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RESEARCH ARTICLE

Evaluation of the adequacy of phase equilibria modeling based on various sets of experimental data

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Abstract

Objectives. *The purpose of the paper is to compare the adequacy of mathematical models of vapor–liquid equilibrium (VLE) and their ability to reproduce the phase behavior of the ternary system benzene–cyclohexane–chlorobenzene using different experimental data sets to evaluate binary interaction parameters.*
Methods. *The research methodologies were mathematical modeling of VLE in the Aspen Plus V.10.0 software package using activity coefficient models (Non-Random Two-Liquid (NRTL), Wilson) and the Universal quasichemical Functional-group Activity Coefficients (UNIFAC) group model, which allows for independent information. For the benzene–cyclohexane–chlorobenzene ternary system, the use of the NRTL equation is warranted because it provides a better description of the VLE experimental data.*
Results. *The diagram construction of the constant volatility of cyclohexane relative to benzene lines revealed three topological structures. Only one of them can be considered reliable because it corresponds to the experimental data and coincides with the UNIFAC model diagram constructed based on independent UNIFAC model data. The results indicate that to study systems containing components with similar properties, it is necessary to improve the description quality of the available data sets (the relative error should not exceed 1.5%).*
Conclusions. *The reproduction of the thermodynamic features of various manifolds in the composition simplex obtained by processing direct VLE data can be used to supplement the adequacy of the model. For the cyclohexane–benzene–chlorobenzene system, the best NRTL equation parameters are those regressed from the extensive experimental VLE data available in the literature for the ternary system as a whole.*

Keywords: *mathematical modeling, binary interaction parameters, vapor-liquid equilibrium, experimental data, components relative volatility*

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НАУЧНАЯ СТАТЬЯ

Оценка адекватности моделирования фазовых равновесий на основе различных наборов экспериментальных данных

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Аннотация

Цели. *Сравнительный анализ адекватности математических моделей парожидкостного равновесия (ПЖР) и их возможности воспроизводить особенности фазового поведения тройной системы бензол–циклогексан–хлорбензол при использовании разных наборов экспериментальных данных для оценки параметров бинарного взаимодействия.*
Методы. *В качестве методов исследования выбрано математическое моделирование ПЖР в программном комплексе AspenPlus V.10.0. с использованием уравнений локальных составов (NRTL, Wilson) и групповой модели UNIFAC, позволяющей получить независимую информацию. Для системы бензол–циклогексан–хлорбензол обоснован выбор уравнения NRTL, обеспечивающего более высокое качество описания экспериментальных данных ПЖР.*
Результаты. *Построение диаграммы хода линий постоянной летучести циклогексана относительно бензола выявило три топологических структуры, из которых только одна может считаться достоверной, поскольку соответствует данным натурного эксперимента и совпадает с диаграммой, построенной на основе независимых данных модели UNIFAC. Полученные результаты свидетельствуют о том, что при исследовании систем, содержащих близкие по свойствам компоненты, необходимо повышать качество описания имеющихся массивов данных (относительная ошибка не должна превышать 1.5%).*
Выводы. *Воспроизведение термодинамических особенностей хода различных многообразий в концентрационном симплексе, полученных обработкой прямых данных ПЖР, может служить дополнительной оценкой адекватности модели. Для системы циклогексан–бензол–хлорбензол наилучшим является набор параметров уравнения NRTL, которые оценены по обширным экспериментальным данным ПЖР, имеющимся в литературе для тройной системы в целом.*

Ключевые слова: *математическое моделирование, параметры бинарного взаимодействия, парожидкостное равновесие, экспериментальные данные, относительная летучесть компонентов*

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INTRODUCTION

Computational experimentation with software products is currently one of the most accessible, widely used, and fast methods for studying phase equilibria and various phase processes, especially the distillation process. The choice of a mathematical model that allows reproducing the physicochemical properties of the object under study with an acceptable error margin is crucial (usually, this margin of error should not exceed 3–6%, depending on the complexity of the system under consideration).

The creation of an adequate mathematical model and the selection of its parameters should be based on experimental data (ED) that has undergone thermodynamic consistency tests [1–4]. Depending on the phase behavior features of the system and the number of components in it, the researcher may have different information for carrying out the parameter estimation procedure: data on different types of equilibrium (liquid–vapor, liquid–liquid, liquid–liquid–vapor, liquid–solid, etc.); boiling points at fixed pressure and azeotrope compositions; data for its overall system or its constituents. Moreover, the values of the binary interaction parameters of the models can be obtained, depending on the data used, their volume, and quality, reproducing the known properties of the system with varying accuracy. The model has good predictive capabilities if it satisfactorily describes not only direct ED but also the course diagram of various isolines of scalar properties obtained on their bases, such as the distribution coefficients of components between phases or the coefficients of relative volatility. These properties are important in the development of flowsheets for distillation separation of mixtures using sharp distillation [5] or extractive distillation [6–9]. The presence of an adequate mathematical model allows for the planning of a computational experiment with a wide range of device operating parameters to determine the optimal modes for separation with the least amount of energy consumption.

The present work aims at comparing description results of the phase behavior of the benzene (B) – cyclohexane (CH) – chlorobenzene (CB) system using Non-Random Two-Liquid (NRTL) and Wilson equations [10], of which binary interaction parameters are determined from various ED sets, as well as the equation of the Universal quasichemical Functional-group Activity Coefficients (UNIFAC) group model.

RESULTS AND DISCUSSION

The B–CH–CB system is well studied in the literature, including experimental vapor–liquid equilibrium (VLE) data for three binary constituents [11–13] and extensive data for the ternary system in the entire composition simplex [13]. All data were checked for thermodynamic consistency using the Herington and Van Ness tests [1, 2].

To evaluate the parameters of the binary interaction of the equations of local compositions, three ED sets will be considered: ED (2) for the VLE of binary constituents; ED (3) for the VLE of a ternary system; ED (2 + 3) for the entire volume of available data. For each set, the parameters of the NRTL equation (1) and the Wilson equation (2) [5] are evaluated in the AspenPlus V.10.0 software package:

$$\ln \gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ji}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right), \quad (1)$$

where γ_i is an activity coefficient of the *i*th component;

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij})\,; \quad \tau_{ij} = \alpha_{ij} + {b_{ij}}/{T} + e_{ij}\ln T + f_{ij}T\,;$$

$$\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15)\,; \quad \tau_{ii} = 0\,; \quad G_{ii} = 1.$$

$$\ln \gamma_i = 1 - \ln\left(\sum_j A_{ij} x_j \right) - \sum_j \frac{A_{ji} x_j G_{ji}}{\sum_k A_{jk} x_k}\,, \quad (2)$$

where $\ln A_{ij} = \alpha_{ij} + {b_{ij}}/{T} + c_{ij}\ln T + d_{ij}T + {e_{ij}}/{T^2}\,.$

Tables 1 and 2 show the average relative errors in describing the VLE (ΔT—by boiling point, ΔY—by vapor phase composition) at a pressure of 101.3 kPa, as well as binary interaction parameters (A_{ij}, A_{ji}, B_{ij}, B_{ji}, C_{ij}). The maximum errors in the description of the phase equilibrium of binary systems do not exceed 3%, and the ternary system is less than 6%.

A comparison of the parameter estimation results shows that both models are capable of accurately describing the VLE of the system under study. However, the NRTL model parameters provide a more accurate description, thus further calculations will be performed using this model.

In the software package, the UNIFAC group model was used to calculate the VLE of the ternary system and its binary constituents at a pressure of 101.3 kPa. The errors in the phase equilibrium description in Table 3 also indicate a high reproduction quality of the VLE ED of the ternary system and its binary constituents.

In most cases, the evaluation of the quality of a mathematical model is complete when the values are absolute and relative errors in the description of direct ED are calculated. However, for systems characterized by small differences in components and mixtures, such as the boiling points of benzene and cyclohexane (80.10 and 80.75°C) and the volatility of benzene relative to cyclohexane [13] (in the composition simplex, the range of variation of these values is 0.8–1.4), additional characteristics must be attracted to confirm the adequacy of the model. The course structure diagram of the constant relative volatility lines of components *i*, *j* is chosen as such a characteristic. In the AspenPlus software package, the VLE in the B–CH–CB system was calculated using three sets of binary interaction parameters of the NRTL equation (Table 1). The values of the relative volatility coefficients of the α_{ij} cyclohexane (*i*)–benzene (*j*) pair are determined by the formula:

$$\alpha_{ij} = \frac{y_i x_j}{x_i y_j}, \tag{3}$$

where $y_{i(j)}$ is the concentration of component *i*(*j*) in the vapor phase, $x_{i(j)}$ is the concentration of component *i*(*j*) in the liquid phase.

Isolines are constructed in the composition triangle, along which the relative volatility takes constant values (α_{ij}-lines). The resulting diagrams are shown in Fig. 1.

Table 1. Binary interaction parameters of the NRTL equation and description results of various ED

Binary system	A_{ij}	A_{ji}	B_{ij}	B_{ji}	C_{ij}	Δ*T*, %	Δ*Y*, %
ED (2)							
B–CH	−8.20751	−8.1266	1779.9	4156.59	0.01906	0.16	1.66
B–CB	−10.9556	2.22538	3832.44	−231.437	0.3	0.67	0.49
CH–CB	0.776229	2.52749	−690.951	−564.789	0.028905	1.23	1.21
ED (3)							
B–CH	0.00252441	−8.85555	88.8179	3108.78	3.16605	0.92*	3.15* (4.11)*
B–CB	2.6802	−4.01723	−514.445	1050.66	0.3		
CH–CB	−4.43646	2.34578	−409.339	1641.97	0.0303645		
ED (2 + 3)							
B–CH	−3.67734	−4.80805	1744.96	1426.44	0.3	1.01	2.09
B–CB	0.354308	0.345032	−170.497	−132.059	0.3	0.77	0.86
CH–CB	−4.32852	0.619341	1216.07	537.117	0.3	1.03	1.97
B–CH–CB	The sets of binary interaction parameters are the same					1.41*	5.02* (5.14)*

*Average errors in the description of the boiling point and benzene (B) (cyclohexane (CH)) concentration in the vapor phase of the ternary system. CB – chlorobenzene.

Table 2. Binary interaction parameters of the Wilson equation and description results of various ED

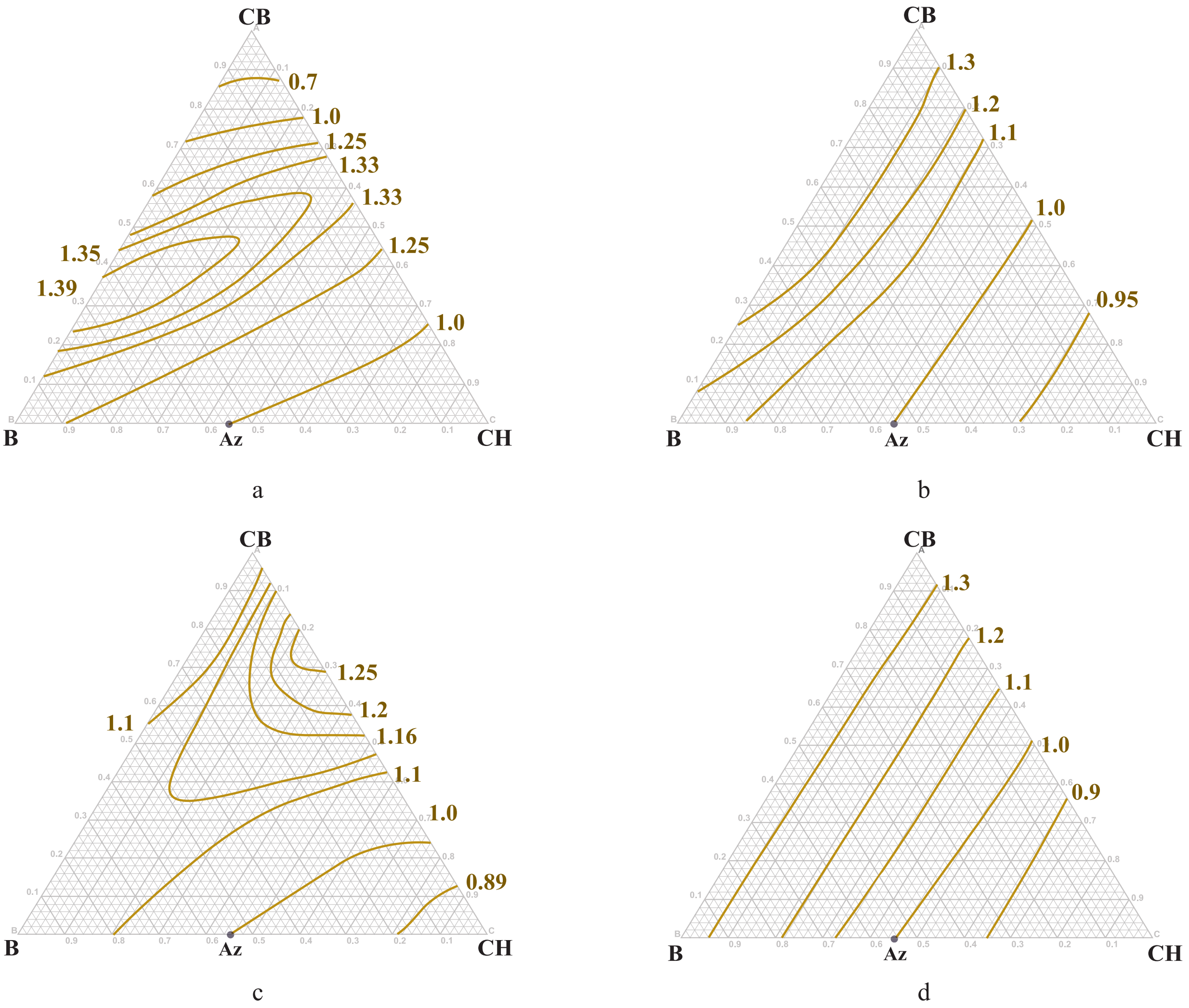
Binary system	A_{ij}	A_{ji}	B_{ij}	B_{ji}	ΔT, %	ΔY, %
ED (2)						
B–CH	2.22465	9.39094	−781.052	−3432.02	0.10	1.43
B–CB	−0.2853	−0.2629	−420.976	421.622	0.65	1.41
CH–CB	−5.21084	8.4696	584.647	−2928.92	1.20	1.49
ED (3)						
B–CH	3.50955	1.8551	−1006.89	−1079.4	1.25*	4.79* (6.14)*
B–CB	0.0317	−0.0239	11.4715	44.8354		
CH–CB	0.701629	2.71709	−1041.94	−696.601		
ED (2 + 3)						
B–CH	2.74451	5.25204	−781.05	−2202.57	1.19	2.29
B–CB	−0.2853	−0.2629	122.157	127.361	0.8	0.89
CH–CB	−0.4298	3.62262	−490.08	−1078.44	1.00	1.99
B–CH–CB	The sets of binary interaction parameters are the same				1.45*	5.06* (5.31)*

*Average errors in the description of the boiling point and benzene (B) (cyclohexane (CH)) concentration in the vapor phase of the ternary system. CB – chlorobenzene.

Table 3. ED description results of the VLE by the UNIFAC equation

Binary system	ΔT, %	$\Delta Y_{\mathrm{B\ (CH)}}$, %
B–CH	0.20	3.36
B–CB	0.38	2.35
CH–CB	0.87	1.94
B–CH–CB	3.88	3.56 (0.23)

As seen, the structures of the stroke α_{ij}-line diagram differ. Figure 1a shows two singular points on binary constituents: elliptical type (constituent B–CB) and hyperbolic type (constituent CH–CB); in Fig. 1b, there are also two binary singular points, however, an elliptical type point belongs to the CH−CB constituent and a hyperbolic one belongs to the B–CB; there are no singular points on the binary constituents in Fig. 1b and 1d (these diagrams are similar not only qualitatively, but also quantitatively).



a b

c d

Fig. 1. Diagram of the relative volatility isolines of a cyclohexane (CH)–benzene (B) pair, constructed using the NRTL equation parameters obtained based on ED: (a) ED (2); (b) ED (3); (c) ED (2 + 3), as well as the UNIFAC equation (d).

It is worth noting that the structures of the diagram for the last two systems are topologically equivalent to the structure of the relative volatility contour diagram constructed from ED of the VLE [13].

This fully concerns the recommendations of works [13] on the use of chlorobenzene as a potential separating agent in the extractive distillation process of a binary benzene–cyclohexane mixture and the fact that chlorobenzene has high selectivity. The use of the ED (2) and ED (2 + 3) parameter sets will lead to incorrect column performance and energy consumption values of the extractive distillation complex. Thus, for the B–CH–CB system, the best is a set of NRTL equation parameters determined using extensive ED of the VLE available in the literature for the entire ternary system.

In the absence of the ED, the UNIFAC group model has become widely used in modeling the properties of mixtures. It satisfactorily describes relatively simple objects, as evidenced by practice [14–16]. Simultaneously, with the presence of many liquid phases in the system [17], an increase in the number of azeotropes and their components, and the emergence of biazeotropic constituents [18–20], the prognostic capabilities of the model decrease rapidly. The use of the UNIFAC model becomes impractical when the system significantly deviates from the ideal behavior.

CONCLUSIONS

It has been demonstrated that different sets of binary interaction parameters of the NRTL equation accurately reproduce the VLE ED, on the basis of which they were obtained. However, the phase equilibrium calculation of the ternary system and the constant relative volatility isoline construction of the cyclohexane–benzene pair revealed the presence of three different topological structures of diagrams α_{ij}-lines, of which only one (Fig. 1b) can be considered reliable because it corresponds to the field experiment data and coincides with the diagram constructed using independent data from the UNIFAC model. The findings indicate that to study systems with components with similar properties, the description quality of the available data arrays must be improved (the relative error should not exceed 1.5%). It is also crucial to reproduce thermodynamic features of phase behavior. The latter includes the VLE data-processed course structures of various characteristic manifolds. Only in this case can the obtained model parameters be used for further regularities investigation and calculation of the distillation process. Unfortunately, ED for the ternary systems VLE is limited and is not available for most systems. In conditions of limited experimental information, it is necessary to conduct at least a local full-scale experiment to confirm the adequacy of mathematical modeling.

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Authors' contributions

A.V. Frolkova – calculation of vapor-liquid equilibrium, construction and analysis of diagrams, writing the paper;

V.G. Fertikova – estimation of binary interaction parameters, verification of the adequacy of mathematical modeling;

E.V. Rytova – evaluation of binary interaction parameters; verification of the adequacy of mathematical modeling;

A.K. Frolkova – analysis of diagrams, formulation of conclusions, writing the paper.

The authors declare that there is no conflict of interest.

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