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Microsoft Excel Solver-assisted Composition Determination to Improve the Experiment of Liquid-Vapor Phase Diagram Construction

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Abstract Since liquid-vapor equilibrium is one of the essentials in thermodynamics to design and optimize separation processes, and phase equilibria require a good understanding of phase diagrams, "Constructing Liquid-Vapor Phase Diagram for Two Completely Miscible Components Systems" often serves as a common experiment in physical chemistry course. In the experiment, the compositions of the binary system, determined both from the liquid and the vapor phases at equilibrium, are regarded as the key data in deriving the overall system point in phase diagram. Here, a practical computer-assisted data processing protocol by using Microsoft Excel Solver is introduced for obtaining the system composition. Combined with the measured refractive index of a standard mixture of the binary system, the composition of any sample mixture of the system can be optimally solved from its refractive index for the phase diagram construction. The paper presents the attempt to improve the experiment, displaying the optimally-solving procedure. The accuracy and feasibility of the approach are verified, and its expanding application prospect in differential refractive index detection are discussed.

Keywords Phase Diagram, Excel Solver, Composition Determination, Refractive Index

1. Introduction

Phase equilibria have great significance in chemical engineering and chemical process technology. Liquid-vapor equilibrium is one of the most common phase equilibria in practical applications, such as in chemical, petrochemical, pharmaceutical and food industries. Liquid-vapor equilibrium data, graphically presented in phase diagrams, are the basis of developing distillation (or rectification) technique for separating liquid mixtures into pure substances. As a common experiment in physical chemistry laboratory, "Constructing Liquid-Vapor Phase Diagram for Two Completely Miscible Components Systems" helps students learn to determine the liquid-vapor equilibrium (i.e., boiling point) parameters, so as to enhance both the comprehension of solution thermodynamics theory and the skills of experimental operation. In view of the phase equilibrium data being the basis of phase separation, the composition determination of the binary mixture is believed to be one of the key steps in the experimental practice [1-5].

Determining the composition or components amount of the binary mixture at phase equilibrium is generally based on the refractive index (RI) measurement or via using chromatography analysis, of which, the former is widely used due to its simplicity in operation and low capital investment [1-2]. The method used to measure the refractive indices (RIs) of a series of binary standard solutions at a certain temperature, and establish a "Correlation Table of RIs against Compositions" (e.g., RIs *vs.* mole fraction x, as refer to Table S1 in the Supplementary Material (1) used in Zhejiang University); thus, the composition of the binary sample solution, either in the liquid or vapor phase, can be determined depending on its measured RI value (the RI of vapor obtained from its condensate solution). However, limited by various factors such as analytical instrument accuracy, measurement temperature and sample size, etc., it is impossible to experimentally collect all arbitrary data into the correlation table, so those unmeasured data often need to be supplemented through interpolation. If simple piecewise linear interpolation is used, the RI of binary mixture should preferably be one that varies apparently and smoothly over its entire composition range. If more complex interpolation model, such as Newton or Lagrange interpolation is employed, typically relevant mathematical and software skills are required, which hardly matches majority of undergraduate students. In practice, however, once the RI of a sample solution is measured, the student experimenters always just look up the correlation table to find its

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composition without the comprehension of where the data in the table come from or how the interpolations are carried out, and thus they are not really involved in all of the phase equilibrium data acquisition and processing.

RI measurement is one of the essentials for determination of composition of binary mixtures, usually for non-ideal mixtures where direct experimental measurements are performed over the entire composition range. The widely used rules for predictivity of refractivity in case of binary liquid mixtures are Arago-Biot, Gladstone-Dale, Lorentz-Lorenz, Eykman, Weiner, Heller, Newton, Oster and Eyring-John [6]. Among them, the most reliable empirical equation over a wide range of concentration is the Lorentz-Lorenz equation (i.e., L-L equation) [7-10] as follows,

$$\frac{n^2-1}{n^2+2}=\sum\nolimits_{i=1}^{k}\frac{n_i^2-1}{n_i^2+2}\varphi_i \tag{1}$$

where n is the RI of the mixture; φ_i is the volume fraction of component i in the mixture, and n_i is the RI of the pure component i. For the binary liquid mixture consisting of just i and j (i.e., volume fraction $\varphi_i+\varphi_i\equiv1$), it can be simply expressed as

$$n=\sqrt{[1/(\frac{\varphi_i}{n_i^2+2}+\frac{\varphi_j}{n_j^2+2})]-2} \tag{2}$$

Nevertheless, the RI (n) is not a univariate function of the composition of a non-ideal binary solution, but also related to some other parameters of the components, such as the component's molecular weight (M_i, M_j), density (ρ_i, ρ_j) and RI (n_i, n_j), etc. Previous studies have shown that for non-ideal binary solutions, the error between the measured RI and the RI calculated from empirical formulas is often related to the excess volume (V^E) [11]. Especially for binary systems where the component volume fraction is around 0.5, the relative error becomes larger [12-14]. Moreover, since the L-L equation is rather suitable for less-nonideal system [15], for RI-related calculation according to the L-L equation, it is more necessary to consider excess volume and actual density of the system [12], which requires higher experimental precision and accuracy, and quite challenging for the student experimenters.

From the perspective of reducing difficulty, it is a feasible idea to modify the L-L equation to the L-L transformation equation (i.e., L-T equation [15,16], see Eq. 3) without emphasizing the nonideality of the system and regardless of its excess volume.

$$n=\sqrt{[1/(\frac{\varphi_i}{n_i^2+2}+\frac{\varphi_j}{n_j^2+2})]-2}+(\frac{\varphi_i\varphi_j}{\varphi_iM_j/\rho_j+\varphi_jM_i/\rho_i})\times D \tag{3}$$

where n is the RI of the mixture; n_i, n_j, φ_i, φ_j, M_i, M_j, ρ_i, ρ_j are the RIs, the volume fractions, the molecular weights and the densities of the components i and j, respectively.

On the basis of the L-L equation, the L-T equation adds a correction term related with D-value of a binary standard mixture, of which the known volume fraction is near 0.5, expanding into the following formula,

$$D=\frac{\varphi_{(0.5)i}M_j/\rho_j+\varphi_{(0.5)j}M_i/\rho_i}{\varphi_{(0.5)i}\varphi_{(0.5)j}}\{n_{0.5}-\sqrt{[1/(\frac{\varphi_{(0.5)i}}{n_i^2+2}+\frac{\varphi_{(0.5)j}}{n_j^2+2})]-2}\} \tag{4}$$

where $n_{0.5}$, $\varphi_{(0.5)i}$, $\varphi_{(0.5)j}$ are the RI and the component volume fractions of the standard mixture, respectively.

Previous studies have shown that the L-T equation has the advantages of reducing error and enhancing applicability for many binary systems [15,16]. In this work, the L-L equation and the L-T equation are compared in determining the compositions of binary systems, which will be discussed in following 3.1 section.

Solving nonlinear equation without approximation, such as inversely solving the L-T equation (to find the composition with the known RI) usually requires computer optimization programming using mathematical modeling and specific professional software, such as MATLAB. Although such software has a wide range of applications and powerful functions, it also has the disadvantage of large and complex plug-ins, taking up a lot of computing resources. Particularly, the barrier for mastering such software is relatively high, requiring considerable programming skills. However, Microsoft Excel Solver, as an intuitive software that virtually available for all college students, helps users quickly solve optimization models without the need to write a bunch of program code. In previous reports, Excel Solver has already been employed to simulate various optimization problems related to chemical education [17-19].

In this paper, by virtue of the L-T equation, Excel Solver is exploited to optimally solve the composition of two completely miscible components system for phase diagram construction. With the obtained composition of the sample mixture, the accuracy and practicality of the proposed approach are verified by comparisons between the actually-prepared compositions and the optimally-solved results, demonstrating it not only improves the experiment and enhances the students' comprehension of more aspects of the experiment, but also shows its further expanding application prospects in differential refractive index detection as well.

2. Optimally-Solving Procedure

Simulation of various mathematical models via Excel Solver to obtain the optimal solution (i.e., the "Variable" to be solved) can be accepted as a simple and practical means by setting the "Decision Variable" of the "Objective Function" under various conditions (such as maximum, minimum and specified). Especially, when the "Objective Function" is specified as zero, it becomes solving an

equation. But to avoid computational overfitting, such "Objective Function specified as zero" is usually replaced by "square of the Objective Function specified as minimum". Sometimes, certain additional constraints are attached as well to discard the unreasonable solved results.

For this work of inversely solving the L-T equation to find the composition with known RI of the sample mixture, taking measured RI (n) as the "Decision Variable", the difference between the solved RI (n_{solved}) and the measured RI (n) as the "Objective Function" to be minimized (i.e., $(\Delta n)^2 \approx 0$), then with some additional "Constraints" to derive a reasonable result, the "Variable" to be optimally solved (i.e., the composition φ_i) can be obtained via Excel Solver programming.

Specifically, taking ethanol−cyclohexane mixture as an example, the optimally-solving procedure is described as follows and shown in Figure 1 (also with an Excel template file attached as the Supplementary Material (2)).

1. An Excel spreadsheet is established with all relevant data included.
2. Click the Solver icon on the "Data Toolbar" to start the Solver, the "Solver Parameter" window is opened up wherein the blanks of "Set Objective" and "By Changing Variable Cells" are needed to be filled with specific cell info to define the "Objective Function" and the "Variable (Decision Variable to be solved)". Then, set some additional "Constraints" in the blank of "Subject to the Constraints", because the composition should be limited in the range of 0 to 1.
3. Calculate the D-value of the L-T equation according to Eq. 4 with a series of relevant parameters of a standard ethanol−cyclohexane mixture and its components (e.g., $n_{(0.5)}$, $\varphi_{(0.5)eth}$, $\varphi_{(0.5)cyc}$, M_{eth}, M_{cyc}, ρ_{eth}, ρ_{cyc}, n_{eth}, n_{cyc}, specifically with the known $\varphi_{(0.5)eth}$ or $\varphi_{(0.5)cyc}$ near 0.5).
4. Set the "Objective Function" $(\Delta n)^2$ to be minimized.
5. Preassign an arbitrary initial value of composition (e.g., φ_{eth}=0.5) and execute Solver process to obtain the solved composition of the ethanol−cyclohexane sample mixture (i.e., φ_{eth}, φ_{cuc}, x_{eth}, x_{cyc}) based on the measured RI (n) of sample mixture, the calculated D-value and the components parameters (e.g., M_{eth}, M_{cyc}, ρ_{eth}, ρ_{cyc}, n_{eth}, n_{cyc}). Noted for the "Select a Solving Method" option, choose "Nonlinear GRG" (suitable for the nonlinear "Objective Function" of this work).

3. Results and Discussion

3.1. Comparative Features of the Composition Determination

To verify the feasibility of the proposed approach, seven binary systems with various components that were hopefully suitable for student experiments were prepared. All reagents used were of analytical grade (see CAS numbers in Table S2 in the Supplementary Material (1)) and the RIs were obtained at 298.15 K with an Abbe refractometer (Shanghai INESA Scientific Instrument Co., Ltd., China) carried out at the standard wavelength of 589.3 nm (n_D) as the light source. The optimally-solved compositions obtained via Excel Slover programming, either based on the L-T or the L-L equation (taking the latter as the control), were compared with the actually-prepared compositions (see Table S3, S4 in Supplementary Material (1) for data) as depicted in Figure 2 and Figure 3.

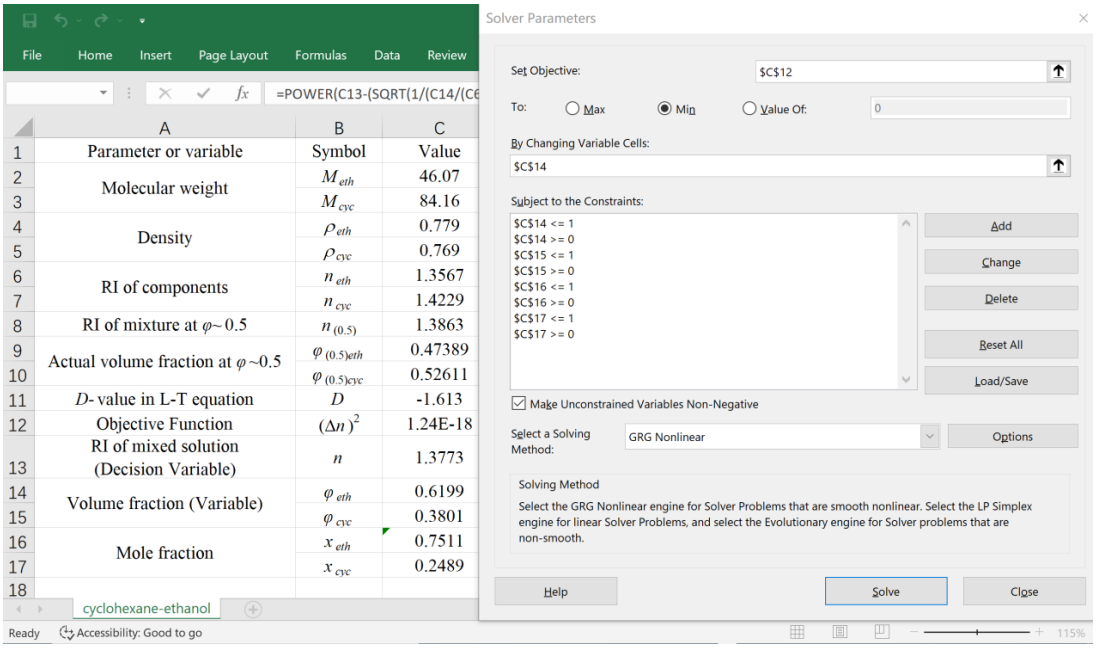

Figure 1. Excel spreadsheet with Solver dialog window for solving the composition of ethanol−cyclohexane mixture (assumed as ideal solution in φ and x conversion $x_{\mathrm{eth}} = \frac{\rho_{\mathrm{eth}}\,\varphi_{\mathrm{eth}}\,/M_{\mathrm{eth}}}{\rho_{\mathrm{eth}}\,\varphi_{\mathrm{eth}}\,/M_{\mathrm{eth}} + \rho_{\mathrm{cyc}}\,\varphi_{\mathrm{cyc}}\,/M_{\mathrm{cyc}}}$

For the following six binary mixtures, including ethanol−cyclohexane, ethanol−isopropanol, ethanol−ethyl acetate, 1,4-dioxane−water, 1,4-dioxane−ethanol, and methylcyclohexane−n-propanol, the correlation between the RIs and the compositions (φ_i of the former in the two components) of both actually-prepared and optimally-solved (either based on the L-T or the L-L equation) are illustrated in Figure 2, indicating the actually-prepared compositions are more consistent with those solved based on the L-T equation, as compared with those based on the L-L equation. Further statistically comparison of the actually-prepared compositions and the solved ones based on the L-T equation, by means of root-mean-square deviation (RMSD) or normalized root-mean-square deviation (NRMSD) or Paired Samples t-Test ($P<0.05$), showed no significant difference (see Table S5, S6 in Supplementary Material (1) for data). Apparently, for the overall agreement with those actually-prepared ones, the optimally-solved compositions based on the L-T equation were superior to those based on the L-L equation. Therefore, for above six binary systems, the optimally-solved composition based on the L-T equation could be accurately solved from the measured RI (n) of the mixture.

However, for ethanol−water mixture, the optimally-solved compositions based on the L-T equation were in good agreement with those actually-prepared at the low ethanol concentration ($\varphi_{eth}<0.5$), but not so good if the ethanol concentration was high ($\varphi_{eth}>0.5$) (see Figure 3, trace blue *vs.* red). Despite not fully matched, for overall agreement with those actually-prepared, the solved compositions based on the L-T equation were still superior to the ones based on the L-L equation (see Figure 3, trace blue and/or green *vs.* red). Furthermore, it showed the RI of the actually-prepared ethanol-water mixture increased with the increasing of water content, but reached a maximum at $\varphi_{eth}\approx0.8$ and then decreased, which was related to the monotonicity of the RI function as well. Formula derivations (see Proof 1 and 2 in Supplementary Material (1)) prove that the RI (n) and the composition (φ_i) of a binary system has a strictly monotonic relationship according to the L-L equation, but according to the L-T equation, they can be either monotonic (e.g., for ethanol−cyclohexane system) or non-monotonic (e.g., for ethanol–water system) depending on the specific system. As shown in Figure 2, for the system with monotonic RI distribution over the entire composition range (e.g., the above six binary mixtures), the image of the RI function according to the L-T equation (i.e., equivalenting to the optimally-solved result based on the L-T equation) matches well with the actually-prepared composition (trace blue *vs.* red), demonstrating the feasibility of our approach for such systems. But for the system with non-monotonic RI distribution in a particular composition range (e.g., ethanol−water mixture), as shown in Figure 3, despite the image of the RI function according to the L-T equation relatively matches the actuality, with some individual RIs correspond to two different compositions (see trace magenta *vs.* red, especially as $\varphi_{eth}>0.5$). But such kind of multi-valued attribute disagrees with the single-valued simulation via Excel Slover of our approach, suggesting the limitation of the proposed approach for the system with non-monotonic RI distribution.

It is clear that the difference of calculated RI from the L-L equation and from the L-T equation depends upon both the composition and the D value of the binary system, of which, the latter mainly depends on the difference between the measured RI of the standard binary solution (with known φ near 0.5) and the RI calculated from the L-L equation. Although it is difficult to fully speculate on all the factors affecting such difference, it should theoretically be related to the difference between the interaction among solvent/solute molecules and among pure solvent molecules, which can also be testified somehow by the data of this work. Some binary systems, such as homologous mixture of ethanol and isopropanol, tend to have smaller D value because they are closer to ideal solutions.

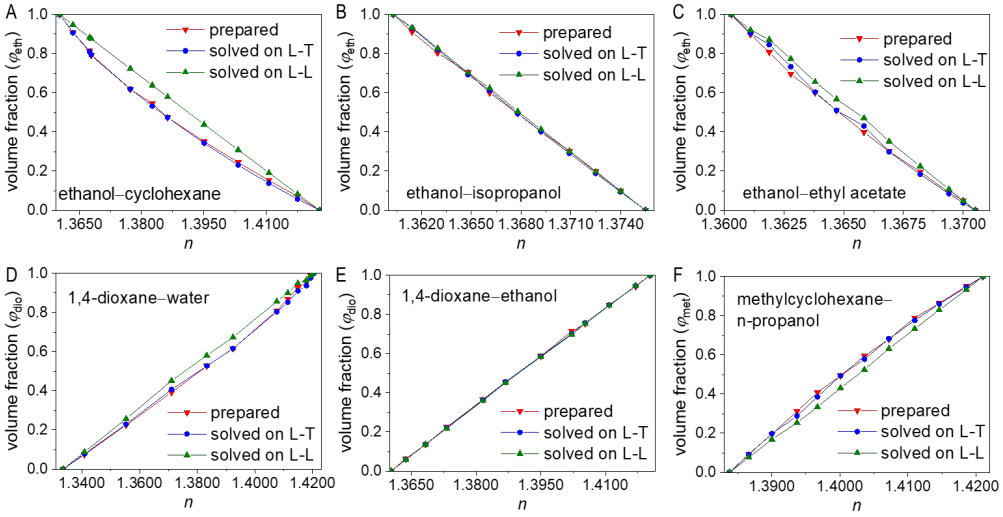

Figure 2. Comparison of the actually-prepared compositions of six binary mixtures with those optimally-solved based on the L-T or the L-L equation

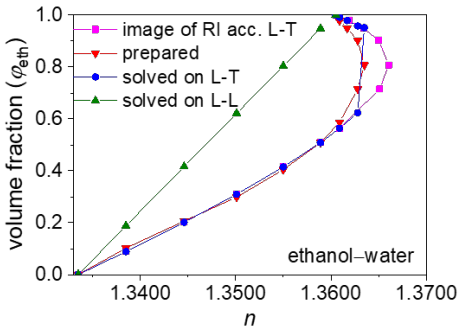

Figure 3. Comparison of the actually-prepared compositions of ethanol-water mixture with those optimally-solved based on the L-T or the L-L equation, and those from the image of the RI function according to the L-T equation (Note: for optimally-solving on the L-T equation to obtain trace blue, it needs to be carried out separately on both sides of the RI maximum, i.e., $0 \le \varphi_{eth} \le 0.8$ and $0.8 \le \varphi_{eth} \le 1$, respectively.)

3.2. Phase Diagram Construction Practice

According to previous practice, the experiment "Constructing Liquid-Vapor Phase Diagram for Two Completely Miscible Components Systems" generally relies on the "Correlation Table of RIs against Compositions" of the system. The more accurate the experiment is expected, the more standard solutions need to be prepared. However, to save the class time, such correlation table is actually provided in advance, which might give students a misconception that the experiment should be performed on binary system with known RI/composition correlation, so they cannot generalize the experiment from one system to the other.

The proposed approach, by using Excel Solver to solve the composition, brings two changes. First, instead of preparing a series of standards to establish the RI/composition correlation table, it requires just one standard solution. Then, the composition of the binary mixture at phase equilibrium, either in liquid or in vapor phase, can be easily solved via entering the RI of the solution (or condensate solution) into Excel spreadsheet. Here, as shown in Figure 4, the phase diagrams of three binary systems have been constructed, including ethanol−cyclohexane, ethanol−ethyl acetate, and ethanol−isopropanol, selected for their mild operation temperature, green and less corrosive solvents for safe experimentation. The phase diagrams constructed from the compositions solved on the L-T equation via Excel Solver (see Table S7 in Supplementary Material (1) for data) are in good consistent with those reported previously [20-22], demonstrating the feasibility of the proposed approach for student's experiment.

The proposed experimental process is largely similar to previous practice. But instead of simply looking up the "Correlation Table of RIs against Compositions" without knowing where the data come from and how to supplement them with interpolation, Excel Solver is used to optimally solve the composition of the mixture at phase equilibrium, which is also expected to attract students' participation.

4. Expanding Application Prospect

In fact, determination of analyte concentration in a mixed sample solution from its measured RI is also a common type of quantitative analysis, such as during HPLC separation. Differential refractive index (DRI) detector offers attractive characteristics as non-destructive and universal sensor, estimating analyte concentration (φ_a) by monitoring the difference of RIs (n_{Dif}) between the sample (n_S, the RI of analyte−eluent mixed solution) and the reference (n_R, the RI of blank eluent) [23]. In previous studies based on DRI detection, two quantitative formulas have been proposed successively from the perspective that the detected signal (n_{Dif}) shows linearity in a certain analyte concentration range.

Yeung et al. [24,25], by derivation of the L-L equation, proposed a protocol for determining the volume fraction of analyte (φ_a) in a flowing system, involving a variety of binary systems with the solvents, such as n-hexane, benzene, chloroform, carbon tetrachloride and carbon disulfide. The quantification equation is as follows,

$$n_{Dif} \cdot K' = \varphi_a \cdot (F_a - F_R) \tag{5}$$

where K' is a constant term related to the RI of the blank eluent (n_R); $F_a = \frac{n_a^2-1}{n_a^2+2}$ and $F_R = \frac{n_R^2-1}{n_R^2+2}$ are equivalent to the molar refractivities per unit molar volume (R_m/V_m) of the analyte and the blank eluent, respectively. Obviously, the formula shows the n_{Dif} is proportional to the φ_a of the sample solution, as well as to the difference of molar refractivities between the analyte and the eluent that affects the linear slope. Actually, this formula results from the substitution of n_R for n_S during its derivation [24], suggesting it can just be applicable to the system with low analyte concentration ($\varphi_a \le$ 5%) [26].

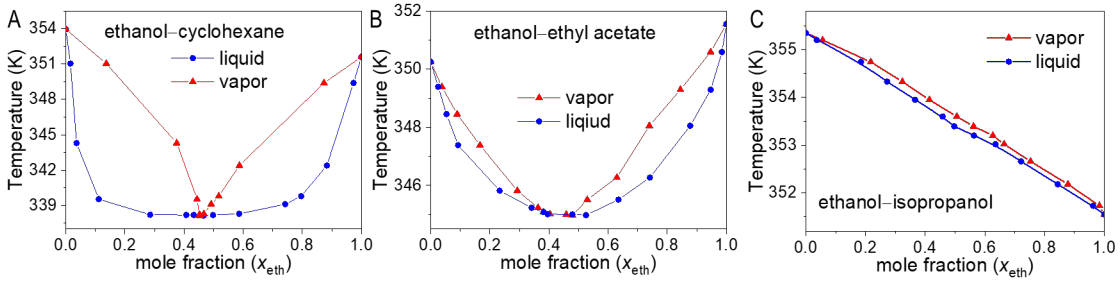

Figure 4. Phase diagrams constructed from the optimally-solved compositions based on the L-T equation

Then, Dorschel et al., the scientists from the Waters Chromatography Division, modified the above formula (Eq. 5) according to their practice of DRI detector to obtain a revised equation [26],

$$n_{Dif} = \varphi_a \cdot (n_a - n_R) \quad (6)$$

where n_a is the RI of the pure analyte. Obviously, it, simplifying molar refractivity (F_a and F_R) to refractive index (n_a and n_R), is an empirical modification [27,28]. Despite both of the above two formulas have their further applications, the problem of the limited linear range is unavoidable anyway. Therefore, for cases in which nonlinearity occurs (e.g., with high analyte concentration), an "almost linear" solution had been proposed further to correct exponentially both of the slope and the concentration terms [26] in above empirical linear equation.

Since n_s can be readily obtained from the DRI detector signals n_{Dif} and n_R, it is also expected that φ_a might be optimally solved via our proposed approach. Compared with Eq. 5 and 6 based on the linear standard curve to determine the analyte concentration, the proposed approach of Excel Solver-assisted composition determination simplifies the quantification procedure without tedious steps dealing with a series of standard solutions, especially free from the upper limit of analyte concentration. Therefore, it is conceivable that the expanding application prospect in DRI detector is promising.

5. Conclusions

As students develop their cognitive learning abilities and scientific process skills, computational formulas, content, and procedures have become increasingly integrated. The data processing in chemical experiment course, often due to its complexity or cumbersomeness, calls for computer-assisted calculation to replace some repetitive experimental operations or manual calculation, becoming one of the important requirements. Here, we show how to use spreadsheet modeling of Microsoft Excel Solver to solve a nonlinear optimization problem, making it easy to determine the composition of a completely miscible binary system. The paper proposes a protocol to improve the experiment "Constructing Liquid-Vapor Phase Diagram for Two Completely Miscible Components Systems", reducing errors caused by individual operational differences. The approach helps students to better understand the principle of phase diagram construction with improved data processing capability, and also shows its expanding application prospect worthy of study further.

Supplementary Material (1)

Table S1. Correlation of RIs (in grey cells) against compositions (x_{cyc}) of ethanol−cyclohexane mixture

n[a]	0	1	2	3	4	5	6	7	8	9
1.357	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
1.358	0.012	0.013	0.014	0.015	0.016	0.017	0.018	0.020	0.021	0.022
1.359	0.023	0.024	0.025	0.026	0.028	0.029	0.030	0.031	0.032	0.033
1.360	0.035	0.036	0.037	0.038	0.039	0.040	0.041	0.042	0.044	0.045
1.361	0.046	0.047	0.048	0.049	0.051	0.052	0.053	0.054	0.055	0.056
1.362	0.057	0.059	0.060	0.061	0.062	0.063	0.064	0.065	0.067	0.068
1.363	0.069	0.070	0.071	0.072	0.073	0.074	0.076	0.077	0.078	0.079
1.364	0.080	0.081	0.082	0.084	0.085	0.086	0.087	0.088	0.089	0.090
1.365	0.092	0.093	0.094	0.095	0.096	0.097	0.098	0.100	0.101	0.102
1.366	0.103	0.104	0.105	0.106	0.108	0.109	0.110	0.111	0.112	0.113
1.367	0.114	0.116	0.117	0.118	0.119	0.120	0.121	0.122	0.124	0.125
1.368	0.126	0.127	0.128	0.129	0.130	0.132	0.133	0.134	0.135	0.136
1.369	0.137	0.138	0.139	0.141	0.142	0.143	0.144	0.145	0.146	0.147
1.370	0.149	0.150	0.151	0.152	0.153	0.154	0.155	0.157	0.158	0.159
1.371	0.160	0.161	0.162	0.164	0.165	0.166	0.167	0.169	0.170	0.171
1.372	0.172	0.173	0.175	0.176	0.177	0.178	0.180	0.181	0.182	0.183
1.373	0.184	0.186	0.187	0.188	0.189	0.191	0.192	0.193	0.194	0.195
1.374	0.197	0.198	0.199	0.200	0.201	0.203	0.204	0.205	0.206	0.208
1.375	0.209	0.210	0.211	0.212	0.214	0.215	0.216	0.217	0.219	0.220
1.376	0.221	0.222	0.224	0.225	0.226	0.228	0.229	0.230	0.232	0.233
1.377	0.234	0.236	0.237	0.238	0.239	0.241	0.242	0.243	0.245	0.246
1.378	0.247	0.249	0.250	0.251	0.253	0.254	0.255	0.257	0.258	0.259
1.379	0.261	0.262	0.263	0.265	0.266	0.267	0.269	0.270	0.271	0.272
1.380	0.274	0.275	0.276	0.278	0.279	0.280	0.282	0.283	0.284	0.286

1.381	0.287	0.288	0.290	0.291	0.293	0.294	0.295	0.297	0.298	0.299
1.382	0.301	0.302	0.304	0.305	0.306	0.308	0.309	0.310	0.312	0.313
1.383	0.315	0.316	0.317	0.319	0.320	0.322	0.323	0.324	0.326	0.327
1.384	0.328	0.330	0.331	0.333	0.334	0.335	0.337	0.338	0.339	0.341
1.385	0.342	0.344	0.345	0.346	0.348	0.349	0.350	0.352	0.353	0.355
1.386	0.356	0.358	0.359	0.361	0.362	0.364	0.365	0.367	0.368	0.370
1.387	0.371	0.373	0.374	0.376	0.378	0.379	0.381	0.382	0.384	0.385
1.388	0.387	0.388	0.390	0.391	0.393	0.395	0.396	0.398	0.399	0.401
1.389	0.402	0.404	0.405	0.407	0.408	0.410	0.411	0.413	0.415	0.416
1.390	0.418	0.419	0.421	0.422	0.424	0.425	0.427	0.429	0.430	0.431
1.391	0.433	0.435	0.436	0.438	0.440	0.441	0.443	0.444	0.446	0.448
1.392	0.449	0.451	0.453	0.454	0.456	0.458	0.459	0.461	0.463	0.464
1.393	0.466	0.467	0.469	0.471	0.472	0.474	0.476	0.477	0.479	0.481
1.394	0.482	0.484	0.485	0.487	0.489	0.490	0.492	0.494	0.495	0.497
1.395	0.499	0.500	0.502	0.504	0.505	0.507	0.508	0.510	0.512	0.513
1.396	0.515	0.517	0.518	0.520	0.522	0.524	0.525	0.527	0.529	0.531
1.397	0.532	0.534	0.536	0.538	0.539	0.541	0.543	0.545	0.546	0.548
1.398	0.550	0.552	0.553	0.555	0.557	0.559	0.560	0.562	0.564	0.565
1.399	0.567	0.569	0.571	0.572	0.574	0.576	0.578	0.579	0.581	0.583
1.400	0.585	0.586	0.588	0.590	0.592	0.593	0.595	0.597	0.599	0.600
1.401	0.602	0.604	0.606	0.608	0.610	0.611	0.613	0.615	0.617	0.619
1.402	0.621	0.623	0.625	0.626	0.628	0.630	0.632	0.634	0.636	0.638
1.403	0.640	0.641	0.643	0.645	0.647	0.649	0.651	0.653	0.655	0.657
1.404	0.658	0.660	0.662	0.664	0.666	0.668	0.670	0.672	0.673	0.675
1.405	0.677	0.679	0.681	0.683	0.685	0.687	0.688	0.690	0.692	0.694
1.406	0.696	0.698	0.700	0.702	0.704	0.706	0.708	0.710	0.712	0.714
1.407	0.716	0.718	0.720	0.722	0.724	0.726	0.728	0.730	0.732	0.734
1.408	0.736	0.738	0.740	0.742	0.744	0.746	0.749	0.751	0.753	0.755
1.409	0.757	0.759	0.761	0.763	0.765	0.767	0.769	0.771	0.773	0.775
1.410	0.777	0.779	0.781	0.783	0.785	0.787	0.789	0.791	0.793	0.795
1.411	0.797	0.799	0.801	0.803	0.806	0.808	0.810	0.812	0.814	0.816
1.412	0.819	0.821	0.823	0.825	0.827	0.829	0.832	0.834	0.836	0.838
1.413	0.840	0.842	0.845	0.847	0.849	0.851	0.853	0.855	0.857	0.860
1.414	0.862	0.864	0.866	0.868	0.870	0.873	0.875	0.877	0.879	0.881
1.415	0.883	0.886	0.888	0.890	0.892	0.894	0.896	0.899	0.901	0.903
1.416	0.905	0.907	0.910	0.912	0.914	0.916	0.919	0.921	0.923	0.925
1.417	0.928	0.930	0.932	0.934	0.937	0.939	0.941	0.943	0.946	0.948
1.418	0.950	0.952	0.955	0.957	0.959	0.961	0.963	0.966	0.968	0.970
1.419	0.972	0.975	0.977	0.979	0.981	0.984	0.986	0.988	0.990	0.993
1.420	0.995	0.997	1.000							

[a] The RIs at 303.15 K are listed in the first column, while the digits in the fourth decimal digit of each RI are listed sequentially in the heading row. The Table commences with pure ethanol (x_{cyc}=0) and ends with pure cyclohexane (x_{cyc}=1).

Table S2. CAS numbers of all reagents used in this work

Solvent	CAS
Ethanol	64-17-5
Cyclohexane	110-82-7
Isopropanol	67-63-0
Ethyl Acetate	141-78-6
1,4-Dioxane	123-91-1
Water	7732-18-5
Methylcyclohexane	108-87-2
N-Propanol	71-23-8

Table S3. The Optimally-Solved Compositions[a] Compared with The Actually-Prepared Ones Corresponding to The Same RI (n) in Following Six Binary Systems

Systems	n	φ_{pre}	x_{pre}	$\varphi_{L\text{-}L}$	$x_{L\text{-}L}$	$\varphi_{L\text{-}T}$	$x_{L\text{-}T}$	D-value[b]
Ethanol–Cyclohexane	1.3635	0.9085	0.9483	0.9478	0.9711	0.9076	0.9478	−1.613
	1.3675	0.8146	0.8905	0.8828	0.9331	0.8111	0.8822	
	1.3679	0.7909	0.875	0.8763	0.9291	0.7945	0.8774	
	1.3773	0.6185	0.75	0.7241	0.8293	0.6198	0.7511	
	1.3826	0.5464	0.6903	0.6388	0.7659	0.5324	0.6781	
	1.3863	0.4739	0.625	0.5794	0.7182	0.4739	0.625	
	1.3951	0.3508	0.5	0.4387	0.5912	0.3428	0.4912	
	1.4033	0.2449	0.375	0.3084	0.4521	0.2308	0.357	
	1.4107	0.1527	0.25	0.1915	0.3047	0.1377	0.2281	
	1.4176	0.0717	0.125	0.083	0.1434	0.0575	0.1014	
Ethanol–Isopropanol	1.3740	0.0984	0.1247	0.0982	0.1223	0.0938	0.1170	−0.04773
	1.3725	0.1999	0.2459	0.1965	0.2384	0.1888	0.2295	
	1.3709	0.3024	0.3613	0.3015	0.3559	0.2913	0.3447	
	1.3692	0.4038	0.4692	0.4132	0.4741	0.4016	0.4621	
	1.3678	0.4936	0.5599	0.5053	0.5666	0.4935	0.5550	
	1.3671	0.5397	0.6002	0.5514	0.6114	0.5397	0.6002	
	1.3660	0.6118	0.6729	0.6238	0.6796	0.6129	0.6696	
	1.3648	0.7040	0.7564	0.7029	0.7517	0.6933	0.7431	
	1.3629	0.8038	0.8424	0.8282	0.8605	0.8218	0.8551	
	1.3613	0.9112	0.9305	0.9339	0.9476	0.9311	0.9454	
Ethanol–Ethyl Acetate	1.3700	0.0503	0.0816	0.0489	0.0793	0.0379	0.0620	−0.1836
	1.3694	0.0910	0.1438	0.1075	0.1680	0.0849	0.1346	
	1.3682	0.1970	0.2914	0.2249	0.3272	0.1838	0.2741	
	1.3669	0.3010	0.4192	0.3522	0.4768	0.2985	0.4164	
	1.3655	0.3984	0.5262	0.4893	0.6164	0.4308	0.5593	
	1.3647	0.5105	0.6361	0.5678	0.6877	0.5105	0.6361	
	1.3638	0.6008	0.7162	0.6561	0.7618	0.6037	0.7186	
	1.3626	0.6962	0.7935	0.7739	0.8526	0.7336	0.8219	
	1.3616	0.8077	0.8756	0.8722	0.9196	0.8466	0.9025	
	1.3611	0.8979	0.9365	0.9213	0.9515	0.9048	0.9409	

[a] Composition is represented by φ (volume fraction) and/or x (mole fraction) of the former of the two components
[b] D-value in the L-T equation

Table S3. (continued)

System	n	φ_{pre}	x_{pre}	$\varphi_{L\text{-}L}$	$x_{L\text{-}L}$	$\varphi_{L\text{-}T}$	$x_{L\text{-}T}$	D-value
1,4-Dioxane–Water	1.3409	0.0743	0.0167	0.0876	0.0199	0.0777	0.0175	0.9332
	1.3553	0.2254	0.0580	0.2568	0.0681	0.2292	0.0592	
	1.3721	0.3918	0.1200	0.4521	0.1486	0.4070	0.1269	
	1.3833	0.5274	0.1911	0.5810	0.2269	0.5274	0.1911	
	1.3914	0.6153	0.2529	0.6737	0.3041	0.6162	0.2536	
	1.4076	0.8101	0.4746	0.8574	0.5599	0.8042	0.4651	
	1.4114	0.8703	0.5867	0.9002	0.6563	0.8530	0.5513	
	1.4149	0.9275	0.7302	0.9593	0.7668	0.9109	0.6813	
	1.4172	0.9570	0.8249	0.9653	0.8549	0.9379	0.7617	
	1.4193	0.9886	0.9481	0.9888	0.9493	0.9767	0.8988	
	1.3409	0.0743	0.0167	0.0876	0.0199	0.0777	0.0175	
1,4-Dioxane–Ethanol	1.3637	0.0630	0.0440	0.0578	0.0403	0.0585	0.0408	−0.06671
	1.3683	0.1354	0.0968	0.1357	0.0971	0.1374	0.0983	
	1.3732	0.2241	0.1651	0.2185	0.1607	0.2210	0.1626	
	1.3816	0.3655	0.2828	0.3598	0.2778	0.3632	0.2808	

	1.3871	0.4556	0.3642	0.4518	0.3607	0.4556	0.3642	
	1.3950	0.5874	0.4935	0.5834	0.4849	0.5873	0.4934	
	1.4019	0.7145	0.6314	0.6978	0.6125	0.7012	0.6164	
	1.4053	0.7534	0.6765	0.7539	0.6771	0.7570	0.6808	
	1.4109	0.8500	0.7950	0.8463	0.7901	0.8483	0.7929	
	1.4170	0.9438	0.9199	0.9461	0.9232	0.9470	0.9244	
Methylcyclohexane–n-propanol	1.3866	0.0938	0.0577	0.0762	0.0465	0.0908	0.0558	–0.7920
	1.3900	0.1951	0.1254	0.1685	0.1070	0.1978	0.1273	
	1.3923	0.3122	0.2116	0.2308	0.1507	0.2682	0.1781	
	1.3956	0.4087	0.2902	0.3200	0.2177	0.3662	0.2547	
	1.4001	0.4942	0.3662	0.4414	0.3185	0.4942	0.3662	
	1.4032	0.5943	0.4641	0.5248	0.3951	0.5785	0.4480	
	1.4072	0.6809	0.5579	0.6321	0.5039	0.6825	0.5597	
	1.4110	0.7904	0.6904	0.7337	0.6198	0.7763	0.6724	
	1.4146	0.8639	0.7897	0.8298	0.7425	0.8607	0.7851	
	1.4185	0.9512	0.9201	0.9336	0.8927	0.9472	0.9139	

Table S4. The Optimally-Solved Compositions[a] Compared with The Actually-Prepared Ones Corresponding to The Same RI (n) in Ethanol-Water System

System	n	φ_{pre}	x_{pre}	$\varphi_{L\text{-}L}$	$x_{L\text{-}L}$	$\varphi_{L\text{-}T}$	$x_{L\text{-}T}$	D-value[b]
Ethanol –Water	1.3385	0.1022	0.0340	0.1879	0.0668	0.0887	0.0292	1.791
	1.3446	0.2065	0.0745	0.4164	0.1807	0.2016	0.0724	
	1.3501	0.2986	0.1163	0.6215	0.3367	0.3099	0.1219	
	1.3550	0.4045	0.1735	0.8037	0.4414	0.4149	0.1798	
	1.3589	0.5089	0.2426	0.9482	0.8498	0.5089	0.2426	
	1.3609	0.5867	0.3050	N/A[c]	N/A	0.5636	0.2854	
	1.3628	0.7155	0.4374	N/A[c]	N/A	0.6235	0.3386	
	1.3631	0.8078	0.5650	N/A[c]	N/A	0.9513[d]	0.8596	
	1.3628	0.9026	0.7412	N/A[c]	N/A	0.9582[d]	0.8766	
	1.3617	0.9492	0.8525	N/A[c]	N/A	0.9787[d]	0.9341	
	1.3609	0.9786	0.9340	N/A[c]	N/A	0.9914[d]	0.9726	

[a] Composition is represented by φ (volume fraction) and/or x (mole fraction) of ethanol
[b] D-value in the L-T equation
[c] Not applicable, as RIs in actually-prepared mixture is higher than those in either pure ethanol or pure water, which makes the composition cannot be optimally-solved based on the L-L equation.
[d] For optimally-solving the compositions based on the L-T equation (refer to trace blue in Figure 3 in the manuscript), it needs to be carried out separately on both sides of the RI maximum, i.e., $0 \le \varphi_{eth} \le 0.8$ and $0.8 \le \varphi_{eth} \le 1$, respectively.

Table S5. RMSD and NRMSD of Optimally-Solved Compositions[a] Based on the L-T Equation *vs.* Actually-Prepared Ones

Systems	RMSD		NRMSD	
	from φ	from x	from φ	from x
Ethanol–Cyclohexane	1.12%	1.05%	0.112%	0.105%
Ethanol–Isopropanol	0.844%	1.01%	0.0844%	0.101%
Ethanol–Ethyl Acetate	0.833%	0.980%	0.0833%	0.0980%
1,4-Dioxane–Water	0.508%	0.548%	0.0508%	0.0648%
1,4-Dioxane–Ethanol	0.492%	0.539%	0.0492%	0.0539%
Methylcyclohexane–n-Propanol	0.612%	0.688%	0.0612%	0.0688%

Table S6. Paired Sample t-Test of Optimally-Solved Compositions on the L-T Equation *vs.* the Ones Actually-Prepared

Systems	t_φ	t_x	$t_{\alpha=0.05, f=9}$
Ethanol–Cyclohexane	1.21	0.12	2.26
Ethanol–Isopropanol	0.80	2.18	
Ethanol–Ethyl Acetate	0.04	0.75	
1,4-Dioxane–Water	1.41	1.26	
1,4-Dioxane–Ethanol	1.04	0.84	
Methylcyclohexane–n-Propanol	2.14	2.09	

Table S7. Optimally-Solved Liquid-Vapor Equilibrium Data Based on the L-T Equation

Systems	Boiling Point (K)	n_{liquid}	x_{liquid}[a]	n_{vapor}	x_{vapor}[a]
Ethanol–Cyclohexane	353.95	1.4229	0.000	1.4229	0.000
	351.04	1.4221	0.0153	1.4153	0.1367
	344.30	1.4209	0.0362	1.4016	0.3752
	339.49	1.4167	0.1114	1.3975	0.4438
	338.21	1.4069	0.2853	1.3971	0.4517
	338.18	1.3997	0.4075	1.3970	0.4531
	338.16	1.3982	0.4327	1.3970	0.4518
	338.14	1.3962	0.4656	1.3970	0.4523
	338.19	1.3942	0.4980	1.3969	0.4538
	338.28	1.3887	0.5864	1.3961	0.4671
	339.11	1.3786	0.7422	1.3946	0.4919
	339.79	1.3750	0.7965	1.3930	0.5174
	342.39	1.3689	0.8832	1.3868	0.5873
	349.40	1.3650	0.9733	1.3682	0.8736
	351.60	1.3603	1.0000	1.3603	1.0000
Ethanol–Ethyl Acetate	351.55	1.3603	1.3603	1.0000	1.0000
	350.60	1.3605	1.3610	0.9851	0.9471
	349.29	1.3610	1.3623	0.9471	0.8445
	348.05	1.3619	1.3635	0.8779	0.7395
	346.27	1.3635	1.3647	0.7412	0.6293
	345.51	1.3647	1.3661	0.6349	0.5294
	344.98	1.3658	1.3663	0.5250	0.4789
	345.00	1.3663	1.3665	0.4789	0.4583
	345.01	1.3670	1.3671	0.3951	0.4036
	345.08	1.3672	1.3672	0.3816	0.3808
	345.23	1.3676	1.3674	0.3409	0.3628
	345.82	1.3685	1.3680	0.2327	0.2928
	347.38	1.3697	1.3691	0.0923	0.1666
	348.45	1.3700	1.3698	0.0530	0.0892
	349.39	1.3703	1.3702	0.0250	0.0374
	350.25	1.3705	1.3705	0.0000	0.0000
Ethanol–Isopropanol	351.55	1.3603	1.3603	1.0000	1.0000
	351.73	1.3610	1.3606	0.9626	0.9838
	352.18	1.3631	1.3625	0.8436	0.8780
	352.66	1.3652	1.3646	0.7210	0.7531
	353.02	1.3665	1.3661	0.6354	0.6644
	353.20	1.3677	1.3667	0.5629	0.6266
	353.40	1.3687	1.3677	0.4972	0.5619
	353.60	1.3692	1.3685	0.4586	0.5056
	353.95	1.3706	1.3699	0.3658	0.4137
	354.33	1.3719	1.3712	0.2721	0.3235
	354.74	1.3731	1.3727	0.1846	0.2174
	355.20	1.3750	1.3748	0.0362	0.0559
	355.35	1.3755	1.3755	0.0000	0.0000

[a] Composition of the binary mixture is represented by x (mole fraction) of the former of the two components

Proof 1 Proof of monotonic function of compositions (φ) according to the L-L equation.

$$n=\sqrt{\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{\varphi_j}{n_j^2+2}}-2}$$

$$\because \varphi_j=1-\varphi_i$$

$$\therefore n=\sqrt{\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{1-\varphi_i}{n_j^2+2}}-2}$$

$$\frac{\partial n}{\partial \varphi_i}=-\frac{1}{2\sqrt{\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{1-\varphi_i}{n_j^2+2}}-2}}\times\left(\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{1-\varphi_i}{n_j^2+2}}\right)^2\times\left(\frac{1}{n_i^2+2}-\frac{1}{n_j^2+2}\right)$$

With $0\le\varphi_i\le 1$, if $n_i>n_j$, $\frac{\partial n}{\partial \varphi_i}>0$. And in the opposite, if $n_i>n_j$, $\frac{\partial n}{\partial \varphi_i}>0$.

Proof 2. Proof of either monotonic or non-monotonic function of compositions (φ) according to the L-T equation.

$$n=\sqrt{\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{\varphi_j}{n_j^2+2}}-2}+D\times\left(\frac{\varphi_i\varphi_j}{\varphi_i M_j/\rho_j+\varphi_j M_i/\rho_i}\right)$$

$$\because \varphi_j=1-\varphi_i$$

$$\therefore n=\sqrt{\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{(1-\varphi_i)}{n_j^2+2}}-2}+D\times\left(\frac{\varphi_i(1-\varphi_i)}{\varphi_i M_j/\rho_j+(1-\varphi_i)M_i/\rho_i}\right)$$

$$\frac{\partial n}{\partial \varphi_i}=-\frac{1}{2\sqrt{\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{1-\varphi_i}{n_j^2+2}}-2}}\times\left(\frac{1}{\frac{\varphi_i}{n_i^2+2}+\frac{1-\varphi_i}{n_j^2+2}}\right)^2\times\left(\frac{1}{n_i^2+2}-\frac{1}{n_j^2+2}\right)+D\times\frac{-M_j/\rho_j\times\varphi_i^2+M_i/\rho_i\times(1-\varphi_i)^2}{[M_j/\rho_j\times\varphi_i+M_i/\rho_i\times(1-\varphi_i)]^2}$$

(1) For ethanol–cyclohexane system, component *i* is ethanol.

$$\frac{\partial n}{\partial \varphi_i}=-\frac{1}{2\sqrt{\frac{1}{\frac{\varphi_i}{3.8504}+\frac{1-\varphi_i}{4.0246}}-2}}\times\left(\frac{1}{\frac{\varphi_i}{3.8504}+\frac{1-\varphi_i}{4.0246}}\right)^2\times\left(\frac{1}{3.8507}-\frac{1}{4.0246}\right)+(-1.613)\times\frac{-109.38\times\varphi_i^2+58.39\times(1-\varphi_i)^2}{[109.38\times\varphi_i+58.39\times(1-\varphi_i)]^2}$$

With $0<\varphi_i<1$, $\frac{\partial n}{\partial \varphi_i}>0$ and the RI of the mixture decreases with the increase of mole fraction of ethanol.

(Refer to **Table S3** for *D* value)

(2) For ethanol–water system, component *i* is ethanol.

$$\frac{\partial n}{\partial \varphi_i}=-\frac{1}{2\sqrt{\frac{1}{\frac{\varphi_i}{3.8504}+\frac{1-\varphi_i}{3.7782}}-2}}\times\left(\frac{1}{\frac{\varphi_i}{3.8504}+\frac{1-\varphi_i}{3.7782}}\right)^2\times\left(\frac{1}{3.8504}-\frac{1}{3.7782}\right)+1.791\times\frac{-18.05\times\varphi_i^2+58.39\times(1-\varphi_i)^2}{[18.05\times\varphi_i+58.39\times(1-\varphi_i)]^2}$$

If $0<\varphi_i<0.8127$, $\frac{\partial n}{\partial \varphi_i}>0$ and the RI of the mixture increases with the increase of mole fraction of ethanol.

If $\varphi_i = 0.8127$, $\frac{\partial n}{\partial \varphi_i} = 0$.

If $0.8127 < \varphi_i < 1$, $\frac{\partial n}{\partial \varphi_i} < 0$ and the RI of the mixture decreases with the increase of mole fraction of ethanol.

(Refer to **Table S4** for *D* value)

Supplementary Material (2)

Parameter or variable	Symbol	Value
Molecular weight	M_{eth}	46.07
	M_{cyc}	84.16
Density	ρ_{eth}	0.779
	ρ_{cyc}	0.769
RI of components	n_{eth}	1.3567
	n_{cyc}	1.4229
RI of mixture at φ~0.5	$n_{(0.5)}$	1.3863
Actual volume fraction at φ~0.5	$\varphi_{(0.5)eth}$	0.47389
	$\varphi_{(0.5)cyc}$	0.52611
D-value in L-T equation	D	-1.613
Objective Function	$(\Delta n)^2$	1.24E-18
RI of mixed solution (Decision Variable)	n	1.3773
Volume fraction (Variable)	φ_{eth}	0.6199
	φ_{cyc}	0.3801
Mole fraction	x_{eth}	0.7511
	x_{cyc}	0.2489

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