Knowledge of the health effects of simultaneous exposure to two or more chemical components is important because more than 80% of the organic solvents used in work environments are mixtures of several components [1, 2]. The biological reactions resulting from simultaneous exposure are also known to be different from those resulting from single component exposure [3–5]. In general, the volatility of a solvent depends on its saturated vapor pressure expressed as a function of temperature. For multicomponent solvents, the equilibrated vapor pressures of the components depend on the mole fractions of the liquid solvents in the mixture. Because the physical and chemical properties, such as the saturated vapor pressure and the polarity of the pure components, vary from solvent to solvent, the fractions of solvents in the liquid and vapor phases at equilibrium also tend to vary.

Hori et al [6] reported that the relationship between the concentrations in both phases can be obtained according to the vapor-liquid equilibrium (VLE) of two-component organic solvents in the presence of air. In our previous work [7], we discussed the availability of the UNIFAC (Universal Quasichemical Functional Group Activity Coefficient) model [8, 9], which is based on the group-contribution method. The calculated values for the binary, ternary, and quaternary systems commonly used as thinners are generally in good agreement with experimentally determined values. On the other hand, the mass transfer rate [10] and fluid dynamics [11] are necessary for estimating vapor concentrations in the work environment accurately, because workplaces are not closed spaces and
vapor concentrations change with time because organic solvents evaporate continuously. However, when the concentration in the work environment is estimated using both methods, information on the VLE at room temperature and atmospheric pressure is required. In this study, the tetrachloroethylene-chlorobenzene system was chosen from among the two-component systems that cannot be calculated using the UNIFAC model because UNIFAC group interaction parameters in the system have not yet been determined, and the equilibrated vapor concentrations were measured at 25°C in the presence of air to investigate the utility of the model in detail.

**Data Analysis**

**Equilibrated Vapor Concentrations**

When several organic solvents are placed in a closed vessel and the VLE is established, the liquid phase can be assumed to be incompressible, and the vapor phase can be approximated as an ideal gas mixture. In this case, the equilibrated vapor pressure of components i, and $P_i^0 \left( \frac{\text{mmHg}}{\text{K}} \right)$ can be expressed as follows:

$$P_i = \gamma_i x_i P_i^0 \left( T \right)$$  \hspace{1cm} (1)

where $x_i$ is the molar fraction in the liquid phase, $P_i^0 \left( T \right)$ is the saturated vapor pressure at absolute temperature $T \left( \text{K} \right)$, and $\gamma_i$ is the activity coefficient. The saturated vapor pressure was calculated using the Antoine equation [12]. The equilibrated vapor concentration, $C_i \left( \text{ppm} \right)$, can be determined as follows:

$$C_i = \frac{P}{P} \times 10^6 = \frac{\gamma_i x_i P_i^0 \left( T \right)}{P} \times 10^6$$  \hspace{1cm} (2)

where $P$ is the total pressure. The activity coefficients are thus experimentally determined using the following equation.

$$\gamma_i = \frac{C_i P \times 10^{-6}}{x_i P_i^0 \left( T \right)}$$  \hspace{1cm} (3)

The molar fraction in the vapor phase, $y_i$, can be expressed as follows:

$$y_i = \frac{C_i}{\sum_j C_j}$$  \hspace{1cm} (4)

**Estimation of the Activity Coefficients**

For an ideal solution, the activity coefficient $\gamma_i$ is unity (Raoult's law) [9]. However, many solutions cannot be regarded as ideal. Several models have been described for estimating the activity coefficient. In this study, the UNIFAC model [8, 9] based on the group-contribution method was applied to calculate the activity coefficient $\gamma_i$. Although thousands of compounds are used in the chemical industry, the number of functional groups that constitute these compounds is much smaller. The UNIFAC model assumes that a fluid's physical properties can be expressed as the sum of the contributions of the molecule's various functional groups. This expression is arbitrarily divided into two parts:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R$$  \hspace{1cm} (5)

where $\ln \gamma_i^C$ is the combinatorial term that depends on the volume and surface area of each molecule and $\ln \gamma_i^R$, the residual term, is directly related to energy differences.

The combinatorial term is given by

$$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + \left( \frac{z}{2} \right) q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j$$  \hspace{1cm} (6)

where

$$l_i = (z/2) \left( r_i - q_i \right) - \left( r_i - 1 \right) \quad \text{and} \quad z = 10$$  \hspace{1cm} (7)

$$\phi_i = \sum_j r_i x_j \quad \text{and} \quad \theta_i = \sum_j q_i x_j$$  \hspace{1cm} (8)

where $\theta_i$ is the area fraction and $\phi_i$ is the segment fraction, which is similar to the volume fraction. The pure-component parameters $r_i$ and $q_i$ are molecular van der Waals volumes and molecular surface areas, respectively, and can be calculated as the sum of the group volume and area parameters $R_k$ and $Q_k$, respectively.

$$r_i = \sum_k \nu_k^{(i)} R_k \quad \text{and} \quad q_i = \sum_k \nu_k^{(i)} Q_k$$  \hspace{1cm} (9)

where $\nu_k^{(i)}$, which is always an integer, is the number of groups of type $k$ in molecule $i$. 
The residual term is given by
\[
\ln Y_i^k = \sum_k \nu_i^{(k)} \left( \ln \Gamma_k^R - \ln \Gamma_k^{(i)} \right)
\]  
(10)
where \( \Gamma_k^R \) is the group residual activity coefficient and \( \Gamma_k^{(i)} \) is the residual activity coefficient of group \( k \) in a reference solution containing only molecules of type \( i \). The group residual activity coefficient \( \Gamma_k \) can be expressed as below.

\[
\ln \Gamma_k = Q_k \left[ 1 - \ln \left( \sum_m \Theta_n \Psi_{mn} \right) - \sum_m \sum_n \Theta_n \Psi_{mn} \right]
\]  
(11)

where

\[
\Theta_n = \frac{Q_m X_m}{\sum Q_m X_m} \quad \text{and} \quad X_m = \sum_i \sum_j \nu_i^{(j)}
\]  
(12)

\[
\Psi_{mn} = \exp \left( -\frac{a_{mn}}{T} \right)
\]  
(13)

where \( \Theta_n \) is the area fraction of group \( m \), \( X_m \) the mole fraction of group \( m \) in the mixture, and \( a_{mn} \) represents the group interaction parameters between groups \( m \) and \( n \), which must be determined based on experimental phase-equilibrium data. Additionally, \( a_{mn} \) has units of kelvin, \( a_{mn} \neq a_{nm} \), and \( a_{nn} = 0 \).

The above equations include three parameters: \( R_k \), \( Q_k \), and \( a_{mn} \). The combinatorial term of Eq. (6) can be calculated from Eq. (7)–(9) using the parameters \( R_k \) and \( Q_k \). The residual term of Eq. (10) can be calculated from Eq. (11)–(13) using the parameter \( a_{mn} \). The activity coefficient can be calculated by substituting Eq. (6) and Eq. (10) into Eq. (5). Therefore, the equilibrated vapor concentration (Eq. (2)) and the molar fraction in the vapor phase (Eq. (4)) can be determined.

Combination of Two-Component Organic Solvents and Group Assignments

Figure 1 shows the combination of two-component organic solvents listed in the Ordinance on Prevention of Organic Solvent Poisoning and the Ordinance on Prevention of Hazards due to Specified Chemical Substances (Industrial Safety and Health Law, Japan). The UNIFAC groups of 47 organic solvents are also shown in this figure as the main groups. Eighteen types of UNIFAC groups (e.g. CH₂, CH₂CO in Fig. 1) are included in the 47 organic solvents. The filled cells (gray) indicate that the systems can be analyzed using the UNIFAC model; that is, the values of the UNIFAC parameters are known [9]. However, 25 systems cannot be calculated using the UNIFAC model because the parameters are unknown.

The Japan Industrial Safety and Health Association (JISHA) investigated the combination of two-component systems used in the workplaces (1092 samples from 336 offices) in Japan [2]. Their results are shown in Fig. 1 (black triangles). In this study, the tetrachloroethylene-chlorobenzene system (No.13 × No.33 in Fig. 1) was chosen because the combination of these solvents appears (black triangle) in JISHA’s study, and its UNIFAC parameters are not confirmed (white cell). The tetrachloroethylene-chlorobenzene system includes four functional groups: ACH, ACCl, C=C, and Cl-(C=C), where AC indicates aromatic carbon. The parameter that relates the ACCl and Cl-(C=C) groups has not yet been determined. Therefore, we measured the VLE of the tetrachloroethylene-chlorobenzene system at 25°C, and the parameter relating the ACCl and Cl-(C=C) groups was experimentally determined.

Experimental

Special-grade tetrachloroethylene and chlorobenzene were supplied by Wako Pure Chem. Ind. Ltd. (Osaka, Japan) and used as received. Two types of solvents (total volume: 1–2 mℓ) were added to vials (5 mℓ) at various mass fractions of tetrachloroethylene (\( w \)), and then placed in a thermostatic bath (25°C) for 1 h. The vapor concentration was measured with a gas chromatograph (GC) (GC-17A, Shimadzu, Kyoto) equipped with a flame ionization detector (FID). The 0.5 mℓ of air in the headspace of the vials was removed using a gastight syringe, which was placed in a 50°C oven before sampling, and injected into the GC. An integrator (C-R7A plus, Shimadzu, Kyoto) was used to determine the vapor concentration. The column used was a DB-WAX capillary column (J&W, 0.25 mm diameter, 30 m length, Agilent Technologies, Tokyo). The column temperature was 100°C, and the injection and detec-
| No | Organic solvents                  | Main group        | 01 | 02 | 03 | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 |
|----|----------------------------------|-------------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|---...
ation port temperatures were both 230°C. Nitrogen was used as the carrier gas with a flow rate of 190 ml/min (split-ratio 110).

Results

Table 1 lists the experimental data of the tetrachloroethylene (1)-chlorobenzene (2) system at 25°C in the presence of air: the equilibrated vapor concentrations \(C_1\) and \(C_2\) at various mass fractions of tetrachloroethylene in the liquid phase \(w_1\), the molar fraction in the vapor phase \(y_1\) determined by Eq. (4), and the activity coefficients \(\gamma_1\) and \(\gamma_2\) determined by Eq. (3). The total pressure \(P\) was assumed to be equal to the atmospheric pressure (760 mmHg).

Figure 2 shows the relationship between the mass fraction \(w_1\) and the equilibrated vapor concentrations \(C_1\) and \(C_2\) for this system. The tetrachloroethylene vapor concentration increased and the chlorobenzene vapor concentration decreased monotonically as the mass fraction of tetrachloroethylene in the liquid phase increased.

Figure 3 shows the experimental VLE in the presence of air for the same system, i.e., the relationship between the liquid molar fraction \(x_1\) and the vapor molar fraction \(y_1\). The vapor molar fraction of tetrachloroethylene increased monotonically as the liquid phase molar fraction increased.

The tetrachloroethylene-chlorobenzene system includes four functional groups: ACH, ACCl, C=C, and Cl-(C=C). The group volume parameter \(R_k\) and area parameter \(Q_k\) have been reported previously [9]; therefore, Eq. (6) can be solved easily. The twelve UNIFAC interaction parameters \(a_{mn}\) are required to solve Eq. (10). These parameters can be obtained from the literature [9], except for the \(a_{mn}\) relating the ACCl and Cl-(C=C) groups. In this study, therefore, the interaction parameters between the ACCl and Cl-(C=C) groups were determined using a nonlinear least-squares method to obtain the best fit for the experimental data using EQUATRAN-G (Omega Simulation, Japan). The values of the parameters obtained are listed in Table 2.

As shown in Table 1 (UNIFAC model) and Figs. 2 and 3 (solid lines), where the results were calculated using EQUATRAN-G, the correlation appears to be accurate.

<table>
<thead>
<tr>
<th>Mass fraction (w_1) (-)</th>
<th>Concentration (C_1) (ppm)</th>
<th>Concentration (C_2) (ppm)</th>
<th>Molar fraction (x_1) (-)</th>
<th>Molar fraction (y_1) (-)</th>
<th>Activity coefficient (\gamma_1)</th>
<th>Activity coefficient (\gamma_2)</th>
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<tbody>
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<td>0.047</td>
<td>767</td>
<td>14045</td>
<td>0.033</td>
<td>0.052</td>
<td>0.966</td>
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<td>0.973</td>
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<table>
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<tr>
<th>Activity coefficient (\gamma_1)</th>
<th>Concentration (C_1) (ppm)</th>
<th>Concentration (C_2) (ppm)</th>
<th>Molar fraction (y_1) (-)</th>
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<td>1.001</td>
<td>23603</td>
<td>528</td>
<td>0.978</td>
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UNIFAC: Universal Quasichemical Functional Group Activity Coefficient, subscript 1: tetrachloroethylene, subscript 2: chlorobenzene, \(w\): liquid mass fraction, \(C\): vapor concentration, \(x\): liquid molar fraction, \(y\): vapor molar fraction, \(\gamma\): activity coefficient
Discussion

The availability of UNIFAC model information for the VLE under room temperature and atmospheric pressure was discussed in our previous work [7]. The UNIFAC interaction parameters were determined for a system consisting of solvents only; that is, air was not included in the vapor phase. However, the presence of air in the vapor phase will not influence the relationship of the VLE. The UNIFAC parameters obtained in this study listed in Table 2 can therefore be applied to other systems that consist of the same functional groups.

In general, for an ideal system that consists of solvents with similar chemical structures, Raoult’s law ($\gamma_i = 1$) can be applied, and the equilibrated vapor concentration can be calculated easily. However, the actual solution cannot be regarded as ideal. For example, the VLEs of the methanol-toluene system and the methanol-xylene system are substantially different from the ideal solutions [6] because the polarities of each component are quite different and their interactions are significant. Therefore, collecting the VLE data of non-ideal solutions is very important in conducting risk assessments of work environments in which organic solvents are used. Generally, combinations of solvents with different chemical structures tend to deviate from ideal systems. In this study, however, although the tetrachloroethylene-chlorobenzene system consists of solvents with different chemical structures, the experimentally determined activity coefficients for both solvents were close to 1, as shown in Table 1. Furthermore, the values calculated using Raoult’s law were also in good agreement with the experimental ones, as shown in Figs 2 and 3. However, to predict the VLE of multicomponent systems (i.e., those involving three or more components), including the tetrachloroethylene-chlorobenzene system, UNIFAC interaction parameters are necessary. Therefore, the unknown UNIFAC parameters should be determined.

Figure 1 shows 47 organic solvents subject to safety and health management regulations, including working environment measurement and specified health examination by Japanese law, and 18 types of UNIFAC groups. Among these solvents, the VLEs of 25 systems could not be calculated using the UNIFAC model; that is, 13 UNIFAC group interaction parameters have not yet been determined. In this study, the parameter relating the ACCl and Cl-(C=) groups was determined experimentally. For the remaining other 24 systems, that is, 12 UNIFAC interaction parameters are still unknown. These parameters may also be determined using the method demonstrated in this study.

**Fig. 2.** Equilibrated vapor concentrations of the tetrachloroethylene (1)-chlorobenzene (2) system at 25°C. Symbols indicate experimental data; ○: tetrachloroethylene, □: chlorobenzene, solid line: UNIFAC (Universal Quasichemical Functional Group Activity Coefficient) model, and broken line: Raoult’s law.

**Fig. 3.** Vapor-liquid equilibria of the tetrachloroethylene (1)-chlorobenzene (2) system at 25°C in the presence of air. Symbols: experimental data, solid line: UNIFAC (Universal Quasichemical Functional Group Activity Coefficient) model, and broken line: Raoult’s law.
Estimation of Equilibrated Vapor Concentrations

Conclusion

Vapor-liquid equilibrium data of the tetrachloroethylene-chlorobenzene system were obtained at 25°C in the presence of air, and the unknown UNIFAC parameter was determined by a nonlinear least-squares method. The results of this study suggest that most of the VLEs of two-component systems used in workplaces nationwide in Japan can be estimated. In addition, because the UNIFAC model can be calculated by molecular structure information and applied to multicomponent systems, the group-contribution method described in this study can be used to perform risk assessments of organic solvents.

Conflict of Interest

None of the authors have any conflict of interest to declare.

References

UNIFACモデルを用いたテトラクロロエチレン－クロロベンゼン系の平衡蒸気濃度の推定

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要   旨：混合有機溶剤を取り扱う作業環境において、環境気中の濃度分布を知ることは労働衛生管理上重要であり、そのためには各成分の平衡蒸気濃度を知る必要がある。本研究では、まず、テトラクロロエチレン－クロロベンゼン系を取り上げ、その平衡蒸気濃度を25℃、空気の存在下で測定した。次に、気液平衡論に基づくUNIFAC（Universal Quasichemical Functional Group Activity Coefficient）式を用いて相関を行った。この系には、4対のUNIFAC式のグループ間相互作用パラメータが存在し、すでに3対は決定されていた。本研究では、実測値を非線形最小二乗法で相関することにより、未決定であったACCIおよびCI-(C=C)間の相互作用パラメータを決定した。その結果、実測値と計算値は良好な一致を示した。

キーワード：有機溶剤、平衡蒸気濃度、テトラクロロエチレン、クロロベンゼン、UNIFACモデル。