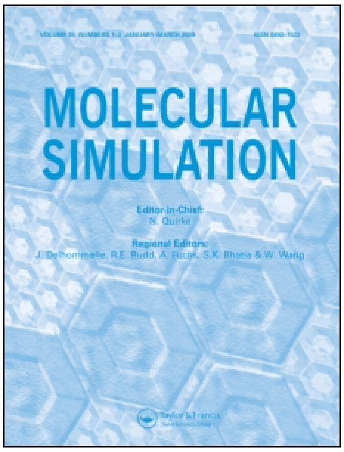

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Prediction of the Liquid Viscosities of Pure Components and Mixtures Using Neural Network and ASOG Group Contribution Methods

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This study proposes a simple method for predicting liquid viscosities of pure components and mixtures from chemical structures only. Initially, the constants B and T_0 used in a modified Andrade equation for pure liquid viscosity were predicted using a three-layer neural network method with an error back-propagation learning algorithm. The network was trained using 194 data sets and information concerning 29 chemical groups was used as descriptors of input. The components covered were paraffines, olefins, alkynes, aromatic hydrocarbons, chlorides, bromides, alcohols, ketones, esters, ethers, aldehydes and organic acids. The temperature range is approximately the melting point to the bubble point of the compounds and the average and maximum deviations of viscosity are 9.5 and 14.3%, respectively.

The viscosities of binary systems were predicted using the ASOG-VISCO group contribution method. This study covers mixtures composed of CH_2, ArCH, CyCH, OH, H_2O, CO and COO groups with a temperature range of 293.15–303.15 K. and an average deviation of viscosities of 4.5%.

Keywords: Liquid viscosity; Neural network; ASOG-VISCO group method; Pure component viscosity

INTRODUCTION

The viscosity of liquids is one of the key transport properties required in many scientific studies and engineering applications. Predictive methods of viscosity could be useful in designing chemical processes or new materials [1]. A predictive method of kinematic viscosities called the ASOG-VISCO group contribution method, which uses information of pure component viscosities and group pair parameters, has already been proposed [2]. Furthermore, a predictive method of thermophysical properties using a three-layer neural network (NN) method with an error back-propagation learning algorithm has also been proposed [3,4].

This paper proposes a predictive method for calculating pure liquid viscosities using a NN method. The components covered are paraffines, olefins, alkynes, aromatic hydrocarbons, chlorides, bromides, alcohols, ketones, esters, ethers, aldehydes and organic acids. The temperature range is approximately the melting point to the bubble point of the compounds. A predictive method for calculating mixture viscosities is secondarily proposed using ASOG-VISCO group interaction parameters. The predicted results are compared with those using the well known Grunberg and Nissan method [1,5].

THE PREDICTION OF PURE COMPONENT VISCOSITY USING A NN

In order to propose a predictive method of viscosity, which is applicable in relatively wide temperature ranges, the following viscosity [mPa s]–temperature [T] equation was used [1,6]:

$$\ln \eta = B\left(\frac{1}{T} - \frac{1}{T_0}\right) \tag{1}$$

This equation is a modified version of the equation commonly referred to as the Andrade equation.

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TABLE I Group classification used as input of NN method

CH_3	$CH_2{=}C$	M	CHO (aldehyde)
CH_2	$CH{=}C$	P	CO
C	$C{=}C$	CCl	COOH
OH	ArCH	CCl_2	COO
GOH	ArH	CCl_3	CH_3COO
$CH_2{=}CH$	ArCl	Cl(C=C)	CHO (ether)
$CH{=}CH$	O	Br	

The two constants B and T_0 have some physical meanings and were predicted using a NN method.

The NN Method

The three-layer NN of the back-propagation method was used in the reconstruction learning method [3,7] to evaluate B and T_0. The equation for calculating B or T_0 is given below:

$$B \text{ or } T_0 = \left\{\sum W_{k,j}\left(\frac{1}{\exp\left(-4.0\sum W_{ij}X_j\right)+1}\right)\right\} \times (Y_{\max} - Y_{\min}) + 0.9\,Y_{\min} - 0.1\,Y_{\max} \quad (2)$$

where

$$X_j = \frac{0.8\,X_{im,j} + 0.1\,X_{\max,j} - 0.9\,X_{\min,j}}{\text{abs}\,(X_{\max,j} - X_{\min,j})}; \quad (2a)$$

i is the type of functional group; j, the number of hidden neuron (number of Sigmoid function); $X_{\min,j}$, the minimum value of functional group j; $X_{\max,j}$, the maximum value of functional group j; $X_{im,j}$, the number of functional group j; X_j, the scaled input j; $Y_{\min}$, the minimum value of B or T_0; $Y_{\max}$, the maximum value of B or T_0; $W_{k,j}$, the Weight matrix (Tables II and III) and $W_{i,j}$, the Weight matrix (Tables II and III).

The parameters necessary for the calculation are $W_{k,j}$, $W_{i,j}$, $Y_{\max}$, $Y_{\min}$, $X_{\max,j}$ and $X_{\min,j}$.

The Two Constants B and T_0

The two constants in Eq. (1) were predicted using the NN method. The number of datasets of B and T_0 [6] are 194 for learning and 33 for prediction data,

TABLE II Weight matrix for evaluating B obtained using NN method

W_{ij}

	j								
i	*1*	*2*	*3*	*4*	*5*	*6*	*7*	X_{min}	X_{max}
1 (CH_3)	0.951	1.351	0.990	− 0.842	− 1.386	− 0.341	− 0.002	0	6
2 (CH_2)	0.180	0.547	− 0.195	− 0.081	− 0.003	1.392	0.298	0	19
3 (C)	− 0.149	− 0.787	0.001	0.436	− 1.263	− 0.418	− 0.326	0	3
4 ($CH_2{=}CH$)	0.324	0.174	0.043	− 0.055	− 0.109	− 0.161	− 0.260	0	2
5 ($CH{=}CH$)	0.001	0.004	− 0.084	− 0.101	0.000	0.093	− 0.043	0	1
6 ($CH_2{=}C$)	0.004	− 0.004	− 0.214	0.092	− 0.003	0.126	− 0.005	0	1
7 ($CH{=}C$)	0.003	− 0.002	− 0.015	0.001	− 0.002	0.000	0.002	0	1
8 ($C{=}C$)	0.004	− 0.070	− 0.109	0.004	− 0.003	− 0.001	0.002	0	1
9 (Ar)	0.327	0.821	− 0.665	− 0.019	0.000	− 0.330	− 0.894	0	6
10 (ArCH)	0.133	− 0.709	− 0.003	0.550	0.274	− 0.025	0.001	0	3
11 (GOH)	− 0.001	− 0.001	0.258	1.268	0.862	− 0.001	0.000	0	3
12 (OH)	− 0.443	1.517	0.566	− 0.041	− 0.150	− 1.999	− 0.896	0	2
13 (ArCl)	− 0.004	− 0.598	0.001	0.205	0.000	0.004	− 0.064	0	2
14 (COOH)	0.000	0.669	− 0.003	0.593	− 0.243	0.003	0.799	0	1
15 (CH_3CO)	0.005	− 0.024	− 0.041	− 0.080	− 0.264	− 0.002	− 0.170	0	1
16 (CHO)	− 0.002	− 0.341	− 0.157	− 0.009	0.008	0.038	− 0.263	0	1
17 (COO)	− 0.341	− 0.144	0.058	− 0.057	− 0.253	0.005	− 0.060	0	1
18 (CH_3COO)	0.086	− 0.001	− 0.005	− 0.025	− 0.030	0.081	− 0.196	0	1
19 (CHO)	0.002	− 0.177	− 0.110	− 0.373	− 0.080	0.088	− 0.324	0	2
20 (CCl)	− 0.467	0.923	− 0.026	0.302	− 0.186	0.001	0.271	0	3
21 (CCl_2)	− 0.042	− 0.112	0.368	− 0.290	− 0.404	0.025	− 0.001	0	1
22 (CCl_3)	− 0.002	0.000	0.001	0.063	− 0.055	0.003	− 0.115	0	1
23 ($C{=}C{-}Cl$)	− 0.001	0.000	0.000	0.164	− 0.003	0.002	− 0.053	0	4
24 (Br)	− 0.002	0.001	0.002	0.002	− 0.001	0.001	− 0.252	0	2
25 (*o*)	0.004	− 0.181	− 0.003	0.221	0.416	0.151	0.001	0	3
26 (*m*)	0.003	− 0.137	0.000	0.042	0.105	− 0.794	− 0.004	0	3
27 (*p*)	0.000	− 0.001	0.000	− 0.163	0.009	0.281	0.000	0	2
28 (baias)	− 0.956	− 1.366	− 0.751	− 0.807	− 0.394	− 0.041	0.000	1	0

W_{kj}

	j								
k	*1*	*2*	*3*	*4*	*5*	*6*	*7*	Y_{min}	Y_{max}
1	− 0.709	0.740	0.477	1.497	− 1.525	0.357	− 0.617	227.9	3337.1

TABLE III Weight matrix for evaluating T_0 obtained using NN method

W_{ij}							
	j						
i	*1*	*2*	*3*	*4*	*5*	X_{min}	X_{max}
1 (CH_3)	−0.907	2.766	−0.370	−1.999	0.842	0	5
2 (CH_2)	−0.402	−4.711	−3.936	1.910	0.754	0	18
3 (C)	−0.078	−1.506	−0.615	1.563	−0.563	0	2
4 ($CH_2{=}CH$)	−1.166	0.937	−0.571	−0.461	0.564	0	2
5 ($CH{=}CH$)	0.000	−0.244	−0.260	0.000	0.198	0	1
6 ($CH_2{=}C$)	0.154	0.084	−0.161	−0.003	−0.004	0	1
7 ($CH{=}C$)	0.328	0.000	−0.001	−0.419	0.003	0	1
8 ($C{=}C$)	0.000	0.000	0.000	0.001	−0.001	0	1
9 (Ar)	−0.371	−0.159	−0.735	0.604	0.333	0	6
10 (ArCH)	0.399	1.144	0.052	−0.278	−0.289	0	3
11 (GOH)	2.291	1.571	−1.271	0.698	0.032	0	3
12 (OH)	0.938	−0.002	−0.916	1.204	−0.759	0	2
13 (ArCl)	0.200	0.590	−0.002	0.023	0.443	0	2
14 (COOH)	0.422	−0.380	−1.975	−0.132	0.494	0	1
15 (CH_3CO)	−0.160	0.010	−0.737	0.053	0.026	0	1
16 (CHO)	0.587	0.883	−0.111	−0.735	0.096	0	1
17 (COO)	0.336	0.386	−0.416	−0.118	−0.596	0	1
18 (CH_3COO)	0.787	−1.015	−0.905	−0.550	0.242	0	1
19 (CHO)	1.558	−1.362	−0.384	−0.490	−0.048	0	1
20 (CCl)	0.811	0.042	−1.007	0.408	0.001	0	3
21 (CCl_2)	0.234	0.005	−0.296	0.673	0.000	0	1
22 (CCl_3)	0.003	0.001	−0.795	0.005	0.000	0	1
23 ($C{=}C{-}Cl$)	1.072	0.004	−0.841	0.004	0.001	0	4
24 (Br)	−0.176	0.498	−1.233	0.001	−1.158	0	2
25 (*o*)	−0.404	−0.005	−0.390	−0.068	0.025	0	2
26 (*m*)	0.003	0.002	0.000	0.082	−0.002	0	3
27 (*p*)	0.000	−0.415	−0.193	0.000	−0.001	0	2
28 (baias)	−0.338	−0.611	2.135	−0.123	−0.948	1	0

W_{kj}							
	j						
k	*1*	*2*	*3*	*4*	*5*	Y_{min}	Y_{max}
1	0.394	0.454	−0.780	0.491	0.716	93.9	426.7

respectively. Table I shows the group classification used as input for the NN method. Tables II and III show the weight matrix for B and T_0. Figure 1(a),(b) shows the comparison between the calculated and experimental B and T_0 values. The correlation factors are 0.9999 and 0.9998, respectively.

Liquid Viscosity

Using the B and T_0 values predicted by the NN method, liquid viscosity was calculated using Eq. (1) and the results were then compared with the experimental values [6,8]. The components discussed covered paraffines, olefins, alkynes, aromatic hydrocarbons, chlorides, bromides, alcohols, ketones, esters, ethers, aldehydes and organic acids.

Learning Data

Figure 2(a) shows the comparison between the predicted and the experimental viscosity data [6].

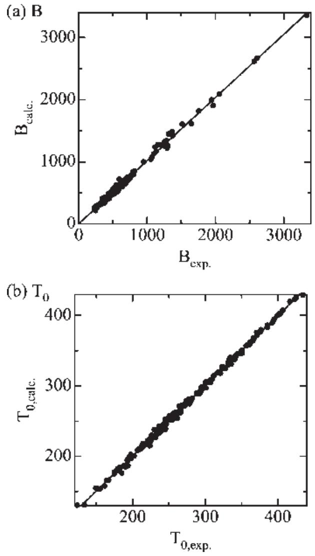
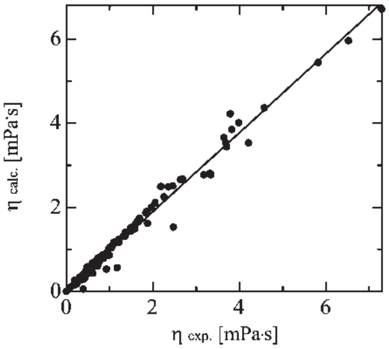


FIGURE 1 Comparison between the experimental and calculated B and T_0 in modified Andrade equation using the proposed NN method.

(a) learning



(b) prediction

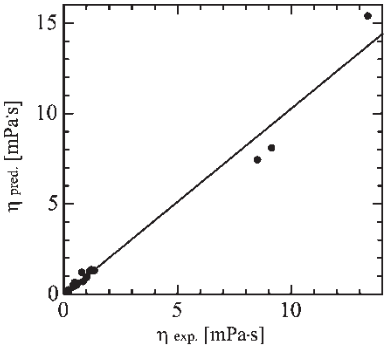


FIGURE 2 Comparison between the experimental and calculated viscosities for (a) learning and (b) prediction data using the proposed NN method.

The correlation factor is 0.9931 and the average relative deviation is 6.51%. Table IV(a) shows the calculated results.

Prediction Data

The ability of the predictive equation was checked using prediction data sets. Table IV(b) and Fig. 2(b) show the comparison between the predicted and the experimental viscosities. The correlation coefficient and the average relative deviation for liquid viscosity are 0.9899 and 9.51%, respectively. As an example, Fig. 3 shows the predicted results for 2-heptanone with an average deviation of 3.20%.

TABLE IV Calculated results of liquid viscosity

Compounds	*NDS*	*ARD*
(a) *Learning data*		
Alkanes	45	6.07
Alkenes	38	6.25
Alcohols	24	13.83
Aromatic hydrocarbons	24	4.67
Chlorides	16	3.81
Bromides	2	2.07
Carbonyls	45	7.97
(b) *Prediction data*		
Alkanes	3	16.9
Alkenes	6	3.55
Alcohols	6	6.02
Aromatic hydrocarbons	2	9.83
Chlorides	1	11.32
Bromides	1	1.80
Carbonyls	14	14.3

NDS, number of data sets; ARD, average relative deviation (%).

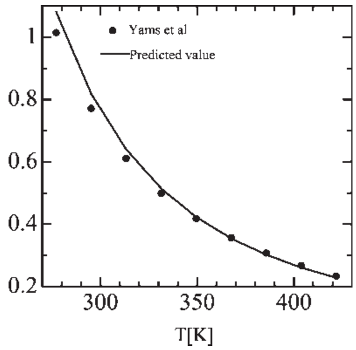


FIGURE 3 Comparison between the experimental and predicted viscosities for 2-heptanone using the proposed NN method.

THE PREDICTION OF MIXTURE VISCOSITY USING THE ASOG-VISCO GROUP CONTRIBUTION METHOD

Equations for Calculating Viscosity

Eyring's theory of absolute reaction rate [2,9,10] gives the kinematic viscosity of liquid mixtures of pure components and excess free energy at the activated state:

$$\ln(\nu M) = \sum_i x_i \ln(\nu_i M_i) + \frac{\Delta^* G^{\mathrm{E}}}{RT} \tag{3}$$

In this paper, we assume the following equation [2]:

$$\Delta^* G^{\mathrm{E}} / \Delta G^{\mathrm{E}} = k \tag{4}$$

Here k is an adjustable parameter whilst the meaning of k is $-(1/A)$ as in Eyring's paper [9]. The kinematic viscosity can be calculated by the known values of excess Gibbs free energy with the given k:

$$\ln(\nu M) = \sum_i x_i \ln(\nu_i M_i) + k\frac{\Delta G^{\mathrm{E}}}{RT} \tag{5}$$

For calculating viscosity, the following equation was constructed from Eq. (6):

$$\ln \eta = \sum_i x_i \ln \eta_i - \left(\ln V - \sum_i x_i \ln V_i\right) + k\frac{\Delta G^{\mathrm{E}}}{RT} \tag{6}$$

When $\ln \nu$ is assumed to be equal to $\sum x_i \ln \nu_i$, Eq. (6) is reduced to the following equation:

$$\ln \eta = \sum_i x_i \ln \eta_i + k\frac{\Delta G^{\mathrm{E}}}{RT} \tag{7}$$

TABLE V ASOG-VISCO group pair parameters (283.15–333.15 K)

(a) $m_{k/l}$

[m]	*l*						
k	*CH_2*	*ArCH*	*CyCH*	*OH*	*H_2O*	*CO*	*COO*
CH_2	0	0.2779	0	− 0.357	− 9.006	0	0.3682
ArCH	1.2817	0	− 1.565	0	NA	− 1.109	0.2418
CyCH	0	− 1.543	0	1.0616	NA	3.4974	0
OH	14.146	0	− 4.676	0	− 13.11	5.9432	− 40.2
H_2O	0.0879	NA	NA	0.204	0	0.2318	NA
CO	0	3.7286	13.184	− 11.32	− 0.968	0	0
COO	0.0952	− 0.902	0	19.131	NA	0	0

(b) $n_{k/l}$

[n]	*l*						
k	*CH_2*	*ArCH*	*CyCH*	*OH*	*H_2O*	*CO*	*COO*
CH_2	0	− 418.5	0.1004	469.65	2216.5	265.39	112.59
ArCH	− 187.4	0	510	280.63	NA	678.02	140.35
CyCH	1	368.21	0	0.9436	NA	− 765.5	− 183.8
OH	− 6137	− 1247	456.72	0	2964.1	− 2071	11583
H_2O	528	NA	NA	537.65	0	94.521	NA
CO	− 460.5	− 1922	− 4657	3240.5	− 0.968	0	− 108.3
COO	− 383.6	− 107.2	36.378	− 5747	NA	99.719	0

NA, not available.

From preliminary studies, -1 is treated as the value of k as seen in the procedures of Tochigi *et al.* [2] and Novak [10].

The Predicted Results of Viscosity using ASOG-VISCO Group Pair Parameters

The ΔG^{E} used in Eqs. (6) and (7) was evaluated using the ASOG group contribution method [11], which is given by the following equations:

$$\Delta G^{\mathrm{E}} = \sum_i x_i \ln \gamma_i = \sum_i x_i \left(\ln \gamma_i^{\mathrm{FH}} + \ln \gamma_i^{G}\right) \tag{8}$$

$$\ln \gamma_i^{\mathrm{FH}} = \ln \frac{\nu_i^{\mathrm{FH}}}{\sum_j \nu_j^{\mathrm{FH}} x_j} + 1 - \frac{\nu_i^{\mathrm{FH}}}{\sum_j \nu_j^{\mathrm{FH}} x_j} \tag{9}$$

$$\ln \gamma_i^{G} = \sum_k \nu_{k,i} \left(\ln \Gamma_k - \ln \Gamma_k^{(i)}\right) \tag{10}$$

$$\ln \Gamma_k = -\ln \sum_l X_l a_{k,l} + 1 - \sum_l \frac{X_l a_{l,k}}{\sum_m X_m a_{l,m}} \tag{11}$$

$$X_l = \frac{\sum_i x_i \nu_{l,i}}{\sum_i x_i \sum_k \nu_{k,i}} \tag{12}$$

$$a_{k,l} = \exp\left(m_{k,l} + \frac{n_{k,l}}{T}\right) \tag{13}$$

In Eq. (13), $m_{k/l}$ and $n_{k/l}$ are the ASOG-VISCO group pair parameters and depend only on the kinds of group pairs and not on temperature. $\nu_{\mathrm{i}}^{\mathrm{FH}}$ is the number of atoms (other than hydrogen atoms) in molecule i, and $\nu_{k,i}$ is the total number of atoms (other than hydrogen atoms) in group k of molecule i. Table V shows some parts of the group pair parameters [2], those related to the CH_2, ArCH, CyCH, OH, H_2O, CO and COO groups. They were determined using the kinematic viscosity data. The parameters cover paraffines, aromatic hydrocarbons, cycloparaffines water, alcohols, ketones and esters and the temperature range is 283.15–333.15 K.

The viscosities for binary systems were evaluated for 50 datasets. Table VI shows the predicted results obtained using Eqs. (6) and (7). The overall average deviations are 4.5 and 5.7%, respectively. Table VI also shows the predicted results using the Grunberg and Nissan method [1,5]. ASOG-VISCO is better than Grunberg and Nissan method for the overall deviation, though the accuracy by Grunberg and Nissan method is better for cyclohexane + alkanes systems. Further, ASOG-VISCO covers water which is an important compound. Figure 4 shows the comparison between the experimental [12,13] and predicted results for acetone + cyclohexane, methanol + water and ethanol + water systems at 298.15 K.

CONCLUSIONS

This study shows that it is possible to calculate viscosity using a structural equation with the NN

TABLE VI Comparison between the experimental and predicted viscosity using ASOG-VISCO and Grunberg and Nissan methods

	System			*ARD*		
	(1)	*(2)*	*T (K)*	*Eq. (6)*	*Eq. (7)*	*G&N*
1	*n*-Butanol	Butyl acetate	298.15	3.6	3.8	–
2	*n*-Butanol	Ethyl benzene	298.15	6.4	7.2	6.0
3	*n*-Butanol	*p*-Xylene	298.15	7.7	8.6	8.6
4	Acetone	Cyclohexane	298.15	5.3	4.0	11.8
5	Acetone	Ethyl acetate	298.15	0.3	0.9	–
6	Acetone	Propyl propionate	298.15	2.6	0.4	–
7	Acetone	Water	298.15	17.8	31.4	–
8	Benzene	Ethyl butyrate	303.15	3.0	2.7	–
9	Benzene	Hexane	298.15	2.8	4.0	2.1
10	Benzene	*n*-Propyl acetate	303.15	2.7	2.8	–
11	Benzene	Toluene	298.15	0.4	0.3	4.9
12	*n*-Butanol	Pentane	298.15	2.7	2.9	9.3
13	Cyclohexane	Benzene	298.15	1.0	0.7	19.3
14	Cyclohexane	Decane	298.15	4.4	8.1	4.9
15	Cyclohexane	Ethanol	298.15	4.7	2.0	6.2
16	Cyclohexane	Heptane	298.15	10.7	12.6	2.4
17	Cyclohexane	Hexane	298.15	17.1	13.2	1.9
18	Cyclohexane	Nonane	298.15	6.8	9.6	14.8
19	Cyclohexane	Octane	298.15	9.4	11.5	3.0
20	Cyclohexanone	*n*-Butanol	303.15	1.7	1.7	–
21	Cyclohexanone	*n*-Hexanol	303.15	6.0	6.3	–
22	Cyclohexanone	*n*-Pentanol	303.15	6.8	6.8	–
23	Cyclohexanone	*n*-Propanol	303.15	2.8	3.7	–
24	Cyclopentanone	*n*-Butanol	303.15	3.6	3.6	–
25	Cyclopentanone	*n*-Hexanol	303.15	3.3	4.5	–
26	Cyclopentanone	*n*-Pentanol	303.15	5.0	5.4	–
27	Cyclopentanone	*n*-Propanol	303.15	2.4	2.7	–
28	Ethanol	Water	298.15	6.1	9.2	–
29	Ethyl acetate	1,2-Dimethyl cyclohexane	298.15	2.4	0.9	–
30	Ethyl acetate	Benzene	298.15	3.0	3.0	–
31	Ethyl acetate	Cyclohexane	298.15	2.2	3.3	–
32	Ethyl acetate	*o*-Xylene	298.15	3.0	3.4	–
33	Ethyl acetate	Toluene	298.15	1.7	1.8	–
34	Ethyl benzene	2-Butanone	298.15	9.0	9.8	–
35	Methanol	Acetone	298.15	15.9	13.5	7.5
36	Methanol	Water	298.15	2.3	5.0	–
37	Methylcyclohexane	*n*-Butanol	303.15	2.1	3.3	2.5
38	Methylcyclohexane	*n*-Hexanol	303.15	1.0	1.1	3.2
39	Methylcyclohexane	*n*-Pentanol	303.15	3.6	4.1	2.9
40	Methylcyclohexane	*n*-Propanol	303.15	1.3	3.7	3.5
41	2-Butanone	Ethyl acetate	298.15	1.3	1.4	–
42	2-Butanone	Propyl propionate	298.15	0.8	0.7	–
43	*n*-Butyl acetate	2-Hexanone	298.15	1.1	1.2	–
44	*n*-Butyl acetate	*n*-Amyl acetate	298.15	0.4	0.3	–
45	Propyl propionate	1,2,4-Trimethyl cyclohexane	298.15	1.0	1.6	–
46	Propyl propionate	Benzene	298.15	3.5	3.1	–
47	Propyl propionate	Methylcyclohexane	298.15	1.9	1.8	–
48	Propyl propionate	Toluene	298.15	8.0	7.5	–
49	Toluene	Acetone	298.15	6.6	7.6	6.0
50	Toluene	Ethylbenzene	298.15	0.9	0.8	6.3
	Overall			4.5	5.7	6.3

ARD, average relative deviation (%); G&N, Grunberg and Nissan method.

method based on the reconstruction learning theory and the ASOG group contribution method. If the quantity of data on viscosity were to increase and the ASOG group pair parameters were to be stored, it may become possible to make remarkable progress in the accuracy and application of these calculations.

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NOMENCLATURE

Δ^*G	free energy of activation (J/mol)
ΔG^{E}	excess Gibbs free energy (J/mol)
k	parameter defined by Eq. (4)
M	molecular weight (g/mol)
R	gas constant (J/mol K)

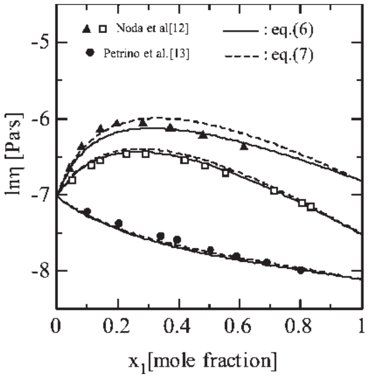

FIGURE 4 Comparison between the experimental and predicted viscosities for (•) acetone + cyclohexane, (▲) methanol + water and (□) for ethanol + water at 298.15 K using ASOG-VISCO method.

T	absolute temperature (K)
ν	kinematic viscosity (m^2/s)
η	viscosity (mPa·s)
Subscript	
i	pure component i
Superscript	
E	excess property

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