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Article

Estimation of Two-Component Activities of Binary Liquid Alloys by the Pair Potential Energy Containing a Polynomial of the Partial Radial Distribution Function

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Abstract: An investigation of pair partial radial distribution functions and molecular pair potentials within a system has established that the existing potential functions are rooted in the assumption of a static arrangement of atoms, overlooking their distribution and vibration. In this study, Hill's proposed radial distribution function polynomials are applied for the pure gaseous state to a binary liquid alloy system to derive the pair potential energy. The partial radial distribution functions of 36 binary liquid alloy systems reported in literature were examined and then validated using four thermodynamic models. Results show that the molecular interaction volume model (MIVM) and regular solution model (RSM) outperform other models when an asymmetric method is used to calculate the partial radial distribution function. The MIVM exhibits a mean standard deviation (SD) of 0.095 and a mean absolute relative difference (ARD) of 32.2%. Similarly, the RSM demonstrates a mean SD of 0.078 and an ARD of 32.2%. The Wilson model yields a mean SD of 0.124 and a mean ARD of 226%. The nonrandom two-liquid (NRTL) model exhibits a mean SD of 0.225 and a mean ARD of 911%. On applying the partial radial distribution function symmetry method, the MIVM and RSM outperform the other approaches, with a mean SD of 0.143 and a mean ARD of 165.9% for the MIVM. The RSM yields a mean SD of 0.117 and an ARD of 208.3%. The Wilson model exhibits the mean values of 0.133 and 305.6% for SD and ARD, respectively. The NRTL model shows an average SD of 0.200 and an average ARD of 771.8%. Based on this result, the influence of the symmetry degree on the thermodynamic model is explored by examining the symmetry degree as defined by the experimental activity curves of the two components.

Keywords: pair potential; partial radial distribution function; binary liquid alloy

1. Introduction

Pair potentials play a fundamental role in comprehending the static and dynamic properties of gases, liquids, and solids [1]. The main objective of studying pair potentials is to develop accurate and reliable models that describe intermolecular interactions and enable simulation, prediction, and explanation of the behavior and properties of molecular systems. Various computational simulation studies, such as for protein folding, drug–receptor interactions, and material property prediction, are conducted using molecular pair potentials to ascertain the underlying mechanisms of molecular interactions, explore novel material properties, and optimize drug design. Materials science and surface science researchers have investigated molecular potentials to thoroughly understand phenomena such as material structure, stability, crystal defects, and surface adsorption. Understanding intermolecular interactions is essential in material design, catalyst development, and comprehending material interfaces and surface phenomena. Molecular pair potential models encompass widely used semiempirical potentials such as the Lennard–Jones potential [2], Morse potential [3], and Born–Mayer potential [4] as well as molecular force fields, quantum mechanical

descriptions, and statistical mechanics methods. Different factors affect the selection and examination of these models, including application needs and accuracy considerations [5–7]. Accurate pair potentials provide a comprehensive description of energy, geometric structure, and spectral properties of molecules and serve as the basis for investigating collision and chemical-reaction dynamics, such as those for molecular collisions. Thus, an in-depth study of potential pair functions holds significant physical implications and offers broad applications. This study reveals a direct correlation between the radial distribution function (RDF) and molecular pair potential. Herein, we establish a unified approach by exploiting the analogy between the computational procedure for the RDF in a pure gas and its application to the molecular pair potential in a binary liquid system. To substantiate our framework, we rigorously analyzed the RDF using 36 binary liquid alloys.

2. Thermodynamic Model

2.1. Regular Solution Model (RSM)

Hildebrand proposed the RSM in 1929 [8]. According to this model, the molar excess volume and mixing entropy are zero and the molar excess mixing Gibbs free energy is equal to the molar excess mixing enthalpy [9]. The expression for the molar excess Gibbs free energy for a binary system is as follows; the activity coefficient of the component i is $\ln \gamma_i$.

$$\Delta G_m^E = \Delta H_m = \Omega_{ij} x_i x_j \quad (1)$$

$$\ln \gamma_i = \Omega_{ij} x_j^2 \quad (2)$$

Here, x_i and x_j are the mole fractions of components i and j , respectively, and Ω_{ij} is the interaction parameter between components i and j . Ω_{ij} is only related to temperature and does not change with the composition of components.

2.2. Wilson model

In 1964, Wilson [10] introduced a semiempirical and semitheoretical model based on the local concept. This model assumes that “local concentrations” (represented as volume fractions) primarily determine molecular interactions. These concentrations are defined in relation to the Boltzmann distribution probability term for energy. The excess free energy associated with the concentrations can be expressed as follows.

$$\frac{G_m^E}{RT} = -x_i \ln(x_i + A_{ji}x_j) - x_j \ln(x_j + A_{ij}x_i) \quad (3)$$

$$\ln \gamma_i = -\ln(x_i + A_{ji}x_j) + x_j \left(\frac{A_{ij}}{x_i + A_{ij}x_j} - \frac{A_{ji}}{x_j + A_{ji}x_i} \right) \quad (4)$$

Here, A_{ij} and A_{ji} are the interaction parameters between components i and j , which are only related to temperature and do not change with the composition of components [11].

2.3. Nonrandom two-liquid (NRTL) model

The NRTL model, introduced by Renon and Prausnitz in 1968 [12], has been extensively used in correlating thermodynamic data, computing thermodynamic properties, and predicting phase equilibrium for diverse fluid systems in chemical processes. This model, based on the concept of local concentration, permits the determination of molar excess Gibbs free energy. The activity coefficient of the component i is $\ln \gamma_i$.

$$\frac{G_m^E}{RT} = x_i x_j \left(\frac{\tau_{ji} G_{ji}}{x_i + x_j G_{ji}} + \frac{\tau_{ij} G_{ij}}{x_j + x_i G_{ij}} \right) \quad (5)$$

$$\ln \gamma_i = x_j^2 \left[\frac{\tau_{ji} G_{ji}^2}{(x_i + x_j G_{ji})^2} + \frac{\tau_{ij} G_{ij}}{(x_j + x_i G_{ij})^2} \right] \quad (6)$$

$$\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT} \quad \tau_{ji} = \frac{g_{ji} - g_{ii}}{RT} \quad (7)$$

$$G_{ij} = \exp(-\alpha \tau_{ij}) \quad G_{ji} = \exp(-\alpha \tau_{ji}) \quad (8)$$

Here, A_{ij} and A_{ji} are energy parameters characterizing the interaction between components i and j ; α is related to nonrandomness in the mixture, independent of temperature and composition of a solution. Moreover, the characteristic parameter of a solution depends on the solution type. When the mixture is entirely random, many binary system experimental data show that α varies from 0.2 to 0.47. In this study, $\alpha = 0.3$.

2.4. Molecular Interaction Volume Model (MIVM)

In 2000, Tao introduced the volume model of molecular interaction [13], which uses statistical thermodynamics and fluid phase equilibrium theory to describe the motion of liquid molecules. This model yields the following expression:

$$\frac{G_m^E}{RT} = x_i \ln \left(\frac{V_{mi}}{x_i V_{mi} + x_j V_{mj} B_{ji}} \right) + x_j \ln \left(\frac{V_{mj}}{x_j V_{mj} + x_i V_{mi} B_{ij}} \right) - \frac{x_i x_j}{2} \left(\frac{Z_i B_{ji} \ln B_{ji}}{x_i + x_j B_{ji}} + \frac{Z_j B_{ij} \ln B_{ij}}{x_j + x_i B_{ij}} \right) \quad (9)$$

The activity coefficients of the components i is $\ln \gamma_i$.

$$\ln \gamma_i = 1 + \ln \left(\frac{V_{mi}}{V_{mi} x_i + V_{mj} B_{ji} x_j} \right) - \frac{x_i V_{mi}}{V_{mi} x_i + x_j V_{mj} B_{ji}} - \frac{x_j V_{mi} B_{ij}}{V_{mj} x_j + x_i V_{mi} B_{ij}} - \frac{x_j^2}{2} \left[\frac{Z_i B_{ji}^2 \ln B_{ji}}{(x_i + x_j B_{ji})^2} + \frac{Z_j B_{ij} \ln B_{ij}}{(x_j + B_{ij} x_i)^2} \right] \quad (10)$$

Here, Z_i and Z_j are the first coordination numbers of i and j pure substances, respectively, and V_{mi} and V_{mj} are the molar volumes of i and j , respectively. B_{ij} and B_{ji} are the interaction parameters of $i-j$ and $j-i$, respectively. k is the Boltzmann constant, and T is the temperature.

3. Pair potential energy polynomials of the binary liquid

In an extremely diluted pure gas, the correlation between the intermolecular potential energy and RDF can be expressed as follows [14]:

$$\lim_{\rho_0 \rightarrow 0} g_{12}(r) = \exp \left(-\frac{\epsilon_{12}}{kT} \right) \quad (11)$$

However, in practical scenarios, the RDF and intermolecular potential energy strongly depend on the number density of the system. The relation between the RDF and pair potential energy can be expanded using a polynomial expression in terms of the number density ρ_0 :

$$g_{12}(r, \rho_0, T) = e^{-\epsilon/kT} \left[1 + \rho_0 g_1(R, T) + \rho_0^2 g_2(R, T) + \dots \right] \quad (12)$$

In this case, we consider a pure gas system comprising three molecules labeled 1, 2, and 3 (Figure 1). These molecules afford six molecular distributions: 1-1, 1-2, 1-3, 2-2, 2-3, and 3-3. Among these distributions, the RDF of 1-2 represents the spatial distribution of molecule 1 around molecule 2. However, $g_{12}(r, \rho_0, T)$ is influenced by molecule 3 and is centered around this molecule, thereby affecting molecules 1 and 2 in $g_{12}(r, \rho_0, T)$. Consequently, based these observations, a connection can be established between the RDF and pair potential energy.

$$g_{12}(r, \rho_0, T) = e^{-\epsilon_{12}/kT} \exp \left\{ \rho_0 \int_V [e^{-\epsilon_{13}/kT} - 1][e^{-\epsilon_{23}/kT} - 1] dr_3 \right\} \\ = e^{-\epsilon_{12}/kT} \left\{ 1 + \rho_0 \int_V [e^{-\epsilon_{13}/kT} - 1][e^{-\epsilon_{23}/kT} - 1] dr_3 \right\} \quad (13)$$

Consequently, the expansion based on ρ_0 is $1 + \rho_0 \int_V [e^{-\epsilon_{13}/kT} - 1][e^{-\epsilon_{23}/kT} - 1] dr_3$. Equation (13) is compared with Equation (12).

$$g_1(r_{12}, T) = \int_V [e^{-\epsilon_{13}/kT} - 1][e^{-\epsilon_{23}/kT} - 1] dr_3 = \int_V [e^{-\epsilon_{13}/kT} e^{-\epsilon_{23}/kT} - e^{-\epsilon_{23}/kT} - e^{-\epsilon_{13}/kT} + 1] dr_3 \\ = \int_V e^{-\epsilon_{13}/kT} e^{-\epsilon_{23}/kT} dr_3 - \int_V e^{-\epsilon_{23}/kT} dr_3 - \int_V e^{-\epsilon_{13}/kT} dr_3 + \int_V dr_3 \quad (14)$$

This knowledge is applied to binary liquid alloys based on the understanding of molecular interactions in pure gases. The molecular distribution in the binary liquid system is characterized by three scenarios: $i-i$, $i-j$, and $j-j$. The RDF $i-j$ describes the distribution of molecule i around molecule j in a binary system (Figure 1). However, the remaining molecule i influences the i molecule in the RDF $i-j$, while the remaining molecule j affects the j molecule in the RDF $i-j$. Unlike pure gas centered on the remaining molecules 3 affecting the RDF 1-2. In a binary system, the spatial positioning of the remaining molecules i and j influences the RDF $i-j$ for molecules i and j . That is, the i molecule in the RDF affecting $i-j$ is centered on the other i molecules, while the j molecule in the RDF affecting $i-j$ is centered on the other j molecules.

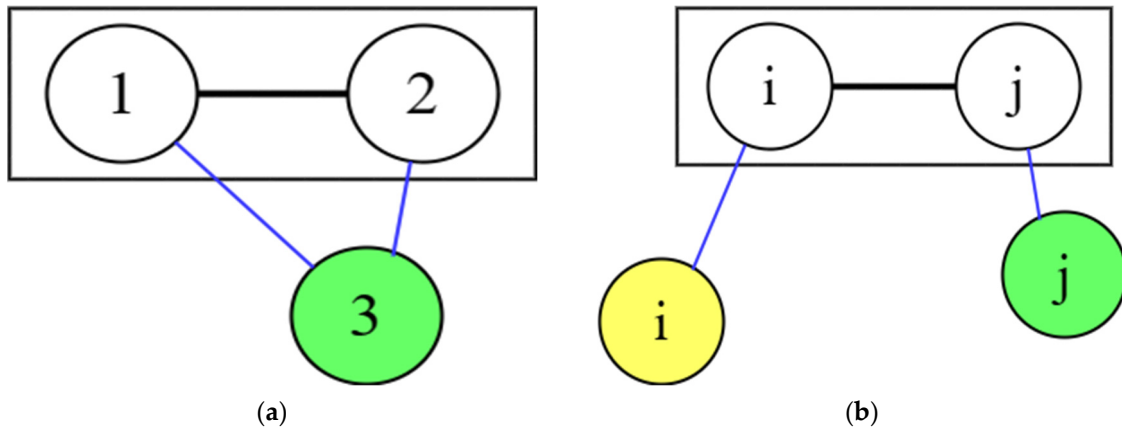


Figure 1. (a) is the molecular distribution diagram of pure substance, (b) is the molecular distribution diagram of the binary system.

If the RDF in a binary liquid system can be expanded as a polynomial based on number density, then Equation (14) takes the following form:

$$g_1(r_{ij}, T) = \int_V e^{-\epsilon_{ii}/kT} dr \times \int_V e^{-\epsilon_{jj}/kT} dr - \int_V e^{-\epsilon_{ii}/kT} dr - \int_V e^{-\epsilon_{jj}/kT} dr + \left(\int_V dr_{ii} + \int_V dr_{jj} \right) \quad (15)$$

Suppose that the subradial distribution function $g_i(r_{ij}, T)$ of the principal RDF $g_{ij}(r, \rho_0, T)$ conforms to $\rho_0 \rightarrow 0$, i.e., $i-j$ is the primary RDF, then $i-i$ and $j-j$ conform to $\rho_0 \rightarrow 0$ and the subradial distribution function is:

$$g_{ii}(r) = \exp \left(-\frac{\epsilon_{ii}}{kT} \right) \quad g_{jj}(r) = \exp \left(-\frac{\epsilon_{jj}}{kT} \right) \quad (16)$$

Substituting Equation (16) into Equation (15), we obtain:

$$g_1(r_{ij}, T) = \int_V g_{ii}(r) dr \times \int_V g_{jj}(r) dr - \int_V g_{ii}(r) dr - \int_V g_{jj}(r) dr + \left(\int_V dr_{ii} + \int_V dr_{jj} \right) \quad (17)$$

Then substituting Equation (17) into Equation (13), we obtain:

$$\begin{aligned}
g_{ij}(r, \rho_0, T) &= e^{-\varepsilon_{ij}/kT} \exp \left\{ \rho_0 \left[\int_V g_{ii}(r) dr \times \int_V g_{jj}(r) dr - \int_V g_{ii}(r) dr \right. \right. \\
&\quad \left. \left. - \int_V g_{jj}(r) dr + \left(\int_V dr_{ii} + \int_V dr_{jj} \right) \right] \right\} \\
&= e^{-\varepsilon_{ij}/kT} \left\{ 1 + \rho_0 \left[\int_V g_{ii}(r) dr \times \int_V g_{jj}(r) dr - \int_V g_{ii}(r) dr \right. \right. \\
&\quad \left. \left. - \int_V g_{jj}(r) dr + \left(\int_V dr_{ii} + \int_V dr_{jj} \right) \right] \right\}
\end{aligned} \tag{18}$$

The relation between the RDF and potential energy can be obtained using Equation (18):

$$-\frac{\varepsilon_{ij}}{kT} = \ln \frac{g_{ij}(r, \rho_0, T)}{\left\{ 1 + \rho_0 \left[\int_V g_{ii}(r) dr \times \int_V g_{jj}(r) dr - \int_V g_{ii}(r) dr \right. \right.} \tag{19}$$

Pair potential energy between molecules can be accurately calculated using the RDF. This function represents the ratio of the probability of finding another molecule at a distance r to the random distribution [15]. In the double distribution function, for a system with N molecules and volume V , the probability of a molecule appearing in the element dr_i is $(N/V)dr_i$, the probability of a molecule appearing at the distance dr_j is $(N/V)dr_j$, and the probability of molecular pairs appearing at a distance r is $(N/V)^2 dr_i dr_j$. The double distribution function is given as follows:

$$p^{(2)}(r)dr_i dr_j = \left(\frac{N}{V}\right)^2 dr_i dr_j \tag{20}$$

In the system, the average potential energy ε between each molecule is:

$$\varepsilon = \iint_V \varepsilon_{ij}(r) p^{(2)}(r) dr_i dr_j \tag{21}$$

However, in the RDF of binary systems, the probability of having molecule i in dr_i at r_i and molecule j in dr_j at r_j is $p^{(2)}(r)dr_i dr_j$. The potential energy is ε , and the average value of ε is the sum of all possible times of the probabilities:

$$\begin{aligned}
\overline{\varepsilon_{ij}} &= \frac{1}{V^2} \iint_V \varepsilon_{ij}(r) g_{ij}(r) dr_i dr_j = \frac{1}{V^2} \int dr_i \int \varepsilon_{ij}(r) g_{ij}(r) dr_j = \frac{1}{V} \int \varepsilon_{ij}(r) g_{ij}(r) 4\pi r^2 dr \\
&= \frac{4\pi \int \varepsilon_{ij}(r) g_{ij}(r) r^2 dr}{4\pi \int r^2 dr} = \frac{\int \varepsilon_{ij}(r) g_{ij}(r) r^2 dr}{\int r^2 dr}
\end{aligned} \tag{22}$$

Substituting Equation (19) into Equation (22) yields the potential energy between molecules:

$$-\frac{\overline{\varepsilon_{ij}}}{kT} = \frac{\int g_{ij}(r) r^2 \left\{ \ln \frac{g_{ij}(r)}{1 + \rho_0 \left[\int_V g_{ii}(r) dr \times \int_V g_{jj}(r) dr - \int_V g_{ii}(r) dr \right. \right.} \right\} dr}{\int r^2 dr} \tag{23}$$

The peak value of the RDF signifies the disparity between the local and bulk molar fractions. As the mole fraction increases, the contributions of the second and third RDF peaks diminish while the contribution of the first peak amplifies. The pair potential energy is then calculated using Equation (23) and the area of the first peak of the skewed RDF. The biased RDF used in this study is defined by three key coordinates: r_0 (which represents the starting point of $g(r)$ before reaching zero), r_m (the transverse coordinate of the first peak of $g(r)$), and r_1 (the transverse coordinate of the first valley of $g(r)$). The asymmetric method of calculating the RDF involves integrating the area between r_0 and r_1 , while the symmetric method involves integrating the area between r_0 and r_m (Figure 2). The

trapezoidal method [16] is used to compute these areas (Equation (24)). Table 1 lists the references for the partial RDFs of 36 binary liquid alloys.

$$\int_{r_1}^{r_0} g(r) dr \approx \frac{b-a}{2N} \sum_{n=1}^N [g(r_n) + g(r_{n+1})] = \frac{b-a}{2N} [g(r) + 2g(r_2) + \dots + 2g(r_N) + g(r_{N+1})] \quad (24)$$

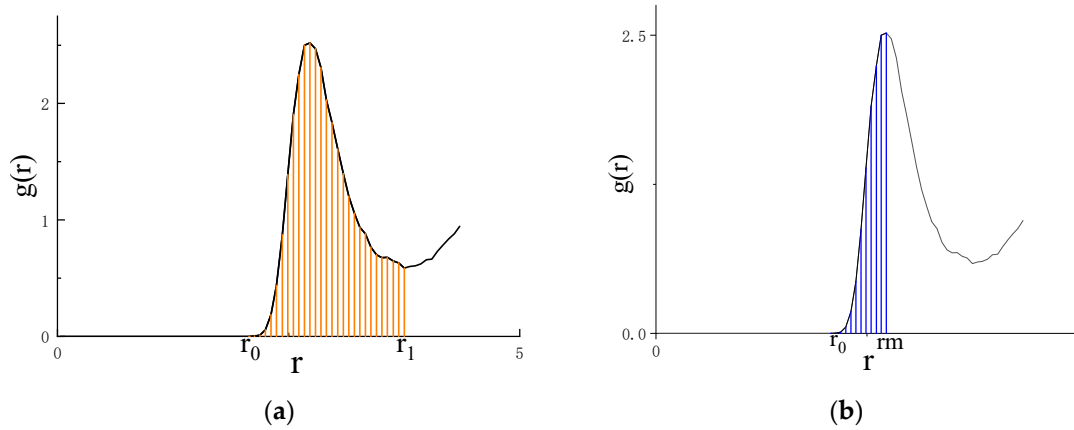


Figure 2. an illustration of the non-symmetric method of integration of radial distribution functions, b graphical representation of the non-symmetric method of integration of a radial distribution function.

Table 1. Partial radial distribution function of binary liquid alloys References.

System	Co-Ni [17]	Al-Zn [18]	Cu-Ni [19]	Al-Ni [20]	Cu-Fe [21]	Ge-Sn [22]	Ag-Cu [20]	Pb-Sb [23]	Al-Si [24]	Al-Co [25]
System	Li-Mg [26]	Sb-Sn [27]	Cu-Zr [28]	K-Na [29]	Pb-Sn [30]	Al-Mg [31]	Cs-K [32]	Li-Na [33]	Au-Cu [34]	Al-Li [35]
System	Nb-Zr [36]	Ni-Pd [37]	Cu-Mg [38]	Al-Ca [39]	Ni-Zr [40]	Al-Sn [41]	Al-Cu [42]	Nb-Ni [43]	Cu-Sn [44]	Au-Si [45]
System	Li-Sn [46]	Fe-Si [47]	Ag-In [48]	Ge-Te [49]	Al-Au [50]	Cu-Sb [51]				

The RSM has a tunable parameter Ω_{ij} . The average coordination number $\bar{Z}$ [52] is obtained using the pure coordination number of the two components. Additionally, the temperature T documented in literature and the calculated parameter Ω_{ij} can be referred to calculate the parameter Ω_{ij}' at the desired temperature T' .

$$\bar{Z} = \frac{1}{2}(Z_i + Z_j) \quad (25)$$

$$\Omega_{ij} = kT \left\{ \bar{Z} \left[\bar{\epsilon}_{ij} - \frac{1}{2}(\bar{\epsilon}_{ii} + \bar{\epsilon}_{jj}) \right] \right\} \quad (26)$$

$$T \ln \Omega_{ij} = T' \ln \Omega_{ij}' \quad (27)$$

The parameters A_{ij} and A_{ji} of Wilson equation are given. Additionally, the values of parameters A_{ij}' and A_{ji}' at the desired temperature T' can be obtained using the temperature T from the literature that was employed to calculate the corresponding parameters A_{ij} and A_{ji} .

$$A_{ij} = \frac{V_i}{V_j} \exp \left(-\frac{\bar{\epsilon}_{ij} - \bar{\epsilon}_{jj}}{RT} \right) \quad A_{ji} = \frac{V_j}{V_i} \exp \left(-\frac{\bar{\epsilon}_{ji} - \bar{\epsilon}_{ii}}{RT} \right) \quad (28)$$

$$T \ln A_{ij} = T' \ln A_{ij}' \quad T \ln A_{ji} = T' \ln A_{ji}' \quad (29)$$

The NRTL has two parameters τ_{ij} and τ_{ji} . These parameters obtained using the temperature T mentioned in the literature are employed to calculate the parameters τ_{ij}' and τ_{ji}' , respectively, at the required temperature T' .

$$\tau_{ij} = -\frac{\overline{\varepsilon_{ij}} - \overline{\varepsilon_{jj}}}{kT} \quad \tau_{ji} = -\frac{\overline{\varepsilon_{ji}} - \overline{\varepsilon_{ii}}}{kT} \quad (30)$$

$$T \ln \tau_{ij} = T' \ln \tau_{ij}' \quad T \ln \tau_{ji} = T' \ln \tau_{ji}' \quad (31)$$

The MIVM involves parameters B_{ij} and B_{ji} , representing the interaction parameters for i - j and j - i interactions, respectively. Using B_{ij} and B_{ji} values obtained at temperature T , the corresponding parameters B_{ij}' and B_{ji}' can be calculated at the desired temperature T' .

$$B_{ij} = \exp\left(-\frac{\overline{\varepsilon_{ij}} - \overline{\varepsilon_{jj}}}{kT}\right) \quad B_{ji} = \exp\left(-\frac{\overline{\varepsilon_{ji}} - \overline{\varepsilon_{ii}}}{kT}\right) \quad (32)$$

$$T \ln B_{ij} = T' \ln B_{ij}' \quad T \ln B_{ji} = T' \ln B_{ji}' \quad (33)$$

4. Result analysis

4.1. Symmetry

Figure 3 shows the molar fraction $x_i = x_j = 0.5$ of the two components as the symmetry axis of their activity curve. The symmetry degree of the activity curve can be defined as the average absolute value of the activity difference between the two components at the same concentration. In this context, S represents the measure of symmetry.

$$S_{ij} = \frac{\sum_{l=1}^m |(a_i - a_j)_{x_i=x_j}|_l}{m} \quad (34)$$

The symmetry increases as the S value decreases. At $S=0$, the system exhibits complete symmetry, where a_i and a_j denote the experimental activity of components i and j , respectively, and m represents the number of experimental activities. This definition also applies to similar geometric figures. Table 3 presents the symmetry degrees of the activity curves for the 36 systems based on the aforementioned definitions.

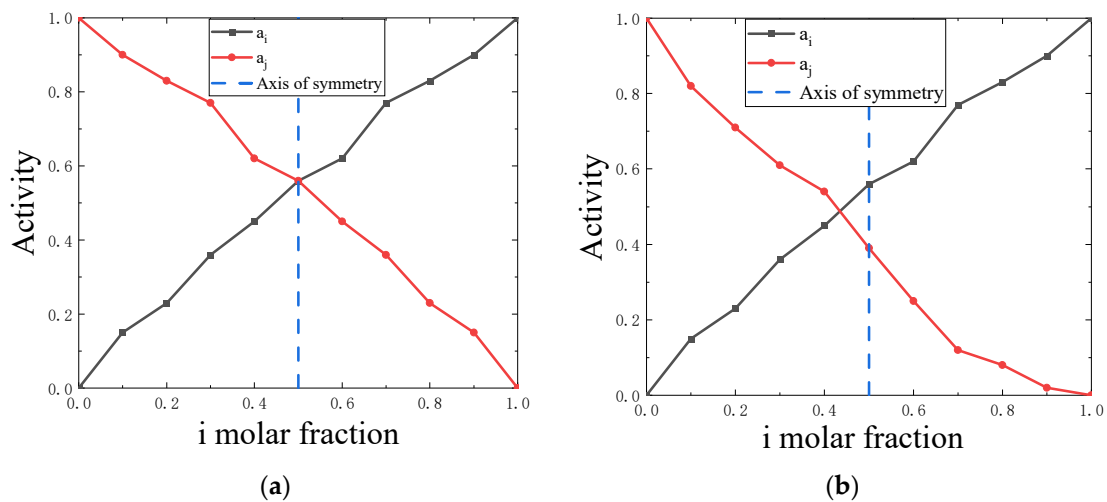


Figure 3. (a) means that the activity curve is entirely symmetric, (b) means that the activity curve is asymmetric.

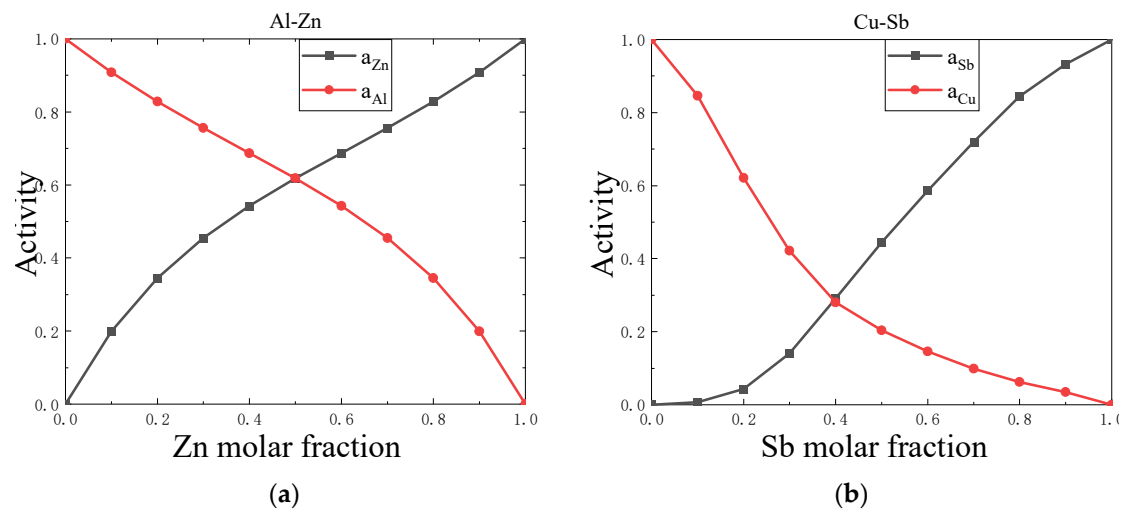


Figure 4. (a) is an entirely symmetric system, (b) is the system with the worst symmetry in this paper.

Table 3. Symmetry of the 36 systems from highest to lowest.

System	Co-Ni	Al-Zn	Cu-Ni	Al-Ni	Cu-Fe	Ge-Sn	Ag-Cu	Pb-Sb	Al-Si	Al-Co
S_{ij}	0	0	0.0028	0.0034	0.0048	0.007	0.0088	0.0096	0.0102	0.0114
System	Li-Mg	Sb-Sn	Cu-Zr	K-Na	Pb-Sn	Al-Mg	Cs-K	Li-Na	Au-Cu	Al-Li
S_{ij}	0.0114	0.0115	0.0119	0.0136	0.0158	0.0177	0.0228	0.0336	0.0364	0.0452
System	Nb-Zr	Ni-Pd	Cu-Mg	Al-Ca	Ni-Zr	Al-Sn	Al-Cu	Nb-Ni	Cu-Sn	Au-Si
S_{ij}	0.0473	0.0494	0.0597	0.0724	0.0807	0.0823	0.1116	0.1334	0.1342	0.139
System	Li-Sn	Fe-Si	Ag-In	Ge-Te	Al-Au	Cu-Sb				
S_{ij}	0.14	0.1454	0.1483	0.1548	0.160	0.208				

4.2. Asymmetric method for calculating the RDF

The asymmetric method uses the area between r_0 and r_1 presented in Figure 2 and Equation (23) to determine the parameters for each model. Tables 4 and 5 and Figure 5 demonstrate that among the first 12 systems, the RSM performs better than other models for 7 systems. The average standard deviation (SD) is 0.033, and the average absolute relative deviation (ARD) is 8.9%. In case of the 12 systems with moderate symmetry, the RSM outperforms the other three models in 8 systems, resulting in a mean SD of 0.054 and a mean ARD of 13.7%. Notably, the MIVM also performs well, with a mean SD of 0.084 and an average ARD of 25.5%. For the 12 systems with low symmetry, the RSM outperforms the other three models in 6 systems, yielding an average SD of 0.115 and an average ARD of 36%. Additionally, the RSM outperforms the other three models in 5 systems when the systems have even lower symmetry, with an average SD of 0.103 and an average ARD of 41.5%. Considering the average performance across all 36 binary liquid alloy systems, the Wilson and NRTL models exhibit the poorest performance, displaying larger SD and ARD values than the other models. As shown in Figure 5, the SD and ARD values generally increase with decreasing symmetry, albeit not significantly. Further analysis of high, medium, and low-symmetry systems reveals a strong correlation between the RSM and symmetry.

Table 4. Model parameters of the non-symmetric method.

System	MIVM		RSM	Wilson		NRTL	
	$B_{ij}^{'}$	$B_{ji}^{'}$	$\Omega_{ij}^{'} = \Omega_{ji}^{'}$	$A_{ij}^{'}$	$A_{ji}^{'}$	$\tau_{ij}^{'}$	$\tau_{ji}^{'}$
Co-Ni	0.964	0.977	0.343	0.964	0.977	-0.036	-0.023
Al-Zn	1.246	0.743	0.423	1.166	0.795	0.220	-0.297
Cu-Ni	1.086	0.863	0.374	0.999	0.938	0.082	-0.147
Al-Ni	1.493	1.649	-5.203	0.991	2.485	0.401	0.500
Cu-Fe	0.943	0.805	1.512	0.943	0.805	-0.059	-0.217
Ge-Sn	0.740	1.273	0.266	1.214	0.776	-0.302	0.241
Ag-Cu	0.675	1.194	1.225	0.471	1.709	-0.394	0.177
Pb-Sb	1.558	0.517	1.046	1.457	0.553	0.443	-0.660
Al-Si	1.405	1.077	-1.856	1.226	1.235	0.340	0.074
Al-Co	1.112	1.884	-4.213	0.802	2.612	0.106	0.633
Li-Mg	1.357	0.914	-1.095	1.469	0.844	0.305	-0.090
Sb-Sn	0.769	1.545	-0.847	0.735	1.618	-0.262	0.435
Cu-Zr	0.908	1.669	-2.277	1.782	0.851	-0.096	0.512
K-Na	0.700	1.176	1.018	0.366	2.252	-0.357	0.162
Pb-Sn	1.044	0.912	0.267	0.932	1.021	0.043	-0.092
Al-Mg	0.820	1.123	0.459	1.162	0.793	-0.198	0.116
Cs-K	1.204	0.635	1.310	0.801	0.955	0.185	-0.454
Li-Na	0.764	0.999	1.347	1.416	0.539	-0.270	-0.001
Au-Cu	1.163	1.444	-2.877	0.812	2.068	0.151	0.368
Al-Li	1.136	1.379	-2.356	1.485	1.055	0.128	0.321
Nb-Zr	0.814	1.255	-0.110	1.048	0.975	-0.206	0.227
Ni-Pd	1.168	1.087	-1.307	1.590	0.798	0.153	0.080
Cu-Mg	1.312	1.258	-2.781	2.575	0.641	0.272	0.230
Al-Ca	2.202	1.259	-5.761	5.826	0.476	0.789	0.230
Ni-Zr	1.522	1.730	-5.373	3.247	0.811	0.420	0.548
Al-Sn	0.624	1.440	0.598	1.024	0.877	-0.471	0.365
Al-Cu	1.568	1.530	-5.209	2.192	1.152	0.476	0.450
Nb-Ni	1.772	1.071	-3.558	1.070	1.774	0.572	0.069
Cu-Sn	1.987	0.849	-2.904	0.874	1.932	0.687	-0.163
Au-Si	1.224	1.684	-3.129	1.034	1.993	0.202	0.521
Li-Sn	3.396	2.186	-10.225	4.263	1.742	1.223	0.782
Fe-Si	5.678	1.776	-9.822	4.695	2.148	1.737	0.574
Ag-In	1.595	0.925	-2.227	2.476	0.596	0.467	-0.078
Ge-Te	0.409	1.891	1.285	0.912	0.848	-0.894	0.637
Al-Au	1.680	1.660	-5.740	2.287	1.219	0.519	0.507
Cu-Sb	1.804	0.881	-2.315	0.757	2.098	0.590	-0.127

Table 5. Deviation and relative error of each model in the non-symmetric method.

System	MIVM		RSM		Wilson		NRTL	
	SD	ARD/%	SD	ARD/%	SD	ARD/%	SD	ARD/%
Co-Ni	0.036	10.8	0.029	8.8	0.003	0.8	0.015	4.4
Al-Zn	0.108	22	0.058	12.1	0.100	20.5	0.116	23.7
Cu-Ni	0.085	16.5	0.085	16.5	0.120	23.1	0.134	25.7
Al-Ni	0.044	18.3	0.037	125	0.208	1472	0.398	4520
Cu-Fe	0.106	12.5	0.128	15.1	0.321	37.5	0.375	44
Ge-Sn	0.071	19.4	0.011	3.1	0.016	4.1	0.027	7.5
Ag-Cu	0.062	10.8	0.025	4.6	0.143	26.1	0.167	30.5
Pb-Sb	0.044	9.9	0.047	10.5	0.070	15.9	0.080	18.1
Al-Si	0.110	40.5	0.058	23.2	0.041	18.5	0.125	63.3
Al-Co	0.080	39.2	0.027	10.5	0.142	341	0.300	1085
Li-Mg	0.056	20.7	0.032	12.3	0.035	14.2	0.082	34.9
Sb-Sn	0.078	29.3	0.012	3.6	0.054	24.5	0.093	44.2
Cu-Zr	0.064	31.6	0.015	8.4	0.098	74.4	0.185	162
K-Na	0.081	15.3	0.012	2	0.144	27.8	0.145	28
Pb-Sn	0.016	3.2	0.009	1.7	0.063	14.3	0.087	19.6
Al-Mg	0.087	32.9	0.092	34.9	0.048	17	0.033	11.2
Cs-K	0.129	36	0.148	41.7	0.016	3.3	0.066	16.9
Li-Na	0.210	22.9	0.192	21.3	0.364	40.5	0.405	45.2
Au-Cu	0.076	34.5	0.038	12.1	0.105	101	0.219	255
Al-Li	0.048	17	0.037	12.2	0.118	115	0.209	236
Nb-Zr	0.089	21.1	0.066	15.1	0.058	13	0.056	12.4
Ni-Pd	0.044	15	0.039	14.1	0.090	53.7	0.140	91
Cu-Mg	0.054	30.2	0.038	12.4	0.104	103	0.226	286
Al-Ca	0.129	64.3	0.087	37.4	0.094	144	0.338	1081
Ni-Zr	0.076	80.2	0.085	266	0.225	1661	0.433	4415
Al-Sn	0.226	34.4	0.142	21.3	0.199	30.4	0.226	34.5
Al-Cu	0.076	43	0.075	30.1	0.158	516	0.343	2031
Nb-Ni	0.128	47.2	0.089	64	0.161	540	0.288	1478
Cu-Sn	0.131	51.2	0.103	33.3	0.135	48	0.524	544
Au-Si	0.116	44	0.090	45.6	0.147	279	0.290	847
Li-Sn	0.098	59.1	0.117	130	0.216	1347	0.596	7906
Fe-Si	0.259	82.9	0.137	58.3	0.088	186	0.516	5003
Ag-In	0.077	32.8	0.095	30.3	0.095	76	0.185	191
Ge-Te	0.099	27.3	0.333	496	0.195	239	0.150	148
Al-Au	0.149	55.9	0.139	42.7	0.168	405	0.333	1822
Cu-Sb	0.072	28	0.096	30.4	0.122	104	0.196	229
Ave	0.095	32.2	0.078	47.4	0.124	226	0.225	911

$$SD = \sqrt{\frac{\sum (a_{pre} - a_{exp})^2}{N}}; \quad ARD = \frac{1}{N} \sum \left| \frac{a_{pre} - a_{exp}}{a_{exp}} \right| \times 100\%$$
 . a_{pre} —calculated value of the activity; a_{exp}

[53]—experimental activity value.

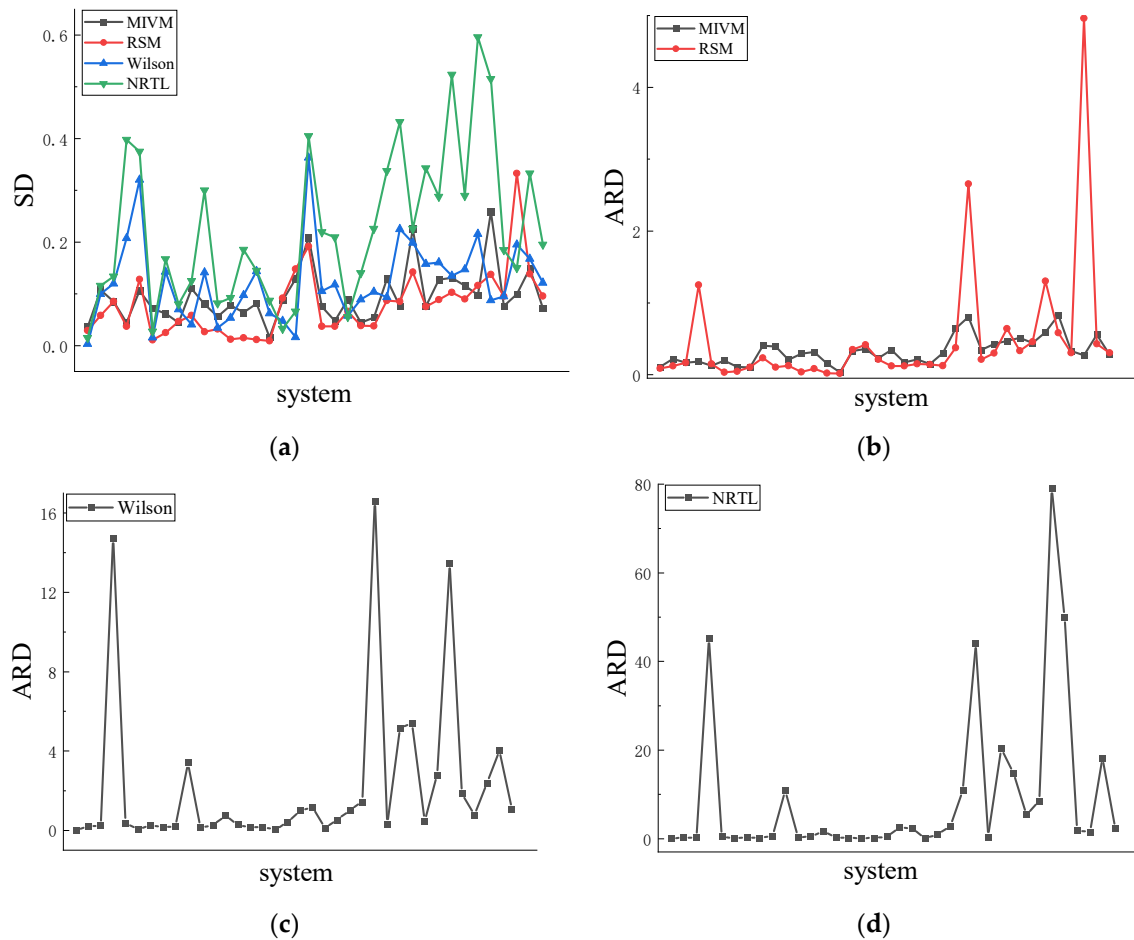


Figure 5. (a) is the SD of 36 systems, (b) is the ARD of MIVM and RSM models of 36 systems, (c) is the ARD of the Wilson equation of 36 systems, and (d) is the ARD of the NRTL equation of 36 systems.

4.3. Symmetric method for calculating the RDF

The methodology based on symmetry involves deriving parameters for each model using the region from r_0 to r_m (Figure 6) and Equation (23). Analysis of data presented in Tables 6 and 7 and Figure 6 reveals that among the 12 systems characterized by high symmetry, the MIVM outperforms the other three models with an average SD of 0.127 and an average ARD of 30.5%. Conversely, the RSM exhibits an average SD of 0.111 and an average ARD of 44.6%. In the 12 systems with medium symmetry, the RSM outperforms the other three models, yielding a mean SD of 0.088 and an ARD of 32.9%. By contrast, the MIVM exhibits a mean SD of 0.118 and an ARD of 36.7%. For the 12 systems with low symmetry, the RSM and MIVM surpass the other three models. The RSM exhibits an average SD of 0.118 and an average ARD of 73.4%, and the MIVM shows a mean SD of 0.159 and a mean ARD of 58.4%. Each model exhibits distinct performance characteristics depending on the system representation. The data comparison indicates an increasing trend in ARD values with decreasing symmetry.

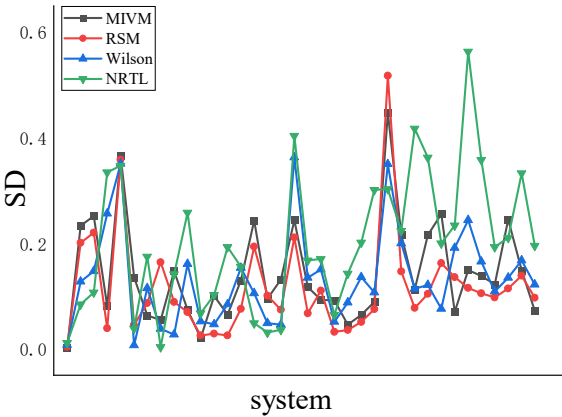
Table 6. Parameters of each model of the weighting method.

System	MIVM		RSM	Wilson		NRTL	
	B_{ij}	B_{ji}	$\Omega_{ij} = \Omega_{ji}$	A_{ij}	A_{ji}	τ_{ij}	τ_{ji}
Co-Ni	1.089	0.900	0.118	1.089	0.900	0.085	-0.106
Al-Zn	1.317	0.938	-1.162	1.232	1.003	0.275	-0.064
Cu-Ni	1.391	0.877	-1.138	1.280	0.953	0.330	-0.132
Al-Ni	1.155	2.099	-5.114	0.766	3.163	0.144	0.742
Cu-Fe	0.890	1.145	-0.103	0.890	1.145	-0.117	0.135
Ge-Sn	0.562	1.573	0.545	0.923	0.958	-0.576	0.453
Ag-Cu	1.309	0.582	1.538	0.914	0.833	0.269	-0.542
Pb-Sb	1.231	0.810	0.017	1.151	0.866	0.207	-0.211
Al-Si	1.534	1.140	-2.499	1.338	1.307	0.428	0.131
Al-Co	0.830	1.774	-2.218	0.551	2.673	-0.186	0.573
Li-Mg	1.087	0.988	-0.363	1.177	0.912	0.083	-0.012
Sb-Sn	0.825	1.576	-1.288	0.788	1.650	-0.192	0.455
Cu-Zr	1.206	1.206	1.206	1.206	1.206	1.206	1.206
K-Na	0.562	1.364	1.390	0.293	2.613	-0.577	0.311
Pb-Sn	1.601	0.830	-1.549	1.430	0.929	0.471	-0.186
Al-Mg	0.808	1.126	0.528	1.144	0.796	-0.213	0.119
Cs-K	1.642	0.660	-0.391	1.092	0.992	0.496	-0.416
Li-Na	0.728	1.069	1.245	1.350	0.577	-0.317	0.067
Au-Cu	2.423	0.515	-1.229	1.692	0.737	0.885	-0.664
Al-Li	0.813	1.374	-0.580	1.062	1.051	-0.208	0.318
Nb-Zr	0.671	1.414	0.279	0.864	1.098	-0.399	0.346
Ni-Pd	1.174	1.105	11.250	-1.445	1.599	0.811	0.159
Cu-Mg	0.882	1.538	-1.689	1.731	0.783	-0.126	0.430
Al-Ca	2.423	0.515	-1.229	1.692	0.737	0.885	-0.664
Ni-Zr	0.607	1.260	1.484	1.296	0.591	-0.499	0.231
Al-Sn	0.649	1.393	0.566	1.065	0.849	-0.433	0.332
Al-Cu	1.963	1.534	-6.647	1.472	2.180	0.714	0.453
Nb-Ni	3.602	1.064	-7.456	2.174	1.763	1.281	0.062
Cu-Sn	4.758	0.617	-5.972	2.091	1.403	1.560	-0.484
Au-Si	1.438	0.875	-0.992	1.214	1.036	0.363	-0.134
Li-Sn	2.077	2.672	-8.741	2.608	2.129	0.731	0.983
Fe-Si	1.534	1.843	-4.414	1.268	2.228	0.428	0.611
Ag-In	1.066	1.467	-2.560	1.654	0.946	0.064	0.384
Ge-Te	0.636	3.025	-3.272	1.419	1.356	-0.452	1.107
Al-Au	1.903	0.844	-2.370	0.799	2.011	0.643	-0.169
Cu-Sb	1.743	1.017	-3.207	1.743	1.017	0.556	0.017

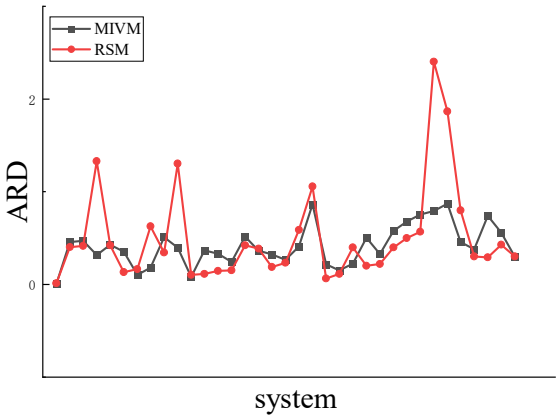
Table 7. Model deviations and relative errors of weighting methods.

System	MIVM		RSM		Wilson		NRTL	
	SD	ARD/%	SD	ARD/%	SD	ARD/%	SD	ARD/%
Co-Ni	0.002	0.4	0.004	1.1	0.007	2.1	0.011	3.3
Al-Zn	0.233	45.8	0.201	40	0.128	26	0.085	17.5
Cu-Ni	0.252	46.9	0.220	41.3	0.147	28.3	0.107	20.8
Al-Ni	0.081	31.7	0.039	133	0.257	2130	0.335	3370
Cu-Fe	0.365	42.8	0.359	42	0.351	41.2	0.347	40.7
Ge-Sn	0.135	35.4	0.045	13.2	0.007	1.6	0.039	10.8
Ag-Cu	0.063	10.2	0.087	16.3	0.115	21.2	0.175	31.8
Pb-Sb	0.054	17.9	0.164	62.6	0.038	13.3	0.004	0.9

Al-Si	0.147	50.8	0.089	34.2	0.027	12.1	0.142	72.6
Al-Co	0.074	39.6	0.070	130	0.161	411	0.258	852
Li-Mg	0.020	7.9	0.026	10.2	0.052	21.7	0.067	28.5
Sb-Sn	0.100	36.5	0.029	11.3	0.046	20.7	0.103	49.6
Cu-Zr	0.065	33	0.026	14.4	0.084	62.1	0.193	171
K-Na	0.130	24.3	0.076	15.2	0.154	29.6	0.156	29.9
Pb-Sn	0.244	51.4	0.194	42	0.105	23.7	0.049	11
Al-Mg	0.095	36.2	0.101	38.4	0.049	17.5	0.031	10.7
Cs-K	0.132	32.3	0.074	18.8	0.046	11.5	0.036	8.9
Li-Na	0.244	26.7	0.211	23.4	0.363	40.4	0.404	45.1
Au-Cu	0.117	40.7	0.067	58.8	0.135	137	0.168	181
Al-Li	0.093	86.2	0.110	106	0.151	156	0.171	182
Nb-Zr	0.092	21.6	0.032	6.3	0.052	11.5	0.065	14.7
Ni-Pd	0.046	15.2	0.036	11.3	0.088	52.4	0.143	93.2
Cu-Mg	0.065	22.3	0.051	40	0.136	144	0.202	245
Al-Ca	0.089	50.3	0.075	20	0.107	175	0.301	901
Ni-Zr	0.447	4520	0.518	5760	0.350	3200	0.303	2560
Al-Sn	0.216	32.8	0.147	21.9	0.200	30.6	0.224	34.3
Al-Cu	0.113	57.6	0.078	39.9	0.114	289	0.417	2930
Nb-Ni	0.216	67.7	0.104	49.9	0.121	302	0.363	2270
Cu-Sn	0.255	75.4	0.163	56.7	0.076	28	0.200	167
Au-Si	0.070	79	0.136	240	0.192	425	0.234	591
Li-Sn	0.150	86.9	0.116	187	0.244	1730	0.564	7420
Fe-Si	0.138	45.8	0.105	79.9	0.165	693	0.358	2900
Ag-In	0.122	37.9	0.097	30.1	0.109	90.8	0.193	204
Ge-Te	0.245	73.9	0.114	29.1	0.135	118	0.211	268
Al-Au	0.149	55.9	0.139	42.7	0.168	405	0.333	1820
Cu-Sb	0.072	29.9	0.097	30	0.122	105	0.196	228
Ave	0.143	165.9	0.117	208.3	0.133	305.6	0.200	771.8



(a)



(b)

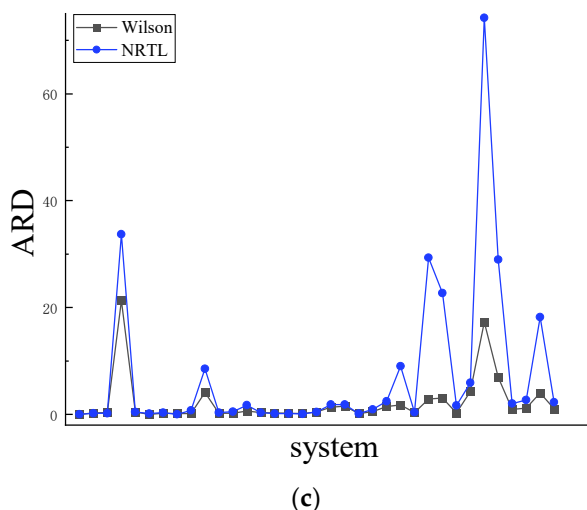


Figure 6. (a) is the SD of 36 systems, (b) is the ARD of MIVM and RSM models of 36 systems, (c) is the ARD of Wilson and NRTL equation of 36 systems.

5. Conclusion

This study uses polynomials to describe the partial RDF in pure gases and extends this approach to binary liquid systems. The primary aim of this study is to characterize the molecular distribution and unravel intermolecular interactions, which are essential for accurate thermodynamic calculations. The RDF exhibits irregularities when the symmetric method is used instead of the asymmetric one for RDF calculation. Notably, the estimation of binary liquid alloy activity favors using the asymmetric method, especially when considering the average results obtained from both methods for the 36 binary liquid alloy systems investigated in this study. We selected and compared four thermodynamic models based on their symmetry degree. Data analysis reveals that the RSM exhibits the highest dependency on the symmetry degree. Conversely, the MIVM demonstrates superior adaptability to symmetric and asymmetric systems.

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