Application of Carnahan-Starling-vdW-β Equation of State for Refrigerant Fluids

S.M. Hosseini

Department of Chemistry, Faculty of Sciences, University of Hormozgan, Bandar Abbas, 71961, Iran
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Herein, the application of Carnahan-Starling-vdW-β equation of state (EoS) for 13 refrigerant fluids was investigated. The EoS could predict the saturated liquid densities of these refrigerants over the temperature range of 100-400 K and pressures from zero up to 187 MPa with the average absolute deviations of 2.66%. The accuracy of Carnahan-Starling-vdW-β EoS in liquid density prediction was also compared with Peng-Robinson EoS and a perturbed hard-sphere-chain EoS. The surface tension and sound velocity of the saturated refrigerants were also calculated using the Carnahan-Starling-vdW-β EoS within 4.76% and 5.66%, respectively. Finally, Carnahan-Starling-vdW-β was employed to predict Joule-Thomson inversion curve for some studied refrigerant fluids.

INTRODUCTION

Pure refrigerants and refrigerant mixtures are widely used as working fluids in industrial applications involving refrigerators and heat pumps. Knowledge of the thermo-physical properties of refrigerant fluids is of importance in the design and fabrication of these devices. In the case of refrigerant mixtures, such knowledge is also of help to take a theoretical insight on the intermolecular forces operating in refrigerant systems. The refrigerants supposed to be investigated here belong to hydrofluorocarbons (HFCs) category. Generally, HFCs have been used as the acceptable alternatives to chlorofluorocarbons (CFCs) and hydro-chlorofluorocarbons (HCFCs), because they contain no chlorine and are harmless to the ozone layer, that is why they have come into focus in both scientific community and refrigeration industries [1-5].

In view of the hazardous aspect of refrigerants for the atmosphere direct measurement of their thermophysical

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*Corresponding author. E-mail: sm.hosseini@hormozgan. ac.ir

properties over a wide range of temperatures and pressures is somewhat impractical. In this regard, equation of state (EoS) method for the correlation and prediction of thermo-physical properties of refrigerant fluids can be highly useful. Numerous studies [6-13] have been carried out to present the analytical equations of state for thermodynamic proprieties of refrigerant fluids based on the various approaches from the work of Fermeglia *et al.* [6] to the very recent work by Hekayati *et al.* [13]. In these efforts, the authors tried to determine the appearing parameters in the EoS using the various approaches such as the critical point criterion, corresponding states correlations, and the lattice-hole theory [14]. Also, some efforts were made to apply the linear isothermal regularity (LIR)-based EoSs [15-17] and computer-aided artificial neural networks [18] to predict the density of various classes of refrigerant.

The preceding work of Papari *et al.* [19] led to the modification of the well-known Carnahan-Starling-vdW EoS [20] to Carnahan-Starling-vdW-*β* for several molecular fluids including non-polar and polar ones. The authors determined two parameters appearing in the EoS by the use of the critical point criterion, where both of first and second

volume derivatives of EoS at critical isotherm are equal to zero [21]. They checked the capability of the modified EoS by the density calculations for several non-polar and polar fluids. However, the performance of that EoS has not been yet well-investigated for the refrigerant fluids, and just two refrigerant fluids have been included in the work of Papari *et al.* [19]. Likewise, Papari *et al.* limited their investigation to the density calculations, and no effort was made to see how accurate the modified EoS is when other thermophysical property data are predicted. This study is going to assess the performance of Papari *et al.* equation for not only various refrigerant fluids, but also the prediction of other thermophysical property data of liquid refrigerants at isothermal and saturated states. Our calculation results are compared with the experimental data [22]. The surface tensions and velocity of sounds of saturated liquid refrigerants are also estimated through some simple relations [23-24].

The inversion curve is defined as the locus of thermodynamic states in which the Joule-Thomson coefficient is zero, under which the temperature of a gas would be invariant with respect to the isenthalpic expansion. Joule-Thomson inversion curve (JTIC) is used widely for refrigeration and for liquefaction of gases under certain conditions, however, this type of expansion may produce heating or cooling. Determination of these conditions is important in the design of cryogenic processes [25]. Due to some difficulties in the direct measurement of JTIC, the application of predictive methods such as EoS can be highly useful. Having an EoS one can easily predict those conditions as several efforts have been devoted to calculate the JTIC of polar and non-polar fluids [26-32]. Generally, the inversion curve is defined as the locus of points along which the inversion conditions is satisfied as follow:

$$T_r \left(\partial P_r / \partial T_r \right)_{V_r} = -V_r \left(\partial P_r / \partial V_r \right)_{T_r} \tag{1}$$

where, P_r, T_r and V_r are, respectively, the reduced pressure, reduced temperature and reduced volume. Agreement with Joule-Thomson inversion curve (JTIC) is a severe test of equations of state [33]. In this study, the EoS previously modified by Papari *et al.* [19] is going to be tested for the prediction of JTIC of some selected refrigerant fluids.

CARNAHAN-STARLING-VDW-β EQUATION

Papari *et al.* [19] have modified the attractive part of some van der Waals (vdW) family of the EoSs. One of them was that well-known Carnahan-Starling-van der Waals (CS-vdW) EoS which is as:

$$Z = \frac{P}{\rho k_B T} = \left(\frac{P}{\rho k_B T} \right)_{CS} + \left(\frac{P}{\rho k_B T} \right)_{vdW} = \frac{1 + \eta + \eta^2 - \eta^3}{(1-\eta)^3} - \frac{a\rho}{k_B T} \tag{2}$$

where P is the pressure, ρ is the number (molar) density, $k_B T$ is the thermal energy per molecule, a is the measure of attractive forces between molecules and η is the packing fraction defined as:

$$\eta = \frac{b\rho}{4} \tag{3}$$

In this equation b is the van der Waals co-volume.
The second term of the right hand of CS-vdW has been modified by Papari *et al.,* as follow [19]:

$$\frac{P}{\rho k_B T} = \frac{1 + \eta + \eta^2 - \eta^3}{(1-\eta)^3} - \frac{a(T)\rho}{k_B T^{(\beta+1)}} \tag{4}$$

where β is introduced as a function of acentric factor of pure fluids as:

$$\beta = c_1 + c_2 \omega + c_3 \omega^2 \tag{5}$$

The different values of coefficients c_1-c_2 were obtained for vapour and liquid phases by Papari *et al.* [19], as reported in Table 1.

When $\beta = 0$, the Carnahan-Starling-vdW EoS is recovered. Papari et al. called Eq. (4) "CS-vdW-β".The parameters a and b were previously obtained by solving the usual critical point equations [19], giving:

$$a = 0.496388 \frac{R^2 T_c^{(2+\beta)}}{P_c} \tag{6}$$

Table 1. The Coefficients that Used in Eq. (5)

Phase	c_1	c_2	c_3
Vapour	-0.0397	0.7619	0.8589
Liquid	0.2606	3.0517	-2.191

Table 2. The Critical Constants along with the Acentric Factors of Studied Refrigerants to be Used in Eqs. (7)-(8) and Taken from Ref. [22]

Refrigerant	T_C (K)	P_C (MPa)	ω
Trichlorofluoromethane (R11)	471.110	4.408	0.188
Dichlorofluoromethane (R12)	385.120	4.136	0.176
1,1,2-Trichloro-1,2,2-trifluoroethane (R113)	487.210	3.392	0.255
1,2-Dichloro-1,1,2,2-tetrafluoroethane (R114)	420.608	3.352	0.246
Chloropentafluoroethane (R115)	353.100	3.129	0.249
Dichlorodifluoromethane (R21)	452.720	5.289	0.202
Chlorodifluoromethane (R22)	369.295	4.990	0.215
1-Chloro-1,2,2,2-tetrafluoroethane (R124)	395.428	3.625	0.300
1,1-Dichloro-1-fluoroethane (R141b)	477.500	4.212	0.217
Tetrafluoromethane (R14)	227.396	3.762	0.176
Hexafluoroethane (R116)	293.030	3.048	0.255
Trifluoromethane (R23)	299.293	4.832	0.253
1,1,1,2-Tetrafluoroethane (R134a)	374.210	4.059	0.326
1,1-Difluoroethane (R152a)	386.410	4.517	0.259
2,2-Dichloro-1,1,1-trifluoroethane (R123)	456.831	36.618	0.2819
Pentafluoroetane (R125)	339.17	3.6177	0.305
Chlorotrifluorometane (R13)	302.0	3.879	0.172
Difluoromethane (R32)	351.25	5.78	0.276
1,1,1,2,3,3,3-Heptafluoropropane (R227ea)	375.95	3.00	0.354

$$b = 0.187294 \ \frac{RT_c}{P_c} \tag{7}$$

The critical parameters of the studied refrigerants of Eqs. (6) and (7) could be taken from the literature, [22] and are reported in Table 2.

RESULTS AND DISCUSSION

Estimation of Liquid Densities

The calculation of density from the given temperature and pressure is one of the most frequently performed operations in phase equilibrium calculations. The ability of the present modified equation of state for predicting the density of studied refrigerants over the temperature range between 100-400 and pressure range from 0.001-1870 bar has been checked. In this work, we have calculated isothermal and saturated liquid densities of pure refrigerants using the proposed EoS. Our calculation results are summarized in Table 3 as the average absolute deviations (AAD%) from the experimental data [22]. For 13 refrigerants, the AAD of the calculated isothermal liquid densities from the experimental values were obtained using the modified EoS. From Table 3, it was found that for 667 data points, the AAD of the calculated densities from the experimental values [22] is 2.16%.

Our calculation results for the isothermal liquid densities were also compared with those obtained from the well-known Peng-Robinson (PR) EoS [34], and the results are reported in Table 3. It was found that the present EoS is favourably superior to PR one. The AAD of calculated isothermal liquid densities from Carnaha-Starling-vdW-β EoS (2.16%) is considerably lower than that obtained from PR EoS (*i.e.*, 6.51%). Furthermore, the accuracy of Carnahan-Starling-vdW-β EoS was compared with the previous work of Eslami-Farrokhnia [7], where a modified perturbed hard-sphere-chain (PHSC) EoS was investigated for refrigerant fluids. Table 4 reveals that the results from Carnahan-Starling-vdW-β EoS were not as accurate as those obtained from the previous work of Eslami-Farrokhnia [7]. From 900 experimental density data points [35-39] examined, the AAD of PHSC EoS [7] was 1.45% which is remarkably lower than that obtained from Carnahan-Starling-vdW-β EoS (*i.e.*, 3.65%).

The densities of saturated liquid refrigerants were also estimated using Eq. (4) over the pressure range from zero up to 1.34 MPa and temperatures within 137-400 K. Our calculation results are shown in Fig. 1 as the relative deviation (in %) of the estimated values from the experimental data [22]. The relative deviation is defined as:

$$\text{Relative deviation} = \left(\frac{\rho^{Cal.}}{\rho^{Exp.}} - 1 \right) \times 100 \tag{8}$$

where superscripts "Cal" and "Exp" stand, respectively, are the calculated and experimental values. The ADD was calculated as 2.66% for 382 data points examined for saturated liquid refrigerants. Figure 1 shows how Carnahan-Starling-vdW-β is near to the experimental data points. As Figure 1 shows, the relative deviations (in %) of the estimated isothermal and saturated liquid densities are within ±5.41%.

The Carnahan-Staring-vdW-β EoS was also employed to predict some known regularities appeared in a typical liquid refrigerant. The pressure dependence of the isotherms of isobaric expansion, α_P, and isothermal compressibility coefficients, κ_T, both of which are passing through a common intersection point. This intersection is a useful tool for evaluating the reliability of a given EoS for producing equilibrium properties of the matter [40]. The Carnahan-Staring-vdW-β EoS was tested for predicting these behaviours for a typical refrigerant, R227ea, for which the experimental results were available in the literature [41]. The results for isotherms of α_P and κ_T are, respectively, shown by Figures 2a and 2b, in which the solid lines are the predicted isotherms from the Carnahan-Staring-vdW-β EoS and the markers represent the experimental isotherms of Pires *et al.* [41]. As Fig. 2a depicts, the EoS could not predict the regularity associated with the isotherms of α_P versus pressure and the results did not reproduce the experimental common intersection point. This can be regarded as the weak point of Carnahan-Staring-vdW-β EoS when isotherms of α_P versus pressure for a typical refrigerant are predicted. However, the EoS could predict the pressure behaviour of κ_T isotherms and the common intersection point of these isotherms with reasonably good accuracies as demonstrated by Fig. 2b which reveals another success of the EoS under consideration.

Table 3. The AAD (in %)[b] of the Calculated Isothermal Liquid Densities from CS-vdW-β (Eq. (4)) [19] and PR EoS [34], Both Compared with Experimental Values [22]

Refrigerant	ΔT (K)	ΔP/MPa	NP[a]	Eq. (4)	PR EoS
Trichlorofluoromethane (R11)	250-380	0.5-30.0	109	1.30	7.05
Dichlorofluoromethane (R12)	200-336	0.5-187	52	1.64	10.44
Chlorotrifluoromethane (R13)	160-260	0.6-32	22	1.92	8.36
Tetrafluoromethane (R14)	110-200	4-49	50	2.11	9.02
Dichlorodifluoromethane (R21)	230-370	0.6-102	30	3.33	6.44
Difluoromethane (R32)	100-175	0.00-70	66	2.77	8.33
1,1,2-Trichloro-1,2,2-trifluoroethane (R113)	230-400	0.002-100	63	1.33	5.01
1,2-Dichloro-1,1,2,2-tetrafluoroethane (R114)	200-320	2.0-80	22	2.55	6.57
Chloropentafluoroethane (R115)	210-315	40-60	15	2.74	8.40
2,2-Dichloro-1,1,1-trifluoroethane (R123)	230-370	4-400	74	2.80	2.69
1-Chloro-1,2,2,2-tetrafluoroethane (R124)	200-330	6-400	37	2.67	2.92
Pentafluoroethane (R125a)	240-330	0.3-600	53	3.25	4.01
Hexafluoroethane (R116)	130-270	4-400	74	2.66	7.45
Overall			667	2.16	6.51

[a]NP represents the number of examined data points.

$$^{b}\,\mathrm{AAD} = 100/\mathrm{NP} \sum_{i=1}^{\mathrm{NP}} \mid \rho_{\mathrm{Cal.}} - \rho_{\mathrm{Lit.}} \mid \Big/ \rho_{\mathrm{Lit.}}$$

Table 4. The AADs (in %) of the Calculated Isothermal Liquid Densities of some Studied Refrigerants from the Experimental Data [35-39], Compared with those Obtained from the Work of Eslami-Farrokhnia (PHSC EoS) [7]

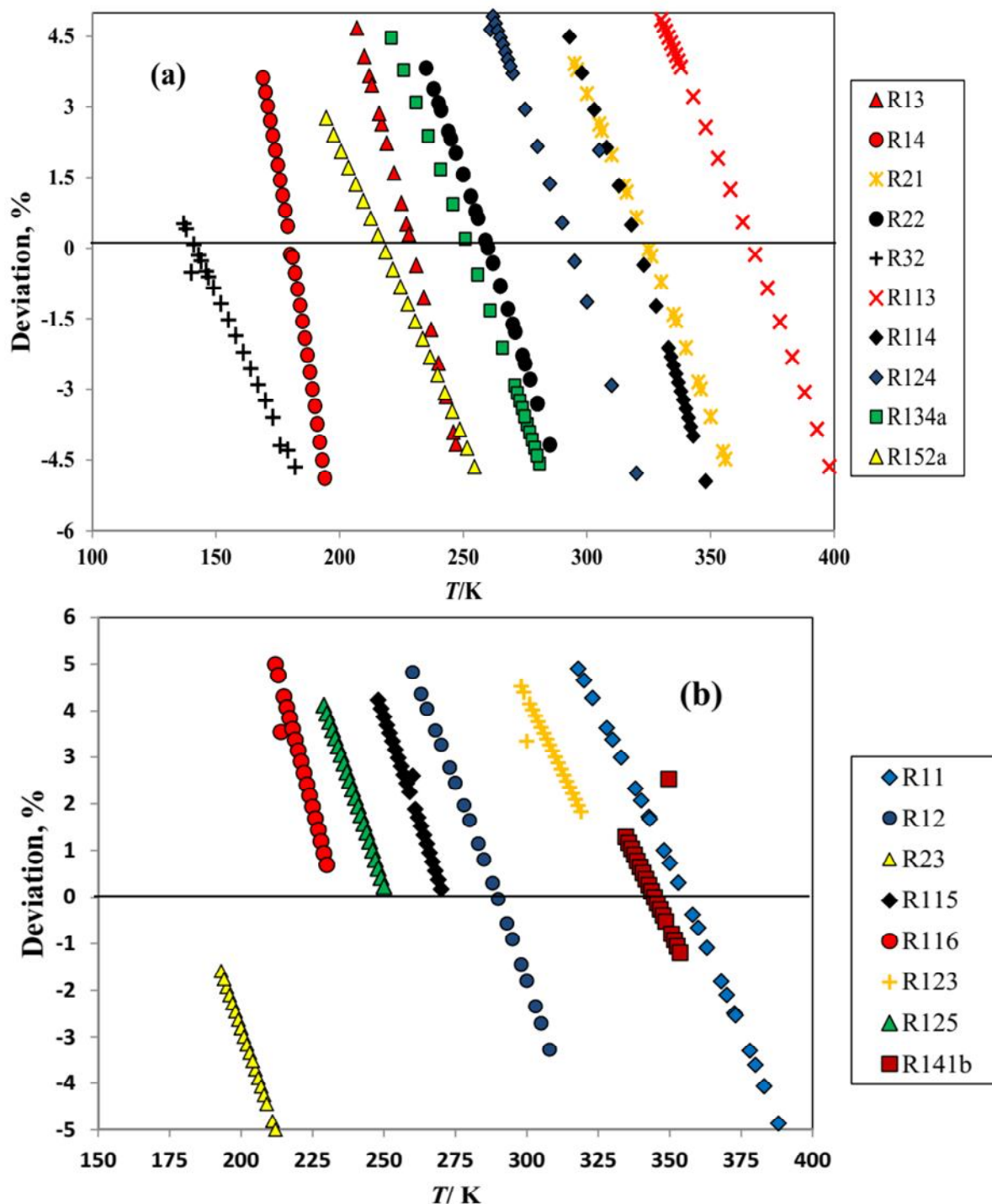| Refrigerant	ΔT (K)	ΔP/MPa	NP	CS-vdW-β	PHSC
R21	273-473	0.1-20	125	5.33	0.56
R124	120-273.8	0.65-4.5	69	3.05	0.45
R134a	170-370	0.01-70	339	4.33	0.96
R152a	243-357.6	0.7-6.5	236	2.29	0.46
R125	180-330	1.24-67.8	131	3.14	0.86
Overall			900	3.65	1.45

Fig. 1. Two deviation plots for the estimated saturated liquid densities of 19 refrigerants by the use of Eq. (4) from the experimental data [22].
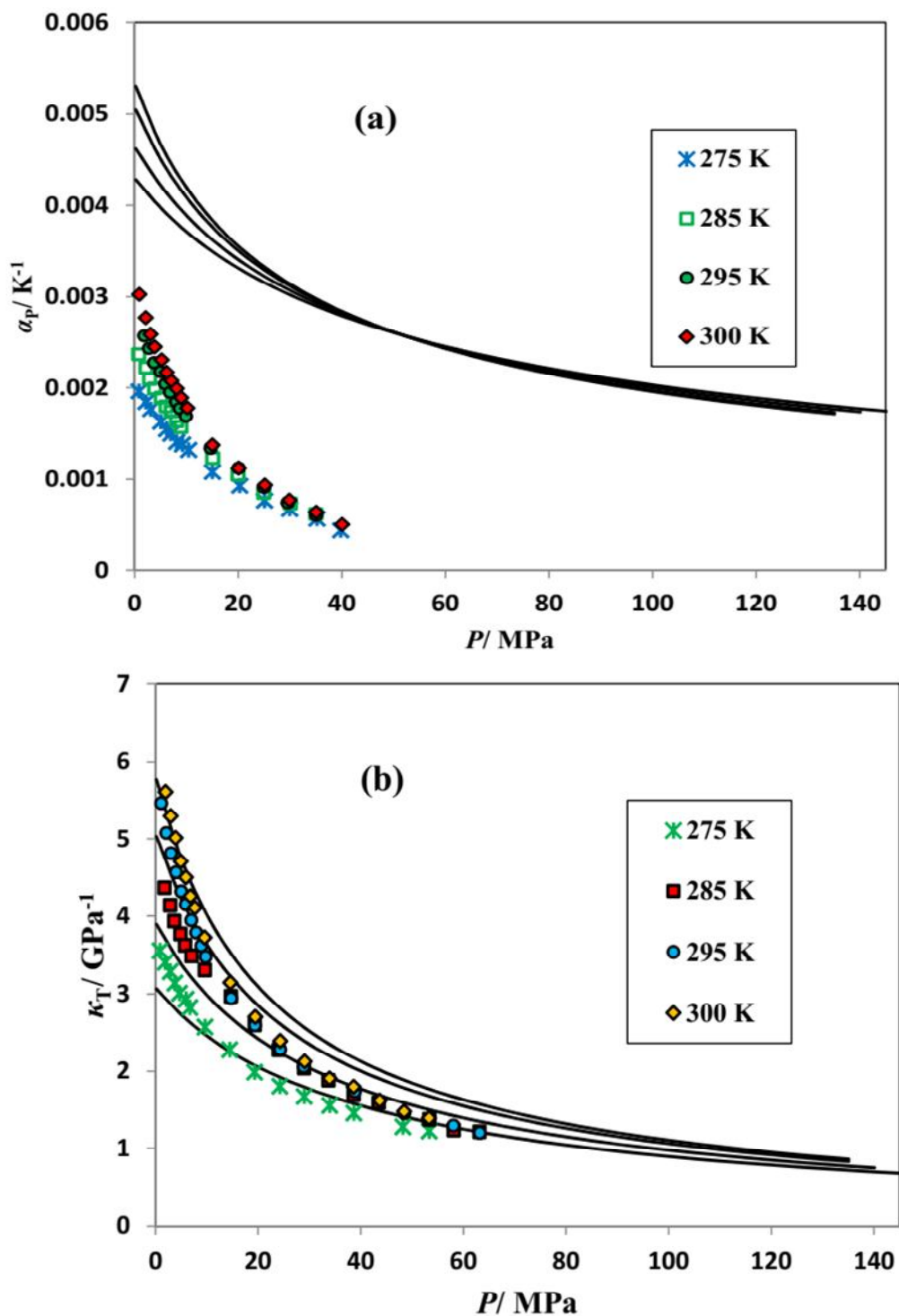
Fig. 2. Isotherms of α_P (a-plot) and κ_T (b-plot) *versus* pressure for R227ea. Solid lines are calculated based on the Carnahan-Starling-vdW-β EoS and markers are experimental isotherms of Pires *et al.* [41].
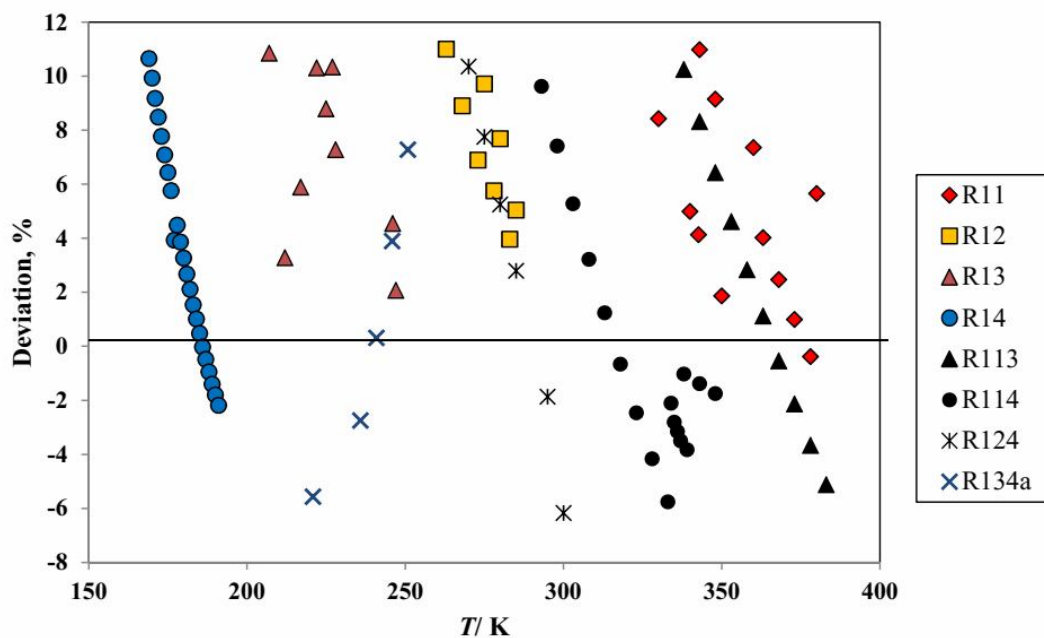
Fig. 3. Deviation plot for the estimated surface tensions of some selected liquid refrigerants using Eq. (9) from the experimental data [22].
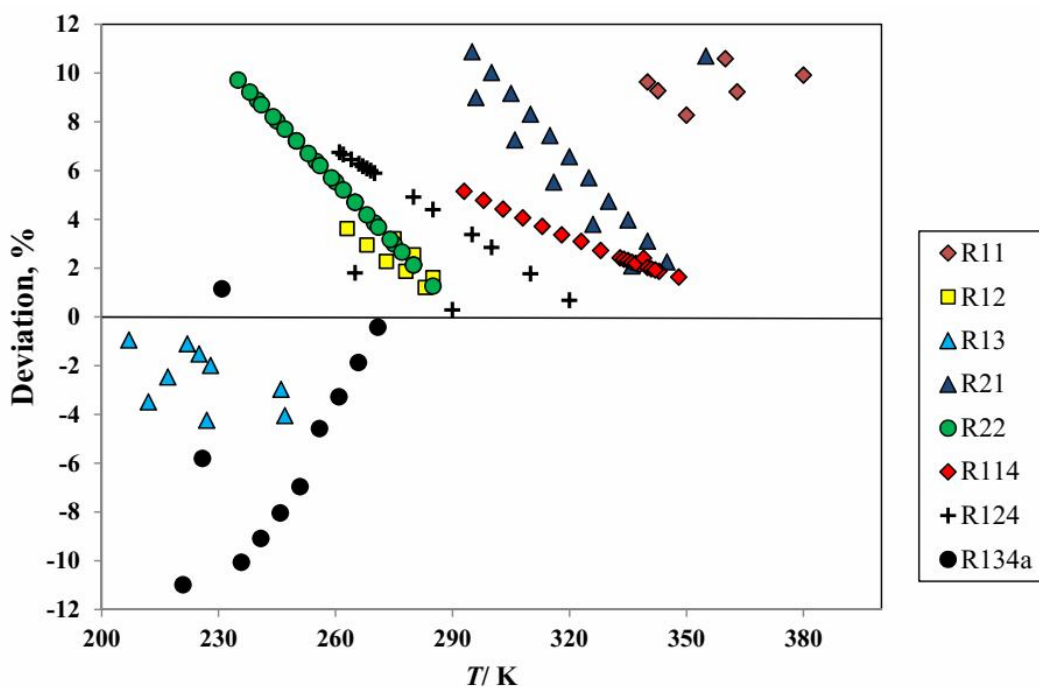

Fig. 4. Deviation plot for the estimated sound velocities of some selected liquid refrigerants using Eq. (11) from the experimental data [22].
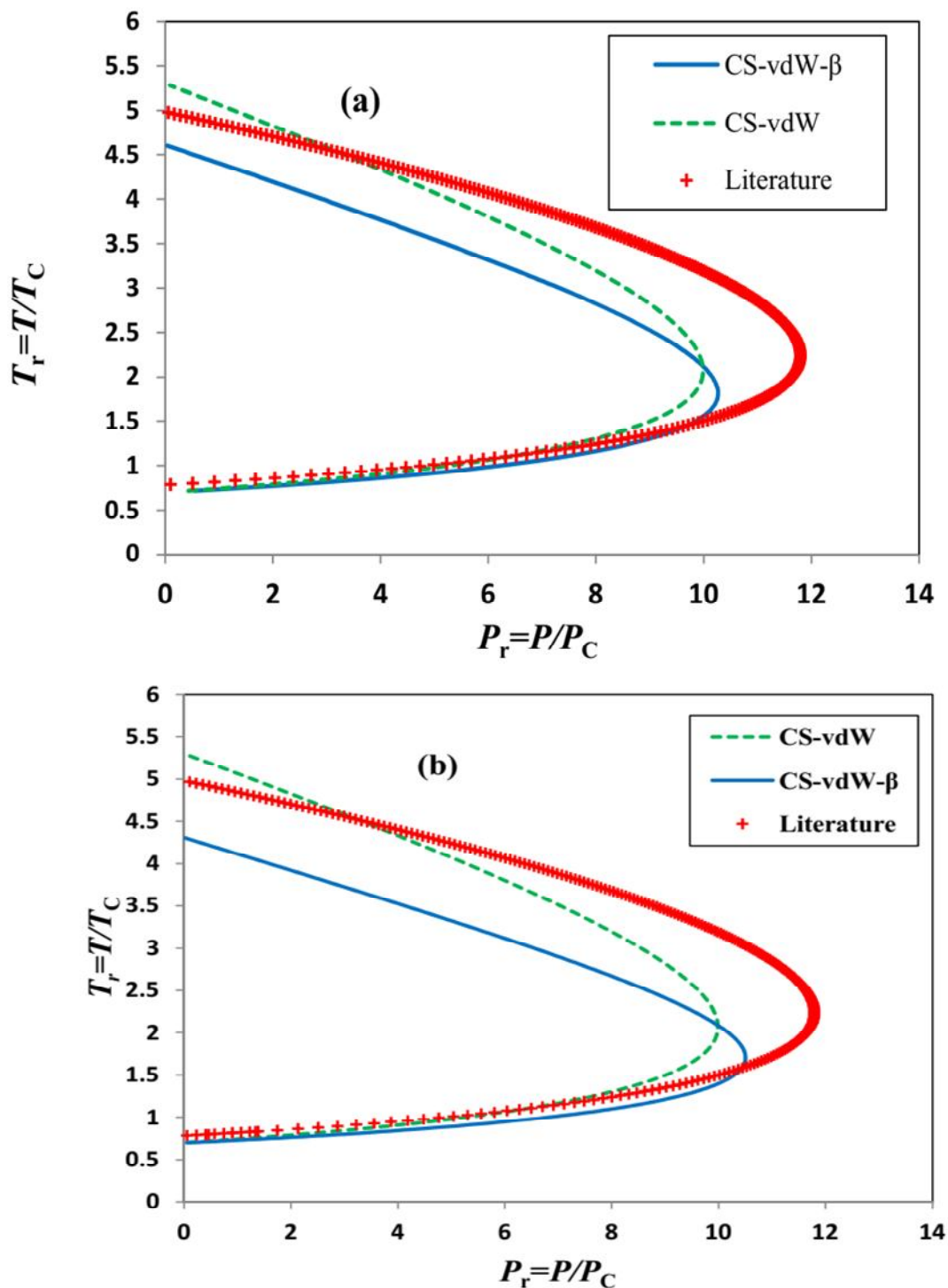
Fig. 5. The estimated JTICs of three selected refrigerant gases including R11 (a-plot), R113 (b-plot) and R134a (c-plot) using CS-vdW-β (solid lines) and that of CS-vdW (dashed lines) Eos, both are compared with JTIC from an empirical correlation [33] (red +).
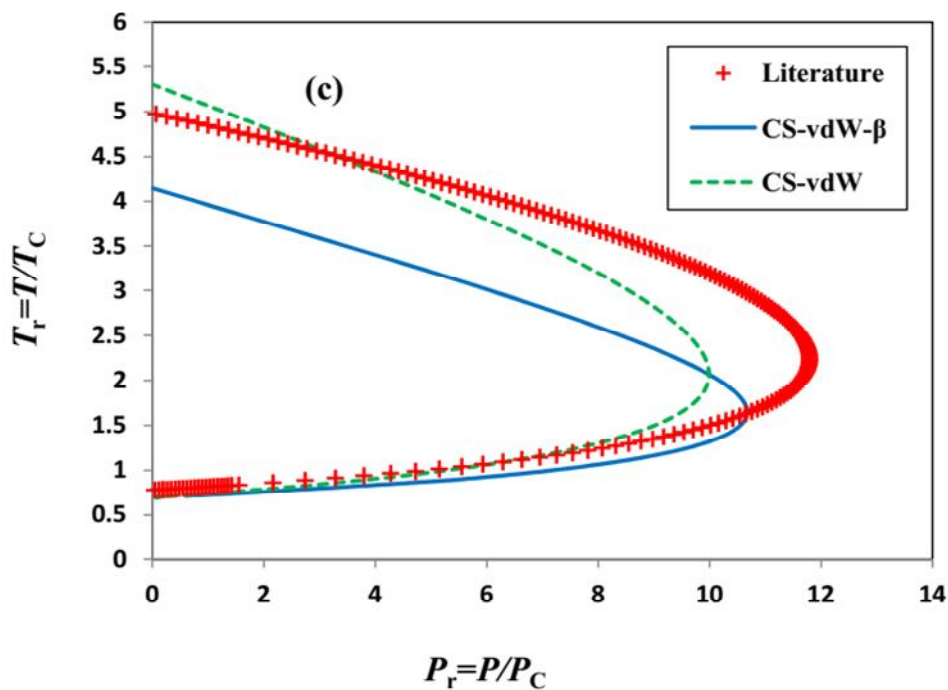
Fig. 5. Continued.

Table 5. The Characteristics of Estimated JTIC of Three Selected Refrigerant Gases Compared with those Obtained from an Empirical Correlation [33]

Refrigerant		$T_{r\,min}$	$T_{r\,max}$	$T_{r\,ip}$	$P_{r\,ip}$
	CS-vdW	0.699	5.28	2.07	9.99
R11	CS-vdW-β	0.716	4.60	1.82	10.27
	Literature [33]	0.772	4.97	2.24	11.79
	CS-vdW	0.70101	5.29	2.07	9.99
R113	CS-vdW-β	0.69896	4.30	1.70	10.50
	Literature [33]	0.78406	4.97	2.24	11.79
	CS-vdW	0.7008	5.29	2.05	9.99
R134a	CS-vdW-β	0.698	4.15	1.64	10.67
	Literature [33]	0.783	4.97	2.24	11.79

Surface Tension Estimation

Having liquid and vapour densities, one can easily estimate the surface tensions of non-polar and polar liquids thorough Escobedo-Mansoori relation [24]:

$$\gamma = \left(P_0 (1 - T_t)^{0.37} T_r Exp \left(0.30066 \, T_r^{-1} + 0.86442 \, T_r^9\right)\left(\rho^l - \rho^v\right)\right)^a$$

(9)

where P_0 is a temperature-independent constant characteristic of the fluid under consideration similar to the Sugden's parachor [42]. In this study, Hugill-Welsenes [43] expression for Sugden's parachor was adopted as follows:

$$P_0 = 40.1684 \left(0.151 - 0.0464 \, \omega\right) T_C^{13/12} / P_C^{5/6}$$

(10)

The surface tensions of 8 saturated refrigerant liquids were estimated by Eqs. (9)-(10) over the temperature range from 169-388 K with the relative deviations from the experimental data [22] of ±10.91%. The value of AAD shows how the proposed EoS is close to the experimental data. A deviation plot is shown in Figure 3. From 98 data points examined, the AAD of estimated surface tension was calculated as 4.76%.

Estimation of Sound Velocity

Having liquid densities and surface tensions, one can easily estimate the sound velocities, u, for non-polar liquids thorough Auerbach's relation [23]:

$$u = \left(\frac{\gamma}{6.33 \times 10^{-10} \cdot \rho}\right)^a$$

(11)

where γ and ρ are the surface tension and the liquid density, respectively. However, Gardas-Coutinho [44] reconsidered this equation for polar liquids by re-evaluating a-power. They estimated value of a- exponent approximately equal to 0.6714. The derived liquid densities from Eq. (4) together with the predicted surface tension values from Eq. (9) were used to estimate sound velocities of 8 refrigerant liquids at saturated states. The corresponding results are shown in Fig. 4 as the relative deviation percentage in the estimated sound velocities from the experimental data [22]. As Fig. 4 shows,

Eq. (11) could estimate the sound velocities of the studied liquid refrigerants over the temperature range of 207-380 K with the relative deviations of 10.96%. The AAD of estimated sound velocities was calculated as 5.66% for 61 data points. It should be noted that, to predict the isothermal and saturated liquid density of refrigerants, the values of coefficients of c_1-c_3 are necessary.

Calculation of Joule-Thomson Inversion Curve

As mentioned earlier, the proposed EoS has also been tested to predict JTIC of fluids of interest. In this regard, Fig. 5 are presented to show the estimated JTIC of three selected refrigerant gases including R11 (5a), R113 (5b) and R134a (5c) using CS-vdW-β and that of CS-vdW EOSs, both were compared with JTIC from an empirical correlation [33]. At the first look, agreement between both EoSs and the literature [33] is reasonably good especially for the case of low reduced temperatures. However, as the temperature gets close to upper reduced temperature, $T_{r,max}$, some significant discrepancies are appeared in those three plots. Figure 6 demonstrates the trend of compression factor ($Z = P/(\rho RT)$) values versus reduced pressure for the selected refrigerant gases including R11 (6a), R113 (6b) and R134a (6c) from $P_r = 0$ up to several decades above the critical pressure (supercritical regions). Also, the characteristics of derived JTICs including minimum and maximum reduced temperatures at $P_r = 0$ as well as the locus of T_r and P_r at inversion point ($T_{r,ip}$ and $P_{r,ip}$) are reported in Table 5. In Figs. 6a-6c, the solid and dashed lines represent, respectively, our estimations form CS-vdW-β and CS-vdW. The markers are those values derived from an empirical correlation [33]. It should be added that, to predict the JTIC of refrigerant fluids, the first set of coefficients c_1-c_3 is taken into account; those were adjusted for "*vapour phase*".

CONCLUSIONS

The most striking aspect observed is the remarkable agreement achieved between the calculated results and the experimental values of volumetric properties of refrigerants using the modified version of CS-vdW EoS. This clearly indicates that the modified CS-vdW EOS is superior to the PR EoS. In sum, the modified CS-vdW EOS behaves well
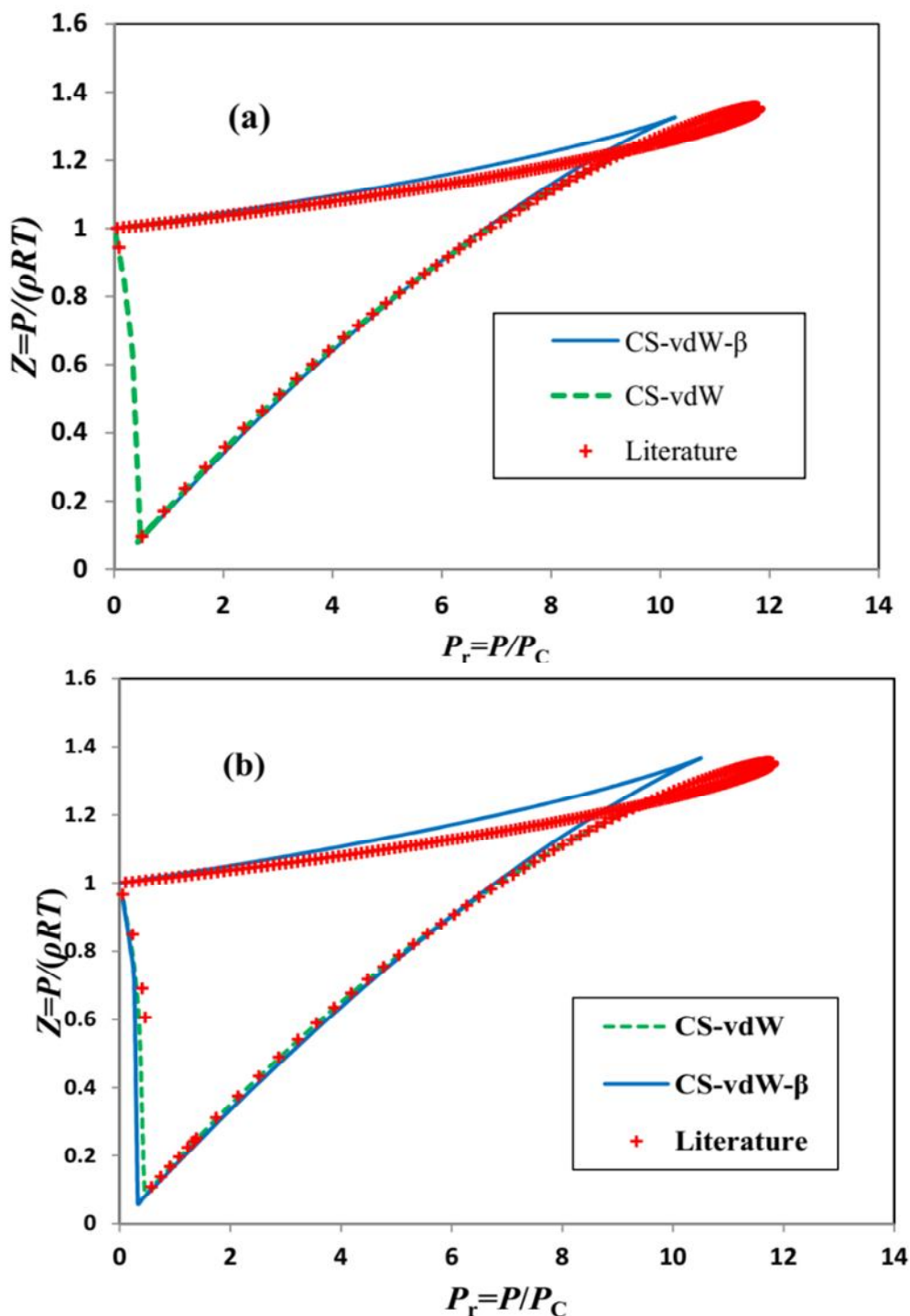
Fig. 6. Three plots for indicating the trend of compression factor ($Z = P/(\rho RT)$)) values *versus* reduced pressure for R11 (a-plot), R113 (b-plot) and R134a (c-plot) using CS-vdW-β (solid lines) and that of CS-vdW (dashed lines) EoSs, both are compared with JTIC from an empirical correlation (+) [33].
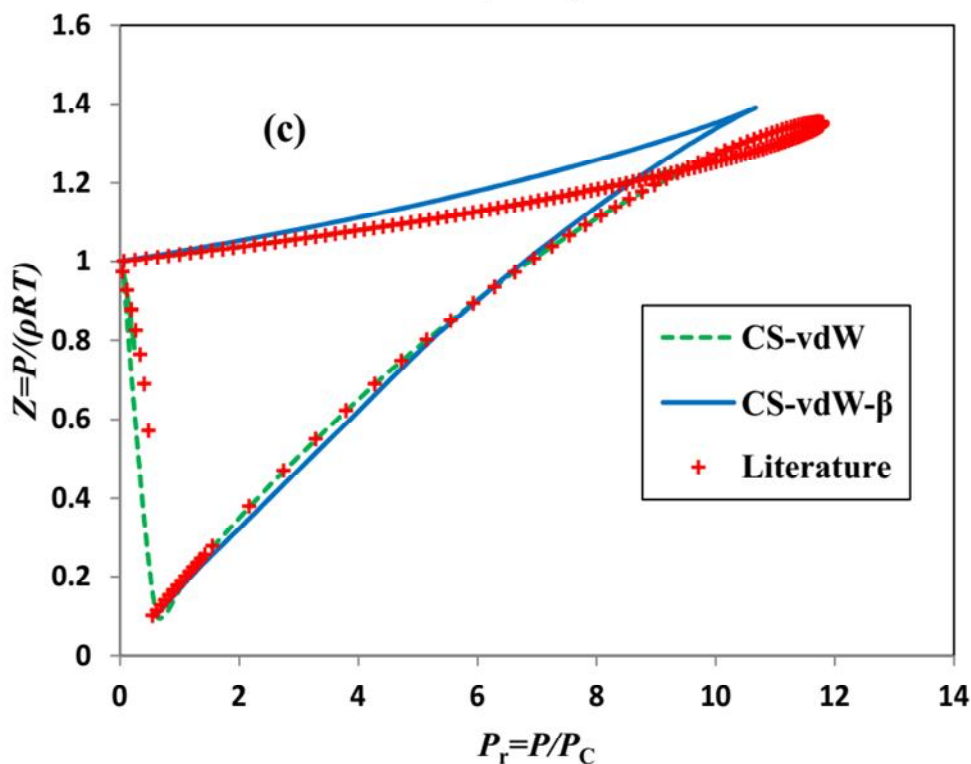
Fig. 6. Continued.

in both isothermal and saturated states. We conclude by pointing out that the attractiveness of the CS-vdW-β EoS made it capable of estimating the surface tensions, sound velocities and JTICs of refrigerant fluids with reasonably good accuracies.

ACKNOWLEDGMENTS

Nomenclature and Units

b	van der Waals co-volume, m^3
P	pressure, Pa
R	Gas constant, $J\,mol^{-1}\,K^{-1}$
T	Absolute temperature, K
k_B	Boltzmann constant, $J\,K^{-1}$
a	Attractive forces between Spheres, $J\,m^{-3}$

Greek letters

γ	Surface tension, N m
u	Sound speed, $m\,s^{-1}$
ω	Acentric factor
ρ	Molar density, $mol\,m^{-3}$

Subscripts

C	Critical

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