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NOTE

Liquid mixture viscosities correlation with rational models

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Abstract: In this paper, twenty two selected rational correlation models for the viscosities of liquid mixtures of organic compounds were tested on 219 binary sets of experimental data taken from the literature. The binary sets contained 3675 experimental data points for 70 different compounds. The Dimitrov–Kamenski X, Dimitrov–Kamenski XII, and Dimitrov–Kamenski XIII models demonstrated the best correlative characteristics for binary mixtures with an overall absolute average deviation of less than 2 %.

Keywords: binary mixture; liquid mixture viscosity; rational correlation models.

INTRODUCTION

The study of the thermodynamic properties of liquid mixtures contributes to an understanding of the behaviour 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 viscosities of liquid mixtures is 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 the viscosities of liquid mixtures. Some of these models are linear or can be linearized per parameters, and others are non-linear. In a previous article, the former were tested on experimental viscosities of liquid mixtures of alkanes, haloalkanes, alcohols, aromatics, amines, ketones, *etc*.[1] Rational models are non-linear per parameters, but these models have the number one as the first term in denominator polynomial, which enables the use of the linear least squares method in correlation. For many

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experimental data sets,[1] models with a rational form resulted in an average error of about 1 %. However, in some instances, the denominator had a very small value resulting in very large percent and average percent errors, making models with a rational form unreliable. This difficulty may be overcome if nonlinear least squares methods Gauss,[2] Levenberg,[3] Marquardt,[4] Law–Bailey,[5] *etc*. are used. In addition, the Hooke–Jeeves,[6] Fletcher–Powell,[7] Nelder–Mead,[8] *etc*. optimization methods can also be used. Selection of the first assumptions for the parameters is critical for successful use of these methods. On the other hand, rational models have many minimums in the parametric area. These problems may be avoided if a global optimizing method, such as the Monte Carlo method, is used. In this article, the linear congruental pseudo-random number generator was used.[9]

The objective function used in the correlation was:

$$OF = \left[\sum_{i=1}^{n} \left(\eta_{\mathrm{lm},i,\mathrm{exp}} - \eta_{\mathrm{lm},i,\mathrm{cal}} \right)^2 / \left(n - np \right) \right]^{1/2} \rightarrow \min \qquad (1)$$

where η_{lm} is the viscosity of a liquid mixture, n is the number of experimental data points per set and np is the number of parameters.

The performance of selected rational models[1] was tested on 219 binary sets of literature experimental data with 3675 experimental data points for 70 different compounds. The selected binary liquid mixtures were presented in a previous article.[1] A deviation from the experimental values is expressed as the absolute average deviation, p_{av}, for each data set point:

$$p_{\mathrm{av}} = (100 / n) \sum_{i=1}^{n} \left| (\eta_{\mathrm{lm},i,\mathrm{exp}} - \eta_{\mathrm{lm},i,\mathrm{cal}}) / \eta_{\mathrm{lm},i,\mathrm{exp}} \right| \qquad (2)$$

The overall absolute average deviation, P_{av}, for each model is defined as:

$$P_{\mathrm{av}} = \sum_{i=1}^{N} n_i \, p_{\mathrm{av},i} / \sum_{i=1}^{N} n_i \qquad (3)$$

where N is the number of data sets.

RESULTS AND DISCUSSION

Results are presented in Table I, where N_{all} is the total number of data points in the correlation. Only sets of experimental data with $n \geq N_{\mathrm{m}} + 2$ were used in the correlation, where N_{m} is number of model parameters. Sets with experimental data at different temperatures and pressures were correlated with only one set of parameters. The results for linear models reported in a previous article[1] are also presented in Table I. The number of experimental data used in the correlations depended on the number of model parameters and on the existence of experi-

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mental data for density. The results presented in Table I indicate that the Dimitrov–Kamenski X, the Dimitrov–Kamenski XII and the Dimitrov–Kamenski XIII, with overall absolute average deviations of 1.74, 1.32 and 1.18 %, respectively, have the best correlation ability of all the considered rational models. These results are slightly better than the results obtained for the linear models (Heric I, Heric–Brewer II and Krishnan–Laddha, with overall absolute average deviations of 1.73 %, 1.23 and 1.76 %, respectively).

TABLE I. Results of viscosity correlation

Entry no.	Correlation model	N_m	P_{av} / %	N_{all}
1	Dolezalek–Schulze	1	6.83	3675
2	Grunberg–Nissan	1	3.37	3675
3	Tamura–Kurata	1	5.14	3360
4	McAllister 3	2	5.29	3264
5	McAllister 4	3	6.07	3249
6	Katti–Chaudri	1	2.45	3264
7	Heric I	2	1.73	3264
8	Heric–Brewer I	3	8.21	3660
9	Heric–Brewer II	3	1.23	3249
10	Krishnan–Laddha	2	1.76	3264
11	McAllister–Soliman–Marschall	2	5.31	3264
12	Mehrotra	1	2.98	3675
13	Baylaucq–Daugé–Boned	3	4.30	486
14	Dimitrov–Kamenski I	2	7.80	3675
15	Dimitrov–Kamenski II	4	6.01	2212
16	Dimitrov–Kamenski III	4	7.69	3576
17	Dimitrov–Kamenski IV	2	2.60	3675
18	Dimitrov–Kamenski V	4	2.58	2212
19	Dimitrov–Kamenski VI	2	2.80	3675
20	Dimitrov–Kamenski VII	6	4.41	2212
21	Dimitrov–Kamenski VIII	3	2.19	3660
22	Dimitrov–Kamenski IX	4	2.05	2212
23	Dimitrov–Kamenski X	2	1.74	3675
24	Dimitrov–Kamenski XI	3	1.88	2212
25	Dimitrov–Kamenski XII	3	1.32	3660
26	Dimitrov–Kamenski XIII	5	1.18	2212
27	Focke–Du Plessis I	4	7.82	3576
28	Focke–Du Plessis II	5	7.86	3401
29	Focke–Du Plessis III	6	6.73	3375
30	Focke–Du Plessis IV	4	7.98	3576
31	Focke–Du Plessis V	5	7.47	3401
32	Focke–Du Plessis VI	6	7.42	3393
33	Focke–Du Plessis VII	5	8.01	3401
34	Focke–Du Plessis VIII	6	8.63	3393
35	Focke–Du Plessis IX	7	7.50	3357

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CONCLUSIONS

Selected rational correlation models were tested on 219 binary mixtures with 3675 experimental data points. The Dimitrov–Kamenski X, the Dimitrov––Kamenski XII and the Dimitrov–Kamenski XIII models have the best correlative characteristics for binary mixtures with overall absolute average deviations of less then 2 %.

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И З В О Д

КОРЕЛИСАЊЕ ВИСКОЗИТЕТА ТЕЧНИХ СМЕША ПОМОЋУ РАЦИОНАЛНИХ МОДЕЛА

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У овом раду тестирана су 22 одабрана рационална модела за корелисање вискозитета течних смеша на литературним експерименталним подацима за 219 бинарних смеша са 3675 експерименталних података за 70 различитих супстанци. Dimitrov–Kamenski X, Dimitrov–Kamenski XII и Dimitrov–Kamenski XIII модели показали су најбоље корелациона својства са укупном средњом процентуалном грешком мањом од 2 %.

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REFERENCES

1. A. B. Knežević-Stevanović, G. M. Babić, M. Lj. Kijevčanin, S. P. Šerbanović, D. K. Grozdanić, *J. Serb. Chem. Soc*. **77** (2012) 1083
2. D. K. Grozdanić, *Numerical methods*, Akademska misao, Belgrade, 2008 (in Serbian)
3. K. Levenberg, *Quart. Appl. Math*. **2** (1944) 164
4. D. W. Marquardt, *J. Soc. Ind. Appl. Math*. **11** (1963) 431
5. V. J. Law, R. V. Bailey, *Chem. Eng. Sci.* **18** (1963) 189
6. R. Hooke, T. A. Jeeves, *J. Assoc. Comp. Mach*. **8** (1961) 212
7. R. Fletcher, M. J. D. Powell, *Computer J*. **6** (1963) 1963
8. J. A. Nelder, R. Mead, *Computer J*. **7** (1964) 308
9. D. K. Grozdanić, A. B. Knežević-Stevanović, B. D. Đorđević, A. Ž. Tasić, S. P. Šerbanović, *J. Serb. Chem. Soc*. **61** (1996) 513.

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