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Short Communication

SHORT COMMUNICATION

Correlation of the liquid mixture viscosities

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Abstract: In this paper, forty-two selected correlation models for liquid mixture viscosities of organic compounds were tested on 219 binary and 41 ternary sets of experimental data taken from the literature. The binary sets contained 3675 experimental data points for 70 different compounds. The ternary sets contained 2879 experimental data points for 29 different compounds. The Heric I, Heric–Brewer II, and Krishnan–Laddha models demonstrated the best correlative characteristics for the binary mixtures (overall absolute average deviation < 2 %). The Heric I, Heric–Brewer II, Krishnan–Laddha and Heric II models demonstrated the best correlative characteristics for the ternary mixtures (overall absolute average deviation < 3 %).

Keywords: binary mixture; ternary mixture; liquid mixture viscosity; correlation model.

INTRODUCTION

The study of thermodynamic properties of liquid mixtures contributes to an understanding of the behavior of various liquids and functional groups. This information is very useful in the design of industrial processes and in the development of the liquid state theories and predictive methods. Knowledge of the liquid mixture viscosities are required for the solution of many engineering problems, including heat and mass transfer, and fluid flow.

A number of correlation models have been developed for liquid mixture viscosities.[1–18] These equations are empirical or at the best semi-theoretical. The aim of this work is to compare the correlation capabilities of these models on the experimental viscosities of binary and ternary liquid mixtures of alkanes, haloalkanes, alcohols, aromates, amines, ketones, *etc*.

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Selection of models

There are numerous correlation models for liquid mixture viscosities. From these, the models Dolezalek–Schulze,[1] Grunberg–Nissan,[2] Tamura–Kurata,[3] McAllister 3,[4] McAllister 4,[4] McAllister–Chandramouli–Laddha,[5] Katti–Chaudhri,[6] Ausländer,[7] Modified Wilson,[8] Heric I,[9] Heric II,[9] Heric–Brewer I,[10] Heric–Brewer II,[10] Krishnan–Laddha,[11] Stephan–Heckenberger,[12] McAllister–Soliman–Marschall (McASM),[13] Mehrotra,[14] Baylaucq–Daugé–Boned,[15] Dimitrov–Kamenski I,[16] Dimitrov–Kamenski II,[16] Dimitrov–Kamenski III,[16] Dimitrov–Kamenski IV,[16] Dimitrov–Kamenski V,[16] Dimitrov–Kamenski VI,[16] Dimitrov–Kamenski VII,[16] Dimitrov–Kamenski VIII,[16] Dimitrov–Kamenski IX,[16] Dimitrov–Kamenski X,[16] Dimitrov–Kamenski XI,[16] Dimitrov–Kamenski XII,[16] Dimitrov–Kamenski XIII,[16] modified Dimitrov–Kamenski,[16] Focke–Du Plessis I,[17] Focke–Du Plessis II,[17] Focke–Du Plessis III,[17] Focke–Du Plessis IV,[17] Focke–Du Plessis V,[17] Focke–Du Plessis VI,[17] Focke–Du Plessis VII,[17] Focke––Du Plessis VIII,[17] Focke–Du Plessis IX,[17] and Focke–Sandrock–Kok,[18] in chronological order, were selected for the present study. The equations related to the selected models are given in the Supplementary material to this paper. The number of parameters in these models varies from one to nine.

McAllister 3, McAllister 4, Stephan–Heckenberger, Dimitrov–Kamenski I–XIII and Focke–Du Plessis I–IX are models for binary mixtures, whereas McAllister–Chandramouli–Laddha, Heric II and Modified Dimitrov–Kamenski are models for ternary mixtures. All models except the Ausländer, Modified Wilson, Stephan–Heckenberger and Focke–Sandrock–Kok are linear or can be linearized per parameters. A preliminary investigation indicated that these non-linear equations do not result in correlations significantly better than those obtained with linear equations with the same number of parameters. The linear models were investigated in this work as correlations with the nonlinear models resulted in problems of convergence and global optima. These models are based on the model of ideal mixture with additional correction terms and therefore their parameters have not physical meaning.

SELECTION OF EXPERIMENTAL DATA POINTS

The performance of selected linear models was tested on 219 binary and 41 ternary sets of literature experimental data. The binary sets contained 3675 experimental data points for 70 different compounds. The ternary sets contained 2879 experimental data points for 29 different compounds. The selected binary and ternary liquid mixtures are presented in Tables SI and SII in the Supplementary material to this paper.

RESULTS AND DISCUSSION

The results for the selected linear models are presented in Table I, where N_{all} is a total number of data points in the correlation. Only sets of experimental data with $n \geq N_m+2$ were used in the correlation, where N_m is the number of model

parameters. Sets with experimental data for different temperatures and pressures were correlated with only one set of parameters. The deviation from the experimental values is expressed as the absolute average deviation p_{av} for each data set point:

$$p_{av} = (100 / n)\sum_{i=1}^{n}\left|(\eta_{l,m,i,exp} - \eta_{l,m,i,cal}) / \eta_{l,m,i,exp}\right| \quad (1)$$

where $\eta_{l,m}$ is the viscosity of a liquid mixture, and n is the number of experimental data points per set. The overall absolute average deviation P_{av} for each model is expressed as:

$$P_{av} = \sum_{i=1}^{N} n_i p_{av,i} / \sum_{i=1}^{N} n_i \quad (2)$$

where N is the number of data sets.

TABLE I. Results for the selected linear models

No.	Correlation model	Binary mixtures		Ternary mixtures	
		P_{av} / %	N_{all}	P_{av} / %	N_{all}
1	Dolezalek–Schulze	6.83	3675	8.32	2879
2	Grunberg–Nissan	3.37	3675	4.24	2879
3	Tamura–Kurata	5.14	3360	8.75	2879
4	McAllister 3	5.29	3264	–	–
5	McAllister 4	6.07	3249	–	–
6	McAllister–Chandramouli–Laddha	–	–	7.84	2861
7	Katti–Chaudhri	2.45	3264	4.18	2879
8	Heric I	1.73	3264	2.91	2879
9	Heric II	–	–	2.62	2861
10	Heric–Brewer I	8.21	3660	9.30	2861
11	Heric–Brewer II	1.23	3249	2.46	2861
12	Krishnan–Laddha	1.76	3264	2.92	2879
13	McAllister–Soliman–Marschall	5.31	3264	7.69	2861
14	Mehrotra	2.98	3675	5.10	2879
15	Baylaucq–Daugé–Boned	4.30	486	12.00	810
16	Dimitrov–Kamenski I	20.72	3675	–	–
17	Dimitrov–Kamenski II	10.48	2212	–	–
18	Dimitrov–Kamenski III	16.03	3576	–	–
19	Dimitrov–Kamenski IV	13.08	3675	–	–
20	Dimitrov–Kamenski V	10.32	2212	–	–
21	Dimitrov–Kamenski VI	20.10	3675	–	–
22	Dimitrov–Kamenski VII	13.72	2212	–	–
23	Dimitrov–Kamenski VIII	3.77	3660	–	–
24	Dimitrov–Kamenski IX	9.42	2212	–	–
25	Dimitrov–Kamenski X	44.67	3675	–	–
26	Dimitrov–Kamenski XI	3.63	2212	–	–
27	Dimitrov–Kamenski XII	32.96	3660	–	–

TABLE I. Continued

No.	Correlation model	Binary mixtures		Ternary mixtures	
		P_{av} / %	N_{all}	P_{av} / %	N_{all}
28	Dimitrov–Kamenski XIII	2.10	2212	–	–
29	Modified Dimitrov–Kamenski	–	–	11.17	2879
30	Focke–Du Plessis I	15.89	3576		
31	Focke–Du Plessis II	9.86	3401		
32	Focke–Du Plessis III	16.96	3375	–	–
33	Focke–Du Plessis IV	20.61	3576	–	–
34	Focke–Du Plessis V	15.64	3401	–	–
35	Focke–Du Plessis VI	11.85	3393	–	–
36	Focke–Du Plessis VII	25.15	3401	–	–
37	Focke–Du Plessis VIII	29.67	3393	–	–
38	Focke–Du Plessis IX	47.03	3357	–	–

The results presented in Table I indicate that the Heric I, Heric–Brewer II, and Krishnan–Laddha models have the best correlation ability for the binary mixtures (with overall absolute average deviations of 1.73, 1.23 and 1.76 %, respectively), while the Heric I, Heric II, Heric–Brewer II and Krishnan–Laddha models demonstrated the best correlation ability for the ternary mixtures (with overall absolute average deviations of 2.91, 2.62, 2.46 and 2.92 %, respectively). These models also have the best correlation results for different group of mixtures, such as *n*-alkane+*n*-alkane (34 data sets), *n*-alkylalcohol+n-alkylalcohol (31 data sets), *etc*. For many experimental data sets, the models with rational form gave average percent errors of about 1 %. However, in some instances, the denominator had a very small value that resulted in very large percent and average percent errors, making the models with rational form unreliable. The large differences in viscosities of the pure substances (2,6,10,15,19,23-hexamethyltetracosane + butane, 2,6,10,15,19,23-hexamethyltetracosane + hexane) resulted in poor correlation results for all models. The experimental data in all sets have monotonically descent or monotonically ascent trend between the viscosities of pure components at constant temperature and constant pressure and therefore models with smaller number of parameters gave better results.

CONCLUSIONS

Selected correlation models were tested on 219 binary and 41 ternary mixtures with 3675 and 2879 experimental data points, respectively. The Heric I, Heric–Brewer II, and Krishnan–Laddha models have the best correlative characteristics (overall absolute average deviations < 2 %) for binary, while the Heric I, Heric–Brewer II, Krishnan–Laddha, and Heric II models (overall absolute average deviations < 3 %) for ternary mixtures.

SUPPLEMENTARY MATERIAL

The equations of the selected correlation models as well as the data of selected binary and ternary liquid mixtures [1–49] are available electronically at http://www.shd.org.rs/JSCS/, or from the corresponding author on request.

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NOMENCLATURE

m	Number of mixture components
n	Number of experimental data points per set
N	Number of data sets
N_{all}	Total number of data points in a correlation
N_m	Number of model parameters
M	Molar mass, g mol^{-1}
T_m	Temperature of mixture, K
p_m	Pressure of mixture, bar
x	Mole fraction
ϕ	Volume fraction
η	Viscosity, mPa s
ρ	Density, g cm^{-3}
v	Molar volume, cm^3 mol^{-1}
p_{av}	Absolute average deviation, %
P_{av}	Overall absolute average deviation, %.

И З В О Д

КОРЕЛИСАЊЕ ВИСКОЗИТЕТА ТЕЧНИХ СМЕША

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У овом раду тестирана су 42 одабрана модела за корелисање вискозитета течних смеша на литературним експерименталним подацима за 219 бинарних и 41 тернерну смешу. Бинарни сетови имају 3675 експерименталних података за 70 различитих супстанци, а тернерни 2879 експерименталних података за 29 различитих супстанци. Heric I, Heric–Brewer II и Krishnan–Laddha модели показали су најбоље корелационе особине са укупном средњом процентуалном грешком мањом од 2 % за бинарне смеше. Heric I, Heric–Brewer II, Krishnan–Laddha и Heric II модели показали су најбоље корелационе особине са укупном средњом процентуалном грешком мањом од 3 % за тернерне смеше.

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