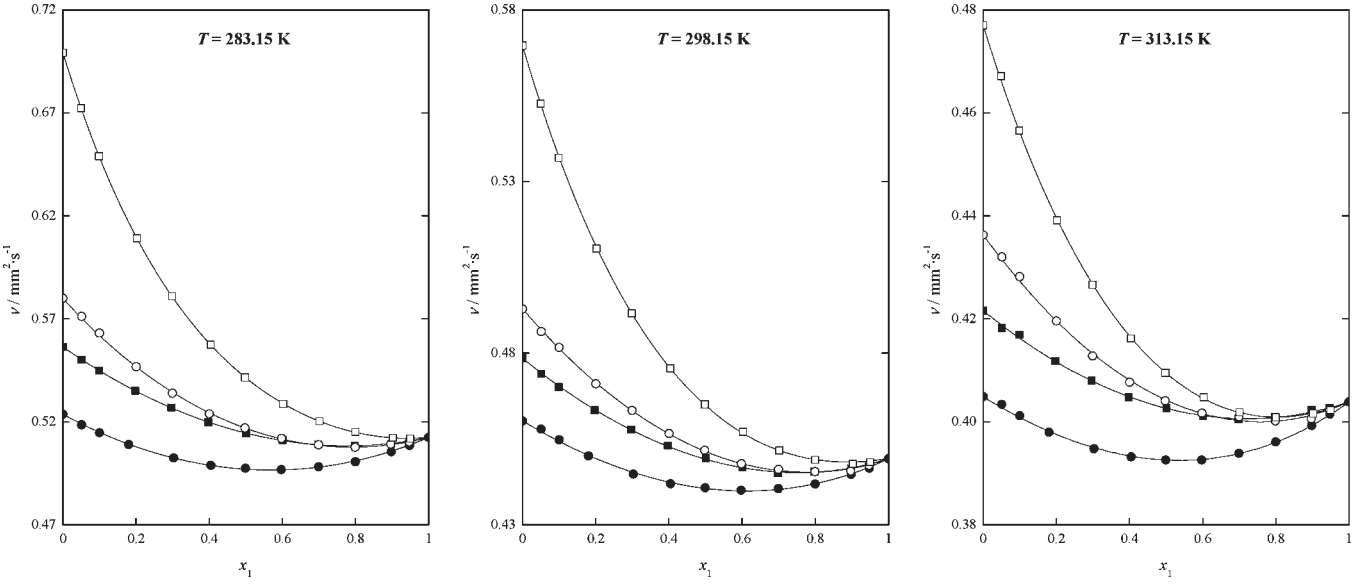

Figure 3. Kinematic viscosities, ν, for *n*-hexane with isomeric chlorobutane: ■, 1-chlorobutane; ●, 2-chlorobutane; ○, 1-chloro-2-methylpropane; □, 2-chloro-2-methylpropane; —, four-body McAllister equation.

the mixtures studied here is below a linear viscosity−composition dependence showing that the weakness of interactions in the pure compounds, especially the dipole−dipole interactions in the isomeric chlorobutanes, is the main contribution to the behavior of the involved systems.[34]

Our viscosity results for the mixture *n*-hexane + 1-chlorobutane are slightly lower than those of Dominguez et al.,[19] the AAD value being equal to 1 %.

■ VISCOSITY PREDICTIONS

The McAllister equation is probably one of the best available correlation methods for the dependence of kinematic viscosity on composition.[35] As we have mentioned above, this equation contains parameters of the pure components and also two adjustable parameters, ν_{12} and ν_{21}; these adjustable parameters mean that this model can be considered only as a correlation method. With the aim of taking advantage of McAllister equation as a predictive model, the Asfour method was proposed. It is based on the effective carbon number for estimating the McAllister three-body model interaction parameters from pure component and molecular properties for liquid binary mixtures, making it possible to predict the dependence of viscosity on composition over the entire composition range. To evaluate the suitability of this method, in this work experimental data have been compared with viscosity prediction values for the studied binary mixtures.

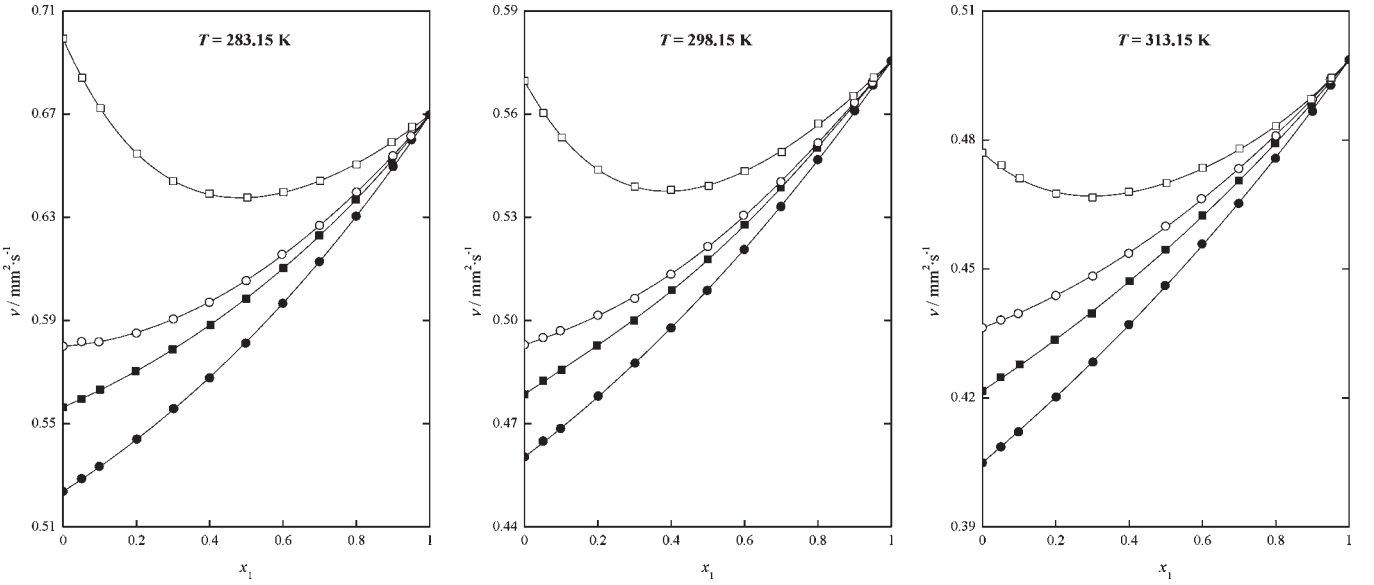

Figure 4. Kinematic viscosities, ν, for *n*-heptane with isomeric chlorobutane: ■, 1-chlorobutane; ●, 2-chlorobutane; ○, 1-chloro-2-methylpropane; □, 2-chloro-2-methylpropane; —, four-body McAllister equation.

Table 3. Parameters of the McAllister Equations and Asfour Method together with the Corresponding Average Absolute Deviations

	three-body McAllister			four-body McAllister				Asfour		
T (K)	ν_{12} (mm^2·s)	ν_{21} (mm^2·s)	AAD (%)	ν_{1112} (mm^2·s)	ν_{1122} (mm^2·s)	ν_{2221} (mm^2·s)	AAD (%)	ν_{12} (mm^2·s)	ν_{21} (mm^2·s)	AAD (%)
				3-Methylpentane + 1-Chlorobutane						
283.15	0.4905	0.5147	0.02	0.4912	0.5021	0.5250	0.02	0.4501	0.4687	4.16
298.15	0.4321	0.4505	0.07	0.4312	0.4449	0.4551	0.05	0.3948	0.4071	4.39
313.15	0.3856	0.3991	0.03	0.3861	0.3925	0.4045	0.03	0.3499	0.3597	4.62
				3-Methylpentane + 2-Chlorobutane						
283.15	0.4789	0.4915	0.04	0.4834	0.4832	0.5004	0.03	0.4396	0.4487	4.13
298.15	0.4281	0.4377	0.07	0.4317	0.4300	0.4449	0.04	0.3885	0.3954	4.63
313.15	0.3786	0.3886	0.05	0.3821	0.3813	0.3938	0.04	0.3441	0.349	4.73
				3-Methylpentane + 1-Chloro-2-methylpropane						
283.15	0.4904	0.5199	0.02	0.4911	0.5046	0.5344	0.02	0.4572	0.4827	3.38
298.15	0.4313	0.4569	0.05	0.4325	0.4440	0.4656	0.05	0.3994	0.4159	3.93
313.15	0.3863	0.4059	0.05	0.3875	0.3944	0.4142	0.05	0.3546	0.3687	4.25
				3-Methylpentane + 2-Chloro-2-methylpropane						
283.15	0.5013	0.5511	0.02	0.4992	0.5255	0.5849	0.02	0.4937	0.5547	0.27
298.15	0.4375	0.4704	0.04	0.4382	0.4518	0.4945	0.03	0.4253	0.4647	0.97
313.15	0.3857	0.4105	0.07	0.3877	0.3952	0.4278	0.06	0.3706	0.3970	1.76
				2,2-Dimethylbutane + 1-Chlorobutane						
283.15	0.5765	0.5673	0.07	0.5893	0.5694	0.5658	0.07	0.5251	0.5056	4.85
298.15	0.4928	0.4832	0.11	0.5036	0.4809	0.4859	0.03	0.4429	0.4306	5.19
313.15	0.4353	0.4269	0.12	0.4444	0.4249	0.4285	0.02	0.3898	0.3792	5.33
				2,2-Dimethylbutane + 2-Chlorobutane						
283.15	0.5666	0.5421	0.06	0.5823	0.5506	0.5394	0.04	0.5167	0.4875	4.57
298.15	0.4888	0.4708	0.09	0.4997	0.4741	0.4711	0.02	0.4389	0.4213	5.05
313.15	0.4325	0.4152	0.07	0.4408	0.4199	0.4146	0.03	0.3861	0.3705	5.24
				2,2-Dimethylbutane + 1-Chloro-2-methylpropane						
283.15	0.5799	0.5835	0.09	0.5921	0.5787	0.5842	0.08	0.5320	0.5194	4.70
298.15	0.4922	0.4943	0.09	0.5022	0.4876	0.4970	0.05	0.4469	0.4388	5.01

Table 3. Continued

	three-body McAllister			four-body McAllister				Asfour		
T (K)	ν_{12} (mm^2·s)	ν_{21} (mm^2·s)	AAD (%)	ν_{1112} (mm^2·s)	ν_{1122} (mm^2·s)	ν_{2221} (mm^2·s)	AAD (%)	ν_{12} (mm^2·s)	ν_{21} (mm^2·s)	AAD (%)
313.15	0.4368	0.4348	0.10	0.4441	0.4319	0.4373	0.04	0.3939	0.3876	5.06
				2,2-Dimethylbutane + 2-Chloro-2-methylpropane						
283.15	0.6132	0.6548	0.07	0.6182	0.6290	0.6683	0.06	0.5665	0.5886	4.34
298.15	0.5100	0.5342	0.06	0.5136	0.5201	0.5439	0.06	0.4692	0.4835	4.26
313.15	0.4423	0.4576	0.07	0.4476	0.4472	0.4639	0.06	0.4060	0.4116	4.46
				n-Hexane + 1-Chlorobutane						
283.15	0.5003	0.5167	0.03	0.5025	0.5098	0.5256	0.03	0.4608	0.4736	3.93
298.15	0.4384	0.4507	0.05	0.4398	0.4469	0.4561	0.03	0.4014	0.4099	4.24
313.15	0.3961	0.4029	0.05	0.3987	0.3983	0.4082	0.05	0.3584	0.3636	4.69
				n-Hexane + 2-Chlorobutane						
283.15	0.4881	0.4926	0.04	0.4926	0.4930	0.4987	0.02	0.4509	0.4542	3.70
298.15	0.4329	0.4394	0.07	0.4371	0.4356	0.4447	0.07	0.3956	0.3988	4.32
313.15	0.3871	0.3906	0.04	0.3920	0.3874	0.3949	0.04	0.3531	0.3534	4.45
				n-Hexane + 1-Chloro-2-methylpropane						
283.15	0.4977	0.5184	0.07	0.5028	0.5053	0.5347	0.07	0.4677	0.4874	2.93
298.15	0.4374	0.4534	0.06	0.4394	0.4471	0.4619	0.05	0.4058	0.4185	3.61
313.15	0.3934	0.4053	0.10	0.3966	0.3981	0.4135	0.10	0.3629	0.3724	3.87
				n-Hexane + 2-Chloro-2-methylpropane						
283.15	0.5116	0.5346	0.09	0.5086	0.5290	0.5680	0.02	0.5033	0.5582	0.75
298.15	0.4439	0.4602	0.05	0.4436	0.4549	0.4836	0.03	0.4305	0.466	0.53
313.15	0.3945	0.4060	0.05	0.3968	0.4001	0.4227	0.05	0.378	0.3995	1.39
				n-Heptane + 1-Chlorobutane						
283.15	0.6125	0.5777	0.02	0.6262	0.5949	0.5721	0.02	0.5544	0.5212	4.69
298.15	0.5322	0.5004	0.07	0.5451	0.5117	0.4971	0.02	0.4765	0.4481	5.14
313.15	0.4657	0.4410	0.04	0.4739	0.4529	0.4362	0.04	0.4152	0.3926	5.34
				n-Heptane + 2-Chlorobutane						
283.15	0.6029	0.5551	0.04	0.6204	0.5760	0.5484	0.02	0.5473	0.5042	4.49
298.15	0.5271	0.4882	0.03	0.5399	0.5054	0.4820	0.02	0.4738	0.4398	4.89
313.15	0.4605	0.4301	0.04	0.4685	0.4471	0.4226	0.03	0.4126	0.3849	5.08
				n-Heptane + 1-Chloro-2-methylpropane						
283.15	0.6172	0.5833	0.04	0.6303	0.5994	05828	0.04	0.5610	0.5348	4.24
298.15	0.5343	0.5028	0.07	0.5463	0.5149	0.5021	0.04	0.4803	0.4561	4.74
313.15	0.4685	0.4470	0.03	0.4753	0.4584	0.4438	0.03	0.4191	0.4009	5.08
				n-Heptane + 2-Chloro-2-methylpropane						
283.15	0.6388	0.6056	0.09	0.6420	0.6295	0.6235	0.03	0.5936	0.6022	1.83
298.15	0.5452	0.5117	0.07	0.5499	0.5329	0.5230	0.04	0.5010	0.4993	2.53
313.15	0.4718	0.4556	0.10	0.4755	0.4687	0.4581	0.05	0.4292	0.4229	3.91

The effective carbon number, N, is an intrinsic property of each compound which can be calculated from the kinematic viscosity of the pure components at the temperature of 308.15 K using the following equation:

$$ln\ \nu = -1.943 + 0.193N \quad (4)$$

The kinematic viscosity at 308.15 K and the calculated effective carbon number values for the studied compounds are collected in Table 4.

Then, the McAllister model interaction parameters can be calculated by means of these expressions:

$$\frac{\nu_{12}}{(\nu_1^2\nu_2)^{1/3}} = 0.8735 + 0.0715\ \frac{(N_2 - N_1)^2}{(N_1^2 N_2)^{1/3}} \quad (5)$$

$$\nu_{21} = \nu_{12}\left(\frac{\nu_2}{\nu_1}\right)^{1/3} \quad (6)$$

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Table 4. Experimental Kinematic Viscosities at 308.15 K and Effective Carbon Number, *N*, for Pure Compounds

compound	ν ($mm^2 \cdot s$)	*N*
3-methylpentane	0.4034	5.36
2,2-dimethylbutane	0.4034	6.24
n-hexane	0.4203	5.56
n-heptane	0.5212	6.69
1-chlorobutane	0.4468	5.89
2-chlorobutane	0.4223	5.60
1-chloro-2-methylpropane	0.4558	6.0
2-chloro-2-methylpropane	0.5087	6.57

Kinematic viscosity can be estimated once the values of the parameters have been obtained. The agreement between experimental and estimated values can be evaluated through the AAD.

The Asfour interactions parameters, ν_{12} and ν_{21}, together with the AADs for each system are collected in Table 2. The overall average deviation is 3.95 % showing a quite good agreement between experimental and predicted values using the Asfour method. The smallest deviations, 0.9 %, are shown for the system *n*-hexane + 2-chloro-2-methylpropane, whereas the largest ones, 5.1 %, are presented for the system 2,2-dimethylbutane + 1-chlorobutane. Taking into account the alkanes, the best predictions are obtained for *n*-hexane; on the other hand, regarding the isomeric chlorobutanes, the best predictions are obtained for 2-chloro-2-methylpropane.

Following the same procedures described above, equations similar to eqs 5 and 6 were obtained by Asfour et al. taking into account the McAllister four-body model. However, the calculation results showed that using the four-body model does not offer any significant improvement over the three-body model. Consequently, the use of the three-body model involving two parameters is recommended for its simplicity relative to the four-body model which involves three parameters.[16]

CONCLUSIONS

Here we present kinematic viscosity measurements of binary mixtures formed by an alkane (3-methylpentane, 2,2-dimethylbutane, *n*-hexane, and *n*-heptane) and an isomeric chlorobutane (1-chlorobutane, 2-chlorobutane, 2-methyl-1-chloropropane, or 2-methyl-2-chloropropane); the results have been satisfactorily correlated using both a three-body and a four-body McAllister equation, with AAD values less than 0.2 % in all cases. The shape of the viscosity−composition curves show that the weakness of interactions of pure chemicals once the mixture is established is the most significant contribution among energetic effects. Finally, the Asfour method has been used to predict the kinematic viscosities of the studied mixtures giving satisfactory results with an overall average deviation of 3.95 %.

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