Journal of Physical Chemistry and Electrochemistry Vol.2 No. 2(2014) 57-65

Islamic Azad University
Marvdasht Branch

Journal of Physical Chemistry and Electrochemistry

Journal homepage: http://journals.miau.ac.ir/jpe

An Analytical Equation of State for Molten Polymers

Seyyed Mostafa Hoseini

Young Researchers and Elite Club, Marvdasht Branch, Islamic Azad University,Marvdasht, Iran

Abstract

An analytical equation of state (EOS) developed by Ihm-Song-Mason (ISM) has been applied to calculate some thermophysical properties of molten polymers including Poly (1-octene) (PO), Poly (vinyl methyl ether) (PVME), Poly (vinyl chloride) (PVC), and Poly (styrene) (PS). Three temperature-dependent parameters of the ISM EOS have been determined based on the alternative scaling constants, dispersive energy parameters between segments/monomers (ε) and segment diameter (σ). The ability of the proposed EOS has been checked by comparing the results with 547 literature data points for the specific volumes over temperature from 311-557 K and pressure ranging from 0.1 up to 200 MPa. The average absolute deviation (AAD) of the calculated specific volumes from literature data was found to be 0.47%. The isothermal compressibility coefficients, κ_T have also been predicted using ISM EOS. From 188 data points examined, the AAD of estimated κ_T was equal to 7.75%. Our calculations on the volumetric and thermodynamic properties of studied polymers reproduce the literature data with reasonably good accuracy.

Keywords: Equation of state, Molten Polymers, thermodynamic properties

1. Introduction

Knowledge of the thermophysical properties of polymers is a prerequisite for the design and optimization of their production plants. They are widely used for industrial and residential purposes. [1-5]. Therefore, accurate knowledge of thermophysical properties of polymeric materials is valuable as it is required to decide whether the use of these fluids could be extended from the laboratory level to large-scale industrial applications. Although some experimental data exist, prediction of thermophysical properties of polymers such as density and isothermal compressibility is still an important task considering they have been in focus as materials offering many highly promising applications. Under this circumstance, the development of equation of state (EOS) methods for the prediction of volumetric and thermodynamic properties of molten polymers can be highly useful.

Several researchers have previously applied the analytical EOSs to describe volumetric properties of molten polymers. For example, Sabzi-Boushehri (S & B) [6] have utilized the original version of Ihm-Song-Mason (ISM) EOS [7] for 4 polymer melts by means of surface tension and the molar density, both at the freezing point for the determination

---

[*] Correspondig Author
E-mail address: smhoseini2000@yahoo.com

of ISM EOS parameters. Recently, Yousefi [8] has employed Tao-Mason (TM) EOS [9] for the estimation of volumetric properties of 8 molten polymers. She determined three temperature-dependent parameters of TM EOS by the help of temperature and liquid density (ρ_g) at the glass transition (T_g), as scaling constants. She has predicted 804 data points for the specific volumes with AAD equal to 0.34%. Yousefi et al. [10] have also applied the above mentioned scaling constants, i.e., temperature and density at glass transition point to ISM EOS for predicting the volumetric properties of 9 polymeric systems. They have predicted 1079 data points for the specific volumes with AAD equal to 0.40%. However, the need for surface tension and liquid density data both at freezing point and glass transition point, respectively, limits the applicability of the above-cited works because these values are not easily available for most polymers,.

In this study, we demonstrate that there is no need for freezing and glass transition data to evaluate three temperature-dependent parameters of ISM EOS. To other word, these parameters will be determined based on the alternative (molecular) scaling constants contrary to the preceding works of Yousefi et al. [8,10], where the required scaling constants were taken from the bulk properties, e.g., liquid density at glass transition point.

Moreover, another distinctive feature of this work is applying the fixed free parameters, λ to ISM EOS [7]. This significance making it possible to reduce the number of input constants to be used in the EOS with respect to the previous works of Yousefi et al. [8,10], in which further inputs are required for each polymer by considering the temperature dependence of λ.

In this paper, the performance of the ISM based on the proposed molecular scaling constants has also been checked by predicting the estimation of isothermal compressibility coefficient of molten polymers with reasonably good AAD which indicates the superiority of proposed method against the previous works of Yousefi et al [8,10] (i.e., AADs of the estimated κ_T were found to be more than 30%).

2. Theory

The general frame of the ISM EOS [7] can be summarized as:

$$\frac{P}{\rho k_B T} = 1 + \frac{(B_2(T) - \alpha(T)\ \rho}{1 + 0.2\ \lambda\ b(T)\rho} + \frac{\alpha(T)\rho}{1 - \lambda b(T)\rho} \qquad (1)$$

where P is the pressure, ρ is the molar (number) density, $B_2(T)$ is the second virial coefficient, $\alpha(T)$ is the contribution of repulsive branch of pair potential function according to Weeks-Chandler-Anderson approach in perturbation theory of liquids [11]. This is based on the recognition that the structure of a liquid is determined primarily by repulsive forces, so that fluids of hard bodies can serve as useful reference states b(T) reflects the van der Waals co-volume, $k_B T$ is the thermal energy per segment. λ is a free parameter which can be varied to get the desired volumetric data of dense fluids at the singular point.

The ISM equation of state requires the usage of the second virial coefficient, B_2(T), along with the parameters α(T) and b(T). For central force fields, the second virial coefficient is related to the intermolecular potential energy $u(r)$ through the following equation:

$$B_2(T) = 2\pi N_A \int_0^\infty (1 - e^{-u(r)/kT})\ r^2 d\,r \qquad (2)$$

Where N_A is the Avogadro's number.

If a two-parameter potential energy function $u(r)$ can describe the nature of the interaction potential between particles of a fluid, the potential can be written in dimensionless form by:

$$\frac{u}{\varepsilon} = F(\frac{r}{\sigma}) \tag{3}$$

where ε is a characteristic energy parameter and σ is a characteristic size parameter, and F is a universal function of the reduced intermolecular separation

This function, $B_2(T)$ can be determined either by a direct correlation of experimental data for the second virial coefficient or by specification of the universal potential function u/ε and integration. In this work, we have taken ε as the energy parameters and σ as the size parameter in the potential energy relation as molecular scaling constants. Because, it was empirically found that σ^3 and ε/k_B both are closely proportional to the reciprocal density and to the inter-molecular energy changes during the phase transitions, respectively.

In this section the temperature-dependant parameters $B_2(T)$. $\alpha(T)$ and $b(T)$ of Eq. (1) are to be evaluated. We have used the alternative scaling constants; i. e., dispersive energy parameter (ε) and segment size (σ) to express $B_2(T)$. $\alpha(T)$ and $b(T)$ in terms of the universal functions of reduced temperature ($T_r = k_B T/\varepsilon$) as the following equations:

$$B_2(T)(N_A\sigma^3) = F_2(k_B T/\varepsilon) \tag{4}$$

$$\alpha(T)(N_A\sigma^3) = F_\alpha(k_B T/\varepsilon) \tag{5}$$

and

$$b(T)(N_A\sigma^3) = F_b(k_B T/\varepsilon) \tag{6}$$

It should be mentioned that the above mentioned temperature-dependent parameters, $B_2(T)$. $\alpha(T)$ and $b(T)$ reflect a measure of pairwise interactions.

3. Results and discussion

3.1. *PVT* properties

To utilize the proposed EOS two pure-component parameters of molten polymers must be characterized. Table 1 has been presented to provide the required pure-component parameters (σ, ε/k_B) for studied systems as well as their monomer molecular weight and glass transition temperature, T_g.

At first, we examined the accuracy of ISM EOS for the prediction of the specific volume of studied molten polymers. For this purpose, the specific data of 4 molten polymers have been taken, for which their measured values were available in the literature [15]. The results for 4 studied polymers were reported in Tables 2-5 as the relative deviations (RD in %) of the predicted specific volumes from the literature data [15]. To show the accuracy of the present work, the maximum deviations (in %) of the predicted specific volumes have also been indicated by bold faces in Tables 2-5.

Table 1. Optimized pure-component parameters of the ISM EOS for studied molten polymers

Polymer	MMW^a (g/mol)	ε/k_B (K)	σ (nm)	λ	T_g ^{b}(k)
PO	112	461.05	0.6135	0.5148	338
PVME	58.00	440.19	0.38299	0.8908	239
PVC	62.50	422.16	0.36499	0.8158	358
PS	104.0	517.86	0.50799	0.6898	373

[a] MMW is the monomer molecular weight.

[b] these values were taken from Refs. 12-14.

Table 2. Relative deviation (in %)[a] of the predicted specific volumes of PS using the proposed EOS at several isotherms, compared with the literature data [15]

P/ MPa	391.45 K	413.75 K	435.55 K	455.75 K	478.55 K	501.05 K	534.95 K	556.25 K	557.25K
0.1	-1.88	-1.73	-1.51	-1.16	-0.62	0.05	1.32	**2.26**[b]	1.38
10	-1.66	-1.54	-1.34	-1.05	-0.60	-0.03	1.02	1.76	0.94
20	-1.45	-1.36	-1.19	-0.95	-0.55	-0.06	0.80	1.41	0.65
30	-1.25	-1.18	-1.06	-0.85	-0.52	-0.11	0.61	1.10	0.39
40	-1.06	-1.01	-0.92	-0.76	-0.48	-0.13	0.47	0.88	0.20
50	-0.89	-0.85	-0.80	-0.67	-0.44	-0.15	0.34	0.68	0.02
60	-0.75	-0.71	-0.67	-0.58	-0.39	-0.14	0.26	0.54	-0.09
70	-0.62	-0.57	-0.56	-0.50	-0.35	-0.15	0.19	0.42	-0.19
80	-0.52	-0.43	-0.45	-0.41	-0.29	-0.14	0.13	0.31	-0.28
90	-0.41	-0.29	-0.33	-0.33	-0.25	-0.11	0.09	0.24	-0.34
100	-0.32	-0.17	-0.23	-0.24	-0.19	-0.09	0.06	0.18	-0.39
110	-0.24	-0.04	-0.12	-0.16	-0.14	-0.07	0.05	0.12	-0.42
120	-0.15	0.07	-0.02	-0.08	-0.08	-0.04	0.02	0.08	-0.45
130	-0.07	0.17	0.08	0.00	-0.02	0.00	0.03	0.06	-0.51
140	0.01	0.27	0.19	0.09	0.03	0.03	0.03	0.03	-0.48
150	0.08	0.35	0.29	0.17	0.10	0.07	0.04	0.02	-0.47
160	0.15	0.44	0.38	0.25	0.17	0.12	0.06	0.02	-0.46
170	0.23	0.52	0.48	0.34	0.24	0.17	0.09	0.03	-0.45
180	0.30	0.59	0.58	0.42	0.31	0.23	0.11	0.04	-0.43
190	0.37	0.67	0.68	0.52	0.38	0.28	0.14	0.07	-0.40
200	0.44	0.73	0.77	0.59	0.45	0.35	0.19	0.09	-0.38

Table 3. Relative deviation (in %)[a] of the predicted specific volumes of PVME using the proposed EOS at several isotherms, compared with the literature data [15].

P/ MPa	311.5K	340.3K	353.5K	374.5K	394.5K	415.5K
0.1	**-1.93**[b]	-1.87	-1.60	-1.01	-0.39	0.41
5	-1.80	-1.73	-1.48	-0.90	-0.32	0.43
10	-1.67	-1.59	-1.35	-0.80	-0.25	0.44
20	-1.42	-1.35	-1.12	-0.60	-0.13	0.50
30	-1.18	-1.10	-0.92	-0.44	-0.02	0.51
40	-0.95	-0.89	-0.73	-0.27	0.11	0.58
50	-0.72	-0.67	-0.54	-0.12	0.22	0.63
60	-0.51	-0.48	-0.37	0.02	0.32	0.66
70	-0.31	-0.29	-0.20	0.16	0.41	0.72
80	-0.10	-0.12	-0.05	0.29	0.51	0.77
90	0.07	0.05	0.10	0.41	0.60	0.81
100	0.25	0.21	0.24	0.53	0.70	0.86
110	0.42	0.37	0.37	0.64	0.77	0.91
120	0.58	0.52	0.49	0.75	0.86	0.96

[a] $RD = \left(\frac{V^{Calc.} - V^{Exp.}}{V^{Exp.}}\right).100$

[b] Bold face is the maximum %RD in the predicted specific volumes.

Table 4. Relative deviation (in %)[a] of the predicted specific volumes of PVC using the proposed EOS at several isotherms, compared with the literature data [15].

P/MPa	373.15K	383.25K	393.25K	403.25K	413.25K	423.15K
0	-0.18	-0.04	0.15	0.41	0.74	**1.14**[b]
10	-0.20	-0.08	0.08	0.31	0.58	0.84
20	-0.20	-0.11	0.03	0.22	0.46	0.75
30	-0.20	-0.13	-0.02	0.15	0.36	0.61
40	-0.21	-0.14	-0.04	0.10	0.27	0.49
50		-0.15	-0.06	0.05	0.21	0.38
60		-0.15	-0.08	0.02	0.15	0.31
70		-0.15	-0.09	-0.01	0.12	0.24
80		-0.15	-0.10	-0.03	0.06	0.19
90			-0.11	-0.04	0.05	0.14
100			-0.11	-0.05	0.02	0.29
110			-0.10	-0.06	0.01	0.08
120			-0.10	-0.07	-0.01	0.06
130				-0.06	-0.02	0.04
140				-0.05	-0.03	0.03
150				-0.04	-0.02	0.02
160				-0.05	-0.02	0.02
170				-0.03	-0.02	0.01
180					-0.01	0.02
190					0.01	0.02
200					0.01	0.02

Table 5. Relative deviation (in %)[a] of the predicted specific volumes of PO using the proposed EOS at several isotherms, compared with the literature data [15]

P/ MPa	455.9K	465.85K	476.1K	485.95K	496.2K	505.75K	516.5K	526.15K	536.75K
0.1	-1.19	-0.89	-0.49	-0.20	0.27	0.71	1.25	1.75	**2.41**
10	-1.00	-0.75	-0.44	-0.18	0.19	0.49	0.92	1.29	1.78
20	-0.81	-0.62	-0.35	-0.11	0.14	0.36	0.72	1.01	1.38
30	-0.69	-0.53	-0.32	-0.12	0.09	0.27	0.49	0.72	1.02
40	-0.57	-0.47	-0.29	-0.13	0.04	0.16	0.37	0.51	0.75
50	-0.46	-0.39	-0.26	-0.16	-0.01	0.08	0.24	0.37	0.52
60	-0.36	-0.31	-0.22	-0.15	-0.03	0.03	0.14	0.23	0.36
70	-0.25	-0.23	-0.17	-0.15	-0.06	-0.02	0.06	0.12	0.21
80	-0.15	-0.16	-0.12	-0.12	-0.06	-0.07	0.01	0.04	0.10
90	-0.07	-0.09	-0.07	-0.10	-0.07	-0.08	-0.05	-0.03	0.01
100	0.03	-0.01	-0.01	-0.06	-0.04	-0.09	-0.07	-0.07	-0.05
110	0.14	0.06	0.04	-0.02	-0.02	-0.09	-0.08	-0.11	-0.11
120	0.25	0.15	0.11	0.02	0.01	-0.07	-0.07	-0.12	-0.13
130	0.34	0.24	0.19	0.09	0.04	-0.04	-0.06	-0.11	-0.15
140	0.44	0.34	0.26	0.15	0.10	-0.01	-0.04	-0.11	-0.16
150	0.56	0.42	0.35	0.22	0.15	0.03	-0.02	-0.10	-0.15
160	0.66	0.53	0.45	0.29	0.20	0.07	0.03	-0.07	-0.13
170	0.76	0.64	0.53	0.36	0.26	0.12	0.06	-0.04	-0.10
180	0.87	0.73	0.61	0.45	0.33	0.17	0.11	0.00	-0.08
190	0.98	0.84	0.71	0.53	0.40	0.24	0.15	0.04	-0.04
200	1.07	0.94	0.79	0.62	0.47	0.30	0.22	0.09	-0.01

Generally, our calculation results over the whole pressure/temperature range were summarized as average absolute deviation percent (AAD in %) from literature data [15] in Table 6. As indicated by Table 6, from 547 data points examined for studied polymers in wide pressure range between 0.1 - 200 MPa and the temperature range from 311 to 557 K, AAD was found to be 0.47%. It should be mentioned that, the range of deviations in the current prediction was of the order of ±2.86%.

Table 6 also compares our prediction results with those obtained from the preceding work of S & B [6] and Yousefi et al. [10], which employed ISM and TM EOSs, respectively, to predict specific volumes of molten polymers based on the scaling constants raised by the bulk properties contrary to the present work, in which the alternative correlation equations based on the molecular scaling constants were presented. As Table 6 shows, our prediction results are almost as accurate as the previous works [6,10].

In order to illustrate how the ISM EOS passes through the experimental points, Figure 1 has been presented. It indicates the specific volume of PVC versus pressure at several isotherms. The markers represent the literature data [15] and the solid lines are those estimated from Eq. (1). As it is obvious from Figure 1, the agreement of the predicted values and literature data is quite good. The maximum RD is not more than 1.14%.

Moreover, it has been found that the predicted specific volumes have been affected by pressure, systematically, as it's impressed

Table 6. Average absolute deviation (AAD in %) of the predicted specific volumes of the molten polymers studied in this work, using the proposed EOS, compared with results from ISM and TM, all were compared with the literature data [15].

Polymer	**ΔP (MPa)**	**ΔT (K)**	**NP** [a]	**this work**	**ISM [6]**	**TM [8]**
PVME	0.1-120	311-415	84	0.88	0.30	0.26
PVC	0-200	373-423	85	0.15	0.14	0.21
PS	0.1-200	391-557	189	0.62	0.51	0.54
PO	0.1-200	456-536.7	189	0.31		
Overall			547	0.47	0.42	0.40

[a] NP represents the number of data points examined

[b] $$\mathrm{AAD} = 100/\mathrm{NP} \sum_{i=1}^{\mathrm{NP}} |V_{i\,\mathrm{Cal.}} - V_{i\,\mathrm{Exp.}}| \big/ V_{i\,\mathrm{Exp.}}$$

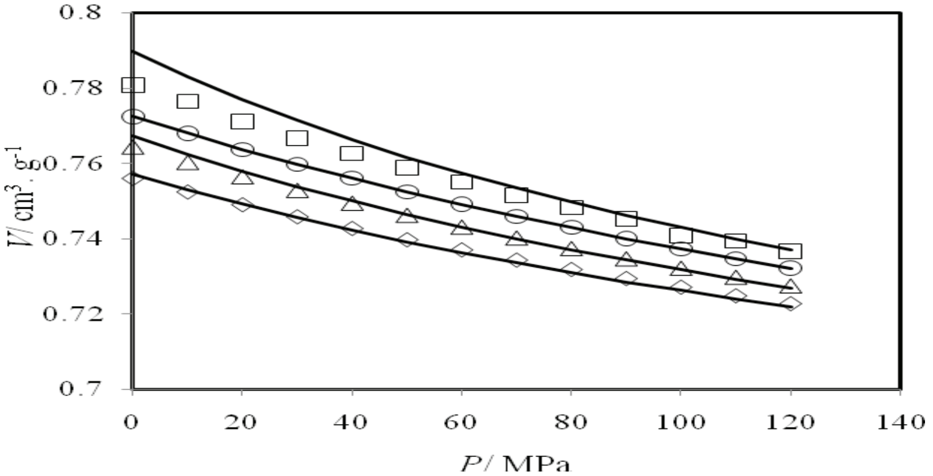

Fig. 1:The specific volume (V in cm^3 g^{-1}) of PVC versus pressure at several isotherms. The markers represent the experimental data [15] and the solid lines are those estimated from ISM EOS; 393.25 K (◊), 403.25 K (Δ), 413.25 K (○), and 423.25 K (□).

from Tables 2-5. Since, the ISM EOS has been parameterized by some PVT data at moderate pressures; the high deviations have been appeared in the current predictions at low and high pressures accordingly.

3.2. First derivative thermodynamic properties

In this section, the relevant thermodynamic properties of molten polymer to the first derivation of ISM EOS were also predicted. Typically, the isothermal compressibility coefficient, κ_T is calculated using the isothermal pressure derivative of density/specific volume according to following equation:

$$\kappa_T = -\left(\frac{1}{V_S}\right)\left(\frac{\partial V_S}{\partial P}\right)_T = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_T \qquad (7)$$

We compared the calculated κ_T of PO using ISM EOS with those obtained from Tait equation [16]. The results were reported in Table 7 as the relative deviations (RD in %) of the predicted κ_T using ISM EOS from those derived by the Tait equation [16]. From 188 data points examined, the AAD of estimated κ_T was equal to 7.75%. According to Table 7, the maximum value of relative deviations (RD) for isothermal compressibility coefficients was found to be 24.38%. Generally, the reason

Table 7. Relative deviation (in %)[a] of the predicted isothermal compressibility coefficients (κ_T) of PO using the proposed EOS at several isotherms, compared with the those obtained from the Tait equation [16].

P/ MPa	455.9K	465.85K	476.1K	485.95K	496K	505.7K	516K	526K	536.7K
0.1	-10.35	-6.25	-1.97	2.18	6.54	10.65	15.33	19.60	24.38
10	-10.00	-6.11	-2.11	1.73	5.70	9.36	13.46	17.12	21.11
20	-9.92	-6.23	-2.46	1.12	4.78	8.14	11.85	15.10	18.61
30	-10.04	-6.52	-2.95	0.41	3.84	6.95	10.36	13.34	16.51
40	-10.30	-6.94	-3.54	-0.36	2.87	5.79	8.97	11.73	14.65
50	-10.66	-7.43	-4.19	-1.17	1.89	4.64	7.64	10.22	12.96
60	-11.08	-7.99	-4.89	-2.00	0.91	3.52	6.36	8.80	11.37
70	-11.56	-8.58	-5.61	-2.84	-0.06	2.43	5.12	7.44	9.88
80	-12.08	-9.21	-6.34	-3.69	-1.03	1.36	3.93	6.14	8.47
90	-12.62	-9.85	-7.09	-4.53	-1.98	0.31	2.78	4.89	7.12
100	-13.18	-10.50	-7.84	-5.37	-2.91	-0.71	1.66	3.69	5.82
110	-13.75	-11.16	-8.58	-6.20	-3.83	-1.71	0.57	2.53	4.58
120	-14.33	-11.82	-9.32	-7.02	-4.73	-2.68	-0.48	1.41	3.39
130	-14.91	-12.47	-10.06	-7.83	-5.61	-3.63	-1.50	0.33	2.24
140	-15.49	-13.13	-10.78	-8.62	-6.47	-4.55	-2.49	-0.72	1.13
150	-16.08	-13.78	-11.50	-9.40	-7.31	-5.45	-3.45	-1.74	0.05
160	-16.66	-14.42	-12.20	-10.17	-8.13	-6.33	-4.38	-2.72	-0.99
170	-17.23	-15.05	-12.90	-10.91	-8.94	-7.18	-5.29	-3.68	-1.99
180	-17.80	-15.68	-13.58	-11.65	-9.73	-8.01	-6.18	-4.61	-2.96
190	-18.37	-16.30	-14.25	-12.37	-10.49	-8.83	-7.04	-5.51	-3.91
200	-18.92	-16.90	-14.91	-13.07	-11.24	-9.62	-7.87	-6.39	-4.83

[a] $RD = \left(\frac{\kappa_T^{Calc.} - \kappa_T^{Tait}}{\kappa_T^{Tait}}\right).100$

[b] Bold face is the maximum %RD in the predicted κ_T.

for such high deviations is that κ_T is nearly related to isothermal EOS derivation against density/volume which resulted serious changes in the original frame of ISM EOS, by which the *PVT* data were predicted well. So, the large deviations related to the prediction of first derivative properties would be expectable.

Figure 2 depicts κ_T (in GPa^{-1} units) versus pressure for PO at several isotherms graphically. The solid lines are our predictions and the markers represent those obtained from the Tait equation [16].

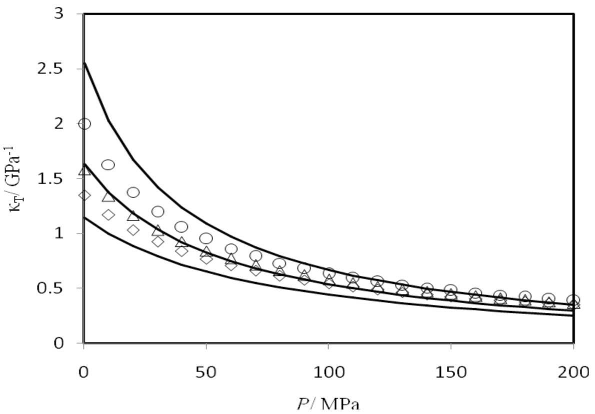

Fig.2: κ_T (in GPa^{-1} units) versus pressure for PO at several isotherms. The solid lines are our predictions and the markers represent those obtained from the Tait equation [13]. 456 K (◊), 486 K (Δ), and 526 K (○).

4. Conclusion

Finally, an analytical EOS has been employed to predict the volumetric and thermodynamic data of molten polymers. Knowing only two molecular scaling constants, ε/k_B and σ, is sufficient to determine the temperature-dependent parameters of the ISM EOS. Our calculations on the volumetric and thermodynamic properties of studied polymers reproduce the literature data over the whole liquid range with reasonably good accuracy.

Acknowledgment

We thank the Young Researchers and Elite Club, Marvdasht Branch for their financial supports.

Nomenclature and units

List of symbols

AAD	average absolute deviation (%)
k_B	Boltzmann's constant (J K^{-1})
NP	number of data points
P	pressure (Pa)
T	Absolute temperature (K)
V	Specific molar volume (m^3 mol^{-1})
MMW	monomer molecular weight (g. mol^{-1})
R	Universal gas constant (J mol^{-1}. K^{-1})
B_2	second virial coefficient/(m^3)
b	co-volume/ (m^3)
α	repulsive contribution to pair potential function/(m^3)
N_A	Avogadro's number

Greek letters

ρ	molar density (mol m^{-3})
σ	segment diameter (nm)
ε	dispersive energy parameter (J)
λ	free parameter

Superscripts

Calc	Calculated values
Exp	Experimental value

References

[1] G. Odian, Principles of polymerization, Wiley, New York (1991).

[2] F. F. Mark, N. Bikales, C. G. Overberger, G. Menges, J. I. Kroschwitz, Encyclopedia of polymer science and engineering. Wiley, New York (1986).

[3] S. Parveen, S. K. Sahoo, Clin. Pharmacokinet., 45 (2006) 965-988.

[4] K. Osada, K. Kataoka, Ad. Polym. Sci., 202 (2006) 113-153.

[5] O. Annunziata, N. Asherie, A. Lomakin, J. Pande, O. Ogun, G. B. Benedek. Proc. Natl. Acad. Sci. U.S.A., 99 (2002) 14165-14170.

[6] Sabzi F., and Boushehri A, Eur. Polym. J., 40 (2004) 1105-1110.

[7] Ihm G., Song Y and Mason E. A. J. Chem. Phys, 94 (1991) 3839-3848.

[8] F. Yousefi, High Temp-High Press, 42 (2013) 211-226.

[9] F. M. Tao, E. A. Mason, J. Chem. Physics 100 (1994) 9075-9084.

[10] F. Yousefi, H. Karimi, R. Ghafarian-Shirazi., M. Gomar, High Temp-High Press, 42 (2013) 451-567.

[11] J. D. Weeks, D. Chandler, H. C. Anderson, J. Chem. Phys. 54 (1971) 5237-5247.

[12] J.E. Mark Polymer Data Handbook, second Ed., Oxford University Press: New York, (1999)

[13] J.E. Mark, Physical Properties of Polymers Handbook, second Ed., Springer, New York, (2007).

[14] S.M. Allen, E.L. Thomas. The Structure of Materials. New York, NY: J. Wiley & Sons, (1999).

[15] C. Wohlfarth, CRC Handbook of Thermodynamic Data of Polymer Solutions at Elevated Pressures, Taylor & Francis, New York, (2005).

[16] J. H. Dymond, R. Malhotra, Int. J. Thermophys., 9 (1988) 941–951.