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Waring and Riedel Functions for the Liquid−Vapor Coexistence Curve

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S *Supporting Information*

ABSTRACT: There exists a minimum in the Waring function, $\psi(T) = -\mathrm{d}(\ln p)/\mathrm{d}(1/T)$, and in the Riedel function, $\alpha(T) = \mathrm{d}(\ln p)/\mathrm{d}(\ln T)$, in the liquid−vapor coexistence curve for most fluids. By analyzing National Institute of Standards and Technology data for the molar enthalpy of vaporization and the compressibility variation at the liquid−vapor phase change of 105 fluids, we find that the temperatures of these minima are linearly correlated with the critical temperature, T_c. Using reduced coordinates, we also demonstrate that the minima are well-correlated with the acentric factor. These correlations are used for testing four well-known vapor pressure equations in the Pitzer corresponding states scheme.

■ INTRODUCTION

The vapor pressure curve of pure fluids provides a fascinating relation between saturation pressures and temperatures from the triple to the critical point. Its shape has been the object of thermodynamics research for about 175 years, since Clapeyron proposed his famous differential equation. Several features of this curve[1−7] are essential not only in the design of practical applications in engineering systems (refrigeration and heat pumping devices, Rankine cycles, and vapor pressure thermometers, etc.) but also in the analysis of environmental problems such as the behavior of new low global warming potential (GWP) fluids.[8]

A plethora of equations have been reported in the literature in order to correlate or to predict vapor pressure experimental data. Several criteria/conditions have been proposed to check thermodynamic consistency of these equations. Perhaps the two more known and used criteria are the Waring criterion and the Riedel condition. The Waring criterion[9] states that the saturation function $\psi(T) \equiv -\mathrm{d}(\ln p)/\mathrm{d}(1/T)$ presents a minimum at a temperature around $T \approx 0.85T_c$, T_c being the critical temperature. The Riedel condition, also known as the Plank−Riedel condition,[10,11] states that the slope of the saturation function $\alpha(T) \equiv \mathrm{d}(\ln p)/\mathrm{d}(\ln T)$ is equal to zero at the critical point. Strictly, this condition is at odds with renormalization-group theory which predicts that $\mathrm{d}^2p/\mathrm{d}T^2$ should diverge at the critical point.

In this work we present an analysis of the Waring and Riedel conditions by using liquid−vapor coexistence data for 105 pure fluids reported by the National Institute of Standards and Technology (NIST) database.[12] This analysis is based on the behavior for these fluids of the so-called Waring and Riedel functions, $\psi(T)$ and $\alpha(T)$, which are two alternative ways of rewriting the Clapeyron differential equation. We show that while the Clapeyron function, i.e., the slope of the natural logarithm of the vapor pressure curve, decreases monotonically with temperature, the Waring function presents a minimum at a given temperature, the Waring temperature, except for fluids with very low critical temperature, such as the quantum fluids. On the other hand, for most fluids, the Riedel function also presents a minimum at a temperature, the Riedel temperature, close to the critical point. The first goal of this paper is to show that both the Waring and Riedel temperatures are linearly correlated with the critical temperature. The second goal is to show that the reduced Waring and Riedel temperatures have a different dependence on the Pitzer acentric factor. We check these dependencies for four well-known vapor pressure equations in the Pitzer corresponding states scheme.

■ WARING AND RIEDEL FUNCTIONS

The Clapeyron equation for vaporization

$$\frac{\mathrm{d}p}{\mathrm{d}T} = \frac{\Delta_v \bar{H}}{T\Delta_v \bar{V}} \tag{1}$$

gives the slope of the vapor pressure curve, $p = p(T)$, in terms of $\Delta_v\bar{H}$, the vaporization molar enthalpy, and $\Delta_v\bar{V}$, the difference between the molar volumes of saturated vapor and saturated liquid. Equation 1 is an exact thermodynamic relation, and it has been rewritten in different, more convenient forms that involve the natural logarithm of the vapor pressure as a function of the temperature. The most usual of these forms is given by

$$f(T) \equiv \frac{\mathrm{d}\ln p}{\mathrm{d}T} = \frac{\Delta_v \bar{H}}{RT^2\Delta_v Z} \tag{2}$$

where Z is the compressibility factor defined as $P\bar{V}/RT$, R being the gas constant. We refer to the saturation function $f(T)$ as the Clapeyron function. Integration of eq 2 requires information about the temperature dependence of $\Delta_v\bar{H}$ and $\Delta_v Z$ or their

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ratio. For all fluids, $f(T)$ decreases monotonically with temperature from the triple to the critical point, where it reaches a finite value $f(T_c)$.

A second form of rewriting eq 1 was proposed by Waring[9]

$$\psi(T) \equiv -\frac{\mathrm{d}\ln p}{\mathrm{d}(1/T)} = \frac{\Delta_v \bar{H}}{R\Delta_v Z} = T^2 f(T) \tag{3}$$

in order to provide a qualitative test for the suitability of various vapor pressure equations. We refer to the saturation function $\psi(T)$ as the Waring function. In contrast to what happens with the Clapeyron function, Waring showed that $\psi(T)$ of many polar and nonpolar fluids presents a minimum at a characteristic temperature T_W in the range of 0.80–0.85 T_c.[9] Ethanol and propanol are recognized exceptions.[13] We note that $\psi(T)$ has dimensions of temperature.

A third alternative form to rewrite eq 1 was proposed by Riedel[11]

$$\alpha(T) \equiv \frac{\mathrm{d}\ln p}{\mathrm{d}\ln T} = \frac{\Delta_v \bar{H}}{RT\Delta_v Z} = Tf(T) \tag{4}$$

We refer to the saturation function $\alpha(T)$ as the Riedel function. From the analysis of experimental vapor pressure data for several fluids, Riedel showed that $\alpha(T)$ decreases as the temperature increases and presents a minimum at the critical point; i.e., it satisfies the condition

$$\left(\frac{\mathrm{d}\alpha}{\mathrm{d}T}\right)_{T=T_c} = 0 \tag{5}$$

Condition 5 implies that the second derivative of the vapor pressure with respect to temperature

$$\left(\frac{\mathrm{d}^2 p}{\mathrm{d}T^2}\right)_{T=T_c} = \left[\left(\frac{\mathrm{d}\ln p}{\mathrm{d}T}\right)_{T=T_c} - \frac{1}{T_c}\right]\left(\frac{\mathrm{d}p}{\mathrm{d}T}\right)_{T=T_c} \tag{6}$$

remains finite at the critical point, contrary to the prescription of the renormalization group theory that $\mathrm{d}^2p/\mathrm{d}T^2$ diverges at this point. However, condition 5 suggests that $\alpha(T)$ could present a minimum at a characteristic temperature T_R very close to the critical point. We note that $\alpha(T)$ is dimensionless.

Parts a–c of Figure 1 show the variation of $f(T)$, $\psi(T)$, and $\alpha(T)$, respectively, with T for propane from the $\Delta_v \bar{H}$ and $\Delta_v Z$ data obtained from RefProp 9.0.[12] These plots show that $f(T)$ decreases monotonically with temperature, $\psi(T)$ presents a minimum at T_W = 302.88 K, and $\alpha(T)$ presents a minimum at T_R = 361.29 K.

We have analyzed the $\psi(T)$ and $\alpha(T)$ functions from the values for $\Delta_v \bar{H}$ and $\Delta_v Z$ of the 105 substances included in RefProp 9.0[12] and listed in Table S1 of the Supporting Information. $\psi(T)$ presents a minimum at a different temperature T_W for all considered fluids except the quantum fluids (helium, hydrogen, orthohydrogen, parahydrogen, and deuterium). We refer to T_W as the Waring temperature. We find that T_W, where $\psi_{\min} = \psi(T_W)$ occurs, bears the following linear relationship with T_c,

$$T_W/\mathrm{K} = -25.9308 + 0.915659T_c \tag{7}$$

with a coefficient of determination R^2 = 0.9891. We note that the above-mentioned quantum fluids for which there is not a minimum in the Waring function have very low critical temperatures that would lead to values below the triple temperature for T_W. This fact is consistent with the correlation presented in eq 7 which is certainly not valid for low values of the critical temperature. Figure 2a shows a plot of T_W vs T_c. The symbols correspond to data obtained from RefProp 9.0[12] and reported in Table S1 of the Supporting Information, and the solid line corresponds to the correlation given by eq 7. The inset of Figure 2a shows the percent relative deviation (Δ_r) of T_W between tabulated values and values obtained using correlation 7. The average absolute relative deviation (AARD) for all fluids is 3.5%. The maximum absolute relative deviation (MARD) is obtained for neon with a value of 45.0%. This large deviation could be due to both the low critical temperature of neon and the influence of quantum effects. We note that from the NIST data, the Waring function for ethanol presents a minimum at T_W = 506.150 K, very close to T_c = 513.9 K, but far from the value T_W = 444.795 K predicted by eq 7. These deviations could be ascribed to the equation of state used in RefProp 9.0[12] for ethanol.[14]

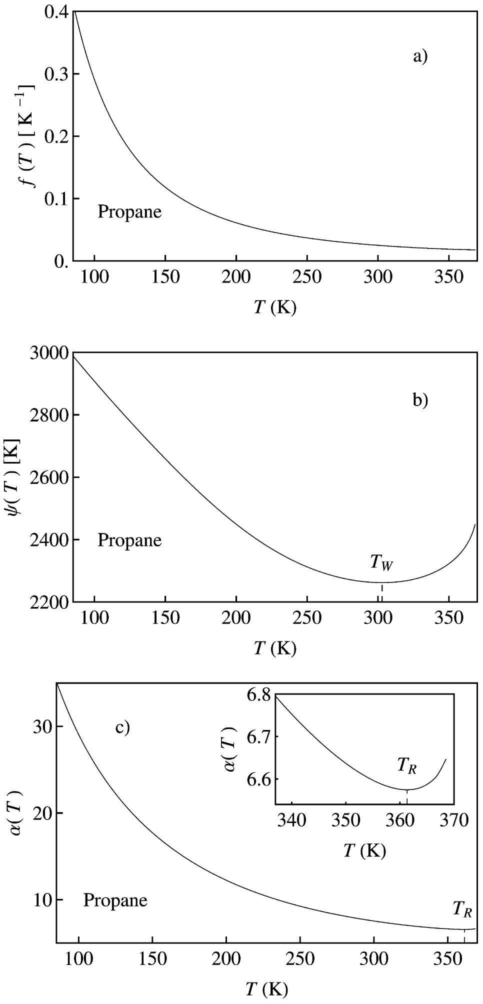

Figure 1. (a) Plot of the Clapeyron function, $f(T)$, vs the temperature, T, for propane. (b) Plot of the Waring function, $\psi(T)$, for propane, indicating the position of the minimum. (c) Plot of the Riedel function, $\alpha(T)$, for propane. The inset is a zoom of the area where the function attains its minimum value.

$\alpha(T)$ presents a minimum at a different temperature T_R for all considered fluids except seven of them (cyclopentane, deuterium, DMC, ethanol, heptane, methanol, and R236ea) for which NIST data do not give a minimum for $\alpha(T)$. The difficulties arising for these seven fluids can be again ascribed to

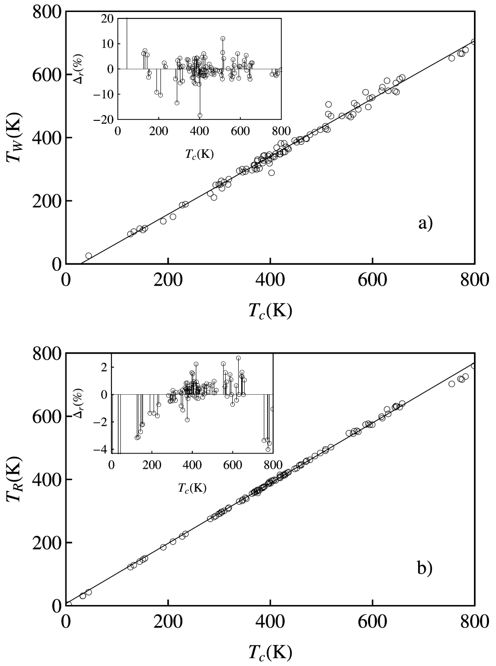

Figure 2. (a) T_W vs T_c. The line represents eq 7. The inset shows the percent relative deviations of T_W. (b) T_R vs T_c. The line represents eq 8. The inset shows the percent relative deviations of T_R. The symbols are the values obtained from RefProp 9.0[12] (see Table S1).

the equations of state used in RefProp 9.0. New equations of state are currently being refitted for which a minimum should occur in the Riedel function in most cases.[14] We refer to T_R as the Riedel temperature. We find that T_R, where $\alpha_{min} = \alpha(T_R)$ occurs, bears the following linear correlation with T_c,

$$T_R/\mathrm{K} = 6.97318 + 0.953554T_c \qquad (8)$$

with $R^2 = 0.9983$. Figure 2b shows a plot of T_R vs T_c. The symbols correspond to data obtained from RefProp 9.0[12] and reported in Table S1, and the solid line corresponds to the correlation given by eq 8. The inset of Figure 2b shows the percent relative deviation of T_R between tabulated values and values obtained using correlation 8. The AARD for all fluids is 3.0%. The MARD is obtained for helium with a value of 139.9%. Again, the large deviation in this case can be due to both the low critical temperature of helium and the influence of quantum effects.

The correlations given by eqs 7 and 8 can be used for predicting purposes for fluids not included in RefProp 9.0. As a check of the predicting performance of these correlations, we have considered perfluorobenzene for which recent experimental results are available.[15] In addition, we have also considered methanol and heptane (two of the fluids for which RefProp 9.0 data do not give a minimum for $\alpha(T)$) but, instead of RefProp 9.0, using other data sources (the Craven and Reuck vapor pressure equation[16] for methanol and the Lemmon and Goodwin equation[17] for heptane). The results of our predictions using eqs 7 and 8 compared with those obtained from other data sources are presented in Table 1, with good agreement.

■ ANALYSIS IN THE REDUCED COORDINATE SCHEME

Waring[9] established that for most fluids $\Delta_v\bar{H}/\Delta_v Z$ presents a minimum at a reduced temperature of about 0.80 or 0.85. To check the Waring finding we have analyzed the values of the reduced Waring temperature, $T_{rW} = T_W/T_c$, and the minimum values of the reduced Waring function, $\psi_{r,min} = \psi_{min}/T_c$, obtained from RefProp 9.0[12] for the 105 fluids considered in the present work and reported in Table S2 of the Supporting Information. Two main conclusions can be drawn from this analysis: (1) the values of T_{rW} vary between 0.6055 for neon and 0.9849 for ethanol, and most of them (76 fluids) are in the range of 0.8−0.9; (2) both T_{rW} and $\psi_{r,min}$ present a clear correlation with the acentric factor, ω, defined by[18]

$$\omega = -1.0 - \log p_r \quad \text{at } T_r = 0.7 \qquad (9)$$

Parts a and b of Figure 3 show plots of T_{rW} and $\psi_{r,min}$ vs ω, respectively. Symbols correspond to tabulated data reported in Table S2. Figure 3a shows that, for low ω, T_{rW} increases as ω increases, reaching a maximum value at around $\omega \approx 0.7$, and then it decreases slightly as ω increases. Figure 3b shows that $\psi_{r,min}$ increases with ω in a practically linear way. Three fluids are shown in Figure 3a that clearly deviate from the correlation: ethanol, propyne, and R41. While the deviations of the two first fluids seem to be due to the equations of state used in RefProp 9.0, it should not be the case for the later.[14]

We have also analyzed the values of the reduced Riedel temperature, $T_{rR} = T_R/T_c$, and the minimum values of the Riedel function, α_{min}, obtained for the 105 fluids considered in the present work and reported in Table S2. Two main conclusions can be drawn from this analysis: (1) the values of T_{rR} vary between 0.9256 for methyl stearate and 0.9925 for R114, and most of them (84 fluids) are in the range of 0.95−0.98 (like in previous cases, the deviations of methyl stearate and R114 from the overall behavior should be related to the equations of state used in RefProp 9.0 for these fluids);[14] (2) both T_{rR} and α_{min} present a clear correlation with ω. Parts a and b of Figure 4 show plots of T_{rR} and α_{min} vs ω, respectively. Symbols correspond to tabulated data reported in Table S2. Figure 4a shows that for low ω values T_{rW} increases as ω increases, reaching a maximum value at around $\omega \approx 0.17$, and then it decreases as ω increases. Figure 4b shows that α_{min} increases with ω in a practically linear way.

Table 1. Comparison of the Predictions of Equations 7 and 8 for the Waring Temperature, T_W (K), and the Riedel Temperature, T_R (K), with Results Calculated from Data Sources Other Than RefProp 9.0 for Perfluorobenzene,[15] Methanol,[16] and Heptane[17]

		T_W (K)			T_R (K)		
fluid	T_c (K)	predicted	calculated	deviation (%)	predicted	calculated	deviation (%)
perfluorobenzene	516.66	447.15	453.65	1.43	499.64	504.00	0.87
methanol	512.6	443.44	461.33	3.9	495.77	503.59	1.6
heptane	540.13	468.64	471.14	0.53	522.02	526.41	0.83

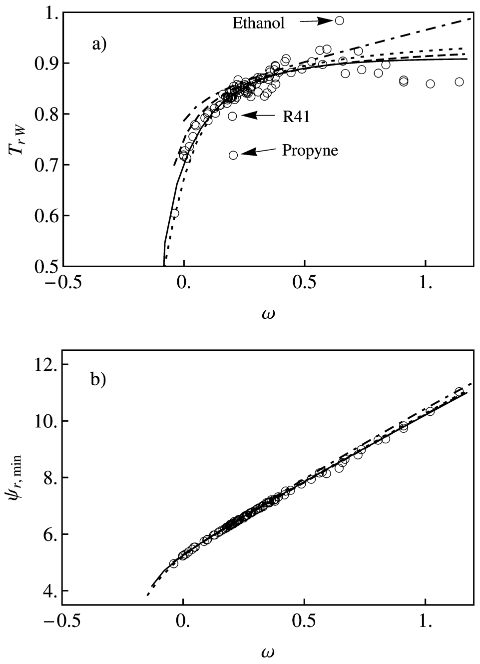

Figure 3. (a) Relationship between $T_{rW} = T_W/T_c$ and ω. (b) Relationship between $\psi_{r,\min}$ and ω. The symbols are the values obtained from RefProp 9.0.[12] (See Table S2.) The lines represent the results of AW (solid line), LK (dashed), B (dotted−dashed), and TCC (dotted).

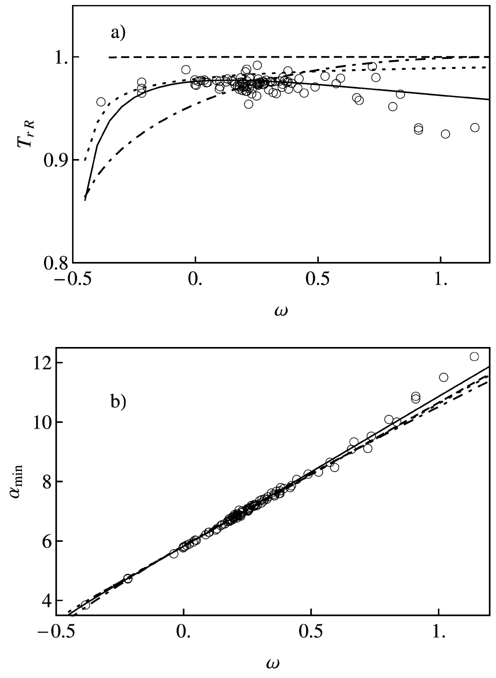

Figure 4. (a) Relationship between $T_{rR} = T_R/T_c$ and ω. (b) Relationship between $\alpha_{\min}$ and ω. The symbols are the values obtained from RefProp 9.0.[12] (See Table S2.) The lines represent the results of AW (solid line), LK (dashed), B (dotted−dashed), and TCC (dotted).

■ WARING AND RIEDEL FUNCTIONS FOR PITZER CORRESPONDING-STATES VAPOR PRESSURE EQUATIONS

The two-parameter corresponding-states principle (CSP) establishes that fluids at equal T_r and p_r behave identically.

More realistic CSP theories include, in addition to the critical temperature and pressure, a third or even a fourth parameter in order to explain the differences appearing in the reduced properties of different fluids. In particular, in the three-parameter CSP the most commonly used third parameter is the Pitzer ω defined by eq 9. In the Pitzer theory a vapor pressure equation has the form

$$\ln p_r = \phi(T_r, \omega) \tag{10}$$

with $\phi(1,\omega) = 0$. Most of the vapor pressure equations of the form of eq 10 proposed in the literature are expressed as a power series of ω,

$$\ln p_r = \sum_{k=0}^{n} \omega^k \phi_k(T_r) \tag{11}$$

where $\phi_k(1) = 1$, and the functions $\phi_k(T_r)$ usually have the same analytical form for different values of k but include different adjustable parameters. The reduced Waring function corresponding to eq 11 is given by

$$\psi_r(T_r) = -\frac{\mathrm{d}\ln p_r}{\mathrm{d}(1/T_r)} = \sum_{k=0}^{n} \omega^k T_r^2 \phi_k'(T_r) \tag{12}$$

and the Riedel function by

$$\alpha(T_r) = \frac{\mathrm{d}\ln p_r}{\mathrm{d}\ln T_r} = \sum_{k=0}^{n} \omega^k T_r \phi_k'(T_r) \tag{13}$$

where $\phi_k'(T_r) = \mathrm{d}\phi_k(T_r)/\mathrm{d}T_r$. Given a vapor pressure equation in the Pitzer CSP scheme, eqs 12 and 13 allow one to obtain the ω dependence of the minima associated with the corresponding Waring and Riedel functions. Comparison of these dependencies with the tabulated data for T_{rW}, $\psi_{r,\min}$, T_{rR}, and $\alpha_{\min}$ reported in Table S2 provides a quantitative tool for checking the suitability of the proposed vapor pressure equation. In this work we consider four of these equations widely used for predicting vapor pressure data. Three of them are linear ($n = 1$) in ω [Lee−Kesler[19] (LK), Brandani,[20] (B), and Twu−Coon−Cunningham[21] (TCC)] and one is quadratic ($n = 2$) in ω [Ambrose−Walton[22] (AW)]. Recently,[23] we have shown the self-consistency of these four vapor pressure equations to reobtain the acentric factor value used as an input.

Lee and Kesler[19] proposed analytical expressions for $\phi_0(T_r)$ and $\phi_1(T_r)$ in the form of a Riedel type of vapor pressure equation

$$\phi_k(T_r) = A_k + \frac{B_k}{T_r} + C_k \ln T_r + D_k T_r^6 \tag{14}$$

Brandani[20] reported his analytical expressions for $\phi_0(T_r)$ and $\phi_1(T_r)$ in the form of a Wagner type of vapor pressure equation

$$\begin{aligned}\varphi_k(T_r) = \frac{1}{T_r}[&A_k(1 - T_r) + B_k(1 - T_r)^{1.5} \\ &+ C_k(1 - T_r)^{2.5} + D_k(1 - T_r)^5 \\ &+ E_k(1 - T_r)^{10}]\end{aligned} \tag{15}$$

Twu et al.[21] also reported their analytical expressions for $\phi_0(T_r)$ and $\phi_1(T_r)$ in the form of a Wagner type of vapor pressure equation

$$\phi_k(T_r) = \frac{1}{T_r}[A_k(1 - T_r) + B_k(1 - T_r)^{1.5} + C_k(1 - T_r)^3 + D_k(1 - T_r)^6] \qquad (16)$$

Finally, Ambrose and Walton[22] proposed analytical expressions for $\phi_0(T_r)$, $\phi_1(T_r)$, and $\phi_2(T_r)$ in the form of a Wagner type of vapor pressure equation

$$\phi_k(T_r) = \frac{1}{T_r}[A_k(1 - T_r) + B_k(1 - T_r)^{1.5} + C_k(1 - T_r)^{2.5} + D_k(1 - T_r)^5] \qquad (17)$$

The values of the coefficients appearing in eqs 14−17 can be found in the corresponding references.[19−22] Only for the LK equation it is possible to explicitly calculate the reduced Waring and Riedel temperatures, obtaining

$$T_{rW}^{(LK)} = \left[-\frac{C_0 + C_1\omega}{42(D_0 + D_1\omega)}\right]^{1/6} \qquad (18)$$

$$T_{rR}^{(LK)} = \left[-\frac{B_0 + B_1\omega}{36(D_0 + D_1\omega)}\right]^{1/6} = 1 \qquad (19)$$

respectively. The result (19) shows that for the LK vapor pressure equation the reduced Riedel temperature is located at the critical point. This is due to the fact that the Riedel condition 5 was used as a constraint for the coefficients in the LK vapor pressure equation so that $B_0 = -36D_0$ and $B_1 = -36D_1$. For the remaining vapor pressure equations T_{rW} and T_{rR} must be calculated numerically.

The variations of T_{rW} vs ω obtained from the considered vapor pressure equations are plotted by lines in Figure 3a. The four vapor pressure equations have a limit value of ω below which T_{rW} becomes negative or imaginary. These values are −0.09565 for LK, −0.029 for B, −0.1462 for TCC, and −0.1292 for AW. This limit agrees with the fact that quantum fluids do not present a minimum for the Waring function. The four vapor pressure equations provide T_{rW} values monotonically increasing with ω. These behaviors agree with the tabulated data for $\omega \lesssim 0.7$, although none of the considered vapor pressure equations predict a decrease of T_{rW} for $\omega \gtrsim 0.7$. The following AARD between theoretical and tabulated data for T_{rW} have been obtained: 2.18% for LK, 3.35% for B, 1.98% for TCC, and 1.70% for AW. These results show that AW fares slightly better than the other vapor pressure equations in the prediction of T_{rW}. We note the excellent agreement for T_{rW} between tabulated data and the results obtained from the AW vapor pressure equation in the range $\omega \approx 0 - 0.8$.

The variations of $\psi_{r,\min}$ vs ω obtained from the considered vapor pressure equations are plotted by lines in Figure 3b. The four vapor pressure equations provide $\psi_{r,\min}$ values increasing with ω in a practically linear way very close to the tabulated data. The following AARD between theoretical and tabulated data for $\psi_{r,\min}$ have been obtained: 0.42% for LK, 0.66% for B, 0.30% for TCC, and 0.27% for AW. These results show a slightly better behavior of AW with respect to the other vapor pressure equations in the prediction of $\psi_{r,\min}$.

The variations of T_{rR} vs ω obtained from the considered vapor pressure equations are plotted by lines in Figure 4a. The LK vapor pressure equation gives $T_{rR} = 1$ (see eq 19). The B vapor pressure equation provides results for T_{rR} that monotonically increase as ω increases, failing to predict the tendency of the tabulated data. The TCC vapor pressure equation yields a good prediction of T_{rR} for $\omega \lesssim 0$, but it overestimates tabulated data for $\omega \gtrsim 0$. The AW vapor pressure equation shows a good qualitative agreement between theoretical and tabulated data; in particular it predicts that T_{rR} decreases as ω increases for $\omega \gtrsim 0.17$. The following AARD between theoretical and tabulated data for T_{rR} have been obtained: 2.86% for LK, 1.38% for B, 1.20% for TCC, and 0.66% for AW. In this case, our results show a clear advantage of AW over the other vapor pressure equations in the prediction of T_{rR}.

The variation of $\alpha_{\min}$ versus ω obtained from the considered vapor pressure equations are plotted by lines in Figure 4b. The four vapor pressure equations provide $\alpha_{\min}$ values increasing with ω in a practically linear way very close to the tabulated data. The following AARD between theoretical and tabulated data for $\alpha_{\min}$ have been obtained: 1.00% for LK, 1.06% for B, 1.04% for TCC, and 0.76% for AW. Again, these results show an advantage of AW over other vapor pressure equations in the prediction of $\alpha_{\min}$. Table 2 presents a summary of these deviations together with other results obtained in this section.

Table 2. Limit ω for T_{rW} and AARD for T_{rW}, $\psi_{r,\min}$, T_{rR}, and $\alpha_{\min}$ for the Vapor-Pressure Equations Considered in This Work

	LK	B	TCC	AW
limit ω for T_{rW}	−0.09565	−0.029	−0.1462	−0.1292
AARD (%) for T_{rW}	2.18	3.35	1.98	1.70
AARD (%) for $\psi_{r,\min}$	0.42	0.66	0.30	0.27
AARD (%) for T_{rR}	2.86	1.38	1.20	0.66
AARD (%) for $\alpha_{\min}$	1.00	1.06	1.04	0.76

■ CONCLUSIONS

The occurrence of minima in the Waring and Riedel functions associated with the liquid−vapor coexistence line of 105 fluids has been analyzed, and two interesting linear empirical relations have been derived between the critical temperature and the temperatures where these functions attain their minimum values. These equations can be then used either for predicting purposes or as a check on equations of state.

In the reduced coordinate scheme we have shown that the temperatures and values of the functions at the minimum present a fairly good correlation with the Pitzer acentric factor. These correlations provide nice examples of the Pitzer three-parameter corresponding-states theory, and they have been used for testing four well-known vapor pressure equations. We have shown the superiority of the Ambrose−Walton equation with respect to the Lee−Kesler, Brandani, and Two−Coon−Cunningham equations for predicting the properties of the minima of the Waring and Riedel functions.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

Table S1 listing critical, Waring, and Riedel temperatures and Table S2 listing acentric factors, reduced Waring temperatures, minium reduced Riedel temperatures with the data used in the figures. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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