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Supplementary Materials

A global transform for the general formulation of liquid viscosities with significant linearizing benefits: A case study on ionic liquid mixtures

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With the objective of further elucidating on the two new models proposed in the current study, which employ the recommended $\mu^{-1/\alpha} - T - x$ space, a pedagogical step-by-step example will be given for estimating the dynamic viscosity of ethanol (1) + 1-methyl-1-(3-(trimethylammonio)propyl)piperidinium dicyanamide (2). Subsequently, the results of both of the new interpolative, as well as extrapolative models will be compared against the experimental values reported by Yang and Fang,[†] which are reproduced here in Table (E.1). As for the selection of the reference temperature required in all of the models, it becomes evident by consulting this table that in the absence of data pertaining to room temperature, the minimum value, which is here $T_{\text{ref.}}$ = 293.15 (K), could be used for this purpose. Accordingly, one would have $\mu_{\text{Pure},\ T_{\text{ref.}}}$ = 4.503 (Pa.s) from the pure IL data reported by Yang and Fang, which are also listed in Table (E.2). These values will be used throughout the following calculations.

1. Extrapolation Mode

For more convenient access, the main working relation of the article, i.e., Eq. (21), is reproduced here in Eq. (E.1):

$$\mu_{\text{mix.}} = \left[\left\{\left(b_8 x_1^8 + b_6 x_1^6 + b_3 x_1^3 + b_1 x_1 + 1\right) \times \mu_{\text{Pure},\ T_{\text{ref.}}}^{-\frac{1}{\alpha}}\right\} + m\left(T - T_{\text{ref.}}\right)\right]^{-\alpha} \tag{E.1}$$

The slope of interest in Eq. (E.1), namely m, could readily be estimated from the experimental pure IL data given in Table (E.2). By employing a simple linear regression on $\mu_{\text{Pure IL}}^{-\frac{1}{\alpha}} = m \times T + c$ one would get a value of m = 0.0145. Moreover, the mixture viscosity data corresponding to the reference temperature could be utilized to fit the adjusted parameters of Eq. (17) of the article, i.e., $\frac{\Delta\mu^*}{\mu^*} = b_8 x_1^8 + b_6 x_1^6 + b_3 x_1^3 + b_1 x_1$, with $\frac{\Delta\mu^*}{\mu^*}$ being defined as in Eq.

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(18) of the article. It should be noted that the global constant of $\alpha = 4.84733$ has been employed throughout the calculations. Doing so, the resulting parameters that could directly be utilized in Eq. (E.1) are determined, which have been tabulated in Table (S2.A) as well. Subsequently, by substituting $b_8 = 1.3191$, $b_6 = -1.2295$, $b_3 = 2.8803$, $b_1 = 0.8869$ in Eq. (E.1), the dynamic viscosity data could be simply calculated at the temperature and composition of interest. Following this approach, the estimated values obtained alongside the respective deviations of each individual data point are listed in Table (E.1). Notice that the Average Relative Deviation (ARD) is defined similar to Eq. (24) of the article.

2. Interpolation Mode

In this approach, all of the adjusted parameters of Eq. (E.1) are taken as pure fitting parameters. In doing so, the fact that several of these parameters could be determined independently or from a much smaller set of experimental data, as done in the above procedure, would not be taken into account. Using $\alpha = 4.1514$, $m = 0.0169$, $b_8 = 1.2005$, $b_6 = -0.7807$, $b_3 = 3.7583$, and $b_1 = 1.0386$, that are also reported in Table (S2.A), one would be able to directly employ Eq. (E.1) for estimation of the dynamic viscosity data of interest. The resulting estimations, as well as their corresponding deviations, are reported in Table (E.1).

Table E.1. Experimental data as well as the ARD (%) for the estimated values of the dynamic viscosities of ethanol (1) + 1-methyl-1-(3-(trimethylammonio)propyl)piperidinium dicyanamide (2).

No.	***T* (K)**	x_1	**Experimental Viscosity (Pa.s)**	**Extrapolation Mode**		**Interpolation Mode**	
				Estimated Value (Pa.s)	**ARD (%)**	**Estimated Value (Pa.s)**	**ARD (%)**
1	293.15	0.10	$2.74\times10^{+00}$	$2.94\times10^{+00}$	7.36	$2.94\times10^{+00}$	7.40
2	293.15	0.20	$1.72\times10^{+00}$	$1.86\times10^{+00}$	8.17	$1.86\times10^{+00}$	8.14
3	293.15	0.30	$1.09\times10^{+00}$	$1.08\times10^{+00}$	0.74	$1.08\times10^{+00}$	1.17
4	293.15	0.40	5.96×10^{-01}	5.65×10^{-01}	5.26	5.59×10^{-01}	6.29
5	293.15	0.50	2.80×10^{-01}	2.69×10^{-01}	4.05	2.64×10^{-01}	5.81
6	293.15	0.60	1.15×10^{-01}	1.18×10^{-01}	2.68	1.15×10^{-01}	0.00
7	293.15	0.70	4.76×10^{-02}	4.92×10^{-02}	3.32	4.76×10^{-02}	0.03
8	293.15	0.80	1.97×10^{-02}	1.92×10^{-02}	2.48	1.86×10^{-02}	5.49
9	293.15	0.90	6.82×10^{-03}	6.85×10^{-03}	0.46	6.82×10^{-03}	0.00

10	303.15	0.10	$1.24\times10^{+00}$	$1.31\times10^{+00}$	5.99	$1.29\times10^{+00}$	4.03
11	303.15	0.20	8.30×10^{-01}	8.88×10^{-01}	7.01	8.81×10^{-01}	6.19
12	303.15	0.30	5.45×10^{-01}	5.56×10^{-01}	1.98	5.56×10^{-01}	2.00
13	303.15	0.40	3.30×10^{-01}	3.14×10^{-01}	4.76	3.16×10^{-01}	4.26
14	303.15	0.50	1.64×10^{-01}	1.62×10^{-01}	1.32	1.63×10^{-01}	0.57
15	303.15	0.60	7.33×10^{-02}	7.67×10^{-02}	4.67	7.73×10^{-02}	5.41
16	303.15	0.70	3.30×10^{-02}	3.42×10^{-02}	3.71	3.44×10^{-02}	4.25
17	303.15	0.80	1.50×10^{-02}	1.42×10^{-02}	5.17	1.43×10^{-02}	4.37
18	303.15	0.90	5.39×10^{-03}	5.37×10^{-03}	0.45	5.55×10^{-03}	2.96
19	313.15	0.10	6.24×10^{-01}	6.59×10^{-01}	5.65	6.49×10^{-01}	4.00
20	313.15	0.20	4.61×10^{-01}	4.68×10^{-01}	1.63	4.69×10^{-01}	1.71
21	313.15	0.30	3.10×10^{-01}	3.10×10^{-01}	0.03	3.15×10^{-01}	1.50
22	313.15	0.40	2.11×10^{-01}	1.86×10^{-01}	11.68	1.91×10^{-01}	9.26
23	313.15	0.50	1.06×10^{-01}	1.02×10^{-01}	3.51	1.06×10^{-01}	0.01
24	313.15	0.60	4.96×10^{-02}	5.16×10^{-02}	4.10	5.38×10^{-02}	8.37
25	313.15	0.70	2.41×10^{-02}	2.44×10^{-02}	1.36	2.55×10^{-02}	5.65
26	313.15	0.80	1.16×10^{-02}	1.07×10^{-02}	7.60	1.12×10^{-02}	3.25
27	313.15	0.90	4.38×10^{-03}	4.25×10^{-03}	2.92	4.56×10^{-03}	4.12
28	323.15	0.10	3.60×10^{-01}	3.60×10^{-01}	0.12	3.60×10^{-01}	0.00
29	323.15	0.20	2.67×10^{-01}	2.66×10^{-01}	0.27	2.71×10^{-01}	1.56
30	323.15	0.30	1.92×10^{-01}	1.84×10^{-01}	4.16	1.91×10^{-01}	0.64
31	323.15	0.40	1.32×10^{-01}	1.16×10^{-01}	11.92	1.22×10^{-01}	7.23
32	323.15	0.50	7.05×10^{-02}	6.73×10^{-02}	4.60	7.17×10^{-02}	1.76
33	323.15	0.60	3.52×10^{-02}	3.58×10^{-02}	1.73	3.85×10^{-02}	9.38
34	323.15	0.70	1.81×10^{-02}	1.78×10^{-02}	1.54	1.92×10^{-02}	6.26
35	323.15	0.80	9.19×10^{-03}	8.20×10^{-03}	10.74	8.90×10^{-03}	3.13
36	323.15	0.90	3.68×10^{-03}	3.41×10^{-03}	7.46	3.78×10^{-03}	2.73
37	333.15	0.10	2.19×10^{-01}	2.11×10^{-01}	3.78	2.15×10^{-01}	1.87
38	333.15	0.20	1.71×10^{-01}	1.61×10^{-01}	6.12	1.67×10^{-01}	2.25
39	333.15	0.30	1.26×10^{-01}	1.15×10^{-01}	8.77	1.22×10^{-01}	3.13
40	333.15	0.40	8.59×10^{-02}	7.56×10^{-02}	11.95	8.18×10^{-02}	4.77
41	333.15	0.50	5.07×10^{-02}	4.57×10^{-02}	9.80	5.02×10^{-02}	0.95
42	333.15	0.60	2.62×10^{-02}	2.55×10^{-02}	2.75	2.83×10^{-02}	7.91
43	333.15	0.70	1.41×10^{-02}	1.33×10^{-02}	6.00	1.48×10^{-02}	4.89
44	333.15	0.80	7.55×10^{-03}	6.37×10^{-03}	15.67	7.15×10^{-03}	5.32
45	333.15	0.90	3.18×10^{-03}	2.75×10^{-03}	13.39	3.16×10^{-03}	0.64
Total:					**5.09**		**3.79**

3. Pure-state viscosity

It is interesting to observe that unlike the current literature models, the relation proposed in the current study, i.e., Eq. (E.1), not only does not take pure-state viscosity or volumetric data as input, but rather, could simply be utilized for estimation of the dynamic viscosity of pure ILs as well. This objective could be fulfilled by simply introducing $x_1 = 0$ to Eq. (E.1) that would ultimately result in:

$$\mu_{\text{Pure IL}} = \left[\mu_{\text{Pure, } T_{\text{ref.}}}^{-\frac{1}{\alpha}} + m\left(T - T_{\text{ref.}}\right) \right]^{-\alpha} \tag{E.2}$$

This method has been undertaken here using the two new approaches discussed beforehand and utilizing their respective adjusted parameters listed above. The final results obtained are reported in Table (E.2) alongside the pertinent deviations that exhibit a satisfactory performance. Notice that an exactly zero deviation is always expected for the results of the interpolation mode at the reference temperature according to the definition of $\frac{\Delta\mu^*}{\mu^*}$ given in Eq. (18) of the article. A similar conclusion could also be drawn for the extrapolation mode, as the reference temperature is essentially the basis of writing the equation of the straight line of interest in this approach in the $\mu^{-1/\alpha} - T$ space, i.e., Eq. (E.2).

Table E.2. Experimental data, as well as the ARD (%), for the estimated values of the dynamic viscosities of pure 1-methyl-1-(3-(trimethylammonio)propyl)piperidinium dicyanamide using the data of Yang and Fang.

No.	***T* (K)**	**Experimental Viscosity (Pa.s)**	**Extrapolation Mode**		**Interpolation Mode**	
			Estimated Value (Pa.s)	**ARD (%)**	**Estimated Value (Pa.s)**	**ARD (%)**
1	293.15	$4.50\times10^{+00}$	$4.50\times10^{+00}$	0.00	$4.50\times10^{+00}$	0.00
2	303.15	$1.84\times10^{+00}$	$1.88\times10^{+00}$	2.45	$1.82\times10^{+00}$	0.71
3	313.15	8.60×10^{-01}	8.99×10^{-01}	4.51	8.69×10^{-01}	1.02
4	323.15	4.60×10^{-01}	4.73×10^{-01}	2.91	4.63×10^{-01}	0.68
5	333.15	2.70×10^{-01}	2.69×10^{-01}	0.47	2.68×10^{-01}	0.66
Total:				**2.07**		**0.61**