

Peng-Robinson equation of state: 40 years through cubics

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ABSTRACT

Since its publication in 1976, the Peng & Robinson equation of state (PR EoS) has become one of the most useful and successfully applied models for thermodynamic and volumetric calculations in both industrial and academic fields. For this reason, we have reviewed this cubic EoS, in order to explore the development around it and some general applications where it has been applied, including its most known modifications. So, a complete time-line of the PR EoS is presented, as a compilation of more than 200 modifications for pure compound applications and about 100 modifications for mixtures.

These modifications to the PR EoS have been grouped in four main categories according to the nature of the modification: (a) by changing the dependence structure of α with temperature or the expressions for parameter a and b , (b) by introducing deviation functions (like volume translation), (c) by incorporating new parameters or terms in the equation of state, and finally (d) by modifying the mixing rules for mixture applications. Although great efforts have been made to improve accuracy and performance of the PR EoS, as demonstrated by the wide range of modifications, the necessity for further development of a universal, simple and accurate model is a rich source for research and discussion, considering the success of most of modifications is restricted to the studied properties and compounds, and therefore, they are limited to be just applied to the studied field. However, after 40 years, PR is still an invaluable and prominent tool, which will be under continuous development and research for next decades.

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1. Introduction

In 1976, the Chemical Engineers Donald B. Robinson, from Canada, [1,2] (1922–1998) and Ding-Yu Peng (1943 – today), from China, presented a new cubic equation of state (CEoS) [3]. Peng & Robinson worked together in a Project for the Natural Gas Processors Association since 1974 to 1975 at the University of Alberta (Canada), they developed the equation of state (EoS) during this period. It is interesting to remember this new expression is the result of a trial to improve the predictive capability of the 1972 Soave modified Redlich-Kwong (SRK) CEoS [4,5]. In 1985, Peng & Robinson [5] pointed out, as they indicated, that their model was born as the result of seeking a modification in the Redlich-Kwong

model, which would preserve the attractive simplicity of the cubic form and yet increase the reliability of its performance in the critical region and along the saturated liquid curve.

Peng et al. [6] showed the high capability of SRK to predict the phase equilibrium in natural gas systems. However, this study also showed that SRK was inaccurate for liquid density calculations and for predicting other properties near the critical point. This notable shortcoming in SRK was common for heavy hydrocarbons, where the deviation increases near the vicinity of the critical point [7]. For this reason, Peng & Robinson began to work in a modified expression for SRK, finding a totally new expression. The Peng-Robinson (PR) EoS acquired its own nature, despite it was built on the same structure of Soave's dependence of α on temperature, as well as the dependence of the limiting volume and attraction factors a and b on T_c and P_c [8], even with the simplicity and predictive capability needed to get better results in the calculation of the studied properties.

Before their EoS was officially published, it was used to estimate the retrograde condensation in natural gas pipelines. When it was

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used by Bergman et al. [9], the equation gave good prediction results of dew points and liquid yield at pipeline conditions, being these better than those obtained by SRK. Later, it was demonstrated that PR could predict retrograde behavior even of near-critical gas-condensate fluids with the same potential [10].

Since its publication, the PR EoS has been widely used and studied in the academic and industrial fields, having a considerable development similar to its predecessor SRK. It has been considered as one of the best two constants third degree equations of state applicable to vapor-liquid equilibria (VLE), and volumetric and thermodynamic properties calculations for pure substances and mixtures [11–16]. Today, there are more than 220 modifications to the PR EoS for pure compounds and uncountable works related with parameter adjustment and extension to mixtures.

In this way, it is necessary to come back to this meaningful EoS and review its progress after 40 years. Many researchers have made comprehensive reviews and studies about this topic although in a general way [14,17–40]. Some of them discuss the PR EoS in depth [12,13,16,41–46], especially Zabaloy & Vera [15], who studied PR and compared it with other equations of state. They found, in 1998, that PR was clearly superior to the other forms considered in their study.

An interesting turn in these path of reviews is the recent work by Wilczek-Vera & Vera [11], who studied the basis for the success of the PR EoS, compared to those of van der Waals (vdW) [47] and Redlich-Kwong (RK). Their work focused on pure substances, included a discussion on the a and b parameter determination based on the van der Waals [47] and Martin & Hou [48] frameworks, besides the replacement of the actual critical volume for a hypothetical critical volume, the root nature, and the critical isotherm behavior. They also explored the Soave [4] and Stryjek & Vera [49,50] approaches on the temperature dependence of α . This last point has been extended by the recent work made by Young et al. [51], who evaluated the performance for P^{sat} prediction of 20 different α functions in PR (including some not originally proposed and applied to PR) for 56 substances, including the estimation of the needed parameters.

However, all these studies focus on the main developments

around the EoS, which do not cover a complete time-line of PR, as it is the aim of the present work. Despite there are numerous studies on PR, this review is presented as an useful EoS data bank for future applications and recognition of all possible uses of the PR EoS. Therefore, the authors try to comprehensively cover the development of the PR EoS and its modifications, as much as possible, like a compendium (including those well-known studies and revisiting those scattered studies with, unfortunately, low dissemination), but without being our scope to do any properties evaluation in order to establish which modification is the best.

Because of its high reputation in the industry, especially petrochemical industry, the PR EoS has been extensively studied and modified in order to improve its predictive capability. Studies have been performed intensively since 1980, even increasing in the last 10 years (see Fig. 1), modifying the original expression at least in four different main ways (as it will be shown later), allowing it to be applied and extended to many substances, fields and applications. Thus, we will focus on those modifications for pure compounds, and we will present some of those that can be applied to mixtures.

2. The PR trip

Liquid volume predicted by the SRK EoS is usually higher than the experimental one [52,53], where deviation increases for compounds with a considerable value of ω . This behavior may be explained by the high-fixed value of the critical compressibility factor (Z_c) equal to $1/3$, which is imposed by the RK EoS (due to the restrictions at the critical point) [24,54].

In considering this, Donald Robinson & Ding-Yu Peng proposed a new equation of state [5]. This equation was based on the improvements of the RK equation of state [55] performed by Giorgio Soave in 1972 [4]. However, the model was different to that of Soave's, having, based on the author's criteria, *significant advantages over other two-parameter models, because ... it was built on rigorous criteria rather than circumstantial respect to RK* [12,56]. In this way, Peng & Robinson kept the dependence of α on temperature, but modified the van der Waals attractive term structure of EoS:

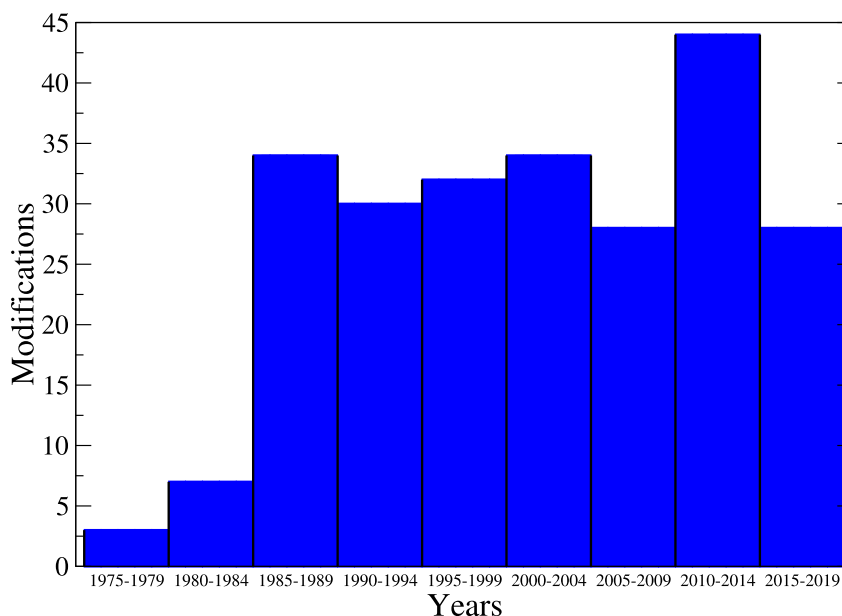


Fig. 1. Published modifications of the PR EoS since 1976 until 2017 (shown by 5 years periods) for pure compounds.

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b) + b(v-b)} \quad (1)$$

with

$$a = a_c \alpha \quad (2)$$

$$\alpha = \left[1 + \kappa \left(1 - \sqrt{T_r} \right) \right]^2 \quad (3)$$

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad (4)$$

$$a_c = \Omega_a \frac{R^2 T_c^2}{P_c} = 0.45724 \frac{R^2 T_c^2}{P_c} \quad (5)$$

$$b = \Omega_b \frac{RT_c}{P_c} = 0.07780 \frac{RT_c}{P_c} \quad (6)$$

Peng & Robinson introduced the term $b(v-b)$, which improves the representation of the attractive pressure forces, and in consequence, the ability of the equation to predict better liquid densities [9,57]. On the other hand, the PR EoS takes the value for Z_c equal to 0.307 at critical point, a more realistic value which, for example, is a closer value to the methane critical compressibility ($Z_c = 0.288$ – considering that Z_c decreases as carbon chain increases) in comparison with the value of the SRK EoS ($Z_c = 0.333$). Therefore, Peng & Robinson [3] also got an equation of state capable of predicting P^{sat} and vapor-liquid equilibria with higher accuracy, as well as performing somewhat better near critical conditions.

As any CEoS, PR can be solved analytically, to give either one or three real roots, depending on the temperature and pressure conditions. The appropriate use of one or other root, except when just one real root exists, rests directly on vapor pressure calculation or physical meaning of the roots [58] (for example, when negative value roots are found).

Peng & Robinson compared the results obtained by their equation with those obtained by Soave equation. Although both equations had similar results at gaseous phase for density (Fig. 2) and enthalpy calculation, the results of Peng & Robinson offered a better correlation of P^{sat} for pure compounds (due to their generalized design) and a better or enhanced estimation of liquid density, with emphasis in heavy compounds (like gasoline fractions). For example, work by Perez et al. [59] shows that PR is more suitable

than SRK for density of C_5 or higher carbon chain hydrocarbons, SO_2 , benzene and toluene. However, Michelsen & Mollerup [60] observed that the fugacity coefficients calculated by SRK were in much better agreement with those obtained by a modified BWR EoS [61,62] (assumed as experimental) than those predicted by PR. This drawback comes from the improvement in the PR Z_c , which decreases to a more realistic value (compared to that of SRK) at the expense of the fugacity coefficient.

Privat et al. [63] compared PR and SRK against an extensive experimental database from the Design Institute for Physical Properties (DIPPR), finding a good performance of PR for predicting enthalpy, liquid heat capacity and second virial coefficient, better than that obtained by SRK. For liquid density, it was observed that PR provides twice more accurate predictions than SRK. But, in general, PR and SRK reproduced VLE and caloric data with similar accuracy, unless a better α function could be obtained, improving the PR EoS performance. Mahmoodi & Sedigh [64,65] also found that PR has a better performance than SRK for predicting experimental P^{sat} of non-hydrocarbon substances, and Z , C_v , C_p , and even fugacity coefficient at supercritical conditions, comparing against simulated data from NIST for the studied substances (e.g. gases and n -alkanes).

3. Modifications for pure compounds

Despite the improvement that PR equation of state allowed, the original model showed significant deviations in the κ function (Eq. (4)), mainly for compounds with high and low ω values, because error in κ increases exponentially with P^{sat} [15]. Besides, the EoS still showed a relative deviation in calculation of density of hydrocarbon liquids [67], and according to Mathias [68], it was slightly worse than RK for the prediction of the high-temperature second virial coefficient. For these and other reasons, many modifications to PR equation of state appeared. Some of them improved the prediction of P^{sat} for heavy hydrocarbons [69], other improved the vapor-liquid equilibria for H_2O [70,71], polar and non-polar compounds [72], and asymmetric hydrocarbons containing systems [73,74], or the liquid volume [75–80], and so on.

Like other equations of state (e.g. RK, Patel-Teja (PT)), PR has been modified in four main ways: (a) by changing the dependence structure of α on temperature or the expressions for a and b parameters, (b) by introducing deviation functions (like volume translation), (c) by incorporating new parameters or terms in the equation of state, and (d) by modifying the mixing rules for mixture applications.

3.1. Modifications for α

The detailed description of the P^{sat} curve for a pure compound is required for phase equilibrium calculations. In consequence, there are many studies that try to improve the modeling of that curve by modifying the α function or the cohesion a parameter (Table 1). The α function has to obey some criteria for its development. In a general way, a first approach [81] considers that it must be:

- Equal to 1 at the critical point (meant to satisfy the corresponding-states principle).
- Positive sign and finite.
- Asymptotic to zero at high temperature to satisfy the ideal gas limit.
- A generalized function to overcome the possible lack of experimental data.

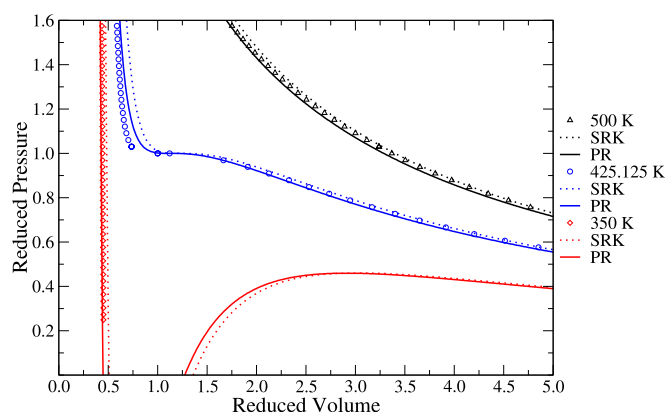


Fig. 2. Calculated isotherms by PR76 and SRK72 equations of state for n -butane at a higher temperature (Δ – 500 K) and a lower temperature (\diamond – 350 K) than critical temperature (\circ – 425.125 K) (experimental data taken from ref. [66]).

Table 1
Modifications of α function (including a parameter) for PR equation of state.

Author(s)	Modification	Improved Properties
Peng & Robinson (1978) [69]	$\alpha = [1 + m(1 - \sqrt{T_r})]^2$ $m = \begin{cases} 0.37464 + 1.54226\omega - 0.26992\omega^2 & \omega \leq 0.491 \\ 0.379642 + 1.48503\omega - 0.164423\omega^2 + 0.016666\omega^3 & \omega > 0.491 \end{cases}$	$psat$
Peng & Robinson (1980) [70]	$\alpha = [1.0085677 + 0.82154(1 - \sqrt{T_r})]^2$	$psat$ H_2O
Mathias & Copeman (1983) [84]	$\alpha = [1 + c_1(1 - \sqrt{T_r}) + c_2(1 - \sqrt{T_r})^2 + c_3(1 - \sqrt{T_r})^3]^2$	$psat$
Wormald (1984) [85]	$a = \left[0.45724 \frac{R^2 T_c^2}{P_c} - R^2 T_c^2 K_{11}(T_c) \right] [1 + m(1 - \sqrt{T_r})]^2 + R^2 T_c^2 K_{11}(T)$	H
Wang (1985) [86]	$\alpha = 0.54 + (1 - 0.54)\exp[0.25(1 - T_r)]$	VLE H_2
Stryjek & Vera (1986) [87]	$\alpha = \{1 + [\kappa_0 + \kappa_1(1 - \sqrt{T_r})(0.7 - T_r)](1 - \sqrt{T_r})\}^2$	$psat$
Stryjek & Vera (1986) [50]	$\alpha = \{1 + \{\kappa_0 + [\kappa_1 + \kappa_2(\kappa_3 - \sqrt{T_r})](1 - \sqrt{T_r})(0.7 - T_r)\}(1 - \sqrt{T_r})\}^2$	$psat$
Kwak & Mansoori (1986) [88]	$\alpha = c + dRT - 2\sqrt{cdRT}$	—
Lielmezs & Merriman (1986) [89]	$\alpha = a_c(1 + pT^{*q})$	$psat$
Perez Casas (1987) [90]	$\alpha = [1 + (0.38085 + 1.49426\omega - 0.10590\omega^2)(1 - \sqrt{T_r})]^2$	v^l, v^v
Yu & Lu (1987) [91]	$10^{[m(A_0A_1T_r + A_2T_r^2)(1 - T_r)]}$	—
Mak (1988) [92]	$\alpha = \begin{cases} 1 + pT^{*q} & T < T_c \\ 1 - pT^{*q} & T \geq T_c \end{cases}$	$psat, v^l, v^v$
Mak (1988) [92]	$\alpha = \sum_{i=0}^7 \frac{\alpha_i}{T_r^i} + \omega \sum_{i=0}^4 \frac{\beta_i}{T_r^i}$	B
Liu & Wang (1989) [93,94]	$\alpha = \exp\{2[1.226(1 - T_r^{0.184})]\}$	VLE H_2
Mak & Lielmezs (1989) [95]	$\alpha = \frac{1}{T_r} \sum_{n=1}^4 C_n T_r^{\left(\frac{1-n}{2}\right)}$	$psat, P_vT, \Delta H_{vap}, S$
Melhem et al. (1989) [96]	$\alpha = \exp[m(1 - T_r) + n(1 - \sqrt{T_r})^2]$	$psat, VLE$
Schwartzentruber et al. (1990) [97,98]	$\alpha = \{1 + [m - \sum_{i=1}^3 \phi_i T_r^{i-1}](1 - \sqrt{T_r})\}^2$	—
Magoulas & Tassios (1990) [99]	$\alpha = [1 + (d_0 + d_1\omega + d_2\omega^2 + d_3\omega^3 + d_4\omega^4)(1 - \sqrt{T_r})]^2$	$P_vT, psat$
Sheng & Lu (1990) [100]	$\alpha = 1 + A_1(1 - T_r) + A_2(1 - T_r)^2 + A_3(1 - T_r)^3$	$psat$
Du & Guo (1990) [101]	$\alpha = [1 + m(1 - \sqrt{T_r}) - p(1 - T_r)(q - T_r)]^2$	$psat, H_2O, Methanol$
Almeida et al. (1991) [102,103]	$\alpha = \exp\left[m \operatorname{sign}(1 - T_r) \left 1 - T_r\right ^{\Gamma} + n\left(\frac{1}{T_r} - 1\right)\right]$	$psat$
Qunlai & Wenchuan (1991) [104,105]	$\alpha = T_r^{2(m-1)} \exp[l(1 - T_r^{2m})]$	$psat$
Kwak & Anderson (1991) [106]	$\alpha = \frac{a+bT_r}{1+cT_r}$	VLE, $psat$ NaCl containing systems
Khalil (1992) [107]	$\alpha = \frac{A+BT_r}{1+CT_r+DT_r^{0.2}}$ $\alpha = \frac{A+BT_r^{2.5}+CT_r}{1+DT_r^{0.2}} \exp[G(1 - T_r)]$	$psat$
Søreide & Whitson (1992) [108]	$\alpha = \left\{1 + 0.4530[1 - T_r(1 - 0.0103c_{sw}^{1.1})] + 0.0034\left(\frac{1}{T_r^2} - 1\right)\right\}^2$	$psat, NaCl-H_2O$
Daridon et al. (1993) [109]	$\alpha = \exp[m(1 - T_r)]$	VLE
Takagi (1994) [110]	$\alpha = 5.8772bRT \left[\frac{1}{T_r^2} + m\left(\frac{1}{T_r} - 1\right) \right]^2$	v^l
Twu et al. (1995) [111]	$\alpha = \alpha^{(0)} + \omega(\alpha^{(1)} - \alpha^{(0)})$	$psat$
Danesh et al. (1995) [112]	$\alpha = [1 + 1.21(0.3796 + 1.485\omega - 0.1644\omega^2 + 0.01667\omega^3)(1 - \sqrt{T_r})]^2$	$psat$
Shtepani et al. (1996) [113]	$\alpha = 0.662415 \frac{RT_c}{P_c} (\alpha_0 - \alpha_T)^2$	P_vT
Zabaloy & Vera (1996) [114]	$\alpha = f_1(f_2 + \kappa_1 f_3 + \kappa_2 f_3)$	$psat$
Hewitt et al. (1996) [115, 116]	$\alpha = 1 + (1 - T_r) \left(0.6122 + \frac{0.2311}{T_r} \right)$	$P_vT, H, HFC125$
Fotouh & Shukla (1997) [117]	$\alpha = [1 + m(1 - T_r^x)]^2$	$psat$
Colina et al. (1997) [118]	$\alpha = T_r \left[1 + k_1 \left(\frac{1}{T_r} - 1 \right) + k_2 \left(\frac{1}{T_r^2} - 1 \right) \right]$	$psat$

Thorwart & Daubert (1997)/ Pfohl et al. (2000) [119,120] Zabaloy & Vera (1997) [121]	$\alpha = \begin{cases} \left[1 + \kappa(1 - \sqrt{T_r}) + n \frac{1 - \sqrt{T_r}}{\sqrt{T_r}}\right]^2 & \\ bRT_c A_c + 40bRT \left(\sum_{k=1}^{11} K_{k,2} X_2^{E_{k,2}}\right)^2 & 1.06b \leq v \leq v_c \\ bRT_c A_c + 40bRT \left[\sum_{k=1}^{10} K_{k,4} X_3^{\left(\frac{1}{2}\right)}\right]^2 & v_c \leq v \leq 7.474714 \times 10^8 b \end{cases}$	— v^l, v^v
Tsai & Chen (1998) [72] Flöter et al. (1998) [74] Carreira & Rodriguez (1998) [122,123]	$\alpha = [1 + M(1 - T_r) + N(1 - T_r)(0.7 - T_r)]^2$ $\alpha = 0.969617 + 0.20089T_r - 0.3256987T_r^2 + 0.066653T_r^3$ $\alpha = T_r \left\{ 1 + \left(1 - \ln \frac{p_r}{T_r}\right)^{-E} \left(-\ln \frac{p_r}{T_r}\right) \left[H_0 + \sum_{i=1}^9 H_i \left(\ln \frac{p_r}{T_r}\right)^i \right] \right\}$	$psat, v^l, v^v$ VLE CH ₄ —
Oellrich & Althaus (2001) [124,125] Gasem et al. (2001) [126] Gasem et al. (2001) [126]	$\alpha = [1 + A_1(1 - \sqrt{T_r}) + A_2(1 - \sqrt{T_r})^2 + A_3(1 - \sqrt{T_r})^4]^2$ $\alpha = \exp\{(A + BT_r)[1 - T_r^{(C+D\omega+E\omega^2)}]\}$ $\alpha = \begin{cases} [1 + (A + B\omega + C\omega^2)(1 - T_r^D)]^{\left(\frac{1}{2}\right)} & \\ T_r^A \exp[B(1 - T_r^C)] + \omega \{T_r^D \exp[E(1 - T_r^F)] - T_r^A \exp[B(1 - T_r^C)]\} & \end{cases}$	$psat$ H ₂ O $psat$ —
Yokozeki (2001) [127]	$\alpha = \sum_{k=0}^3 \beta_k \left(\frac{1}{T_r} - T_r\right)^k$	$psat$
Hyprotech (2001) [128]	$\alpha = [1 + m(1 - \sqrt{T_r})]^2$ $m = \begin{cases} 0.37464 + 1.54226\omega - 0.26992\omega^2 & \omega \leq 0.49 \\ 0.379642 + [1.48503 - (0.164423 + 1.016666\omega)\omega]\omega & \omega > 0.49 \end{cases}$	$psat$
Barragán-Aroche et al. (2002) [13] Coquelet et al. (2004) [129,130]	$\alpha = 1 + A(1 - T_r) + B(1 - T_r^2) + C(1 - T_r^3)$ $\alpha = \begin{cases} \exp[c_1(1 - T_r)][1 + c_2(1 - \sqrt{T_r})^2 + c_3(1 - \sqrt{T_r})^3]^2 & T_r < 1 \\ \exp[c_1(1 - T_r)] & T_r \geq 1 \end{cases}$	H $psat$
Figueira et al. (2005) [122,131–135]	$\alpha = T_r \left[1 + \frac{m}{n-1} \left(1 - \frac{1}{T_r^{n-1}}\right) \right]$	$psat$
Sabbagh et al. (2006) [136]	$\alpha = \left \sqrt[3]{1 + c(1 - T_r)^3} \right \frac{RT_c^2}{P_c}$	LLE Asphaltenes
Faradonbeh et al. (2008) [137] Joshipura et al. (2009) [138]	$\alpha = T_r^{n(m-1)} \exp[l(1 - T_r^m)]$ $\alpha = \begin{cases} [1 + m_1(1 - \sqrt{T_r})]^2 & \\ \exp[m_2(1 - T_r)] & \end{cases}$	P_vT , VLE —
Nji et al. (2009) [139] Wemhoff (2010) [140] Kud et al. (2010) [141]	$\alpha = [1 + f_\omega(1 - \sqrt{T_r})]^2$ $\alpha = 1 + 1.7409(1.2762\zeta)^{(1.7312\exp[5.5493(1-T_r)])}$ $\alpha = \exp\left[\Theta_1\left(1 - \frac{1}{T_r}\right) + \Theta_2 \ln T_r + \Theta_3(T_r - 1)\right]$	$psat$ σ $psat, P_vT$
Joshipura et al. (2010) [142]	$\alpha = \begin{cases} [1 + m_1(1 - \sqrt{T_r})]^2 & m_1 = \begin{cases} s_1 + s_2\omega \\ p_1 + p_2\omega + p_3\omega^2 \end{cases} \\ \exp[m_2(1 - T_r)] & m_2 = \begin{cases} s_1 + s_2\omega \\ p_1 + p_2\omega + p_3\omega^2 \end{cases} \end{cases}$	$psat$
Li & Yang (2011) [143] Hajipour & Satyro (2011) [144] van der Stelt et al. (2012) [145]	$\alpha = \exp\{k_1(1 - T_r) + l \ln[1 + k_2(1 - \sqrt{T_r})]^2\}$ $\alpha = [1 + (a_1 + a_2\omega + a_3\omega^2 + a_4\omega^3)(1 - \sqrt{T_r})]^2$ $\alpha = \{1 + [\kappa_0 + \kappa_1(\sqrt{[A - D(T_r + B)]^2 - E + A - D(T_r + B)}\sqrt{T_r + C})(1 - \sqrt{T_r})]\}^2$	$psat$ $psat$ P_vT, S
Kumar & Okuno (2012) [146]	$\alpha = \left\{ 1 + \left[0.4707 + 2.4831M_w^{\left(\frac{-39.933}{M_w}\right)} \right] \left(1 - \sqrt{T_r} \right) \right\}^2$	P_vT
Kumar & Okuno (2012) [147,148]	$\alpha = \left\{ 1 + \left[0.51824 + 2.5847(f_m M_w)^{\left(\frac{-43.4572}{f_m M_w}\right)} \right] \left(1 - \sqrt{T_r} \right) \right\}^2$	P_vT
Kumar & Okuno (2013) [149]	$\alpha = \left\{ 1 + \left[0.4707 + 2.4831(f_m M_w d^\gamma)^{\left(\frac{-39.933}{f_m M_w d^\gamma}\right)} \right] \left(1 - \sqrt{T_r} \right) \right\}^2$	P_vT

(continued on next page)

Table 1 (continued)

Author(s)	Modification	Improved Properties
Saffari & Zahedi (2013) [150] Li (2013) [151] Li & Yang (2013) [152]	$\alpha = \exp[k_1 T_r + k_2 \ln T_r + k_3 (1 - \sqrt{T_r})]$ $\alpha = \exp\{k_1 (1 - T_r) + l \ln[1 + k_2 (1 - \sqrt{T_r})^2]\}$ $\alpha = \left[c_1 + c_2 (1 - T_r) - c_3 \left(1 - \frac{1}{T_r} \right) + c_4 \left(1 - \frac{1}{T_r} \right)^2 \right]$	VLE, P_v/T P^{sat} , P_v/T P^{sat} H ₂ O
Hou et al. (2015) [153] Hosseiniifar & Jamshidi (2016) [154] Hekayati et al. (2016) [155] Valiollahi et al. (2016) [156] Forero & Velázquez (2016) [157]	$\alpha = \exp[k_1(\omega)T_r + k_2(\omega)\ln T_r + k_3(\omega)(1 - \sqrt{T_r})]$ $\alpha = (c_1\beta + c_2\gamma)^d$ $\alpha = A_1 + \ln P_r \times (A_2 + A_3 \ln T_r - A_4 \ln^2 T_r - A_5 \sin(A_6 \ln^2 P_r)) - A_7 \sin(\ln T_r)$ $\alpha = [1 + \kappa(1 - \sqrt{T_r})]^2 \times [1 + (\sqrt{T_r} - 1)^{0.5} \times (f_1 f_2 + f_1 f_3 P_r + f_1 f_4 P_r^2)]$ $\alpha = \exp \left\{ \left(\frac{\gamma_c - 1 + \beta_c}{\beta_c - 1 + \beta_c} \right) \left[1 - T_r \right] \right\}$	VLE P^{sat} P_v/T SC-CO ₂ v^l P^{sat}
Li et al. (2016) [158]	$\alpha = \left[1 + \left[k_0(\omega) + \left(p_1 + p_2 \frac{\ln p_r}{T_r} + \frac{p_3}{T_r} + p_4 y^{0.3} \right) \left(1 + \sqrt{T_r} \right) (0.7 - T_r) \right] \left(1 - \sqrt{T_r} \right) \right]^2$	P_v/T CO ₂ -NG
Rostamian & Lotfollahi (2016) [159,160]	$\alpha = \left[1 + m_1 (1 - \sqrt{T_r})^2 \left(\frac{\beta_c - 1}{\beta_c} \right) \right]$	Solubility in SC-CO ₂
Mahmoodi & Sedigh (2017) [161]	$\alpha = \exp \left[2 \times C_1 (1 - \sqrt{T_r}) - (C_2 (1 - \sqrt{T_r}))^2 + \frac{2}{3} C_3 (1 - \sqrt{T_r})^3 \right]$	VLE, C_p , C_v
Mahmoodi & Sedigh (2017) [64]	$\alpha = \exp \left[2c_1 (1 - \sqrt{T_r}) - c_2^2 (1 - \sqrt{T_r})^2 + \frac{2}{3} c_3^3 (1 - \sqrt{T_r})^3 \right]$ $\alpha = \exp \left[2c_1 (1 - \sqrt{T_r}) - c_2^2 (1 - \sqrt{T_r})^2 + \frac{2}{3} c_3^3 (1 - \sqrt{T_r})^3 \right]$	P^{sat} , C_p , C_v

A second and more recent approach [82] states that α must be:

- Monotonically decreasing with temperature ($d\alpha/dT \leq 0$).
- A function with its first ($d\alpha/dT$) and second ($d^2\alpha/dT^2$) derivatives existing and being continuous with temperature.
- Positive sign ($\alpha > 0$).
- Be convex with temperature ($d^2\alpha/dT^2 \geq 0$).
- A function with its third ($d^3\alpha/dT^3$) derivative being less or equal to zero.

These last criteria were developed as a consistency test for evaluating accuracy and physically meaning in the behavior of EoS in both the subcritical and supercritical regions. However, the original PR α function obeys the first approach criteria more than the second approach (in fact, it fails the consistency test as stated).

The PR α function was formulated by using vapor pressure data for each substance from the normal boiling point to the critical point, whereas Soave had worked using only the critical point and the calculated vapor pressure at $T_r = 0.7$ based on the value of acentric factor (which introduces some information on interacting forces and the molecules shape [83]). This framework allowed PR a better representation along the vapor pressure curve [9]. However, in 1978 the same Peng & Robinson presented an improved version of their α function [69]. For this function, coefficients were adjusted and defined according to different intervals for ω , which improved the prediction of P^{sat} applied to heavy hydrocarbons. So, this kind of generalized α functions provides accurate prediction of other non-volumetric VLE data (i.e. heat of vaporization) [63]. Some other modifications are discussed below (see Table 1).

3.1.1. Mathias and Copeman modification (1983)

Five years later, Mathias & Copeman [84] proposed an extended version of the α function:

$$\alpha = \left[1 + c_1 (1 - \sqrt{T_r}) + c_2 (1 - \sqrt{T_r})^2 + c_3 (1 - \sqrt{T_r})^3 \right]^2 \quad (7)$$

The additional parameters c_2 y c_3 were necessary to successfully correlate P^{sat} for highly polar substances (e.g., H₂O and CH₃OH). These parameters are adjustable (determined from vapor-liquid equilibria data) and own to every compound. Some researchers have tried to list, tune or generalize them [129,162,163].

This α function is directly proportional to temperature in the supercritical region. For this reason, it is necessary to employ a second expression when temperature is higher than critical [164,165]

$$\alpha = \left[1 + c_1 (1 - \sqrt{T_r}) \right]^2 \quad (8)$$

However, this second function implies a discontinuity at the critical point and a significant deviation in enthalpy calculations [166]. Even so, the Mathias and Copeman function was successful, being extended to other equations of state (e.g. Predictive Soave-Redlich-Kwong – PSRK EoS [167,168]). Mahmoodi & Sedigh [64] arrived to a similar conclusion, that the discontinuity in the second derivative causes undesirable discontinuity in C_p and C_v curves at T_c . So, in order to fix the discontinuity of the second and even third derivative at T_c , they presented two alternative expressions respectively, as

$$\alpha = \left[1 + c_1(1 - \sqrt{T_r}) + c_2(1 - \sqrt{T_r})^3 + c_3(1 - \sqrt{T_r})^4 \right]^2 \quad (9)$$

$$\alpha = \left[1 + c_1(1 - \sqrt{T_r}) + c_2(1 - \sqrt{T_r})^4 + c_3(1 - \sqrt{T_r})^5 \right]^2 \quad (10)$$

This and other later proposed α functions or cohesion a functions were built on empirical bases, so, in most of the cases, there are compound-specific and characteristic parameters, which are listed just for some compounds and are not correlated based on generalized properties [169]. Besides, this kind of modifications to α are more accurate and successful than generalized α functions as long as a sufficient amount of experimental data distributed on adequate temperature ranges are available to perform parameter regression [63].

3.1.2. Stryjek and Vera modifications: PRSV and PRSV2 (1986)

Stryjek & Vera [87] modified the PR EoS with the aim to extend its applicability to low temperature regions. Their α function was built on the same structure of the original PR (Eq. (3)), but its design was thought by the authors to be as accurate as Antoine's equation [49] for P^{sat} prediction even to 1.5 kPa for hydrocarbons, polar compounds and associative compounds. Stryjek & Vera set a fixed value for T_r equal to 0.7 (a near point to normal boiling point for most of the compounds studied by the authors) in order to consistently adjust κ (Eq. (4)) to available experimental data for P^{sat} . Consequently, Stryjek & Vera defined κ (expressed as κ_0) as:

$$\kappa_0 = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196554\omega^3 \quad (11)$$

with the purpose of further improving the P^{sat} estimation under $T_r = 0.7$, a temperature-dependent term was incorporated inside the definition of κ , which takes the form:

$$\kappa = \kappa_0 + \kappa_1(1 + \sqrt{T_r})(0.7 - T_r) \quad (12)$$

where κ_0 is defined as above (Eq. (11)), and κ_1 is an adjustable parameter which is characteristic to each compound and can be found listed [49,170,171]. Zabaleta-Mercado [172] optimized κ_1 as well as ω (acentric factor was assumed as an adjustable parameter instead of an experimental one) to improve P^{sat} prediction at low temperatures of compounds other than hydrocarbons. Cheluget & Vera [173] correlated κ_1 with T_b using a third order polynomial expression. Later Figueira et al. [169] developed a generalized correlation for estimating these parameters for almost 800 compounds, based on adjustment to P^{sat} data taken from DIPPR database (for hydrocarbons) [174]:

$$\kappa_0 = 0.379368 + 1.459994Z_c - 0.125563\omega^2 \quad (13)$$

$$\kappa_1 = 0.599529 - 1.952083Z_c + 0.080764\omega - 0.209272\omega^2 \quad (14)$$

Another way was tried by Hatami et al. [175], who modeled κ_1 through Artificial Neural Network (ANN) [176] and Adaptive Network-based Fuzzy Inference System (ANFIS) [177] methods from common thermodynamic properties and constants of pure

and pseudocomponents (namely T_c , P_c , ω and M_w), avoiding the use of vapor pressure data sets for this purpose.

Stryjek & Vera [50] tried to improve even more the capability for P^{sat} prediction of their function under $T_r = 0.7$, so they reformulated κ as:

$$\kappa = \kappa_0 + \left[\kappa_1 + \kappa_2(\kappa_3 - \sqrt{T_r}) \right] (1 + \sqrt{T_r})(0.7 - T_r) \quad (15)$$

where κ_0 keeps the original definition (Eq. (11)), and κ_1 , κ_2 , and κ_3 are compound-specific adjustable parameters. This improvement in the dependence of κ on temperature highly reduced deviation on P^{sat} prediction.

3.1.3. Twu et al. modification: a different approach (1995)

According to a later study by Forero & Velásquez [178], it is possible to get a better or adequate representation of the vapor pressure and the saturated vapor volume of pure substances when the original Soave's type α function is replaced by an n-parameter exponential function. This observation was made earlier by Twu et al. [111], who abandoned Soave's type of alpha function and presented a new approach, suggested first by Heyen [179]. Since the principle of corresponding states is very useful for the prediction of the properties of a large class of substances from the knowledge of a few compounds, their aim was to find a way in which the principle of corresponding states could be applied to the alpha function. The way they found was to expand the alpha function as a type of power series in the acentric factor:

$$\alpha = \alpha^{(0)} + \omega(\alpha^{(1)} - \alpha^{(0)}) \quad (16)$$

This approach allowed the α function to become a linear function of the acentric factor at a constant reduced temperature, not a higher order function as suggested by Soave and other researchers, which is an advantage in the extrapolation of the alpha function to heavy hydrocarbons, petroleum fractions, and gas condensates, according to Twu et al. [111] who then used an appropriate α function, proposed previously by Twu et al. [180] in 1991 for correlating the vapor pressure data of pure components:

$$\alpha = T_r^{N(M-1)} \exp \left[L(1 - T_r^{NM}) \right] \quad (17)$$

where the parameters L , M , and N are unique to each component and have been determined from the regression of pure component vapor pressure. All critical constants and vapor pressure data correlations from the triple point to the critical point were taken from DIPPR [174].

The new generalized α function allowed the accurate reproduction of the vapor pressure data from the triple point to the critical point for light as well as heavy hydrocarbons compared to the original Peng-Robinson equation or other versions of PR. Even, when it was developed primarily using the data for n-paraffin, it gave relatively high accuracy for P^{sat} prediction for other kinds of hydrocarbons as expected from the corresponding states principle [111]. However, it does not seem to be satisfactory at low temperatures for strongly polar fluids and some chain-like alkanes (even with a moderate length) [181].

Short time ago, Le Guennec et al. [82], with the aim of not only efficiently representing the saturation properties, but also to safely extrapolate in the supercritical temperature region, determined L , M and N for more than 1000 compounds, and developed generalized correlations for these parameters (setting $N = 2$), achieving

very accurate results, i.e. interesting low deviation values for P^{sat} (at least 0.9%), enthalpy and heat capacity (both at least 2%) representation.

3.1.4. Gasem et al. modification (2001)

Gasem et al. [126] modified the cohesion function proposing a reduced temperature and acentric factor-dependent exponential alpha function to predict pure component vapor pressure. Their approach was to avoid using component-specific parameters or switching functions in α , while an appropriate temperature limiting behavior for the function was achieved, in order to get a simple generalized α function. This is because a simple generalized α function facilitates *a priori* predictions, and it does not produce crossover anomalies in derivative properties, as it often occurs when using switching functions [126]. The authors proposed the expression:

$$\alpha = \exp \left\{ (A + BT_r) \left[1 - T_r^{(C + D\omega + E\omega^2)} \right] \right\} \quad (18)$$

Thus, a function with model parameters based solely on pure component properties was developed, which improved predictions for the pure fluid vapor pressures of simple, normal and slightly polar fluids, including heavy hydrocarbons, with an absolute average deviation of 1.1 %, being better compared to original PR (Soave-type) α function and Twu's logarithmic-type α function [126].

3.1.5. Generalized, adjustable definition and group contribution methods approach for α

Because α functions can be defined as generalized expressions (when parameters can be correlated to other known parameters, such as ω), like the original Peng-Robinson α function, or parameterizable functions (when compound-specific parameters are fitted to experimental data), like the Mathias & Copeman α function, Privat et al. [63] tried to establish the possibility to use group contribution methods to estimate those adjustable parameters. They studied a modified form of Mathias & Copeman (Eq. (19)) and Twu [182] (Eq. (20)) α functions:

$$\alpha = \left[1 + c_1 (1 - \sqrt{T_r}) \right]^2 \quad (19)$$

$$\alpha = T_r^{2(M-1)} \exp \left[L (1 - T_r^{2M}) \right] \quad (20)$$

where the parameters c_1 , L and M can be empirically correlated by

$$PP = a_p + \sum_k N_k \Gamma_{p,k} \quad (21)$$

PP represents each adjustable parameter in both α functions and $\Gamma_{p,k}$, N_k , and a_p are group contribution parameters following Marrero & Gani group-decomposition scheme [183]. They found this methodology can be successfully applied when ω is not available, giving accurate predictions of liquid density and liquid heat capacity. However, this methodology loses accuracy for P^{sat} , ΔH_{vap} and B prediction. Even so, this method has a predictive potential that could be interesting for process or product development when no vapor-liquid equilibria data is available [63].

3.2. Modifications for a and b parameters

Danesh et al. [112] proposed to determine the PR parameters based on VLE data for binary systems, improving inversion curve locus prediction at low temperatures [184], for example. Based on the same information, κ (Eq. (4)) has also been adjusted for halo-carbons and highly asymmetric n-alkane mixtures by Meskel-Lesavre et al. [185] and Ting et al. [186], respectively. The latter ones even found interesting behavior and trend between regressed a , b and κ , and carbon number. In the same line, Zhang et al. [187,188] and Louli & Tassios [189] adjusted a and b for molten salts and their mixtures (based on pseudo-volumes of the same salts at atmospheric pressure), and for polymer and their mixtures respectively; while Schmitt & Reid [190] adjusted a and b in order to improve solubility prediction of solute compounds in supercritical solvents, and de Loos et al. [191] calculated a and b from P_v isotherms at different temperatures for ethylene and some n-alkanes. Other example was performed by Hosein et al. [192–194], who tuned $\Omega_{a,b}$ and k_{ij} for constant volume depletion prediction for gas condensates, following similar works [195,196].

A different way was followed by Rijkers [197], who adjusted the critical properties for methane with the purpose of reproducing the volumetric data for this substance in the studied region, even sacrificing the experimental critical data. Like Rijkers, Castellanos Días et al. [198] tuned the critical properties and acentric factor of fatty acid methyl esters for predicting P^{sat} and C_p^l . Derevich et al. [199] also tuned (developed by correlations) the same parameters for vapor-liquid equilibria prediction in Fischer-Tropsch synthesis products. So, a and b were modified in specific ways, by adjustment of equation parameters although there were no correlations to describe them. Though optimizing a and b parameters is an old method, it still attracts attention in the aim of improving the representation of compositional and volumetric behavior.

On the other hand, it is interesting that accuracy of $P_v T$ data calculated by the EoS using parameters from a correlation is lower than with individually fitted parameters. However, correlations eases the calculation process avoiding the use and lack of needed tabulated data. In this way, many correlations have been proposed in the literature. Xu & Sandler [200], studied the temperature dependence of a and b , indicating *a priori* this approach lead to greater accuracy in vapor pressure and density predictions, based on previous observations from other authors. So, they correlated Ω_a and Ω_b with quadratic polynomial functions as:

$$\Omega_a = \sum_{i=0}^2 a_i T_r^i \quad (22)$$

$$\Omega_b = \sum_{i=0}^2 b_i T_r^i \quad (23)$$

These functions of T_r have different sets of parameters in the subcritical and supercritical temperature regions and are connected by a continuous cubic-spline function in the critical region which satisfies the critical conditions. But these functions were still specific to each fluid (fluid specific coefficients), so later Wu & Sandler [201] proposed generalized correlations, also in the subcritical and supercritical regions, for Ω_a and Ω_b in terms of T_r and ω . Other approach was proposed in 1988 by Carrier et al. [202], who, under the concept of a pseudovolume- and pseudocovolume-based EoS, reformulated a and b as

$$a = a(T_b) \left[1 + m_1 \left(1 - \sqrt{\frac{T}{T_b}} \right) - m_2 \left(1 - \frac{T}{T_b} \right) \right] \quad (24)$$

$$b = -2.40086 + \sum_{j=1}^{13} B_j G_j \quad (25)$$

where m_1 , m_2 , B_j and G_j parameters were intended to be correlated through an also proposed group contribution method. This modification improved the vapor pressure prediction for compounds encountered in petroleum fractions. Then Coniglio et al. [203], in 1993, estimated b based on the Bondi's method [204], while keeping the structure performed by Carrier. Feyzi et al. [205,206] considered a and b like temperature-dependent functions.

Another example is a more recent modification by Kumar & Okuno [207], who through a method for reservoir fluid characterization, directly perturbed a and b parameters of pseudocomponents from the n -alkanes values, systematically adjusting both parameters of all pseudocomponents within a given reservoir fluid through a few adjustable parameters, specially a ψ parameter, which is used to ensure the proper interrelationship between a and b parameters, as

$$\psi = \frac{a}{b^2} \quad (26)$$

Like those of Xu & Sandler or Carrier et al. and Kumar & Okuno, correlations could keep the basic structure of PR a and b functions or take new forms (see Table 2).

3.3. Pilot cases: modifications for b parameter

In 1988, Moshfeghian et al. [245] assumed that b parameter was a function of temperature, while keeping the original expression for a . They defined b with an adjustable parameter own to each compound, taking the form

$$b = 0.07780 \frac{RT_c}{P_c} [1 - \eta(1 - T_r)] \quad (27)$$

A second modification to b was performed by Fitzgerald et al. [246,247] in order to improve the predictive capability of the Simplified Local Density–Peng–Robinson model (SLD–PR – density and attractive parameter are functions of position [248–250]) dealing with near-critical and supercritical adsorption of gases on coals. Such a modified model incorporated a deviation factor for b :

$$b = 0.07780 \frac{RT_c}{P_c} (1 + \Lambda_b) \quad (28)$$

where Λ_b is an adjustable parameter [247,251]. This and some other modifications to the SLD model [249,250,252,253], allowed it to accurately represent the adsorption of pure methane, nitrogen, and CO at coal-bed conditions [254].

However, this methodology applied to PR did not represent a significant improvement by itself, because, for example in the case of Moshfeghian et al. [245] modification, the average deviation for the studied property (liquid density ρ^l) was reduced from 5.5% to 3.5% [100]. In fact, even when an improvement in volume calculation can be achieved, it is at the expense of deteriorating P^{sat} prediction [255], since modification of this parameter influences directly in pure compound P_{sat} calculations. Besides, according to Michelsen & Møllerup [60], this kind of modification can likely

violate the condition of thermal stability ($T/C_v > 0$), specially at high densities, where v tends to b , and the repulsive term outweighs the attractive term.

3.4. Volume translation

The second kind of modification (see Table 3) consists in a correction to the v value predicted by the equation of state, through new terms or deviation or adjustment factors addition, which follows the generalized structure:

$$v = v_{EoS} + c \quad (29)$$

This concept was proposed by Pénéloux et al. [53] in 1982, originally for the SRK EoS, in order to solve the common weakness in cubic equations of state related to deviation between predicted liquid density values and experimental ones. So, when applied to the PR EoS, it takes the form:

$$P = \frac{RT}{v + c - b} - \frac{a}{(v + c)(v + c + b) + b(v + c - b)} \quad (30)$$

The volume translation coupled to PR improved the v^l prediction, through a method easy to apply, as SRK. The c parameter, which does not affect phase equilibrium, is a deviation measure between the predicted (originally conceived as a pseudovolume) and experimental v or ρ value evaluated at $T_r = 0.7$, so:

$$c = v_{calc} - v_{exp} \quad (31)$$

In other words, c was used, initially, as a shift to volume prediction along an isotherm, which can be expressed by the generalized expression [80,256]:

$$c = -0.252 \frac{RT_c}{P_c} (1.5448Z_c - 0.4024) \quad (32)$$

where Z_c is the experimental compressibility factor of the pure compound at critical point. The same Pénéloux, later proposed a non-published relation for c applicable to PR [257] as

$$c = \frac{RT_c}{P_c} (0.1154 - 0.4406Z_{RA}) \quad (33)$$

Le Guennec et al. [258] advised to calculate the volume translation with the experimental liquid molar volume at $T_r = 0.8$ using the corresponding Rackett compressibility factor (Z_{RA}), as

$$c = v_{PR}^l(T_r = 0.8) - \frac{RT_c}{P_c} Z_{RA}^{(1+0.2^{2/7})} \quad (34)$$

Two years later to Pénéloux work, in 1984 Jhaveri & Youngren [259,260], and later Chien & Monroy 80 applied first this methodology to PR. In order to improve the prediction of volumetric properties for hydrocarbon fluids, Jhaveri & Youngren began defining a dimensionless parameter s , as

$$s = \frac{c}{b} \quad (35)$$

which has negative values for lighter hydrocarbons, decreasing as the carbon number increases. For heavier than n -heptane hydrocarbons, the authors correlated s with molecular weight, as

Table 2
Modifications to a and b parameters.

Author(s)	Modification to a	Modification to b	Improved Properties
Panagiotopoulos & Kumar (1985) [208]	$a = bRT \sum_i B_i (\ln Z^i)^i$	$b = \frac{RT_c}{P_c} \left[\frac{\sum_i B_i (\ln Z^i)^i}{1 + \sum_i B_i (\ln Z^i)^i} \right]$	PvT
Mohamed & Holder (1987) [209]	$a = [1 + C_a k(1 - \sqrt{T_r})]^2$	$b = 0.0778 \frac{C_a RT_c}{P_c}$	p^{sat}, v^l
Xu & Sandler (1987) [200,210]	$\Omega_a \alpha = \sum_{i=0}^2 a_i T_r^i$	$\Omega_b = \sum_{i=0}^2 b_i T_r^i$	p^{sat}, PvT
Carrier et al. (1988) [202]	$a = a(T_b) \left[1 + m_1 \left(1 - \sqrt{\frac{T_r}{T_b}} \right) - m_2 \left(1 - \frac{T_r}{T_b} \right) \right]$	$b = -2.40086 + \sum_{j=1}^{13} B_j G_j$	p^{sat}
Dorhn & Brunner (1988) [211]	$a = a_c \left[1 + x_0 \left(1 - 2.4243 \sqrt{\frac{RT_c}{a_c}} \right) \right]^2$	$b = b_1 v_{20} c + b_2$	PvT, VLE
Wu and Sandler (1989) [201]	$\Omega_a \alpha = [\sum_{i=1}^3 a_i (1 - \sqrt{T_r})^{i-1}]^2$	$\Omega_b = [\sum_{i=1}^3 b_i (1 - \sqrt{T_r})^{i-1}]^2$	PvT, p^{sat}
Sugie et al. (1989) [212]	$\Omega_a = \text{constant}$	$\Omega_b = \text{constant}$	v^l
Rogalski et al. (1990) [213]	$a = X a_{PR} + (1 - X) a_{CRP}$	$b = 0.045572 \frac{RT_c}{P_c}$	PvT, p^{sat}
Ahmed (1991) [214]	$a = a_c \left[1 + m \left(1 - \sqrt{\frac{520}{T_r}} \right) \right]^2$	$a_c, b = \sum_{i=0}^3 C_i D^i + \frac{C_6}{D} + \sum_{i=5}^6 C_i \gamma^{i-4} + \frac{C_7}{\gamma}$	PvT, VLE, C_{1-7+}
Bian et al. (1992) [215]	$\Omega_a = 0.457235528921$	$\Omega_b = 0.0777960739039$	Z_c
Dorhn (1992) [216]	$a_c = \Omega_a a_1 \left(\frac{b_c T_c}{\Omega_b} \right)^{a_2}$	$b = \Omega_b (b_1 v_{10} v_{20} c + b_2)$	p^{sat}, v^l
Coniglio et al. (1993) [203]	$a = a(T_b) \left\{ 1 + m_1 \left[1 - \left(\frac{T_r}{T_b} \right)^x \right] + m_2 \left[1 - \left(\frac{T_r}{T_b} \right)^y \right] \right\}$	$b = b_{CH_4} \left(\frac{\sum_{j=1}^7 (V_{Wj} N_j) + \sum_{k=1}^3 (\delta V_{Wk} k_k)}{V_{WCH_4}} \right)$	p^{sat}, v^l
Kalospiros & Tassios (1995) [217]	$a = M_{w,poly} \exp \left(A_1 + \frac{A_2}{T^{A_3}} \right)$	$b = 0.975 M_{w,poly} \exp[a_g(T - T_g)]$	Polymer PvT
Li et al. (1996) [218]	$\alpha = \left[1 + \left(\kappa_{0,RSV} + \sum_i \frac{\phi_i}{T_r^{i+1}} \right) \left(1 - \sqrt{T_r} \right) \right]^2$	$b = \Omega_b \frac{RT_c}{P_c} \sum_i \frac{d_i}{T_r^{i+1}}$	R32, R125 and R134a PvT, VLE
Orbey et al. (1998) [219]	$a = \frac{RT_b \left[\left(\frac{T_r}{T_b} \right)^2 + 2 \left(\frac{T_r}{T_b} \right) - 1 \right]}{\left(\frac{T_r}{T_b} \right) - 1}$	$b = \left(\frac{M_{w,poly}}{\rho} \right) \left[0.95 - \frac{\exp \left(-\frac{1000}{T_r} \right)}{1 + \exp \left(-\frac{1000}{T_r} \right)} \right]$	Polymer p^{sat}, v^l
Feyzi et al. (1998) [220]	$a = a_c \{ 1 + [m_1 + m_2(1 - T_r) + m_3(1 - T_r)^2][1 - \exp(-100 T_r - 1)] \}^2$ $b = b_c \{ \sqrt{n_1} + [n_2 + n_3(1 - T_r) + n_4(1 - T_r)^2][1 - \exp(-n_5 T_r - 1)] \}^2$	$b = 0.45713317 - 1.1260406 \times 10^4 T$	ρ^l
Ahmed (2000) [221]	$a = 1.7639581 \times 10^4 - 21.150287T$		p^{sat}, v^l, CO_2
Coniglio et al. (2000) [222]	$a = a(T_b) \exp \left\{ 1 + f_1 \left[1 - \left(\frac{T_r}{T_b} \right)^{0.4} \right] + f_2 \left[1 - \left(\frac{T_r}{T_b} \right)^{2.5} \right] \right\}$	$b = b_{CH_4} \left(\frac{\sum_{j=1}^7 (V_{Wj} N_j) + \sum_{k=1}^3 (\delta V_{Wk} k_k)}{V_{WCH_4}} \right)$	p^{sat}, v^l
Mutelet (2001) [223,224]	$a = a(T_b) \exp \left\{ 1 + f_1 \left[1 - \left(\frac{T_r}{T_b} \right)^{0.4} \right] + f_2 \left[1 - \left(\frac{T_r}{T_b} \right)^{2.5} \right] \right\}$	$b = b_1 v_X + b_2$	PvT
Eubank & Wang (2003) [225]	$a = \frac{\left[\frac{p^{sat}(T^* - T^l)}{RT} - 2 \sqrt{2} RT \frac{\Delta H_{vap}}{RT} \right]}{\ln \frac{(T^l + b(1 - \sqrt{2}))^{a^*} + b(1 - \sqrt{2})}{(T^* + b(1 - \sqrt{2}))^{a^*} + b(1 - \sqrt{2})}}$	$b = \frac{v^* - v^l \exp \left(\frac{\Delta H_{vap}}{RT} \right)}{1 - \exp \left(\frac{\Delta H_{vap}}{RT} \right)}$	$p^{sat}, \Delta H_{vap}$
Tada et al. (2003) [226]	$a = N_A^2 \epsilon d^3 (13.978 - 1.2734 \hat{T}_r - 2.0054 \exp \hat{T}_r) \left(1 + \frac{\hat{\Delta T}_{ra}}{\hat{T}_{ra} - \hat{T}_r} \right)$ $b = N_A d^3 (0.67981 + 0.71789 \hat{T}_r - 0.063637 \exp 2.1984 \hat{T}_r) \left(1 + \frac{\hat{\Delta T}_{ra}}{\hat{T}_{ra} - \hat{T}_r} \right)$		p^{sat}, v^l
Crampon et al. (2004) [227]	$a = a(T_b) \exp \left\{ 1 + m_1 \left[1 - \left(\frac{T_r}{T_b} \right)^{0.4} \right] + m_2 \left[1 - \left(\frac{T_r}{T_b} \right)^{2.5} \right] \right\}$	$b = b_{CH_4} \left(\frac{\sum_{j=1}^{N_g} V_j N_j}{V_{CH_4}^*} \right)$	p^{sat}
Amorim et al. (2006) [228,229]	$a = c \left[1 + k \left(1 - \sqrt{\frac{T_r}{T}} \right) \right]^2$	$b = 0.07779607 \frac{RT_c}{P_c}$	ρ
Vahid et al. (2006) [205,230]	$a = 0.4572355289 \frac{RT_c^2}{P_c} \alpha(T_r)$	$b = 0.0777960739 \frac{RT_c}{P_c} \beta(T_r)$	VLE, PvT

Tada et al. (2007) [231]	$a = a_0 p f_{c_0} + N_2^2 d^3 \left[13.82 - 1.824 \left(\frac{v_r}{T_c} \right) - 1.738 \exp \left(\frac{v_r}{T_c} \right) \right] (1 - f_{c_0})$	p^{sat}, v^l
Hinojosa-Gómez et al. (2010) [232]	$b = b_0 p f_{c_0} + N_2^2 d^3 \left[0.7489 - 0.9151 \left(\frac{v_r}{T_c} \right) - 0.1531 \exp \left(1.699 \frac{v_r}{T_c} \right) \right] (1 - f_{c_0})$	v^l
Staudt et al. (2010) [233,234]	$a = a_c \alpha'$	Polymer $P_v T$
Ahmed & Meehan (2010) [235]	$a = \left(\frac{RT}{v_0 - b} \right) (v_0 + \epsilon b) (v_0 + \sigma b)$	$P_v T, VLE C_{7+}$
Haghtalab et al. (2011) [236]	$a = a_c \left[1 + m' \left(1 - \sqrt{\frac{v_r}{T_c}} \right) \right]^2$	VLE
Martynov et al. (2013) [237]	$a = a_c \exp(1 - n^{m' r})$	SVE
Shestova et al. (2013) [238,239]	$a = a_0 \left(1 - \frac{T}{T_c} \right)$	$p^{sat}, P_v T$
Kumar & Okuno (2015) [207]	$a = (A + B \exp \theta)^2$	$P_v T$
Eslami & Khadem-Hamedani (2015) [240]	$a = b^2 \Psi$	
Al-Malah (2015) [241,242]	$b = -14.6992113939827 + 1.36977232166027 M_w - 0.0000912089276536298 M_w^2$	p^{sat}, v^l
Kaviani et al. (2016) [243]	$a = a_c [a_0 v + a_1 (1 - T_r) + a_2 (1 - T_r)^2]$	VLE He
Myint et al. (2016) [244]	$a = 0.024362 C_{fac}^{-0.2172} M_w^{1.505}$	$P_v T$
	$a = a_c \{ 1 + [a_1 + a_2 (1 - T_r) + a_3 (1 - T_r)^2 + a_4 (1 - T_r)^3 + a_5 (1 - T_r)^4] [1 - \exp(-100 T_r - 1)] \}^2$	p^{sat}, v^l
	$b = b_c [b_1 + b_2 (1 - T_r) + b_3 (1 - T_r)^2 + b_4 (1 - T_r)^3 + b_5 (1 - T_r)^4]$	VLE He
	$a = \begin{cases} a_1 T + a_0 & \text{solid RDX and solid TNT} \\ (a_1 T + a_0)^2 & \text{liquid TNT} \\ \exp(a_1 T + a_0) & \text{liquid RDX} \end{cases}$	$P_v T$
	$b = \begin{cases} \text{constant} & \text{special case} \\ b_3 T^3 + b_2 T^2 + b_1 T + b_0 & \end{cases}$	$P_v T$

$$s = 1 - \frac{d}{M_w^e} \quad (36)$$

where d and e are correlation coefficients. Following Jhaveri & Youngren, Whitson & Brulé [261] determined s for selected compounds by matching saturated liquid density at $T_r = 0.7$. Other volume translation was proposed by Magoulas & Tassios [99], who extended to PR a volume translation proposed by Watson et al. [262,263] originally for a volume translated van der Waals EoS model (vdW-711 model). Their work, including a modification of α , was conceived for improving predictions of vapor pressures, saturated liquid volumes and enthalpies of vaporization for heavy n -alkanes.

Volume translations like these have been extensively studied in the literature. For example, Bezerra et al. [262] compared some volume translation for PR, especially in the saturation region. A different study approach was proposed in a universal way by Twu et al. [264], who proposed a different methodology for volume translation applicable over the entire temperature range from the triple point to the critical point. Their work was based on deviation c parameter calculation at T_b

$$c = \frac{RT_c}{P_c} \left\{ \frac{b_c^*}{2} \left[\left(\frac{a^*}{b^*} - 1 - 0.9999 \right) - \sqrt{\left(1.9999 \frac{a^*}{b^*} \right)^2 - 4 \left(0.9999 + \frac{a^*}{b^*} \right)} \right] - Z_{RA} \left[1 + \left(1 - \frac{T_b}{T_c} \right)^{2/7} \right] \right\} \quad (37)$$

Recently, Shi & Li [265] developed a concise criterion to judge whether a volume-translated EoS will result in crossover issues (crossing of pressure-volume isotherms for a pure compound), and Young et al. [255] concluded that the simplest and most efficient way to improve the volumetric predictions was the utilization of temperature-dependent volume translation functions. They suggested that the advantage of these functions is not only the best results presented for density, but also the fact that such functions do not interfere in P_{sat} calculation and, consequently, in VLE. In contrast, Jaubert et al. [257] studied the effect of the temperature-independent and temperature-dependent volume translation over different properties to understand which experimental data the volume translation should be fitted on, concluding that the dependence on temperature of c was not advised since it affects not only the volume, but also the enthalpy and the speed of sound, among others.

Nevertheless, the key point regarding volume translation concept, is to well understand that the problem of reproducing both experimental phase equilibrium and thermodynamic properties can be separated from the problem of reproducing experimental liquid densities. Working with the PR EoS, it is advised to determine first the parameters of the α function on many diversified experimental data except densities (vapor pressure, heat of vaporization, heat capacities) and in a second step to determine the value of c on liquid densities and possibly speed of sound experimental data [258]. In fact, Salimi & Bahramian [266] suggested to use the prediction of speed of sound as a consistency test for any EoS, previously. Besides, the influence of the volume translation has been studied for mixtures [267].

Table 3

Volume translation and volume correction applied to PR.

Author(s)	Modification	Improved Properties
Chien & Monroy (1986) [80]	$v = v_{PR} - sb$ $s = 1.077 - 1.644 \left(\frac{V_0}{b} \right) + (0.4878 \times 10^{-4} 0.5156 \times 10^{-7} M_w) \left(\frac{M_w}{b} \right)$	v^f
Watson et al. (1986) [268,269]	$v = v_{PR} - t$ $t = t_0 + (t_c - t_0) \exp(\beta 1 - T_r)$	—
Yu & Lu (1987) [91]	$v = v_{PR} + c \quad b = b_{PR} + c$ $c = 0.25(2 - u)b$	v^f
Jhaveri & Youngren (1988) [260]	$v = v_{PR} + c$ $c = sb$	P_vT , VLE
Carrier et al. (1988) [202]	$v = v_{PR} + c$ $c = -0.03222 \frac{RT_c}{P_c}$	$psat$
Søreide (1989) [270]	$v = v_{PR} - sb$ $s = \begin{cases} T_r - a_1 ^{a_2} + a_3 + a_4\omega + a_5 \exp[a_6(T_r - 1)] & T_r \leq 1 \\ a_1 + a_2 T_r & T_r > 1 \end{cases}$	P_vT
Mathias et al. (1989) [79]	$v = v_{PR} + s + f_c \left(\frac{0.41}{0.41 + \delta} \right)$	v^f
Sheng & Lu (1990) [100]	$v = v_{PR} + c \quad b = b_{PR} + c$ $c = 0.25 \{ 2 - [u_0 + u_1(1 - T_r)^{0.1} + u_2(1 - T_r) + u_3(1 - T_r)^2] \} b$	v^f, v^v
Magoulas & Tassios (1990) [99]	$v = v_{PR} - t$ $t = t_0 + (t_c - t_0) \exp(\beta 1 - T_r)$	P_vT , $psat$, ΔH_{vap}
Rogalski et al. (1990) [213]	$v = v_{PR} - c$ $c = \begin{cases} c_{T_b} + 85.8m^2[1 - T/T_b]^2 & T \leq T_b \\ c_{T_b} + 85.8m^2[1 - T_b/T]^2 & T > T_b \end{cases}$	v^f
Kokal & Sayegh (1990) [271]	$v = v_{PR} - c$ $c = \begin{cases} v - \frac{RT_c}{P_c} Z_{RA}^{[1+(1-T_r)^{2/7}]} & T \leq T_r \\ \frac{RT_c}{P_c} (0.307 - Z_{RA}) & T > T_r \end{cases}$	v^f
Coniglio (1993) [203,272]	$v = v_{PR} - c$ $c = C[1 + \alpha(1 - Y) + \beta(1 - Y)^2]$	P_vT
Deo et al. (1993) [273]	$v = v_{PR} - c$ $c = \text{constant}$	P_vT
Voros et al. (1994) [274]	$v = v_{PR} - t$ $t = (d_0 + d_1\omega + d_2\omega^2 + d_3\omega^3 + d_4\omega^4)(RT_c/P_c)$	H , S
Alkan et al. (1995) [275]	$v = v_{PR} - c$ $c = c_i(T_0)[1 + \alpha(T - T_0)]$	v H ₂ O
Satyro & Trebble (1996) [276]	$v = v_{PR} + v_{trans}$ $v_{trans} = \exp(7.07453 \times 10^{-2} - 6.08271 \times 10^{-4} M_w)$	$psat$, v^f
Ungerer & Batut (1996) [78,277]	$v = v_{PR} - c$ $c = AT + B$ $C = -130.031 + 0.95924 \frac{M_{C7+}}{M_{C7+}} - 0.15229T$	v^f
Al-Mehaideb et al. (1996) [278]	$v = v_{PR} - v_{trans}$	ρ
Fotouh & Shukla (1997) [117]	$v_t = v_t^{(0)} + \sum_{i=0}^5 C_i T_i^i$	v^f
Monnery et al. (1998) [77]	$v = v_{PR} + c$ $c = c_1 + \frac{c_4}{\sqrt{2\pi c_2}} \exp \left[-0.5 \left(\frac{T_r - c_1}{c_2} \right)^2 \right]$	v^f
Tsai & Chen (1998) [72]	$v = v_{PR} - t$ $t = \left(\frac{RT_c}{P_c} \right) \left[k_1 + k_2(1 - T_r^{2/3}) + k_3(1 - T_r^{2/3})^2 \right]$	$psat$, v^f , v^v
Coniglio et al. (2000) [222]	$v = v_{PR} - c$ $c = C[1 + \alpha(1 - Y) + \beta(1 - Y)^2] + (-1 + \sqrt{2})b$	$psat$, v^f
Hoyos (2000) [279,280]	$v = v_{PR} - c$ $c = C_1 + C_2(T_r - C_3)^2$	v^f
Ghotbi et al. (2000) [281]	$v = v_{PR} - c$ $c = c_1 + c_2\mu_R\omega + c_3(\mu_R\omega)^2 + c_4(\mu_R\omega)^3 \quad \mu_R = \frac{1000\mu P_c}{T_c^2}$	v^f
Li et al. (2001) [282–284]	$v_{PR} = v_{COSTALD}$	VLE
Ahlers & Gmehling (2001) [76]	$c = \delta(RT_c/P_c)(\chi - Z_c)$ $v = \begin{cases} v_{PR} - c & c = (0.3074 - Z - c) \frac{RT_c}{P_c} \left[\frac{0.35}{0.35 - (\eta T_r - \alpha)^{\gamma}} \right] \\ v_{VTPR} - c & \end{cases}$	v^f
Pedersen et al. (2002) [285,286]	$v = v_{PR} - c$ $c = c_0 + c_1(T - 288.15)$	P_vT
Lin & Duan (2005) [287]	$v = v_{PR} - c$ $c = (0.3074 - Z_c) \left(\frac{RT_c}{P_c} \right) \left[\beta + (1 - \beta) \exp(\gamma 1 - T_r) \right]$	v^f
Lin & Duan (2005) [288]	$v = v_{PR} - c$ $(0.3074 - Z_c) \left(\frac{RT_c}{P_c} \right) \left[1 - f_0(1 - T_r)^{f_1} (1 + f_2 \sqrt{1 - T_r}) \right]$	ρ
Laugier et al. (2007) [289,290]	$v = v_{PR} - c$ $c = M_w \left(\frac{1}{\rho_{ANN}} - \frac{1}{\rho_{PR}} \right)$	P_vT , VLE

Table 3 (continued)

Author(s)	Modification	Improved Properties
Amorim et al. (2007) [228]	$v = \left(\frac{M_{a_s} v_{PR}}{a_s} \right)$	ρ
Amorim (2007) [291]	$v = v_{PR} - c$ $c = v_0 + v_1 T + v_2 P^2$	—
Loria et al. (2009) [75]	$v = v_{PR} - v_{real}$ $v_{real} = \frac{M_w}{SG(\rho_{H_2O@60^\circ F})}$	v^l
Wang & Lv (2009) [292]	$v = v_{TPR} + S + \Delta v_c \left(\frac{0.35}{0.35 + 0.5(d_r \alpha_{TPR} - T_r)} \right)$	ρ, μ
Wei et al. (2011) [293]	$v = v_{PR} + S + f_c \left(\frac{0.41}{0.41 + \delta} \right)$	ρ^l, ρ^v
Baled et al. (2012) [294,295]	$v = v_{PR} - c$ $c = A + BT_r$	PvT
Abudour et al. (2012) [296,297]	$v = v_{PR} + \left(\frac{RT_c}{P_c} \right) \left[c_1 - (0.004 + c_1) \exp(-2d) \right] - \delta_c \left(\frac{0.35}{0.35 + d} \right)$	v^l
Pellegrini et al. (2012) [298]	$c = AT_r^2 + BT_r + D$	PvT
Nazarzadeh & Moshfeghian (2013) [299]	$v = v_{PR} - c$ $c = (0.3074 - Z_c) \left(\frac{RT_c}{P_c} \right) \left[\gamma + (1 - \gamma) \exp(\beta \alpha - T_r) \right]$	ρ^l
Motahhari (2013) [300]	$v = v_{PR} - c \quad c = \gamma_0 + \gamma_1 (T - 288.75)$ $v = v_{PR} + \gamma'_0 + \gamma'_1 (T - 288.75) + f_c \left(\frac{0.41}{0.41 + \delta} \right)$	PvT
Wu et al. (2013) [301]	$\mu = \mu_{PR} - c \quad c = c_0 + c'$	μ^v
Singh et al. (2013) [302]	$v = v_{PR} - c$ $c = \left(1.5448Z_c - 0.40244 \frac{RT_c}{P_c} \right) (a_1 + b_1 P + c_1 P^2 + d_1 P^3)$	PvT H ₂ O and CO ₂
Sheikhi-Kouhsar et al. (2015) [303]	$v = v_{PR} - c$ $\frac{1}{c} = a' + b'(1 - x_{ionic})^2 + c'(1 - x_{ionic})^{2.5} + d'(1 - x_{ionic})^3$ $+ e'M_w + fM_w \ln M_w + gM_w^{1.5} + hM_w^{0.5} \ln M_w + i \exp - M_w$	$PvT, PvTx$ ionic liquids
Hekayati et al. (2016) [155]	$v = v_{PR} + A_1 + A_2 (\ln P_r) \left[\frac{A_3 - \ln P_r - A_4 \ln \frac{RT_c}{P_c}}{A_3 - \ln P_r - A_4 \ln \frac{RT_c}{P_c}} \right] - A_5 \ln T_r$	PvT SC-CO ₂
Le Guennec et al. (2016) [258]	$v = v_{PR} - c$ $c = v_{PR}^l (T_r = 0.8) - \frac{RT_c}{P_c} Z_{PRA}^{(1+0.227)}$	PvT
Forero & Velásquez (2016) [157]	$v = v_{PR} - c$ $c = \left[M \cos \left(\theta + \frac{2\pi}{3} \right) - \frac{A_2}{3} \right] \frac{0.7RT_c 10^{(\omega-1)}}{P_c} - v_{DIPPR}^l (T_r = 0.7)$	v^l

3.5. Term and parameter addition

This kind of modification consists in (a) the parameter addition inside the attractive or the repulsive term of the EoS, and (b) the term addition (or term substitution) to the equation of state, which rewrites the structure of the same (see Table 4).

One of the first studies in this field was carried out by Adachi et al. [304] at 1983. They evaluated a set of possible combinations between repulsive and attractive terms of equations of state, in order to get a three-parameter EoS suitable for liquid compressibility prediction. Thus, four PR models (van der Waals [47] (original term), Scott [305], Guggenheim [306], and Carnahan-Starling [307] repulsive terms + PR attractive term) were studied

Although the study concluded in the development of a three-parameter RK EoS, two years later, Adachi et al. [308] developed an analogous model for PR equation of state.

Other modification was performed by Cismondi & Mollerup [320], who developed a three-parameter hybrid model between RK and PR, called RK-PR model, given by

$$P = \frac{RT}{v-b} - \frac{a_c \left(\frac{3}{2+T_r} \right)^k}{(v+\delta b) \left[v + \left(\frac{1-\delta}{1+\delta} \right) b \right]} \quad (39)$$

$$P = \begin{cases} \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2} & \text{van der Waals - PR (original)} \\ \frac{RT(v+b)}{v(v-b)} - \frac{a}{v^2 + 2bv - b^2} & \text{Scott - PR} \\ \frac{RT}{v(v-b)^4} - \frac{a}{v^2 + 2bv - b^2} & \text{Guggenheim - PR} \\ \frac{RT(v^3 + bv^2 + b^2v - b^3)}{v(v-b)^2} - \frac{a}{v^2 + 2bv - b^2} & \text{Carnahan - Starling - PR} \end{cases} \quad (38)$$

Table 4
Parameter and term addition or substitution applied to PR.

Author(s)	Modification	Improved properties
Rauzy (1982) [309]	$P = \frac{RT}{v+c-b} - \frac{a}{(v+c)(v+c+4.82843b)}$	—
Freze et al. (1983) [310,311]	$P = \frac{RT}{v-b} - \frac{a}{(v-r_1)(v-r_2)}$	P_vT
Adachi et al. (1985) [308]	$\frac{RT}{v-b} - \frac{a}{v(v+c)+c(v+c)}$	P_vT
Toghiani & Viswanath (1986) [312]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+cb(v+b)}$	p^{sat}
Yu & Lu (1987) [91]	$\frac{RT}{v-b} - \frac{a}{v(v+c)+b(3v+c)}$	v^I
Xiao & Lu (1988) [313]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} + \frac{RT}{v-b} R(\bar{\Lambda})$	VLE
	$P = \frac{RT}{v-b} \left[1 + \sum_{i=1}^4 D_i \left(\frac{v}{b} \right)^i \right] - \frac{a}{v(v+b)+b(v-b)}$	
Solimando et al. (1993) [314,315]	$P = \frac{RT}{v+c-b} - \frac{a}{(v+c)(v+c+4.82843b)}$	P_vT
	$+ \frac{I_m}{v} \left(\frac{b}{v+c} \eta_m \right)^x \exp \left\{ \frac{x}{2} \left[\left(\frac{b}{v+c} \eta_m \right)^2 - 1 \right] \right\}$	
Wu & Chen (1997) [316]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+0.645b(v-b)}$	P_vT , VLE, JTIC
Nasrifar & Moshfeghian (2001) [317]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-2b)}$	p^{sat} , v^I
Esmailzadeh & Roshanfekr (2004) [318,319]	$P = \frac{RT}{v-b} - \frac{a}{v(v+c)+b(v-c)}$	p^{sat} , v^I , v^J
Cismondi & Mollerup (2005) [320]	$P = \frac{RT}{v-b} - \frac{a_c \left(\frac{3}{2+T_r} \right)^k}{(v+db) \left[v + \left(\frac{1-b}{1+8} \right) b \right]}$	P_vT
Li & Firoozabadi (2009) [321]	$P = \frac{k_B T}{1-4n_{3k}} - \frac{an_{0k}^2}{1+8n_{3k}-16n_{0k}^2}$	σ
Checoni (2009) [322]	$P = \frac{RT(1+y+y^2-y^3)}{v(1-y^3)} - \frac{a}{v(v+b)+b(v-b)}$	P_vT
Papari et al. (2011) [323]	$P = \begin{cases} \frac{RT(1+y+y^2-y^3)}{v(v-y^3)} - \frac{a}{v(v+b)+b(v-b)} \\ \frac{RT(v+b)}{v(v-b)} - \frac{a}{v(v+b)+b(v-b)} \end{cases}$	P_vT
Guria & Pathak (2012) [324]	$P = \frac{RT}{v-b} - \frac{a}{[v+\varepsilon(\omega)b][v+\sigma(\omega)b]}$	P_vT
Novikova & Tyumenkov (2013) [325]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v\pm b)}$	JTIC
Chgeconi & Aznar (2014) [326]	$P = \frac{RT(1+y+y^2-y^3)}{v(1-y^3)} - \frac{a}{v(v+b)+b(v-2b)}$	p^{sat} , P_vT
Abocsky (2014) [327]	$P = \frac{RT}{v-b} - \frac{a}{v(v+c)+c(v-b)}$	—
Hekayati et al., 2016 [155]	$P = \frac{RT}{v+c-b} - \frac{a}{(v+c)(v+c-b)+b(v+c-b)}$	P_vT SC-CO ₂

Through connecting the density dependence of the SRK and PR equations of state a better modeling of P_vT properties of pure fluids was achieved. The aim of their work was to improve the representation of density for different types of compound to consider asymmetric mixtures, for example, hydrocarbon mixtures [328].

However, the hybrid model seems to keep some limitations for prediction of densities although its three-parameter structure, because it is an extension of two different two-parameter models, which are constrained because of their two-parameter nature rather than by their empirical character. These limitations were observed by Aparicio-Martinez & Hall [329], who compared this model with the PT [330] and PC-SAFT [331] equations of state for predicting density and dew point for synthetic natural gas mixtures, concluding that RK-PR has the capability for good dew point predictions, although it underestimates somewhat the cricondenbar pressure (maximum pressure at which two phases can exist in equilibrium) [332].

A last example is the model proposed by Checoni [322], who combined the hard sphere repulsion term by Carnahan & Starling (CS) [307,333], and the PR attractive term. Even, this combination was tested by Harmens & Jeremiah [334], who found that CS-PR is unsuitable for application over a wide range of pressure and temperature, Checoni successfully applied this model to liquid electrolyte-containing solutions.

3.6. Other modifications

Special approaches or applications have allowed PR to be

extended to other fields of study. Although these studies use some of the different frameworks explained here, because of their own nature, these have been independently considered. Some of these modifications are included in Table 5.

3.6.1. The crossover Peng-Robinson equation of state

A special approach was followed first by Magdziarz [343] and Feyzi et al. [341], who developed a crossover EoS based on PR equation of state. The crossover technique was implemented and applied earlier by Kiselev [344–346] to the PT equation of state. In developing crossover CEoS, the Helmholtz energy (A) is first separated into two contributions. The first contribution takes into account the singular behavior of fluids inside the critical region and the second term considers the regular behavior of fluids outside the critical region. Then, the renormalization-group theory [347–350] is applied to transform the Helmholtz energy into a crossover one [341].

The model incorporates the critical scaling laws [351,352] valid asymptotically close to the critical point and reduces to the original PR far away from the critical point, through a crossover function which has the ability to predict the rapid changes of density with the reduced temperature from inside the critical region to the region outside, through renormalization of density and temperature, which become non-analytic scaling functions of the dimensionless distance to the critical point. The crossover function [353–355] is the key variable that ensures that change, changing its value from zero at the critical point to the unit outside the critical region to reproduce the original equation of state.

Table 5

Parameter and term addition or substitution applied to PR.

Author(s)	Modification	Improved properties
Zhou et al. (1994) [335]	$A_s \pi = \frac{\sigma RT}{1 - \beta w} - \frac{\alpha w^2}{1 + 2\beta w - \beta^2 w^2}$	Adsorption isotherm
Guo et al. (1997) [336–339]	$T = \frac{rP}{\mu - b'} - \frac{a}{\mu(\mu + b) + b(\mu - b)}$	μ
Guo et al. (2001) [338]	$T = \frac{rP}{k - b'} - \frac{a}{k(k + b) + b(k - b)}$	k
Fan & Wang (2006) [340]	$T - T_d = \frac{RP}{\mu - b} - \frac{a}{\mu(\mu + b) + b(\mu - b)}$	μ
Feyzi et al. (2010) [341]	$P = \frac{RT}{v_{0c}} \left[-\frac{v_{0c}}{v_c} \left(\frac{\partial \Delta \bar{A}}{\partial \Delta \eta} \right)_T + \bar{P}_0(T) \right]$	VLE
Amooey (2014) [342]	$\pi = \frac{RT}{\sigma - \Omega} \left(1 + m \frac{\Omega}{\sigma} \right) - \frac{a}{\sigma^2 + 2\sigma\Omega - \Omega^2}$	Adsorption isotherm

Thus, a crossover PR EoS is obtained, which contains five component-dependent parameters, four crossover parameters and its inherent and constrained classical compressibility factor. The model is expressed by:

$$P = \frac{RT}{v_{0c}} \left[-\frac{v_{0c}}{v_c} \left(\frac{\partial \Delta \bar{A}}{\partial \Delta \eta} \right)_T + \bar{P}_0(T) \right] \quad (40)$$

The authors concluded that the results presented for the studied pure compounds and mixtures show comparable predictions with the original PR EoS far from the critical point and excellent agreement with experimental data close to the critical point. Other similar models for PR have been proposed in the literature [356,357].

3.6.2. Viscosity focused PR

An interesting turn in the use of the PR EoS was the transport properties prediction. There is similarity between the PvT and the $P\mu T$ relationships, which was first pointed by Philips [358] early in 1912. Since viscosity is an important parameter of compounds and the basic data for transmission and processing systems, as well as for design and operation procedures, many models have been developed for correlating viscosity, including some EoS-based models. Thus, Little & Kennedy [359] developed the first EoS-based viscosity model using the vdW EoS. The main advantages of developing a viscosity model based on an equation of state are that (a) the viscosity of both gas and liquid phases can be described by a single model, achieving smooth transition of liquid/gas viscosity in the near-critical region and (b) both high and low pressure data can be correlated, and density is not involved in evaluating the fluid viscosity [301].

In 1997, Guo et al. [339] proposed two viscosity models based on the PT and the PR equations of state (see Table 5). One year later, Guo et al. revised the viscosity model based on PR and the prediction accuracy was improved [338]. However, the primary shortcoming of Guo's model was that under critical pressure, it could not describe saturated state of PR. This was overcome by Fan & Wang [340], who developed a new PR model that, as a model imitating PR, could get a pair of results for the saturated pressure and viscosity at a specified temperature with satisfactory accuracy. This model was later improved by Wu et al. [301], who employed the critical compressibility factor of each component rather than the PR original fixed $Z_c = 0.3074$, leading to better results in pure hydrocarbon (and mixtures) viscosity prediction.

3.6.3. The confinement extended PR for porous media and the two-dimensional (2-D) PR equations of state

Yet another interesting approach on development of equations of state is the application of these to gas adsorption phenomenon. Travalloni et al. [360] extended the PR equation of state to the modeling of fluids confined in homogeneous and heterogeneous

porous media, applicable to both confined and bulk phases, giving a consistent description of the adsorption system, and expressing it as an explicit function of pore size and the molecule - wall interaction. In this way, PR takes the form:

$$P = \frac{RT}{v - b_p} - \frac{a_p}{v(1 + b_p) + b_p(v - b_p)} - \sum_{i=1} \left\{ x_i \theta_i \frac{x_i b_{p,i}}{v^2} \left(1 - \frac{x_i b_{p,i}}{v} \right)^{\theta_i - 1} (1 - F_{pa,i}) \left\{ RT \left[1 - \exp \left(-\frac{N_A \epsilon_{p,i}}{RT} \right) \right] - N_A \epsilon_{p,i} \right\} \right\} \quad (41)$$

Another approach arises if the interfacial region between a gas phase and a solid surface is visualized to be a two-dimensional non-ideal compressed fluid phase with its own thermodynamic properties, so that, it is possible to use analogs of three-dimensional equations of state, like vdW-type equations of state, to describe the adsorbed phase [361,362]. Based on the work by Vera & Prausnitz [363] for three-dimensional gases, Patrykiewicz et al. [364] extended the PR to a two-dimensional gas EoS, similar to the original form and to an Eyring's repulsive term coupled modified form [365], in order to adapt them to physical adsorption description of single gases on homogeneous solid surfaces. Both suggested equations take the form:

$$\gamma = \frac{Nk_B T}{A_s - N\beta} - \frac{a_s \alpha_s N^2}{A_s(A_s + N\beta) + N\beta(A_s - N\beta)} \quad (42)$$

$$\gamma = \frac{Nk_B T}{A_s - \sqrt{N\beta^* A_s}} - \frac{a_s \alpha_s N^2}{A_s(A_s + N\beta^*) + N\beta^*(A_s - N\beta^*)} \quad (43)$$

Zhou et al. [335] proposed a generalized model for the 2-D vdW-type equations of state, which when it is applied to PR, takes the form:

$$A_s \pi = \frac{wRT}{1 - \beta w} - \frac{\alpha w^2}{(1 + \beta w) + \beta w(1 - \beta w)} \quad (44)$$

where α and β are regressed model parameters, which must be evaluated for pure components and mixtures by correlating with experimental data [366]. Zhou et al. evaluated other 4 equations of state finding that the 2-D EoS models have different behavior from their 3-D analogs. Later, Gasem et al. [367] developed correlations for the 2-D model parameters in order to improve modeling of pure gas adsorption.

Recently, behavior of confined fluids in nanopores has been studied using a modified form of the PR EoS; the model not only shows phase changes due to pore proximity, but also it can capture the changes of critical properties [368,369].

3.6.4. The Peng-Robinson plus association (PRPA) equation of state

Since the original PR model was not enough accurate for reproduction of the liquid densities and the critical region, as well as it had limited applicability for electrolytes and high polar fluids exhibiting hydrogen bondings [370], it is necessary to incorporate or coupling associative models inside PR, in order to the study of associative compounds and their mixtures. Shinta & Firoozabadi [371] mixed PR with an authors's self-modified associative model by Anderko [372]. Also, Peng et al. [373] proposed a set of equations based on the PR EoS to improve the P^{sat} and PvT behavior prediction for H₂O and some alcohols. These and other works follow the Cubic-Plus-Association CPA concept.

Kontogeorgis et al. [374] formulated the CPA concept, which is a model that incorporates the SRK EoS and an associative model. In a similar way, Wu & Prausnitz [370] associated PR with the statistical associating fluid theory (SAFT) model [375]. To get it, the authors assumed that Helmholtz free energy (A) can be understood as the contribution of several types of interactions, so:

$$A = A_{Id} + A_{PR} + A_{Asoc} + A_{Born} + A_{Coulomb} \quad (45)$$

Based on the definition for A :

$$A = RT \int_v^\infty (Z - 1) \frac{dv}{v} \quad (46)$$

The A_{PR} term, the PR-based Helmholtz free energy, can be defined as:

$$A_{PR} = RT \ln \left(\frac{v}{v-b} \right) + \frac{a}{2\sqrt{2}b} \ln \left[\frac{v+b(1-\sqrt{2})}{v+b(1+\sqrt{2})} \right] \quad (47)$$

The contribution of A_{Asoc} , due to hydrogen bridge presence, is based on SAFT model as:

$$A_{Asoc} = RT \sum_A \left(\ln x_A + \frac{1-x_A}{2} \right) \quad (48)$$

The other contributions are based on ideal gas state (Id) and the electrostatic ionic interactions (Born and Coulomb). Wu & Prausnitz [370] studied the H₂O behavior employing a three-sites escheme [375] (two donor sites for equal H atom number and an acceptor site for the O atom in each H₂O molecule), concluding that the associative model improved itself the prediction of properties for H₂O (although the model showed some lack for representing P^{sat} and v^l in wide temperature intervals), even more if a was modified.

PR coupled with SAFT also allowed an acceptable description of hydrocarbon-rich liquid mixtures and gaseous aqueous systems. However, the model was not useful for H₂O-hydrocarbon systems, particularly those water-rich [370,376]. The problem arose in the lack of capability of SAFT for predicting the hydrocarbon solubility in water at low temperatures, where an hydrophobic effect is predominant, which is not included inside the associative model. Even so, the authors got a just five-adjustable parameter model.

In the same framework, Huang et al. [377] considered just association rather than electronic interactions, in order to get a strictly analogous model to CPA. As Kontogeorgis et al. [374], the authors defined the associative term through the use of original Wertheim's thermodynamic perturbation theory of associating fluids [378–381] and SAFT:

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} + \frac{RT}{v^2} \sum_i \left[x_i \sum_{A_i} \left(\frac{1}{X^{A_i}} - \frac{1}{2} \right) \left(\frac{\partial X^{A_i}}{\partial \rho} \right)_{T,x_i} \right] \quad (49)$$

This approach, however, was first visited some years before by Michelsen & Hendriks [382], who found that the association terms of SAFT and CPA were formally identical. Thus, they derived [382,383] a simpler and computationally more efficient expression for the associative term [384]:

$$P = P_{EoS \text{ repulsive term}} - P_{EoS \text{ attractive term}} + \frac{RT}{2v} \left[1 + \frac{1}{v} \left(\frac{\partial \ln g}{\partial \rho} \right) \right] \times \sum_i x_i \sum_{A_i} (1 - X^{A_i}) \quad (50)$$

Eslami & Khadem-Hamedani [240] extended PRPA by modifying the energy a and covolume b parameters through the introduction of correction factors as functions of reduced temperature. A homologous framework was recently proposed by Shojaeian [385], who defined a Peng Robinson - Two-state association model, i.e. PR EoS plus Two-state association model, which was applied to model the PvT behavior of pure ionic liquids and solubility of H₂S. The author defined the model as

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} - RT \sum_i x_i \frac{\sum_j x_j v_{ij} f_{ij}}{v(\nu + \sum_j x_j v_{ij} f_{ij})} \quad (51)$$

Other associative PR models are listed in Table 6.

4. Mixtures: the mixing rule cases

To extend the applicability of equations of state to mixtures, mixing rules are used. Solorzano Zavala et al. [393] highlighted some essential features of a convenient mixing rule, such as [43]: (a) a simple form with few parameters, (b) invariant to the division of a component into identical subcomponents (not suffering from Michelsen-Kistenmacher syndrome [394]), (c) predicting satisfactorily VLE of non-polar and highly non-ideal binary and multi-component mixtures, (d) capable of predicting other properties like enthalpy and entropy, etc., (e) applicable to prediction of liquid-liquid and liquid-liquid-vapor equilibria, and (f) able to use the parameters of a $\gamma - \phi$ model. It may not be possible to meet all these requirements simultaneously, but having most of these characteristics expand the applicability of the EoS.

4.1. Classical mixing rules

Peng & Robinson extended their model to mixtures. To get it, they employed the conventional mixing rules as modified by Zudkevitch & Joffe [395]:

$$a = \sum_{i=1}^n \sum_{j=1}^n x_i x_j a_{ij} \quad (52)$$

$$a_{ij} = \sqrt{a_i a_j} (1 - \delta_{ij}) \quad (53)$$

Table 6
Some modifications to associative models coupled to PR.

Author(s)	Modification
Shinta & Firoozabadi (1995) [371]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} + \frac{RT}{v} \left[\frac{\zeta X_A}{\sqrt{\zeta + \frac{RTK_{SA}}{v} + \beta} \left(\frac{RTK_{SA}}{v} \right)^2} - X_A \right]$
Pfohl et al. (1999) [386]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} + \frac{RT}{v} \left[\frac{\partial \left(\frac{A_{\text{Assoc}}}{RT} \right)}{\partial \rho} \right] \rho$
Silva-Santos (2003) [387]	$P = \frac{RT}{\zeta(v-b)} - \frac{a}{v(v+b)+b(v-b)}$
Peng et al. (2005) [373]	$P = \left[\frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} \right] \left(1 - \frac{X_A}{2} + \frac{X_A}{1 + \sqrt{1 + \frac{8aRTK_{SA}}{v-b}}} \right)$
Zoghi et al. (2011) [388]	$P = \frac{RT}{v-b\beta'} - \frac{a}{v(v+b\beta')+b\beta'(v-b\beta')} - \frac{RT}{2v} \left[1 + \rho \left(\frac{\partial \ln g(\rho)}{\partial \rho} \right) \right] \sum_i [X_i \sum_j (1 - X_{A_{ij}})]$
Ma et al. (2012) [389,390]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} + \frac{RT}{v} \sum_i \left[X_i \left(\frac{1}{X_i} - \frac{1}{2} \right) \rho_0 \left(\frac{\partial X_i}{\partial \rho_0} \right) \right]$
Checoni & Ravagnani (2013) [391]	$P = \frac{RT(1+y+y^2-y^3)}{v(1-y^3)} - \frac{a}{v(v+b)+b(v-b)} - \frac{RT}{2v} \left(1 + \frac{1.9pb}{4-1.9pb} \right) \sum_A (1 - X_A)$
Arvelos et al. (2014) [392]	$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} - \frac{RT}{2v} \left[1 + \rho \left(\frac{\partial \ln g(\rho)}{\partial \rho} \right) \right] \sum_i \sum_{A_i} X_i (1 - X_{A_i})$

$$b = \sum_{i=1}^n x_i b_i \quad (54)$$

where δ_{ij} is an empirical parameter, called binary interaction parameter. It is a correction of the deviation between the EoS prediction and the experimental data, which, without a theoretical basis, accounts for the difference in the interaction between unlike molecules, directly connected to the extent of non-ideality of the mixture [396,397].

4.1.1. Approaches for δ_{ij} estimation

Since the binary interaction parameters δ_{ij} (or k_{ij}) could not be predicted *a priori* from existing theory, they were (and in most of

generalized models to estimate binary interaction parameters using a quantitative structure-property relationship (QSPR) modeling approach [402]. First, binary interaction parameter were determined by fitting on experimental VLE data and then were generalized using QSPR modeling methodology. Results indicated that the generalized model provides bubble-point pressure predictions within two times the errors obtained through direct regressions of the binary interaction parameters [401].

4.1.2. Predictive Peng-Robinson 1978 (PPR78) equation of state

In 2004, Jaubert & Mutelet [457] introduced PPR78, which is a model based on 1978-Robinson & Peng modification [69] that incorporates an own group contribution method [426] for estimating k_{ij} :

$$k_{ij} = \frac{-\frac{1}{2} \sum_{l=1}^{N_g} \sum_{k=1}^{N_g} \left[(\alpha_{ik} - \alpha_{jk}) (\alpha_{il} - \alpha_{jl}) A_{kl} \left(\frac{298.15}{T} \right)^{\left(\frac{b_{kl}}{A_{kl}} - 1 \right)} \right] - \left(\frac{\sqrt{a_i}}{b_i} - \frac{\sqrt{a_j}}{b_j} \right)^2}{2 \frac{\sqrt{a_i a_j}}{b_i b_j}} \quad (55)$$

cases, they are still) fitted on VLE experimental data, and lately on VLLE experimental data, for modeling of complex multiphase equilibrium [398,399]. The above has given many possible correlations according to the studied system (see Table 7). However, also it is possible to use alternate techniques. An example of that approach, Li & Yang [400] developed a hybrid model formed by PR and a genetic algorithm, for the extraction process modeling with supercritical fluids (SCF). This model can find nonlinear binary interaction parameters. In this way, the proposed hybrid model is able to select interaction parameters near the optimal one, in order to adjust prediction to experimental process data. Thus, this model, optimized by genetic algorithms, keeps the structure and physical meaning of a and b , while simultaneously can optimize non-linear binary interaction parameters, achieving a better prediction (until 22% more) than conventional PR model [400].

In a similar way, Abudour et al. [401] developed some

PPR78 can be seen as the combination of the PR78 equation of state with a van Laar-type activity coefficient (G^E) model [458] under infinite pressure (which relies on the Huron-Vidal mixing rules [459]), inside a classic vdW one-fluid mixing rule for a . In this way, it was possible to accurately estimate k_{ij} for saturated hydrocarbon systems at the beginning. Besides, the model improved the description of the critical region for binary systems, as well as VLE for asymmetric mixtures. This model has been successfully extended to several systems [460–474], including mixtures of H₂O, CO₂, N₂ and H₂S, mercaptans, H₂, and alkenes; even, it has been used to convert binary interactions parameters k_{ij} generated by the PPR78 method to the equivalent k_{ij} for a target EoS and α function [475].

Qian [476] extended PPR78 to the Enhanced Predictive Peng-Robinson 1978 (E-PPR78) EoS, with the aim of simultaneously correlating H^E , C_p^E and VLE data better than PPR78 by refitting group

Table 7Some modifications to a_{ij} and δ_{ij} interaction parameters in Eqs. (52) and (53).

Author(s)	Modification
Mulliken & Sandler (1990) [403–405]	$\delta_{ij} = F - GTr - H\gamma - K\omega$
Kato et al. (1981) [406,407]	$\delta_{ij} = a'(T - b')^2 + c'$
Valderrama & Reyes (1983) [408]	$\delta_{ij} = \alpha + \frac{\beta}{T_j}$
Lin (1984) [409]	$\delta_{ij} = 0.122 + 5.3 \times 10^{-4}A$
Stryjek & Vera (1986) [49,410]	$a_{ij} = \sqrt{a_i a_j} (1 - x_i \delta_{ij} - x_j \delta_{ji})$ $a_{ij} = \sqrt{a_i a_j} \left(1 - \frac{\delta_{ij} \delta_{ji}}{x_i \delta_{ij} + x_j \delta_{ji}} \right)$
Varotsis et al. (1986) [411]	$\delta_{ij} = \delta_2 T_r^2 + \delta_1 T_r + \delta_0$
Valderrama & Molina (1986) [412]	$\delta_{ij} = A + BT + CT^2$
Panagiotopoulos & Reid (1986) [413]	$a_{ij} = \sqrt{a_i a_j} [1 - \delta_{ij} + x_i (\delta_{ij} - \delta_{ji})]$
Heidemann & Rizvi (1986) [414]	$\delta_{ij} = A + B \left(\frac{T}{647.29} \right) + C \left(\frac{T}{647.29} \right)^2$
Mohamed & Holder (1987) [209,415]	$\delta_{ij} = \alpha_{ij} + \beta_{ij} \rho$
Nishiumi et al. (1988) [416,417]	$1 - \delta_{ij} = C + D \left(\frac{v_{ci}}{v_{cj}} \right) + E \left(\frac{v_{cj}}{v_{ci}} \right)^2$
Tanishita et al. (1988) [418]	$\delta_{ij} = \left\{ \begin{array}{l} 1 - K_1 - K_2 \left(\frac{v_{ci}}{v_{cj}} \right) - K_3 \left(\frac{v_{cj}}{v_{ci}} \right)^2 - K_4 \left \omega_i - \omega_j \right \\ -K_5 \left \omega_i - \omega_j \right ^2 - K_6 \left(\frac{M_{wi}}{M_{wj}} \right) - K_7 \left(\frac{M_{wi}}{M_{wj}} \right)^2 \end{array} \right\}$
Sandoval et al. (1989) [419]	$\delta_{ij} = \left\{ \begin{array}{l} \bar{k}_{ij} + \Delta k_{ij} x_i + \Delta k_{ji} x_j \\ \bar{k}_{ij} + \Delta k_{ij} x_i + \Delta k_{ji} x_j + l_{ij} [x_i (1 - x_i) + x_j (1 - x_j)] \\ \bar{k}_{ij} + \left(\frac{v^j}{v} \right) (\Delta k_{ij} x_i + \Delta k_{ji} x_j) \\ k_{ij}^0 + \left(\frac{v^j}{v} \right) [(\bar{k}_{ij} - k_{ij}^0) + \Delta k_{ij} x_i + \Delta k_{ji} x_j] \end{array} \right\}$
Slot-Petersen (1989) [10]	$\delta_{ij} = m_i (M_{wi})^n + d_i$
Stryjek (1989) [420]	$\delta_{ij} = \delta_{ij}^{(0)} + \delta_{ij}^{(T)} (T - 273.15)$
Nishiumi & Gotoh (1990) [421]	$1 - \delta_{ij} = \begin{cases} 1.224 - 0.00440T + 3.251 \times 10^{-5} T^2 & T < 461.75 \text{ K} \\ 56.98 - 0.1655T + 1.199 \times 10^{-4} T^2 & T \geq 461.75 \text{ K} \end{cases}$
Valderrama et al. (1990) [422]	$\delta_{ij} = \delta_{ij,0} + \delta_{ij,1} \left(\frac{T}{273.15} - 1 \right)$
Treble & Sigmund (1990) [423,424]	$1 - \delta_{ij} = \left(\frac{v_i v_j}{v_{ij}^2} \right)^\theta - \eta \left[\frac{v_i \mu_j^2 + v_{ij} \mu_i^2}{v_{ij}^2} + \frac{1.5(v_i Q_i^2 + v_j Q_j^2)}{\left(\frac{8}{3} \right)} \right] \frac{1}{v_{ij}}$
Dohrn et al. (1991) [425]	$\delta_{ij} = \delta_{ij,0} + \delta_{ij,1} v^{\vartheta}$
Abdoul et al. (1991) [426]	$\delta_{ij} = \frac{E_{ij} - (\delta_i - \delta_j)^2}{2\delta_i \delta_j}$
Gao et al. (1992) [427]	$\delta_{ij} = 1 - \left(\frac{2 \sqrt{T_{ci} T_{cj}}}{T_{ci} + T_{cj}} \right)^{Z_{ij}}$
Bartle et al. (1992) [428]	$\delta_{ij} = 0.51A(\omega_j - \omega_i) \left(\frac{v_{ci}}{v_{cj}} \right) \left(\frac{P_{cj}}{P_{ci}} \right)^2$
Voros & Tassios (1993) [429]	$\delta_{ij} = a + bP$
Schulze (1993) [430]	$\delta_{ij} = 0.41 \ln(\theta + 1.13) - 0.50$
Avlonitis et al. (1994) [431]	$\delta_{ij} = Q - \frac{T_r^2 + A}{T_r^2 + C}$
Firoozabadi et al. (1994) [432]	$\delta_{ij} = \delta_{ij}^0 \left(1 + \frac{\gamma_{ij}}{\beta + \delta} \right)$
Kordas et al. (1994) [433]	$\delta_{ij} = a + bT_r + cT_r^3$
Arbabi & Firoozabadi (1995) [434]	$\delta_{ij} = a' + b'M_{wi}$
Carroll & Mather (1995) [435]	$\delta_{ij} = A + Bq + Cq^2$
Kordas et al. (1995) [436]	$1 - \delta_{ij} = \begin{cases} -0.13409\omega + 2.28543\omega^2 - 7.61455\omega^3 & N_C \leq 20 \\ +10.46565\omega^4 - 5.2351\omega^5 \\ -0.04633 - 0.04367 \ln \omega & N_C > 20 \end{cases}$
Shinta & Firoozabadi (1997) [437]	$\delta_{ij} = 0.469925 - 3.28256T_r + 3.1679T_r^2$
Enick et al. (1998) [438]	$\delta_{ij} = aT^3 + bT^2 + cT + d$
Stamatakis & Magoulas (2000) [439]	$\delta_{ij} = a + b\omega_j$
Oellrich & Althaus (2001) [124,125,440]	$\delta_{ij} = A + \frac{B}{T_j}$
Mutelet (2001) [224]	$a_{ij} = \left(\alpha_1 + \alpha_2 T + \frac{\alpha_3}{T} + \alpha_4 \ln T \right) F_1 F_2$
Mutelet & Rogalski (2001) [441]	$a_{ij} = \left(\alpha_1 + \alpha_2 T + \frac{\alpha_3}{T} + \alpha_4 \ln T \right) \left(c + rR_2 + s\pi_2^H + b \sum \beta_2^H + l \log L^{16} \right)$
Yarrison et al. (2006) [442]	

Table 7 (continued)

Author(s)	Modification
Chen et al. (2008) [443]	$\delta_{ij} = aT^3 + bT + c$
Chen et al. (2009) [444]	$\delta_{ij} = \delta_i - \delta_j$
Barrios et al. (2011) [445–447]	$\delta_{ij} = A + BT_{b_i}$
	$\delta_{ij} = c - \frac{d}{ 1 - T_{r_j} }$
Escandell et al. (2011) [448]	$\delta_{ij} = \delta_{ij}^{(0)} + \rho_{ij}^{(0)} \left(\frac{b}{\sum_i x_i q_i G_{ij}} + \frac{b}{\sum_j x_j q_j G_{ji}} \right)$
Hu et al. (2012) [449]	$\delta_{ij} = \frac{\omega_j \sqrt{P_{r_j}}}{I_{c_j}} \delta_i - \frac{\omega_i \sqrt{P_{r_i}}}{I_{c_i}} \delta_j$
Fateen et al. (2013) [450]	$\delta_{ij} = 1 - \frac{1}{2} \frac{b_i}{b_j} \sqrt{\frac{a_i}{a_j}} - \frac{1}{2} \frac{b_j}{b_i} \sqrt{\frac{a_j}{a_i}} + \frac{1}{2} \frac{b_i RT}{\sqrt{a_i a_j}} \frac{\theta_1}{T_{r_i}^2 P_{r_i}^2}$
Venkatramanic & Okuno (2014) [451,452]	$\delta_{ij} = c_1 [1 + \exp(c_2 - c_3 M_w)] \left(\frac{-1}{c_4} \right)$
Li et al. (2014) [453,454]	$1 - \delta_{ij} = \begin{cases} a_1 + a_2 C_{sw} + (a_3 + a_4 C_{sw}) T_{r_i} + (a_5 + a_6 C_{sw}) T_{r_i}^2 \\ \quad + [a_7 + a_8 C_{sw} + (a_9 + a_{10} C_{sw}) T_{r_i}] \ln P \\ a_1 + a_2 C_{sw} + (a_3 + a_4 C_{sw}) T_{r_i} + (a_5 + a_6 C_{sw}) T_{r_i}^2 \end{cases}$
Myint et al. (2016) [244]	$\delta_{ij} = k_3 (T - T_{\text{eutectic}})^3 + k_2 (T - T_{\text{eutectic}})^2 + k_1 (T - T_{\text{eutectic}}) + k_0$
Li et al. (2016) [455]	$\delta_{ij} = \frac{c_1 + c_2 T_{r_j} + c_3 T_{r_j}^2 + d_1 \omega_j}{1 + c_4 T_{r_j} + c_5 T_{r_j}^2 + d_2 \omega_j + d_3 \omega_j^2 + d_4 \omega_j^3}$
Zhang et al. (2016) [456]	$\delta_{ij} = w_j \delta_i + w_i \delta_j \ (i \neq j)$

The authors encourage very much to readers to consult the original references for more detailed information on mixing rules and specific applications.

Table 8

Some modifications to a_{ij} or k_{ij} (Eqs. (52) and (53)) and b_{ij} or l_{ij} (Eqs. (56) and (57)) parameters.

Author(s)	Modification
Wenchuang & Kunyuan (1989) [93]	$k_{ij} = 0$
De Leeuw et al. (1992) [492]	$k_{ij} = k_{ij}^0 + m_{ij} T + \frac{o_{ij}}{v}$
Gasem et al. (1993) [493]	$k_{ij} = A_1 + A_2 \omega$
Kordas et al. (1994) [433]	$k_{ij} = a + b T_{r_i} + c T_{r_i}^3$
Chai Kao et al. (1995) [494]	$k_{ij} = \frac{x_i \Delta_{ij} + x_j \Delta_{ji}}{x_i + x_j}$
Gao et al. (2003) [495]	$k_{ij} = 1 - \left(\frac{a_{ij}^{N_{ij}} + a_{ji}^{N_{ij}}}{2} \right)^{\frac{1}{N_{ij}}}$
Abudour et al. (2012) [496]	$k_{ij} = aT^2 - bT - c$
	$b_{ij} = \left(\frac{\sqrt[3]{b_i} + \sqrt[3]{b_j}}{2} \right)^3 \left(1 - I_{ij}^0 - I_{ij}^1 \frac{T}{1000} \right)$
	$l_{ij} = I_{ij}^0 + n_{ij} T + \frac{p_{ij}}{v}$
	$l_{ij} = A_3 + A_4 \omega$
	$l_{ij} = \text{constant}$
	$l_{ij} = \text{constant}$
	$b_{ij} = \left(\frac{b_i^{M_{ij}} + b_j^{M_{ij}}}{2} \right)^{\frac{1}{M_{ij}}}$
	$l_{ij} = AT^2 + BT + C$

contribution parameters. This model has been successfully extended to incorporate new species, such as permanent gases (CO, He, Ar, SO₂, O₂, NO, COS, NH₃, NO₂, N₂O), refrigerants and even pseudocomponents [332,477–480]. Later, Hajiw et al. [481,482] connected PPR78 with the CPA EoS, through a model called GC-PR-CPA. This model was successfully applied to hydrocarbon systems containing methanol and, light and medium hydrocarbon-water mixtures. In the last case, k_{ij} was additionally modified for incorporating of three new interaction parameters for water [481] (see Table 9).

4.2. Conventional and unconventional mixing rules: other methodologies

With classical mixing rules [483], thereby, PR achieves an adequate prediction of the VLE for hydrocarbon mixtures, especially paraffins. For these mixtures, PR also achieves an accurate description of the PvT behavior [3]. However, it is limited to non-polar mixtures by using conventional mixing rules, and in consequence, as PR was applied to new systems (like strongly polar and hydrogen-bonded fluids, or common gases and hydrocarbons mixtures), it was necessary to adjust or improve the existing mixing rules for a (Eq. (52)) and b , such as eq. (54) and:

$$b = \sum_{i=1}^n \sum_{j=1}^n x_i x_j b_{ij} \quad (56)$$

$$b_{ij} = \frac{b_i + b_j}{2} (1 - l_{ij}) \quad (57)$$

where l_{ij} is an empirical binary interaction parameter. For those systems, the assumption of simple (random) mixing is poor because strong polarity and hydrogen bonding can produce significant segregation or ordering of molecules in mixtures [135]. So, required modifications included, besides of the binary interaction parameter δ_{ij} modification [407,412,416,419,426,433,436], the incorporation of the local composition concept [84,484,485], and mixing rules coupled with G^E models [486–491], between others. Some of these modifications are listed in Table 8 and Table 9.

Like happens with other cubic equations of state (i.e., SRK), it is possible to connect mixing rules with G^E models at different conditions and with different activity coefficient (γ) models. For example, Lee & Lin [497] and Hsieh et al. [498] used COSMO-SAC [499,500], while Neau et al. [488,501,502] used NRTL, Tochigi [503] used ASOG [504], and Ahlers & Gmehling [505] and Collinet & Gmehling [506] used UNIFAC [507,508] and LIFAC [509]

Table 9Other modifications to a , b and other parameters.

Author(s)	Modification
Mollerup (1981) [485]	$a = \sum_i^n \left[x_i q_i - \frac{\sum_j \left(\frac{x_i b_j q_{ij}}{q_{ji}} \right)}{\sum_j x_j E_{ji}} \right]$
Cheok et al. (1986) [519]	$a = 0.45724 \frac{RT_{cm}^2}{P_{cm}} [1 + p_m (T_m^*)^{q_m}]$ $b = 0.07780 \frac{RT_{cm}}{P_{cm}}$
Benmekki & Mansoori (1987) [520,521]	$b = \sum_i^n \sum_j^n x_i x_j \left(\frac{\sqrt[3]{b_i} + \sqrt[3]{b_j}}{2} \right)^3 (1 - l_{ij})^3$ $c = \sum_i^n \sum_j^n x_i x_j b_{ij} \sqrt{\frac{c_i c_j}{b_i b_j}} (1 - k_{ij})$ $d = \sum_i^n \sum_j^n x_i x_j \left(\frac{\sqrt[3]{d_i} + \sqrt[3]{d_j}}{2} \right)^3 (1 - m_{ij})^3$
Gangadhara Rao & Mukhopadhyay (1989) [522]	$a = \sum_i^n \sum_j^n x_i x_j a_{ij} \left(\frac{b}{b_{ij}} \right)^m$ $b = \sum_i^n \sum_j^n x_i x_j b_{ij}$ $a = \sum_i^n \sum_j^n x_i x_j \sqrt{a_i a_j}$
Wenchuan & Chongli (1989) [484,523]	$b = \sum_i^n \sum_j^n x_i x_j [1 - k_{b_{ij}} + (k_{b_{ij}} - k_{b_{ji}}) x_i] \left(\frac{\sqrt[3]{b_i} + \sqrt[3]{b_j}}{2} \right)^3$
Michelsen (1990) [515]	$a = b \left\{ \sum_i^n x_i \frac{a_i}{b_i} + \frac{G^E}{q_i} + \frac{RT}{q_i} \sum_i^n x_i \ln \frac{b}{b_i} \right\}$
Kwak & Anderson (1991) [106]	$a = \sum_i^n \sum_j^n \left\{ \frac{x_i x_j a_{ij}}{\sum_i^n \left[x_i \exp \left(\frac{\Delta u_{ik} - \Delta u_{ij}}{RT} \right) \right]} \right\}$
Mathias et al. (1991) [524]	$a = \sum_i^n \{ x_i [\sum_j^n x_j \sqrt{a_i a_j} (1 - k_{ij})] \} + \sum_i^n \{ x_i [\sum_j^n x_j (\sqrt{a_i a_j} l_{ij})^{1/3}]^3 \}$
Wong & Sandler (1992) [517]	$a = b \left(\sum_i^n x_i \frac{a_i}{b_i} + A_{\infty}^E \right)$ $b = \frac{\sum_i^n \sum_j^n x_i x_j \left(\frac{b_{ij} - a_{ij}}{RT} \right)}{1 - \frac{A_{\infty}^E}{RT} - \sum_i^n x_i \frac{a_i}{RT b_i}}$
Boukouvalas et al. (1994) [165,491,525]	$a = b \left\{ \left(\frac{\lambda}{A_v} + \frac{1-\lambda}{A_m} \right) G^E + \frac{RT(1-\lambda)}{A_m} \sum_i^n \left[x_i \ln \left(\frac{b}{b_i} \right) \right] + \sum_i^n \left[x_i \left(\frac{a_i}{b_i} \right) \right] \right\}$ $a = b \left(\sum_i^n x_i \frac{a_i}{b_i} + \frac{A^E}{CRT} \right)$ $b = \frac{\sum_i^n \sum_j^n x_i x_j \left[\frac{b_i + b_j}{2} - \frac{\sqrt{a_i a_j} (1 - k_{ij})}{RT} \right]}{1 - \frac{A^E}{CRT} - \sum_i^n x_i \frac{a_i}{RT b_i}}$
Orbey & Sandler (1995) [490]	$\frac{a}{b} = \sum_i^n x_i \frac{a_i}{b_i} \times \frac{\ln \frac{1 + \sqrt{2} + \frac{a_i}{b_i}}{1 - \sqrt{2} + \frac{a_i}{b_i}}}{\ln \frac{1 + \sqrt{2} + \frac{a_j}{b_j}}{1 - \sqrt{2} + \frac{a_j}{b_j}}} - \frac{2\sqrt{2}}{\ln \frac{1 + \sqrt{2} + \frac{a_j}{b_j}}{1 - \sqrt{2} + \frac{a_j}{b_j}}} \left\{ \frac{G_0^E}{RT} + \sum_i^n x_i \ln \frac{b}{b_i} + \sum_i^n x_i \ln \frac{\sum_j x_j \frac{a_{ij}}{b_j} - 1}{\frac{a_i}{b_i} - 1} \right\}$ $b = \frac{a}{RT} + \sum_i^n \sum_j^n \left[x_i x_j \left(\frac{b_i + b_j}{2} + \frac{\sqrt{a_i a_j}}{RT} \right) \right]$ $b = \sum_i^n x_i b_i + b^E$ $c = \frac{1}{x_{ps}} \sum_i^n x_i c_i$ $a = bF \left(\sum_i^n x_i \frac{a_i}{b_i} + \frac{G_0^E}{C^E} \right) + RT \left[b - \sum_{i=1}^n \left(b_i - \frac{a_i}{RT} \right) \right] (1 - F)$
Tochigi et al. (1995) [503,526]	$a = b \left(\sum_i^n x_i \frac{a_i}{b_i} \right)$ $b = \frac{\sum_i^n \sum_j^n x_i x_j \left(\frac{b_{ij} - a_{ij}}{RT} \right)}{1 - \sum_i^n x_i \frac{a_i}{RT b_i}}$ $a = \left(\sum_i K_i y_i \sqrt{a_i} \right)^2$ $a = b \left(\sum_i^n x_i \frac{a_i}{b_i} - \frac{A_{\infty}^E}{\sigma RT} \right)$ $b = \frac{\sum_i^n \sum_j^n x_i x_j (1 - k_{ij}) \left[\left(\frac{\sqrt[3]{b_i} + \sqrt[3]{b_j}}{2} \right)^3 - \frac{2\sqrt[3]{l_{ij}}}{l_i + l_j} \times \frac{64 b_i b_j}{(\sqrt[3]{b_i} + \sqrt[3]{b_j})^6} \times \frac{\sqrt{a_i a_j}}{RT} \right]}{1 + \frac{A_{\infty}^E}{\sigma RT} - \sum_i^n x_i \frac{a_i}{RT b_i}}$
Chen et al. (1995) [527]	
Ungerer & Batut (1996) [277,528]	
Ioannidis (1996) [529]	
Zhong & Masuoka (1996) [530]	
Young (1997) [531,532]	
Fotouh & Shukla (1998) [489]	
Sun et al. (2001) [533]	

Table 9 (continued)

Author(s)	Modification
Voutsas et al. (2004) [534,535]	$b = \sum_{i=1}^n \sum_{j=1}^n y_i y_j \sqrt{b_i b_j (1 - l_{ij})}$ $a = \frac{RTB}{A} \left(\frac{G_{ac}^E + G_{ac}^E}{RT} + A \sum_i x_i \frac{a_i}{RTb_i} \right)$ $b = \sum_i^n \sum_j^n x_i x_j \left(\frac{b_i^{1/3} + b_j^{1/3}}{2} \right)^2$
Valderrama & Álvarez (2004) [88,536]	$a = \sum_{i=1}^n \sum_{j=1}^n x_i x_j \sqrt{a_i a_j (1 - k_{ij})}$ $b = \sum_{i=1}^n \sum_{j=1}^n x_i x_j \frac{b_i + b_j (1 - \beta_j)}{2}$ $d = \sum_{i=1}^n \sum_{j=1}^n x_i x_j \frac{d_i + d_j (1 - \delta_j)}{2}$
Lazzaroni et al. (2004) [537]	$a = b \left[\sum_i x_i \frac{a_i}{b_i} + \frac{G_{ac}^E}{q_1} + \frac{RT}{q_1} \sum_i x_i \ln \left(\frac{b_i}{b} \right) \right]$
McFarlane et al. (2007) [538,539]	$b = \sum_{i=1}^n \sum_{j=1}^n x_i x_j [(1 - m_{ij})b_{ij} + m_{ij}b_{ij}^*]$
Hsieh & Lin (2008) [540–542]	$a = \frac{b}{C} \Delta G^{chg} \quad b = \sum_i^n x_i b_i$
Foster (2009) [543]	$a = b \left(\sum_i^n x_i \frac{a_i}{b_i} - \frac{G_{ac}^E + G_{ac}^E}{0.53087} \right)$
Neau et al. (2010) [448, 488, 544–546]	$a = b \left[\sum_i^n x_i \frac{a_i}{b_i} - \frac{1}{b} \sum_i^n \left(x_i q_i \frac{\sum_j^n x_j q_j G_{ji}}{\sum_j^n x_j q_j G_{ji}} \right) \right]$
Wei et al. (2011) [293]	$c = \sum_{i=1}^n x_i c_i + c^E$
Maoxing et al. (2011) [547]	$a = \sum_{i=1}^n \sum_{j=1}^n x_i x_j \sqrt{a_i a_j} \{ 1 - (c_{ij} - d_{ij}T) + [c_{ij} - c_{ji} + (d_{ij} - d_{ji})T]x_{ij} \}$
Gomes et al. (2012) [548,549]	$a = \sum_{i=1}^n \sum_{j=1}^n x_i x_j \sqrt{a_i a_j} (1 - k_{ij} M_{wi})$
Costa et al. (2013) [550–552]	$b = \sum_{i=1}^n x_i b_i + x_H \sum_{j=1}^n x_j E_{Hj} M_{wi}$
Colpas Castillo et al. (2013) [553]	$a = b \left[\left(\frac{\lambda'}{A_v} + \frac{1 - \lambda'}{A_m} \right) G^E + \frac{RT(1 - \lambda')}{A_m} \times \sum_i^n x_i \ln \frac{b_i}{b} + \sum_i^n x_i \frac{a_i}{b_i} \right]$
Hajiw et al. (2015) [481,482]	$a = a_1 \quad a_2 = a_1 \alpha^2 \quad b = b_1 \quad b_2 = b_1 \beta$ $a = \sum_{i=1}^n \sum_{j=1}^n x_i x_j \sqrt{a_i a_j} \left(1 - \frac{-\frac{1}{2} \Sigma_{H_2O} - \left(\frac{\sqrt{a_i} - \sqrt{a_j}}{b_i - b_j} \right)^2}{2 \frac{\sqrt{a_i a_j}}{b_i b_j}} \right)$
Han et al. (2015) [554]	$\Sigma_{H_2O} = \sum_{k=1}^{H_2O} (\alpha_{ik} - \alpha_{jk})(\alpha_{iH_2O} - \alpha_{jH_2O})(C_{kH_2O}T^2 + D_{kH_2O}T + E_{kH_2O})$ $+ \sum_{l=1}^{H_2O} (\alpha_{iH_2O} - \alpha_{jH_2O})(\alpha_{il} - \alpha_{jl})(C_{lH_2O}T^2 + D_{lH_2O}T + E_{lH_2O})$ $b = \sum_i^n \sum_j^n x_i x_j \left(\frac{b_i + b_j}{2} \right) (1 - l_{ij})$ $l_{ij} = 1 - \frac{2 \sqrt{b_i b_j}}{b_i + b_j} \times \frac{\sqrt{\theta_i \theta_j}}{\theta_{ij}} \times \frac{\sqrt{\theta_i \theta_j}}{\theta_{ij}}$
Sheikhi-Kuhsat et al. (2015) [303]	$c = \frac{1}{a + bx^2 + cx^{2.5} + dx^3 + fM_w \ln M_w + gM_w^{1.5} + hM_w^{0.5} \ln M_w + i \exp(-M_w)}$
Zhao & Lvov (2016) [555]	$a = RT \left(\sum_i^n x_i \frac{a_i}{b_i RT} - \frac{G^E}{CRT} \right) \frac{\sum_i^n \sum_j^n x_i x_j \left\{ \frac{b_i + b_j}{2} \sqrt{\frac{a_i a_j (1 - d'_{ij} - d'_{ji} - d'_{ij} x_{ij})}{RT}} \right\}}{1 - \sum_i^n x_i \frac{a_i}{b_i RT} - \frac{G^E}{CRT}}$
Neau et al. (2016) [502]	$b = \frac{\sum_i^n \sum_j^n x_i x_j \left\{ \frac{b_i + b_j}{2} \sqrt{\frac{a_i a_j (1 - d'_{ij} - d'_{ji} - d'_{ij} x_{ij})}{RT}} \right\}}{1 - \sum_i^n x_i \frac{a_i}{b_i RT} - \frac{G^E}{CRT}}$ $a = RTb \sum_i^n \frac{a_i}{b_i RT} - \frac{1}{0.53} \left[\frac{\sum_{i=1}^{i=(200)} (x_i X_i^{(2i-1)} - X_i) E_{i(200)}^0 + \sum_i x_i q_i \left(\sum_{j=1}^n \frac{x_j q_j G_{ji} \Gamma_{ji}}{\sum_{m=1}^n x_m q_m \Gamma_{mi}} \right)}{RT} \right]$

respectively. Since the coupling of mixing rules with well-selected G^E models can lead to very accurate results, this kind of connections (EoS/ G^E) is one of the reasons for the popularity of PR (like happens with some other cubic equations of state), especially because of the availability of group contribution schemes which allows the prediction of substance and mixture parameters from chemical structures [510].

The starting point of many but not all EoS/ G^E mixing rules is the equality of excess Gibbs energy (G^E) or the excess Helmholtz energy (A^E) from the CEoS and the external activity coefficient model, which must be set at some suitable pressure [511]; such models are pressure-independent (they only depend on temperature and composition) but the same quantity from an EoS depends on

pressure, temperature and composition, which explains why it is necessary to select a reference pressure before equating both quantities [512]. Huron & Vidal (HV) [459] were the first in presenting this kind of model and they assumed infinite pressure as reference point using the SRK EoS (but other EoS could be used as well). However, a limitation of the HV mixing rule is that it does not permit the use of the large parameter collection of models such as Wilson, UNIQUAC or UNIFAC, due to they are based on low-pressure VLE data [513]; therefore, the zero reference pressure was an alternative solution and it was introduced by Mollerup [514] and Michelsen [515,516].

Wong & Sandler [517] used the HV reference point and they found that for every two-parameter CEoS it was possible to satisfy

the quadratic dependence of B with composition through their own mixing rules. Also, it was possible to get the same results for A_{∞}^E (as a composition-dependent function) obtained by γ models. Thus, Wong-Sandler mixing rules allowed PR to correlate VLE, LLE and gas solubility data in wide temperature and pressure intervals for several complex mixtures, even being better than other thermodynamic models [518]. Three years later, Orbey & Sandler [490] reformulated these mixing rules using UNIFAC as the activity coefficient model. A complete review of the different approaches for EoS/ G^E models applied to PR (and SRK) can be found in Kontogeorgis's works [511,513].

4.2.1. Universal group contribution volume translated Peng-Robinson (GC-VTPR)

Some strong equations of state have been developed through coupling with group contribution methods (like PSRK) with the purpose to get a better phase equilibrium prediction for polar, non-polar and asymmetric mixtures in wide pressure and temperature intervals. However, some limitations of these models (particularly PSRK) led Ahlers and Gmehling [505,556–559] to develop an analogous model based on a volume-translated PR EoS [76], the Twu et al. α function [111], improved mixing rules coupled to UNIFAC (Dortmund) [560,561] and temperature-dependent binary interaction parameters. Thus, a and b were defined by:

$$a = b \left(\sum_{i=1}^n x_i \frac{a_i}{b_i} - \frac{G_{res}^E}{0.53087} \right) \quad (58)$$

$$b = \sum_{i=1}^n \sum_{j=1}^n x_i x_j \left[\frac{b_i \left(\frac{3}{4} \right) + b_j \left(\frac{3}{4} \right)}{2} \right] \left(\frac{4}{3} \right) \quad (59)$$

This model was born as a *substitute* for PSRK, because it achieved a better description of ρ^l for pure compounds and mixtures. Also, the model improved the VLE prediction for symmetric and highly asymmetric systems [505,562], polymer solutions [557], and electrolytes [506,563,564], the solubility of solids and high boiling point liquids in supercritical fluids [556], the solubility of gases in aqueous solutions [565], and the solid-liquid equilibria (SLE) prediction for alkanes, aromatics and esters [566]. The model has been successfully applied to refrigeration cyclic process calculations (such as the Organic Rankine Cycle -ORC- process) [81]. Schmid & Gmehling showed typical applications of GC-VTPR for process development [567].

4.2.2. Electrolyte, salts and CO₂ systems

Other approach applied to mixtures is to use the Helmholtz free energy, as a state function, for modification performing. Sieder & Maurer [568] and Lotfollahi et al. [569–571] extended PR to VLE calculations at high pressures for solvent, supercritical CO₂ and salt containing mixtures. This methodology starts from the Helmholtz free energy definition, as:

$$A = A_{id} + \delta A_{nonionic} + \delta A_{ionic} \quad (60)$$

The term $\delta A_{nonionic}$ is obtained through Melhem's modified PR [96], being equal to:

$$\delta A_{nonionic} = RT \sum_i^n x_i \ln \left(\frac{v}{v-b} \right) + \frac{a}{2\sqrt{2}b} \ln \left[\frac{v+b(1-\sqrt{2})}{v+b(1+\sqrt{2})} \right] \quad (61)$$

In an analogous way, Zoghi et al. [572] used an associative model

for PR [388], to describe the CO₂ solubility in aqueous electrolytic solutions, based on:

$$\frac{A^R}{RT} = \left(\frac{A^R}{RT} \right)_{PR-CPA} + \left(\frac{A^R}{RT} \right)_{F\ddot{u}rst \text{ and Renon}} + \left(\frac{A^R}{RT} \right)_{Born} \quad (62)$$

where A^R contributions from F\ddot{u}rst & Renon [573] and Born [574] describe the studied electrolyte interactions, and PR-CPA contribution is defined by

$$\begin{aligned} \left(\frac{A^R}{RT} \right)_{PR-CPA} = & \frac{a}{2\sqrt{2}bRT} \ln \left[\frac{v+b(1-\sqrt{2})}{v+b(1+\sqrt{2})} \right] \\ & + \sum_i^n \left[x_i \sum_j \left(\ln x_{A_j} - \frac{x_{A_j}}{2} \right) + \frac{M_j}{2} \right] + \ln \left(\frac{v}{v-b} \right) \end{aligned} \quad (63)$$

The success of this approach is based on the choice of a right physical model for describing electrolyte interactions, as showed by Maribo-Morgensen et al. [575]. As stated by the researchers, the incorporation of ion-ion interactions, like Debye-H\ddot{u}ckel model interaction [576], together to Born model [574] interaction, helps and even improves the handling of electrolytes [577,578]. Such an electrolyte-CPA (eCPA) model could be applied to predict VLE, LLE, and SLE in aqueous salt mixtures as well as in mixed solvents, being possible, flexible and feasible to furthermore reduce it to a simple EoS, becoming it also compatible with existing tools for characterized petroleum fractions, and suitable for handling phase equilibrium calculations for mixtures with oil, gas, brine, and other chemicals [578]. However, as much as the authors know, this explicit framework has not been applied to PR-CPA yet. Other PR models for electrolytes based on similar frameworks have been proposed [579,580].

4.2.3. Isomorphism

Other methodology was follow by Abdulkadirova et al. [581] to calculate volumetric and thermodynamic properties for mixtures through the isomorphic thermodynamic behavior principle applied to the PR EoS. Such principle indicates that a mixture, even at critical conditions, can be described through a single-fluid model, keeping constant the chemical potentials rather than compositions. This model is defined by

$$P = \frac{RTh}{v} - RT\hat{A}_{ISO} \quad (64)$$

with

$$h = \ln \left[\exp \left(\frac{\mu_1}{RT} \right) + \exp \left(\frac{\mu_2}{RT} \right) \right], \quad \hat{A}_{ISO} = \frac{P_c}{RT_c} \tilde{A} \quad (65)$$

where \tilde{A} is the Helmholtz free energy density [582] and μ is the chemical potential obtained by PR, which are defined by

$$\tilde{A} = \frac{\rho RT_c}{P_c} \left[\ln \left(\frac{\frac{\rho}{\rho_{cPR}}}{1-\rho b} \right) + \frac{\alpha \rho_{cPR}}{\sqrt{2}RT_c} \arctan \left(\frac{1-\rho b}{\sqrt{2}} \right) \right] + \frac{\rho}{\rho_{cPR}} \tilde{\mu}^{(0)} \quad (66)$$

$$\mu = \frac{P_c T}{\rho_{cPR} T_c} \left[\tilde{A} + \frac{RT}{v-b} - \frac{a}{v(v+b) + b(v-b)} \right] \quad (67)$$

5. What's the next

Considering the hard and wide research around cubic equations of state, especially those successful models like PR, it is interesting that in times when computer simulations of fluid phase systems are so advanced, CEoS are still a working horse, finding widespread acceptance as tools that permit convenient and flexible calculations in the chemical industry [583].

In contrast to early solving methods for equations of state, where predictive or adjusted modes of the PR EoS gave poor agreement with experimental data, data regression was the best necessary choice for the required engineering accuracy in results [196]. However, it was just possible since 1990's, when computational tools became a very useful way to predict, correlate and simulate thermodynamic and volumetric properties of substances either based on experimental data or in lack of it for process and research applications, allowing the development of many complex models in order to accurately predict these properties. Even that, equations of state still provided an efficient and simple means of expressing various thermodynamic functions and relations between temperature, pressure, and phase compositions in binary and multicomponent systems [584], because of their relative inherent simplicity, ease to use, efficiency and reasonable accuracy, being commonly used as both educational tools and, design and simulation tools of industrial separation chemical processes [58,567]. Besides, little computer resources are required through mathematical operations for which reliable and better algorithms exist. In fact, in process simulations and time-consuming optimization studies, for example, CEoS are preferred because of their high and computationally advantageous efficiency [585]. Therefore, it is not astonishing that PR, like other similar models, is frequently used today, directly connected to, or as an input for more complex models, for the calculation of phase equilibrium and later thermodynamic properties (see Fig. 3); although in a general way, cubic

equations of state leave much to be desired from the viewpoint of statistical thermodynamics [510].

In the other hand, it meet one or more of the following criteria [586]: (a) versatility in whole temperature and pressure for target compounds, (b) reasonable accuracy of density of every phase, and (c) accuracy of fugacity of each component in both vapor and liquids phases, especially for liquid-vapor equilibria of mixtures under pressure where the PR EoS find their principal application (for example, Harstad et al. [587] showed that PR could be used to obtain a relatively accurate, non-iterative and computationally efficient correlation of high-pressure fluid mixtures used in gas turbines and rocket engines), and seems at the present time to be irreplaceable [588].

In this way, it is our duty to highlight that the PR EoS is one of the most widely used equation of state applied and studied widespread, its applications are almost unlimited (prediction of pH, solubility in clean fire extinguishing agents, energetic materials, etc. [244,589,590]). Currently PR equation model is frequently applied in chemical engineering process simulation, design, and optimization, being incorporated in many chemical process simulators and software packages, like Aspen HYSYS, Aspen Plus [591], VMGSim [592], ThermoData Engine (TDE) [593] or NIST REFPROP program [594,595] at NIST, which in their data bank provide enhanced equations of state (PR and PRSV) for rigorous treatment of hydrocarbon systems, for example. For oil, gas and petrochemical applications, PR is the most recommended property package [596], whereas for natural gas cryogenic processes (like liquefaction) is PR and modified PR (or PRSV) recommended [128,596–598].

However, in a general way, recommendations about the most proficient use of PR can be found widespread in the literature. The review by Valderrama [12] is one of the most complete and useful in order to know where PR could be expected for reliable application (Table 10).

For mixtures, Valderrama found a good prediction of PR for the next kind of systems (Table 11).

For other applications PR is limited. Perhaps the importance and necessity of an accurate EoS is reflected by the appearance of numerous publications in the literature, but in spite of this high rate of research activities in the area, universally accurate EoS is still lacking, thus necessitating continued research and development [584]. As it was indicated at the beginning, there are more than 200 modifications for pure compound applications and an uncountable number of applications for mixtures (there were showed or listed near of 100 modifications for mixtures in this paper), trying to overpass the disadvantages of the original PR model. However, the success of most of modifications is restricted to the studied properties and compounds, and therefore, they are limited to be just applied to the studied systems in the literature. In consequence, as new processes or mixtures are studied, PR must be extended by modification or tuning, in order to apply it. Other possibility is to get new models based on the structure of PR, such as it happens with PR itself (see Fig. 4).

But, in spite of that discussed above, the success of PR over the

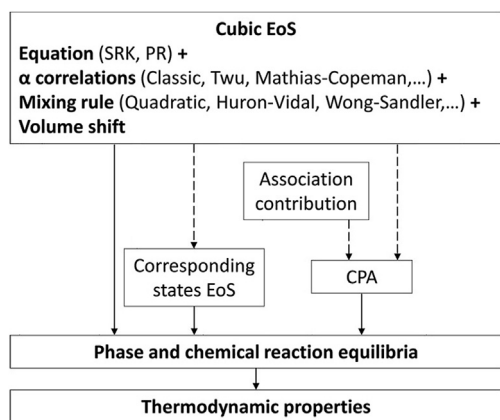


Fig. 3. Connections between CEoS and thermodynamic calculations (based on Wilhelmsson et al. [585]).

Table 10

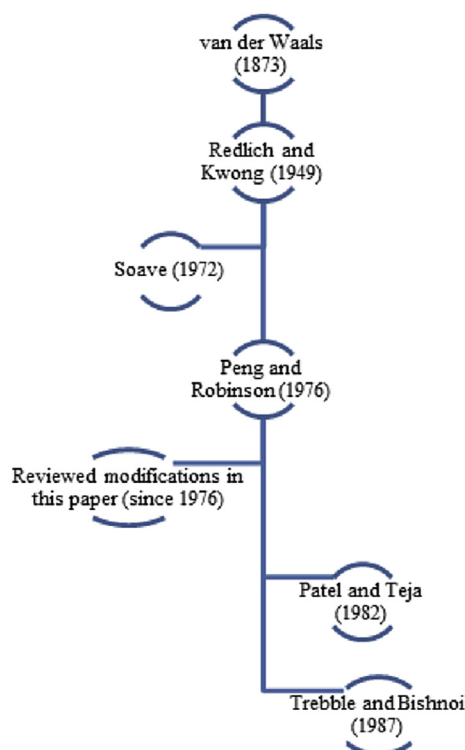
General recommendations for using the PR EoS (based on Valderrama [12]).

Property	Recommendation
Gas volume at moderate/high pressure	—
Gas volume at low temperatures, moderate/high pressure	Adjustment using low temperature data is preferred
Saturated vapor volume	—
Vapor pressure for nonpolar fluids	Use of $\alpha(T)$ functions with specific parameters for nonpolar fluids is preferred
Vapor pressures for polar fluids	Use of complex $\alpha(T)$ functions with specific parameters for polar fluids is preferred
Enthalpy and entropy of gases at low pressure	Use of $\alpha(T)$ functions with specific parameters for polar fluids is preferred
Enthalpy and entropy of gases at moderate/high pressure	Use of $\alpha(T)$ functions with specific parameters for polar fluids is preferred

Table 11

Applicability of the PR EoS for different kind of mixtures at low and, medium and high pressures (based on Valderrama [12]).

Type of mixture	Low pressure (< 10 atm)	Moderate and high pressures (> 10 atm)
Nonpolar + Nonpolar	✓	✓
Nonpolar + Polar	✓	✓
Polar + Polar	✓	✓
Asimetric mixtures	✓	–
Reservoir fluids	–	✓
Polymer solutions	✓	✓
One supercritical fluid	–	✓

**Fig. 4.** EoS tree showing the interrelationship between various equations of state (based on Wei & Sadus [24]).

time, comparable to that of RK, based on its inherent properties, is the key for its continuous application in the short and medium term in the future, even now there is a remarkable maturity in the CEoS field, at least for pure compounds [22]; this until it becomes a book example in a very long time, when another model arises.

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Nomenclature

ANFIS	Adaptive Network-based Fuzzy Interference System
ANN	Artificial Neural Network
ASOG	Analytical Solution of Groups
Aspen	Advanced System for Process Engineering
CEoS	Cubic Equation of State
COSMO-SAC	Conductor like Screening Model- Segment Activity Coefficient
CPA	Cubic-Plus-Associating
CPR	Crossover Peng-Robinson
CRP	Carrier-Rogalski-Péneloux
CS	Carnahan & Starling
DIPPR	Design Institute for Physical Properties
EoS	Equation of State
E-PPR78	Enhanced Predictive Peng-Robinson 1978
GC	Group Contribution
HYSYS	Hyprotech Systems
JTIC	Joule-Thomson Inversion Curve
LLE	Liquid-Liquid Equilibria
NG	Natural gas
NIST	National Institute of Standards and Technology
NRTL	Non-Random Two-Liquid
ORC	Organic Rankine Cycle
PC	Perturbed-Chain
PPR78	Predictive Peng-Robinson 1978
PR	Peng-Robinson
PRPA	Peng-Robinson Plus Association
PRSV	Peng-Robinson Stryjek & Vera
PSRK	Predictive Soave-Redlich-Kwong
PT	Patel-Teja
QSPR	Quantitative Structure-Property Relationship
REFPROP	Reference Fluid Thermodynamic and Transport Properties Database
RK	Redlich-Kwong
SAFT	Statistical Associating Fluid Theory
SCF	Supercritical Fluid
SLD	Simplified Local Density
SLE	Solid-Liquid Equilibria
SRK	Soave-Redlich-Kwong
SVE	Solid-Vapor Equilibria
TDE	ThermoData Engine
UNIFAC	UNIQUAC Functional-group Activity Coefficients
UNIQUAC	Universal Quasichemical
vdW	van der Waals
VLE	Vapor-Liquid Equilibria
VMGSim	Virtual Materials Group Simulator
VTPR	Volume-Translated Peng-Robinson
A	Helmholtz free energy/Dimensionless <i>a</i> parameter/Constant
$A_{M,V}$	Constants of Vidal and Michelsen mixing rules
A_s	Surface area

\bar{A}	Dimensionless Helmholtz free energy	n_{ij}	Temperature-dependent parameter
\bar{A}	Helmholtz free energy density	n_{0k}, n_{3k}	Weighted electronic density
\hat{A}_{ISO}	Modified isomorphous Helmholtz energy density	o	Specific parameter
a	van der Waals attractive parameter/Specific parameter	P	Pressure
B	Virial coefficient/Dimensionless b parameter/Specific parameter	\bar{P}	Dimensionless pressure
b	van der Waals covolume/Specific parameter	PP	Predictive parameter
b_p	Confinement-modified volume parameter	p	Specific parameter
b_0	Universal constant for all polymers	Q	Quadrupole/Specific constant
C	Specific parameter	q	Molecular surface area parameter/Specific parameter/Any specific properties of a pure component
$C_{a,b}$	Correction factors	q_i	Mixing rule constant
C_{frac}	Hydrocarbon fraction	R	Universal gas constant
C_p	Heat capacity at constant pressure	R'	Parameter of the PR_μ model
C_{sw}	NaCl molality	r	Parameter of the PR_k model
C_v	Heat capacity at constant volume	r_1, r_2	Roots of the quadratic equation in volume
c	Deviation between the predicted and experimental volume (pseudovolume)/Specific parameter	S	Entropy
D	Specific parameter	SG	Specific gravity
d	Specific parameter	s	Dimensionless parameter of volume translation/Specific parameter
E	Specific parameter	T	Temperature
E_{Hj}	Interaction parameter	$T_{a,b}$	Specific parameters
e	Specific parameter	T_g	Glass transition temperature
F	Specific parameter	T_d	Specific temperature for correction
F_{pa}	Fraction of the confined molecules subject to the pore wall attractive	\hat{T}	Reduced form of T
f	Specific parameter	T^*	Dimensionless temperature
f_c	Correction factor	t	Translation parameter
f_m	Perturbation factor	ΔU_{ij}	Adjustable binary parameter
f_w	Parametric function	u	Specific parameter
G	Gibbs free energy/Specific constant	$V_{w,j}$	Contribution of group j to the van der Waals volume
G_j	Number of the j th group in a given compound	$\delta V_{w,k}$	Increment in the van der Waals volume
G_{jl}	Non-randomness parameter between molecules l and j	v	Molar volume
ΔG^{*chg}	Total charging free energy of the mixture	X	Junction function/Specific parameter
g	Specific parameter	X^A	Mole fraction of molecules not bonded at site A
$g(\rho)$	Radial distribution function	x	Specific parameter
H	Enthalpy/Specific parameter	x_{A_i}	Mole fraction of molecules i not bonded at site A
ΔH_{vap}	Heat of vaporization	x_H	Mole fraction of hydrogen
h	Specific parameter	x_i	Mole fraction of the component i
I_i	Ionization potential of component i	x_0	Acentric factor-dependent parameter
I_k	Number of corresponding occurrences	Y	Temperature-dependent function
I_m	Temperature-dependent parameter	y	Reduce volume in rigid-phase equations $b/4v$ /Specific parameter
i	Specific parameter	Z	Compressibility factor
K	Equilibrium constant/Specific parameter/Association constant	Z_{RA}	Rackett parameter
K_K	Specific parameter	Greek symbols	
k	Thermal conductivity/Binary contribution parameter/Specific parameter	α	Temperature-dependent function in the attractive term/Specific parameter
k_B	Boltzmann constant	α_i	Boiling point-dependent parameters
k_i	Adjustable parameter	β	Temperature-dependent parameter/Specific parameter
L	Specific parameter	Γ	Contribution group parameter
l	Binary contribution parameter/Specific parameter	γ	Temperature-dependent function/Gradiation parameter/Activity Coefficient/Specific parameter
M	Specific parameter	Δ	Specific parameter
M_j	number of associating sites per molecule j	δ	Specific parameter
M_w	Molecular weight	δ_c	Volume correction at T_c
$M_{C_{7+}}$	Molecular weight of C_{7+} fraction	δ_{ij}	Binary interaction parameter
m	Acentric factor-dependent parameter/Temperature-dependent parameter/Specific parameter	ε	Interaction potential
N	Specific parameter/Number of molecules	ζ	Degree of polymerization/Specific parameter
N_A	Avogadro number	η	Reduce density/Specific parameter
N_C	Carbon number	Θ_i	Specific parameter
N_g	Number of different groups	θ	Specific parameter/Reduce temperature $\ln(T_c/T)$
N_{ij}, M_{ij}	Exponents of the conformational combining rule	κ	Acentric factor-dependent parameter
N_k	Group contribution parameter	Λ_b	Specific parameter
n	Number of components/Specific parameter	λ	Specific parameter

μ	Dynamic Viscosity/Chemical Potential/Dipole moment
π	Spreading Pressure
ρ	Density
σ	Interfacial tension/Area allocated to each molecule
ϕ	Fugacity coefficient/Specific parameter
Ψ	Specific parameter
$\Omega_{a,b}$	Coefficients of the attractive and covolume parameters
ω	Acentric factor/Surface area occupied

Subscripts

A	Association site A
Asoc	Associative contribution term
Born	Born contribution term
b	Boiling
calc	Calculated
Coulomb	Coulomb contribution term
c	Critical
eutectic	Eutectic point
exp	Experimental
i	Component reference letter
Id	Ideal
ionic	Ionic contribution term
j	Component reference letter
k	Component reference letter
l	Component reference letter
m	mixture
n	Alkane/Counter
nonionic	Nonionic contribution term
poly	Polymer
RA	Rackett
r	Reduced by critical parameter
res	Residual part
SG	Staverman-Guggenheim
trans	Translation term
∞	Infinite pressure state
'	Specific constant/Constant for a viscosity/thermal conductivity/ionic model

Superscripts

E	Excess
l	Liquid phase
R	Residual
sat	Saturation
v	Vapor phase
*	Reduced parameter

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