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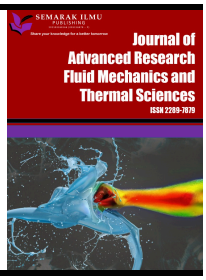


# Prediction of Phase Equilibria and Transport Properties Using ASOG and PRASOG Group Contribution Methods: A Review

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**ABSTRACT**

Half century has passed since the first version of Analytical Solution of Groups (ASOG) model was proposed. Now the ASOG model is well known as a group contribution method as well as UNIFAC. Although the ASOG model was designed for prediction of vapor-liquid equilibrium around the atmospheric pressure, the applications are extended to not only the phase equilibria in the wide temperature and pressure ranges but also the transport properties. The function forms in the ASOG model, basically composed of Flory-Huggins equation and Wilson equation, can be applied for the prediction of the phase equilibria (vapor-liquid, liquid-liquid, solid-liquid and vapor-solid) and the transport properties (kinematic viscosity, thermal conductivity) of the mixtures with some modifications.

## 1. Introduction

The phase equilibria and transport properties are essential to establish new technologies for process development and equipment design in the chemical and mechanical industries [1-11]. In the predictive methods, the group contribution method is an important technique for the thermophysical properties because the parameters can be evaluated just from the molecular structure. UNIQUAC Functional-group Activity Coefficients (UNIFAC) and Analytical Solution Of Groups (ASOG) models are well known group contribution methods to estimate the activity coefficient in the mixtures. The first concept of the ASOG model was proposed by Derr and Deal [12]. Successively, Kojima and Tochigi [13] provided a modified version, and the ASOG model have been applied to predictions not only for phase equilibria but also for transport properties. Figure 1 shows an example of the groups in the ASOG model for a binary mixture, pentane (1) – ethanol (2). In the binary, just two functional groups, -$CH_2$- (including –$CH_3$) and -OH, contribute to an equation for the prediction of thermophysical properties in the mixture. The authors have made the continuing research works on the ASOG model for various thermophysical properties shown in Figure 2. The

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review deals with the prediction of phase equilibria and transport properties using some ASOG models.

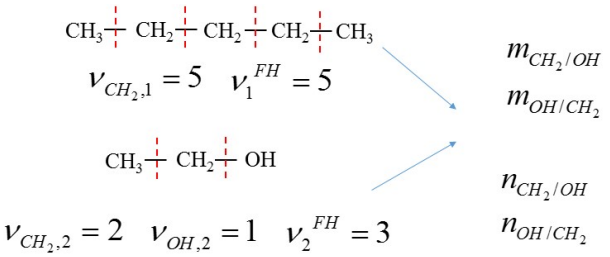


**Fig. 1.** Example of groups for pentane (1) – ethanol (2) based on ASOG model [12,13]


**Fig. 2.** Prediction of phase equilibria and transport properties using ASOG models

## 2. Methodology

In the original ASOG model, the activity coefficient of the component *i* is given by the following equation [12,13]

$$\ln \gamma_i = \ln \gamma_i^{FH} + \ln \gamma_i^{G} \tag{1}$$

The ASOG model is composed of the two activity coefficient models, Flory-Huggins and Wilson. The activity coefficient, based on Flory-Huggins model, is given by the following equation

$$\ln \gamma_i^{FH} = 1 - \frac{\nu_i^{FH}}{\sum_j \nu_j^{FH}} + \ln \frac{\nu_i^{FH}}{\sum_j \nu_j^{FH}} \tag{2}$$

where $\nu_i^{FH}$ is the number of atoms (other than hydrogen atoms) in the component *i*. On the other hand, the activity coefficient, based on Wilson model, is given by the following equation

$$\ln \gamma_i^{G} = \sum_k \nu_{k,i} \left[ \ln \Gamma_k - \ln \Gamma_k^{(i)} \right] \tag{3}$$

$$\ln \Gamma_k = 1 - \sum_l \frac{X_l a_{l/k}}{\sum_m X_m a_{l/m}} - \ln\left(\sum_l X_l a_{k/l}\right) \tag{4}$$

$$X_k = \frac{\sum_j x_j v_{k,j}}{\sum_j x_j \sum_l v_{l,j}} \tag{5}$$

$$\ln a_{k/l} = m_{k/l} + \frac{n_{k/l}}{T} \tag{6}$$

where $v_{k,i}$ is the total number of atoms (other than hydrogen atoms) in group *k* of the component *i.*

The $v_{k,i}$ has exceptions for some groups. For example, the following values are applied to the three groups, $H_2O$, -CH< and >C<

$$v_{H_2O,i} = 1.6; \quad v_{CH,i} = 0.8; \quad v_{C,i} = 0.5; \tag{7}$$

$a_{k/l}$ is the ASOG group parameter. Figure 3 shows the available group parameters provided in a research by Tochigi *et al.,* [14]. The ASOG group parameters have been determined for 43 groups when the literatures by Tochigi *et al.,* [14], Tochigi and Kojima [15], and Tochigi and Gmehling [16] were published. Figure 1 also shows the examples of the ASOG group parameters in Eq. (1) to Eq. (6) for the binary, pentane (1) – ethanol (2).

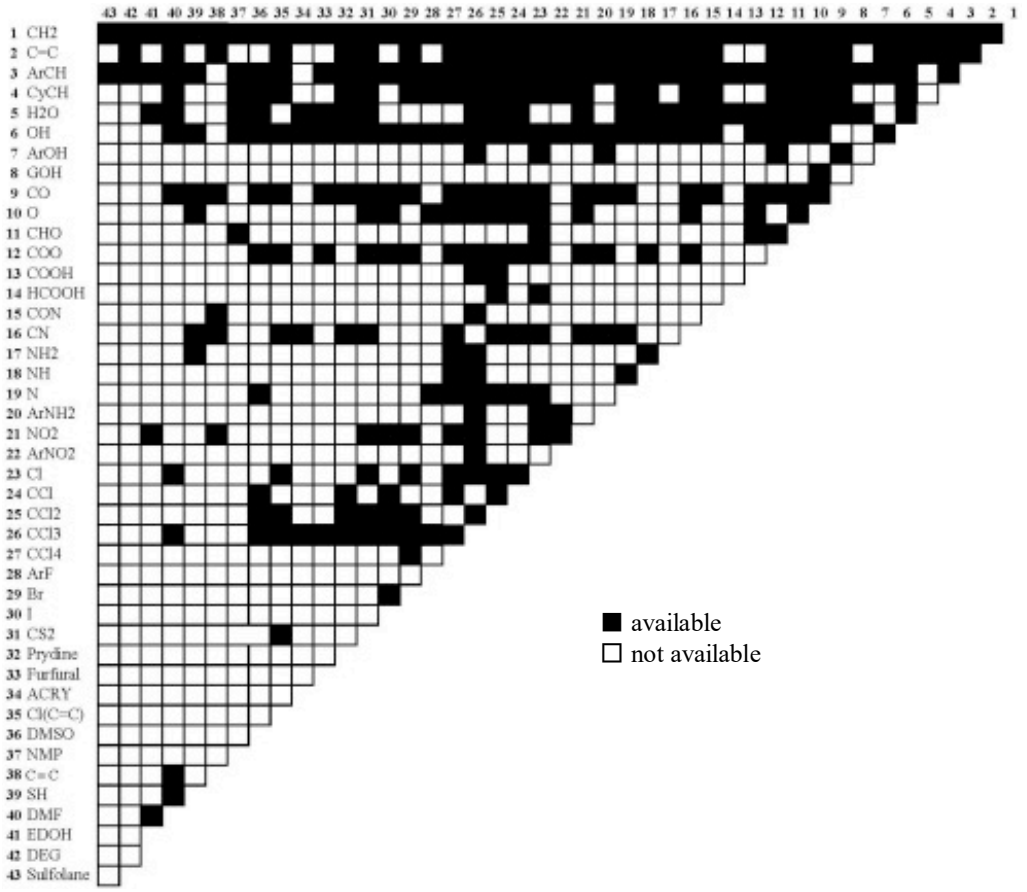


**Fig. 3.** Examples of available parameter in ASOG model [3]

## 3. Prediction of Phase Equilibria using ASOG Model

### *3.1 Vapor-Liquid Equilibria*

#### *3.1.1 Vapor-Liquid Equilibria around the atmospheric pressure*

The vapor-liquid equilibria (VLE), around the atmospheric pressure, will be calculated by using the following equation

$$y_i p = \gamma_i x_i p_i^s \tag{8}$$

where the activity coefficient $\gamma_i$ can be predicted by using the ASOG model. Figure 4 shows the predictive accuracy for VLE, and compared with those by UNIQUAC, UNIFAC and its modifications [17-20]. The average deviations are slightly larger than those by others. However, as described later, the extension to the other physical properties have been well investigated in the ASOG model.

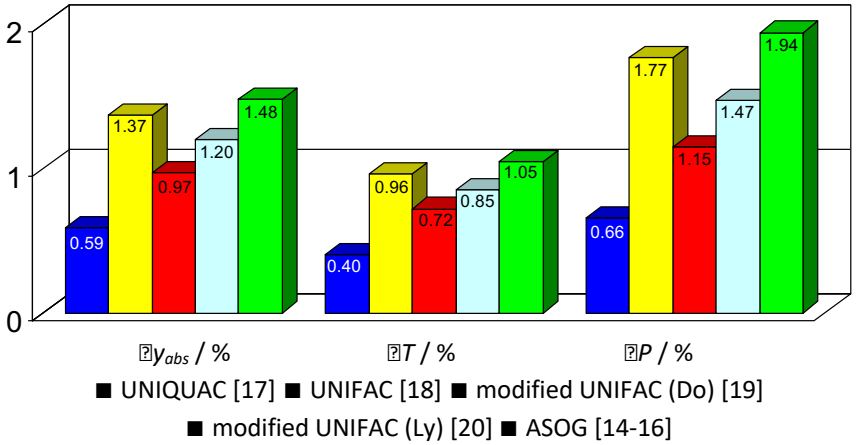


**Fig. 4.** Average deviations of VLE around the atmospheric pressure

The further applications were found for the reactive mixtures of ester, alcohol, water and acetic acid and the mixtures containing hydrofluoroethers [21-24]. The temperature dependences in Eq. (6) were also discussed and improved by using other function forms [25]. The reproducibility for the vapor-liquid-liquid equilibria (VLLE) and the azeotropic point were also reported [26,27].

#### *3.1.2 Gas solubility in liquid*

At the temperature higher than the critical point of the component with the low boiling point, the saturated vaper pressure, $p_1^s$, will not exist. However, the fugacity of the hypothetical liquid can be evaluated by a graphical correlation of Prausnitz and Shair [28]. Then, the Henry constant, derived from Eq. (8), is given by the following equation

$$H_1 = \lim_{x_1 \to 0} \frac{y_1 p}{x_1} = \gamma_1 f_1^{s,hyp} \tag{9}$$

where $f_1^{s,hyp}$ is the hypothetic saturated vapor pressure of the component with the low boiling point. Eq. (9) is known as the ASOG-gas solubility (GS) model [29]. In the ASOG-GS model, Eq. (4) was slightly modified with the following equation

$$\ln \Gamma_k = 1 - \sum_l \frac{X_l a_{l/k}}{\sum_m X_m a_{l/m}} - \ln\left(\sum_l X_l a_{k/l}\right) + \sum_l \sum_m \left( A_{l/k} - \frac{1}{2} A_{l/m} \right) X_l X_m \tag{10}$$

$$A_{k/l} = C_{k/l} + \frac{D_{k/l}}{T} \tag{11}$$

The parameters, $m_{k/l}$, $n_{k/l}$, $C_{k/l}$ and $D_{k/l}$ in Eq. (6) and Eq. (10), have been newly determined for group pairs composed of 7 groups: $CH_2$, OH, Ar, $N_2$, $O_2$, $H_2$, and $CO_2$. The solubilities were evaluated at the gas partial pressure of 101.33 kPa in the temperature range of 283-313 K. The average deviations are 6.0 % for the mole fraction of dissolved gas in pure solvents covering 36 systems [29].

### *3.1.3 Vapor-Liquid Equilibria for systems containing polymers*

In thermodynamics, polymer can be assumed as a liquid with zero saturated vapor pressure and no fluidity. Therefore, in solvent - polymer systems, the total pressure is approximately the same as the partial pressure of solvent. So, Eq. (8) will be converted to the following equation for the solvent

$$p = a_1 p_1^s \tag{12}$$

where $a_1$ is the activity of the solvent in polymer. Considering the compressibility in the polymer, Eq. (1) should be modified as the following equation

$$\ln a_1 = \ln \gamma_1^{FH} + \ln \gamma_1^{G} + \ln a_1^{FV} \tag{13}$$

where $a_1^{FV}$ is come from the free volume effect. Eq. (13) is known as the ASOG-free volume (FV) model, and makes use of Oishi-Prausnitz equation for $a_i^{FV}$ [30,31]

$$\ln a_1^{FV} = c_1 \left[ 3 \ln \frac{\tilde{v}_1^{1/3} - 1}{\tilde{v}_m^{1/3} - 1} + \frac{\tilde{v}_1^{4/3}}{\tilde{v}_1^{1/3} - 1} \left( \frac{1}{\tilde{v}_1} - \frac{1}{\tilde{v}_m} \right) \right] \tag{14}$$

$$\tilde{v}_i = \frac{v_{w,i}}{v_i^*} \tag{15}$$

$$\tilde{v}_m = \frac{\sum_k v_{w,k} w_k}{\sum_k v_k^* w_k} \tag{16}$$

$$c_i = A + B w_i \tag{17}$$

where $w_i$ is the mass fraction of component *i*. The $v_{w,i}$ and $v_i^*$ are the specific volume and the core volume, respectively. $A$ and $B$ are newly determined parameters for solvent (1) – polymer (2). The average deviation of the activity coefficient of solvent, $(a_1/w_1)$, was 2.41 % for the 6 organic solvents in poly (ethylene oxide) with the molecular mass $M_w$ =920,000 and the polydispersity $M_w/M_n = 1.10$ [30]. The ASOG-FV model was also applied for solvent (1) – polystyrene (2) [32].

*3.1.4 Vapor-Liquid Equilibria at high pressure*

VLE at high pressures should be considered by using fugacities, so Eq. (8) will be converted to the following equation

$$\hat{f}_i^{\,V} = \hat{f}_i^{\,L} \tag{18}$$

The fugacity $\hat{f}_i$ is evaluated by the following equations

$$RT\ln\frac{\hat{f}_i^{\,V}}{y_i p} = \int_{V^V}^{\infty}\left[\left(\frac{\partial p}{\partial n_i}\right)_{T,V,n_{j\neq i}} - \frac{RT}{V}\right]dV - RT\ln\frac{pv^V}{RT} \tag{19}$$

$$RT\ln\frac{\hat{f}_i^{\,L}}{y_i p} = \int_{V^L}^{\infty}\left[\left(\frac{\partial p}{\partial n_i}\right)_{T,V,n_{j\neq i}} - \frac{RT}{V}\right]dV - RT\ln\frac{pv^L}{RT} \tag{20}$$

The VLE at high pressures will be calculated from $(\partial p/\partial n_i)_{T,V,n_{j\neq i}}$, $v^V$ and $v^L$ by using the cubic equations of state, Peng-Robinson (PR), Soave-Redlich-Kwong (SRK), Martin and so on, with their mixing rules [33-35]. The PR plus ASOG (PRASOG) model makes use of the followings, PR equation and the mixing rule using excess Gibbs energy $g^E$ [33,36,37].

$$p = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} \tag{21}$$

$$\frac{a}{b} = \sum_i x_i \frac{a_i}{b_i}\left[\frac{\ln\dfrac{1+\sqrt{2}+\dfrac{v_{i0}}{b_i}}{1-\sqrt{2}+\dfrac{v_{i0}}{b_i}}}{\ln\dfrac{1+\sqrt{2}+\sum_j x_j\dfrac{v_{j0}}{b_j}}{1-\sqrt{2}+\sum_j x_j\dfrac{v_{j0}}{b_j}}}\right]$$

$$-\frac{2\sqrt{2}}{\ln\dfrac{1+\sqrt{2}+\sum_j x_j \dfrac{v_{j0}}{b_j}}{1-\sqrt{2}+\sum_j x_j \dfrac{v_{j0}}{b_j}}} \times \left[ \frac{g_0^E}{RT} + \sum_i x_i \ln \frac{b}{b_i} + \sum_i x_i \ln \frac{\sum_j x_j \dfrac{v_{j0}}{b} - 1}{\dfrac{v_{i0}}{b} - 1} \right] \tag{22}$$

$$b - \frac{a}{RT} = \sum_i \sum_j x_i x_j \left[ \frac{b_i + b_j}{2} - \frac{\sqrt{a_i a_j}}{RT} \right] \tag{23}$$

$$\frac{g_0^E}{RT} = \sum_i x_i \ln \gamma_i \tag{24}$$

where $\frac{v_{i0}}{b}$ are the value of $\frac{v_i}{b}$ at $\frac{T}{T_{c,i}} = 0.4$. In the PRASOG model, the original ASOG parameters were applied to the Gibbs free energy $g_0^E$. Together with the original parameters, 31 group parameters were newly determined. The VLE at high pressures have been correlated for 56 binary systems (461 isotherms). Figure 5 and Figure 6 show the examples of predicted results. As well as the PRASOG model, many attempts were done by using the ASOG model with SRK and Martin equations [38-41]. Recently, the availability of the PRASOG model was extended to the systems containing ammonia [42]. Also, the PR equation was combining with the ASOG-FV model, and the predictions were also reported for solvent –polymer [43,44]. Instead of PR equation, Sako-Wu-Prausniz equation of state were also employed and combined with ASOG-FV [45,46].

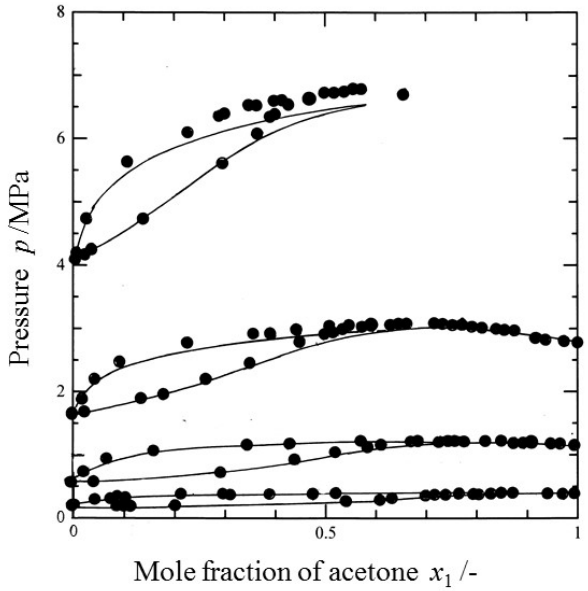


**Fig. 5.** VLE for the acetone (1) – water (2) at various temperatures; (●): Griswold and Wong [50] (373, 423, 473 and 523 K); (———): PRASOG model

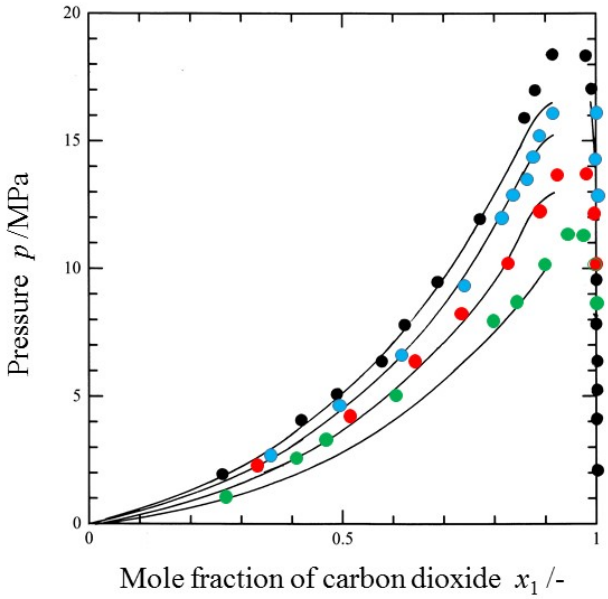


**Fig. 6.** VLE for the carbon dioxide (1) – methyl palmitate (2) at 313-343 K; (●, ●, ●, ●): Inomata *et al.*, [51] (313, 323, 333 and 343 K); (———): PRASOG model

### *3.2 Liquid-Liquid Equilibria*

The liquid-liquid equilibria (LLE) can be calculated by the following equation

$$\left(x_i\gamma_i p_i^s\right)^{L_I} = \left(x_i\gamma_i p_i^s\right)^{L_{II}} \tag{25}$$

where the saturated vapor pressures $p_i^s$ were cancelled in the both sides, because the coexisted liquid phases, $L_I$ and $L_{II}$, are at the same pressure. This model was named as the ASOG-LLE model. However, the pressure dependence on LLE were not evaluated. The LLE for 31 ternary systems has firstly been predicted using the original ASOG parameters in Eq. (8) [47,48]. Figure 7 and Figure 8 show the example of predicted results. It is well known that the parameters, determined from LLE, sometimes will be different from those from VLE in many activity coefficient models. So, later, the ASOG-LLE parameters have been determined using experimental LLE data [49].

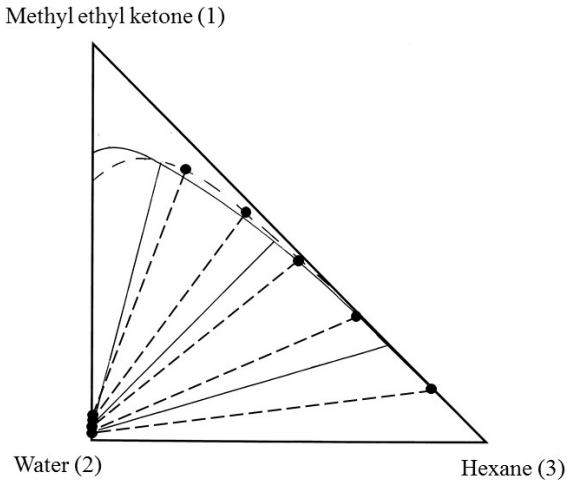


**Fig. 7.** LLE for methyl ethyl ketone (1) – water (2) – hexane (3) at 298 K; ( – – ●– ) : Treybal and Vondrak [52]: ( ——— ) ASOG-LLE model

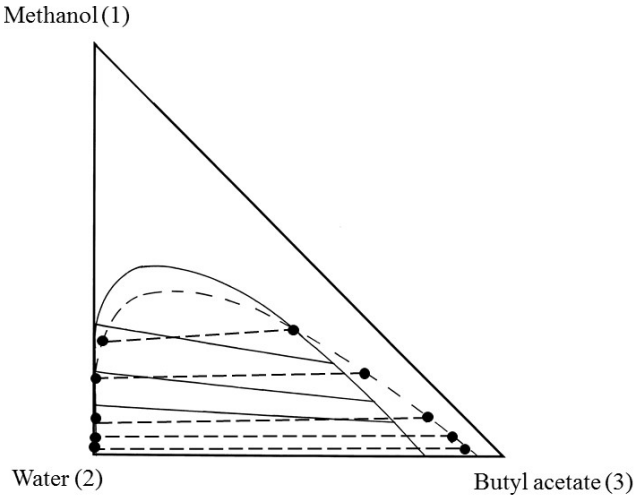


**Fig. 8.** LLE for methanol (1) ‑ water (2) ‑ butyl acetate (3) at 303 K; ( – –●– ) : Rao and Rao [53]: (———) ASOG-LLE model

### *3.3 Solid-Liquid Equilibria*

Simple eutectic systems are important for designing a crystallization process especially in medical industries, because the solid of pure compound can be obtained from solution. The solid-liquid equilibria (SLE) are calculated by the following equation

$$x_i\gamma_i = -\frac{\Delta h_{f,i}}{R}\left(\frac{1}{T}-\frac{1}{T_{m,i}}\right) \tag{26}$$

where $\Delta h_{f,i}$ and $T_{m,i}$ are the latent heat of fusion and the melting point of the pure component *i*, respectively. Ochi *et al.,* [54] have predicted the solid-liquid equilibria using the original ASOG parameters in Eq. (8). This method is called as the ASOG-SLE model. Figure 9 shows the examples of predicted results.

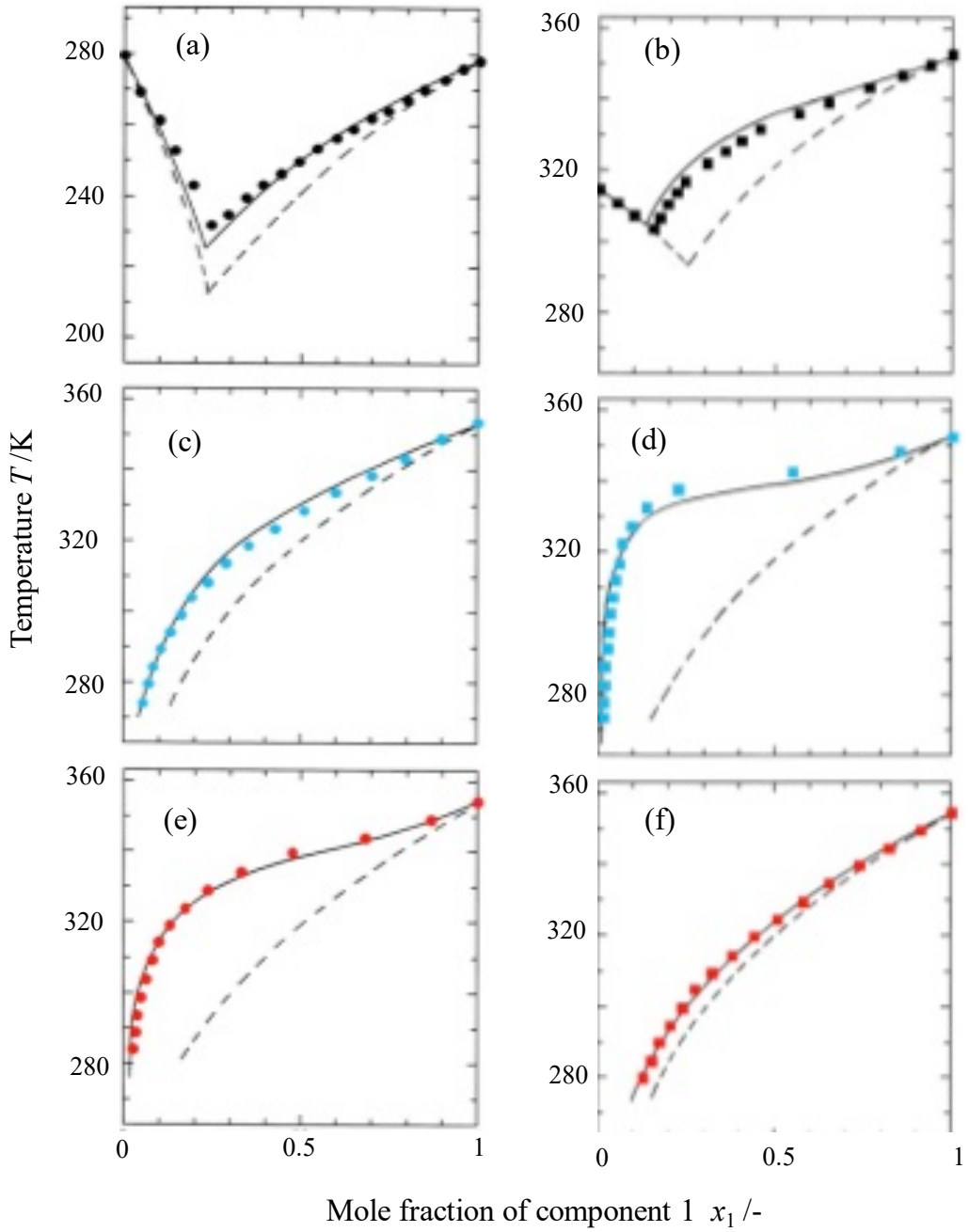


**Fig. 9.** SLE for 6 binaries; (a) benzene (1) – cyclohexane (2), (●): Yoshida *et al.*, [61]; (b) naphthalene (1) –phenol (2), (■) Timmermans [62]; (c) naphthalene (1) –aniline (2), (●) Ward [63]; (d) naphthalene (1) –methanol (2), (■) Ward [63]; (e) naphthalene (1) ‑butanol (2), (●) Sunier [64]; (f) naphthalene (1) – acetone (2), (■) Ward [63]; (———) ideal solution model; (– – – –) ASOG-SLE model

### *3.4 Solid-Vapor Equilibria*

Some interesting solubility data of a solute solid were reported in the vapor phase, especially the supercritical conditions. The solid-vapor equilibria (SVE) can be predicted using the following equation

$$\hat{f}_i^{\,V} = p_i^{\,s} \exp\left[\frac{v_i^{s}\left(p - p_i^{s}\right)}{RT}\right] \tag{27}$$

$p_i^{\,s}$ and $v_i^{\,s}$ are the sublimation pressure and the solid molar volume of solid solute, respectively. The fugacity of the solid in the vapor phase can be calculated using equation of state with the mixing rule. In the method, the fugacity in the vapor phase were calculated from Eq. (19), Eq. (21) to Eq. (23) together with the parameters in the PRASOG model [37]. The PRASOG parameters were available not only for VLE but also SVE. Figure 10 and Figure 11 show the examples of predicted results. As shown in Figure 10 and Figure 11, good reproducibility can be seen not only for the binaries but also for a ternary.

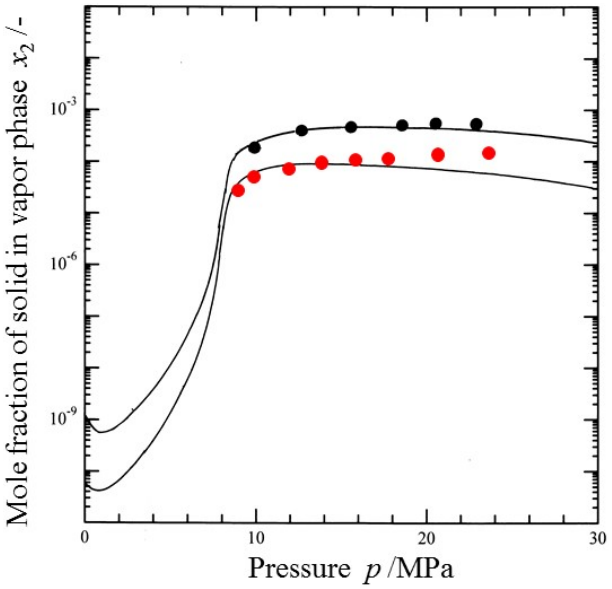


**Fig. 10.** SVE for two binaries, carbon dioxide(1) – palmitic acid (2) and carbon dioxide(1) – stearic acid (2) at 308 K; (●): Iwai *et al.,* [65]; (●): Iwai *et al.,* [66]; (———): PRASOG model

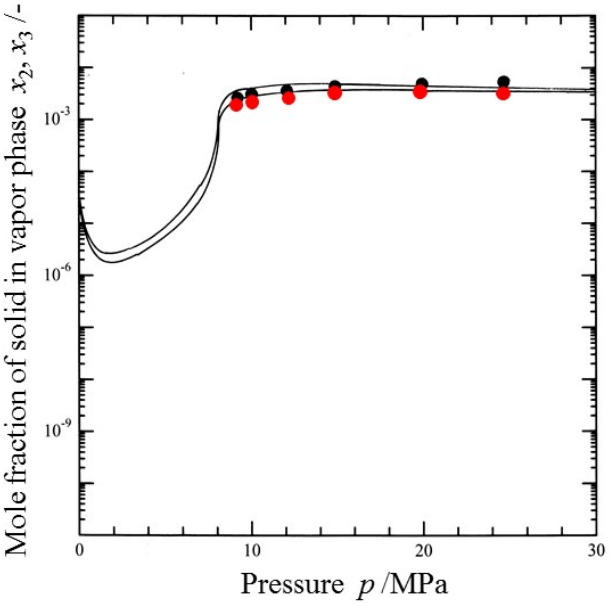


**Fig. 11.** SVE for carbon dioxide(1) – 2,6-dimethylnaphthalene(2) - 2,7-dimethylnaphthalene(3) at 308 K; (●): 2,6-dimethylnaphthalene ; (●): 2,6-dimethylnaphthalene, Iwai *et al.,* [67]; (———): PRASOG model

## 4. Prediction of Transport Properties using ASOG Model

### *4.1 Kinematic Viscosities*

The kinematic viscosity of a liquid is given by the following equation

$$\ln\left(\frac{\eta M}{\rho}\right) = \sum_i x_i \ln\left(\frac{\eta_i M_i}{\rho_i}\right) + \frac{g_{\eta/\rho}^{\pm}}{RT} \tag{28}$$

$$g_{\eta/\rho}^{\pm} = kg^{E} \tag{29}$$

The equation is based on the absolute reaction rate theory. The excess molar Gibbs energy can be calculated not only from the activities calculated by solution models but also from the fugacities calculated by equation of states [11,55-57]. The ASOG-VISCO model was proposed by assuming $k=-1$ [58-60]. The excess Gibbs free energy was estimated by using Eq. (1) to Eq. (6). Although Eq. (1) to Eq. (6) was not changed, the pair parameters, were newly determined [58,59]. The average deviations are 4.15 % for binary systems and 5.03 % for ternary systems using the ASOG-VISCO parameters [59]. Figure 12 shows the predicted results. Instead of Eq. (6), Matsuda *et al.,* [60] improved the prediction and extended to high pressure conditions by using the following equation

$$\ln a_{k/l} = m_{k/l} + \frac{n_{k/l}}{T} + o_{k/l} \ln T \tag{30}$$

Figure 13 shows the predicted results. Even at high pressure the ASOG-VISCO model provides a good reproducibility.

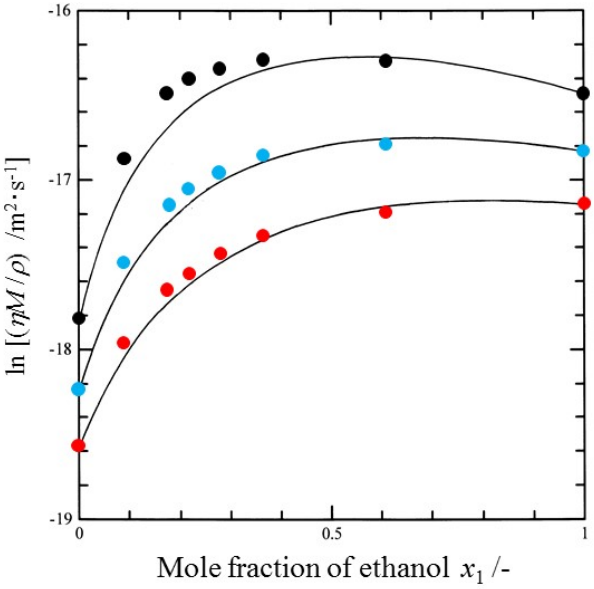


**Fig. 12.** Kinematic viscosity for ethanol (1) – water (2) at 293-333 K using ASOG-VISCO model; (●, ●, ●): Noda *et al.,* [69] (293.15, 303.15 and 333.15 K); (———): ASOG-VISCO model

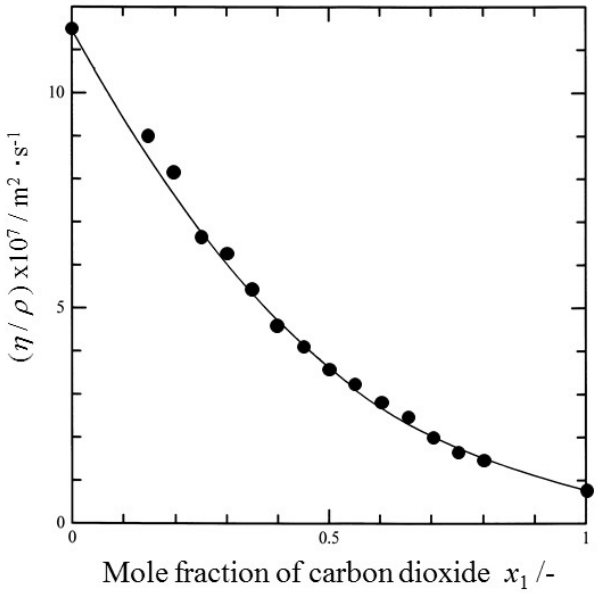


**Fig. 13.** Kinematic viscosity for carbon dioxide (1) – acetone (2) at 308.15 K using ASOG-VISCO model; (●): Sih *et al.,* [70]); ( ——— ): ASOG-VISCO model

*4.2 Thermal Conductivities*

The excess thermal conductivity of a liquid is given by the following equation

$$\ln \lambda M = \sum_i x_i \ln \lambda_i M_i + g_\lambda^E \tag{31}$$

Similar to Eq. (29), the following equation was employed

$$g_\lambda^E = \frac{k g^E}{RT} \tag{32}$$

The Eq. (32) and Eq. (33) was named as ASOG-thermal conductivity (TC) model by assuming $k = -1$ [68]. Then, the pair parameters have been newly determined for the ASOG-TC model [68].

## 5. Conclusions

The ASOG model is one of the predictive methods using activity coefficients based on the group contribution methods. In this review, some predictions have been shown for phase equilibria and transport properties (kinematic viscosity and thermal conductivity). Although the prediction was not shown here, the parameters for the ASOG- excess molar enthalpy ($H^E$) model have been already determined for predicting the heats of mixing. The authors are also thinking to determine some ASOG parameters for predicting the surface tension and permittivity, too.

## Acknowledgement

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