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Modeling vapour pressure using compound specific cohesion factor relationship

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ABSTRACT

Major factor in the success of predictive capability of cubic equations of state (CEOS) is the temperature dependency of the cohesion factor. Accurate prediction of vapour pressure is the yardstick for comparing various cohesion factor relationships. For polar and weekly polar compounds generalized expression fails to perform well in predicting vapour pressure using CEOS. The best alternate to improve this is to introduce compound specific parameter in cohesion factor model. So, four compound specific models were compared in the present study. Two of the models were having single additional parameter and the remaining had two compound specific parameters. We use a simple method to obtain parameters for each compound. Behavior at supercritical conditions was also compared and it was found that the alpha function having exponential form behaves satisfactorily. Modified Trebble–Bishnoi type of cohesion factor model emerged as the best amongst the compared models. Family specific generalized expressions were also proposed. These expressions would be useful in the absence of experimental vapour pressure data. Compound specific parameters for nearly 300 compounds are listed in the paper and can be utilized for the modeling of phase equilibrium of the mixtures of these compounds.

1. Introduction

Amongst various thermodynamic models available, cubic equations of state (CEOS) play a significant role in the representation of phase equilibria of pure fluids and mixtures. Most of the commercial process simulators have numerous equations of state (EOS) ranging from fundamentally strong SAFT (Song and Sadus, 2000) EOS to the algebraic simple CEOS. Over and above being simple in nature, these CEOS offer following advantages:

- Capable of being applied over wide ranges of temperatures and pressures.
- Relatively simple extension to mixtures through use of mixing and combining rules.

There has been extensive effort in improving the predictive capabilities of CEOS through refinements of cohesion factor model and extending their use to wider variety of fluids.

Since van der Waals proposed the first CEOS, a large number of equations were proposed to improve prediction of thermodynamic properties of pure compounds and mixtures. Generic form of any CEOS can be written as

$$P = \frac{RT}{v-b} - \frac{a(v-k_3 b)}{(v-b)\left(v^2 + k_1 bv - k_2 b^2\right)} \quad (1)$$

where a, b, k_i (i = 1–3) may be universal constants, fluid-specific constants or functions of temperatures (but not of pressure or density). The most frequently used CEOS in engineering practice are, without doubt, the Soave–Redlich–Kwong (SRK) EOS (Soave, 1972) and Peng–Robinson (PR) EOS (Peng and Robinson, 1976). In the present work PR EOS, one of most widely accepted two parameter EOS, was selected. PR EOS, as a special case of generic form (k_1 = 2, k_2 = 1, k_3 = 1), can be expressed as

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)} \quad (2)$$

where

$$a(T) = \frac{\psi\alpha(T_r)R^2T_c^2}{P_c} \quad (3)$$

$$b = \frac{\Omega RT_c}{P_c} \quad (4)$$

where Ω and ψ are the parameters for PR EOS and their values are 0.07780 and 0.45724 respectively. $\alpha(T_r)$ is the cohesion function (popularly known as alpha function) and represents the dependency of attractive term a (T) on temperature. Strength of any EOS in predicting phase equilibrium can be judged by how

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Nomenclature

%AAD	percent absolute average deviation (defined in Table 2)
a	attractive parameter of EOS (defined in Eq. (3) for PR EOS)
b	co-volume parameter of EOS (defined in Eq. (4) for PR EOS)
B	EOS parameter defined in Eq. (9)
k_i	universal constants for EOS
m	characteristic constant for the proposed model in present work
n	characteristic constant for the proposed model in present work
N_c	number of compounds
N_p	number of data points
P	pressure (Pa)
P_c	critical pressure (bar)
R	universal gas constant (J/mol K)
T	temperature (K)
T_c	critical temperature (K)
T_r	reduced temperature
v	molar volume (cm^3/mol)
W	error propagation factor defined in Eq. (8)
Z	compressibility factor

Superscripts and subscripts

cal	predicted values
exp	pseudo-experimental data
V	vapour
L	liquid
sat	saturated property

Greek symbols

α	cohesion factor
ω	acentric factor
Ω	EOS parameter
ψ	EOS parameter

precisely it predicts saturation vapour pressure. Accuracy can be increased by proper selection of the expression for the cohesion function in the EOS. Peng and Robinson (Peng and Robinson, 1976) expressed this cohesion function as

$$\alpha = \left[1 + m(1 - T_r^{0.5})\right]^2 \tag{5}$$

The above form was first proposed by Soave (Soave, 1972) who observed that for a given substance the square root of alpha varies linearly with square root of the reduced temperature, to a good approximation. Expression for m to be used with PR EOS is

$$m = 0.3746 + 1.54226\omega - 0.26992\omega^2 \tag{6}$$

where ω is the acentric factor. A large number of cohesion factor models for PR EOS have been proposed there after and their functional forms can be categorized in three basic types as follows:

(i) Polynomial in acentric factor;
(ii) Exponential in acentric factor and
(iii) Corresponding state type, *i.e.* linear in acentric factor ($\alpha = \alpha^0 + \omega(\alpha^1 - \alpha^0)$).

Our previous study (Joshipura *et al.*, 2009) reports comparison of vapour pressure prediction by ten such models covering all functional forms. All the models with their parameters are shown in Table 1. Nearly 300 compounds were considered in the study comprising of more than 25 families. Table 2 shows summary of the results obtained in terms of global %AAD values for the three regions of temperature studied. It was observed that out of ten models studied no single model was capable of representing the large variety of compounds simultaneously. However, some of the families were represented better by some specific models.

The present work, therefore, determines substance specific parameters in cohesion functions as adjustable parameters, instead of from generalized expression in terms of acentric factor. Four models, listed in Table 3, representing above three categories of cohesion factor models were selected. These can be grouped in two sub classes: single additional compound specific parameter and two additional compound specific parameters. Encouraged by performance of compound specific parameters they were used to obtain family specific generalized expressions in terms of acentric factor. Section 2 discusses approaches and techniques for computation of compound specific and family specific parameters. Results and their discussion are given in Section 3 and conclusions are reported in Section 4.

Table 1
Various cohesion function (alpha) models available in the literature.

Model no. (reference)	$\alpha(T_r)$
PR (Peng and Robinson, 1976)	$\left[1 + (A + B\varpi + C\varpi^2)(1 - Tr^D)\right]^{1/E}$; $A = 0.37460$; $B = 1.54226$; $C = -0.26992$; $D = 0.5$; $E = 0.5$
PRG (Gasem *et al.*, 2001)	$\left[1 + (A + B\varpi + C\varpi^2)(1 - Tr^D)\right]^{1/E}$; $A = 0.386590$; $B = 1.50226$; $C = -0.16870$; $D = 0.5$; $E = 0.5$
TWU (Twu *et al.*, 1995)	$T_r^{-0.171813}\exp[0.125283(1 - T_r^{1.77634})] + \varpi[T_r^{-0.607352}\exp[0.511614(1 - T_r^{2.20517})] - T_r^{-0.17183}\exp[0.125283](1 - T_r^{1.77634})]$
TWUG (Gasem *et al.*, 2001)	$Tr^A\exp(B(1 - Tr^C)) + \varpi\left(Tr^D\exp(E(1 - Tr^F)) - Tr^A\exp(B(1 - Tr^C))\right)$ $A = -0.207176$; $B = 0.092099$; $C = 1.94800$; $D = -0.502297$; $E = 0.603486$; $F = 2.09626$;
mTB (modifed Trebble–Bishnoi) (Gasem *et al.*, 2001)	$\exp\left((A + BTr)\left(1 - Tr^{(C + D\varpi + E\varpi^2)}\right)\right)$; $A = 2.00$; $B = 0.836$; $C = 0.134$; $D = 0.508$; $E = -0.0467$;
TB (Trebble and Bishnoi, 1987)	$\exp(m(1 - T_r))$ $m = 0.418 + 1.58\varpi - 0.580\varpi^3 \quad \varpi < 0.4$ $= 0.212 + 2.2\varpi - 0.831\varpi^3 \quad \varpi \geq 0.4$
PR NSM1 (Joshipura *et al.*, 2009)	$\left[1 + (1.3676\omega + 0.4132)(1 - T_r^{0.5})\right]^2$
PR NSM2 (Joshipura *et al.*, 2009)	$\exp[(1.2294\omega + 0.4887)(1 - T_r)]$
PR NSM3 (Joshipura *et al.*, 2009)	$\left[1 + (1.3748\omega + 0.4086)(1 - T_r^{0.5})\right]^2$
PR NSM4 (Joshipura *et al.*, 2009)	$\exp[(1.252\omega + 0.4754)(1 - T_r)]$

Table 2
Global values of average absolute deviation (%AAD)[a] in vapour pressure for all the models.

Model	$T_r < 0.7$	$T_r \geq 0.7$	Entire range
PR	13.9	2.46	8.59
PRG	11.41	2.01	7.06
TWU	9.37	2.61	6.28
TWUG	9.35	2.43	6.13
mTB	10	2.72	6.68
TB	20.89	3.44	12.82
PR NSM1	11.45	2.14	7.14
PR NSM2	19.2	2.99	11.85
PR NSM3	11.44	2.23	7.20
PR NSM4	20.42	2.73	12.51

[a] $\%AAD = 100/N_p \sum abs\left(P_{exp}^{sat} - P_{cal}^{sat}\right)/P_{exp}^{sat}$ with N_p, no. of data points P_{cal}, predicted vapour pressure and P_{exp}, pseudo-experimental vapour pressure.

2. Computation of parameters for cohesion function

Values of the pseudo-experimental cohesion function, α_{exp}, were obtained in terms of reduced temperature for 298 compounds, classified in 29 subfamilies, from pseudo-experimental vapour pressure data generated from the correlations given in the Handbook of Yaws (Yaws, 1992). The generation of the data was done by applying equi-fugacity criteria (Smith *et al.*, 2001), which also gave the values of saturated vapour and liquid volumes. Coding for the same was done in MATLAB®.

2.1. Compound specific parameters

Optimization was done to obtain the compound specific parameters m and n (wherever applicable) for each compound using following objective function:

$$f(m,n) = \min \sum_{\text{all } T_r} \left[W \frac{\alpha(m,n) - \alpha_{exp}}{\alpha_{exp}} \right]^2 \quad (7)$$

where W the error propagation factor is given by Figueira *et al.* (2007),

$$W = 1 - \frac{1}{Z^V - Z^L} \ln\left(\frac{Z^V - B^{sat}}{Z^L - B^{sat}}\right) \quad (8)$$

and

$$B^{sat} = \frac{bP^{sat}}{RT} \quad (9)$$

where Z is the compressibility factor and the superscripts L and V denote the liquid and vapour phase respectively $\alpha(m,n)$ is the cohesion factor value obtained using the model parameters m and n. Optimization was done using *Solver* in Microsoft Excel®. This procedure for obtaining the parameters is nearly as accurate as the computationally much more complex "rigorous method" (Figueira *et al.*, 2007). The compound specific parameter values computed by this procedure are listed in Table 4. The critical properties (T_C, P_c, ω), to be used with these constants, should be obtained from the handbook of Yaws (Yaws, 1992) to maintain consistency.

2.2. Family specific generalized models

The optimized compound specific parameters reported in the present work are recommended for accurate modeling of phase equilibria involving these compounds. For compounds not listed in the present work optimized compound specific parameters may be determined with the help of procedure outlined here, if experimental vapour pressure data are available. However, in the absence of such data a compromise is to develop a family specific generalization for cohesion function model parameters. Two generalized expressions, linear and quadratic, in terms of acentric factor are reported:

$$m = s_1 + s_2\omega \quad (10)$$

$$m = p_1 + p_2\omega + p_3\omega^2 \quad (11)$$

The values of constants (m_{TB} and m_{PR}), reported in Table 4, were plotted against acentric factor and trend line in Excel® was used to get the constants of Eq. (10), s_i (i = 1, 2) and Eq. (11), p_i (i = 1–3).

3. Results and discussion

Any cohesion function (alpha) model should obey/meet certain conditions/requirements (Coquelet *et al.*, 2004; Twu *et al.*, 2002) such as:

i. The value of alpha should be finite and positive for entire range of T_r.
ii. The value of alpha should tend to zero as T_r approaches infinity.
iii. The value of alpha must be unity at $T = T_c$.

It was observed (Joshipura *et al.*, 2009) that the Soave type cohesion factor models do not fulfil condition (ii) and tend to increase after some transition temperature. The models with exponential form fulfil all the above conditions. Soave type models may not thus be suitable beyond a certain transition value of reduced temperature.

3.1. Compound specific parameters

Table 5 lists the percent average absolute deviations (%AAD) in vapour pressure for the cohesion factor models studied in the present work. %AAD values are shown for all the families considered. Based on the global values one could see that the modified TB model is the best model out of the four models studied. Amongst the single additional parameter models, compound specific PR model performs better compared to compound specific TB model. However, one must note that this model may not behave properly after some transition temperature value.

3.2. Family specific generalized models

This generalization is reported here for (i) families containing five or more compounds and (ii) only single parameter models (*i.e.* for original PR and original TB models).

Table 3
Models considered for obtaining compound specific cohesion factor.

Model	Expression	Remarks
Original PR type	$\left[1 + m_{PR}(1 - \sqrt{T_r})\right]^2$	Single additional parameter
Original TB type	$\exp(m_{TB}(1 - T_r))$	Single additional parameter
Twu type	$\alpha = \alpha^0 + \omega(\alpha^1 - \alpha^0)$ with $\alpha^0 = \exp(m_{Twu}(1 - T_r))$ $\alpha^1 = \exp(n_{Twu}(1 - T_r))$	Two additional parameters
Modified TB type (Gasem *et al.*, 2001)	$\exp(m_{mTB}(1 - T_r^{n_{mTB}}))$	Two additional parameters

Table 4
Compound specific parameters for the cohesion factor models studied in the present work.

Compounds	m_{TB}	m_{PR}	m_{TWU}	n_{TWU}	m_{mTB}	n_{mTB}
Neon	0.346947947	0.316520643	0.411183005	1.62262453	0.306924398	1.183081802
Argon	0.410922439	0.382838388	0.410922439	–[a]	0.385930966	1.083773748
Krypton	0.414484304	0.386109214	0.414484304	–	0.400247014	1.045700624
Xenon	0.426583043	0.398108323	0.426583043	–	0.30046356	0.277745799
Mercury	0.135530846	0.101078965	0.135521544	0.135463567	0.163689973	1.770608134
Nitrogen	0.480911031	0.445904976	0.434957969	1.431163289	0.595892243	0.760457332
Oxygen	0.473681321	0.420696618	0.359228047	2.834178115	0.665549996	0.618482623
Fluorine	0.504554334	0.452857569	0.309704976	2.266516188	0.788964155	0.544269927
Chlorine	0.561417189	0.513778495	0.68952218	−3.649978394	1.0553041	0.444895542
Bromine	0.612899439	0.570251933	0.775343061	−1.231774102	0.850141579	0.653096165
Hydrogen	0.02270785	0.018843066	0.349175778	1.401994301	0.011867663	31.92824816
Hydrogen cyanide	0.954620815	0.937510214	0.954618261	0.954623534	0.567314282	2.076421527
Nitro methane	0.883377574	0.842474204	0.883375794	0.883379718	0.834309799	1.087759818
Water	0.892972678	0.85360439	0.905476289	0.869215621	0.888479072	1.007293331
Carbon monoxide	0.508782901	0.474271371	0.508766043	0.509031875	0.419072579	1.302895714
Carbon dioxide	0.730694785	0.715436446	0.847854203	0.308887677	0.731024854	1.000299622
Nitrous oxide	0.638854797	0.611376031	0.877364149	−1.446435663	1.552062853	0.362640722
Sulfur dioxide	0.806790208	0.768213905	1.14712095	−0.789043865	1.254803197	0.568407801
Sulfur trioxide	1.059390368	1.050286298	2.088759185	−1.434119578	17.79995368	0.049107983
Hydrogen sulfide	0.567175635	0.530615684	0.727218408	−2.792900809	1.23295558	0.394292862
Carbon disulfide	0.604914516	0.536035795	0.741316772	−1.475606146	0.7318172	0.740800412
Hydrogen chloride	0.602131033	0.563824854	0.715793596	−0.3239728	0.679536286	0.853378193
Phosgene CCl_2O	0.764721814	0.701076996	1.048619888	−1.415818799	1.186163609	0.533347436
Diborane	0.638287698	0.58324299	0.799979742	−1.233485375	0.80851476	0.714263674
p-Nitrotoulene	1.042445675	1.018833521	1.042450997	1.042441752	0.71927214	1.813529734
Methane	0.434683026	0.398598567	0.413793729	1.886074247	0.510580922	0.809591899
Ethane	0.607436302	0.53940674	0.332819979	2.037666094	0.844778382	0.609055536
Propane	0.710081885	0.624879634	0.315236375	1.938253391	0.933924012	0.633428226
Butane	0.753133306	0.688718781	1.014193147	−1.13100136	1.030481483	0.629022599
Isobutane	0.765365514	0.692574324	1.034601922	−2.334970959	1.303439503	0.459528046
Pentane	0.850500849	0.786723507	1.197538	−1.164850223	1.275725841	0.552092008
Isopentane	0.821379604	0.741430301	1.127547202	−1.357544096	1.129396275	0.598987035
Neopentane	0.701914426	0.675627706	0.701697024	0.702806118	0.685933419	1.028995506
Hexane	0.904575379	0.853440568	1.325415276	−0.76019228	1.453927625	0.518404648
2,2-Dimethyl butane	0.797633946	0.742227199	1.09833231	−0.825392084	1.1170544	0.621021512
Heptane	0.972051146	0.923539017	1.442340321	−0.513762639	1.445281676	0.56843841
2-Methyl hexane	0.958635729	0.898645561	1.401121045	−0.723517016	1.388796954	0.573167469
3-Methyl hexane	0.940057574	0.877406573	1.346164724	−0.562721872	1.248889036	0.644428407
3-Ethyl pentane	0.910603222	0.845481287	1.252957877	−0.31322056	1.092559047	0.746994393
2,2-Dimethyl pentane	0.922184276	0.858152708	0.922183806	0.922184731	0.880588501	1.084817993
2,3-Dimethyl pentane	0.895733745	0.832610988	1.258411683	−0.617575074	1.174723776	0.660011823
2,4-Dimethyl pentane	0.91715473	0.855042329	1.313179064	−0.73621428	1.276167969	0.607225504
3,3-Dimethyl pentane	0.867858309	0.793186531	1.205790543	−0.870689032	1.133898307	0.64997329
2,2,3-Trimethyl butane	0.793558564	0.755745845	1.051568172	−0.228675923	0.983669651	0.753912493
Octane	0.996346845	0.958152059	1.367085642	0.234772871	1.141851347	0.82028992
2-Methyl heptane	1.00525169	0.949741068	1.459415145	−0.241064827	1.282926819	0.684155172
3-Methyl heptane	1.013292998	0.952732842	1.494780994	−0.465602828	1.369399399	0.622852348
4-Methyl heptane	1.015368522	0.955067758	1.49408837	−0.457177083	1.361290204	0.630053902
3-Ethyl hexane	0.939802536	0.911791957	1.261798714	0.234621256	1.096572109	0.816136197
2,2-Dimethyl hexane	0.974756558	0.912128918	1.420642024	−0.646266111	1.346995308	0.605805812
2,3-Dimethyl hexane	0.917398801	0.888026827	1.251604025	0.115282653	1.107306069	0.781935552
2,4-Dimethyl hexane	0.913942187	0.885411328	1.241937851	0.122574606	1.100878249	0.785273087
2,5-Dimethyl hexane	0.974197038	0.924433889	1.414603102	−0.302537821	1.298522749	0.655122195
3,3-Dimethyl hexane	0.95382633	0.885463875	0.95382633	0.95382633	1.327956171	0.594025686
3,4-Dimethyl hexane	0.910822087	0.880483311	1.211149315	0.174828242	1.063471571	0.815117944
2-Methyl-3-ethylpentane	0.896303161	0.867427558	1.223544961	0.176325708	1.062001974	0.802690214
3-Methyl 3-ethyl pentane	0.899667909	0.841038696	1.269201765	−0.483686584	1.17866579	0.666720235
2,2,3-Trimethyl pentane	0.912897542	0.847902108	1.304026524	−0.798190907	1.269648642	0.60391681
2,2,4-Trimethyl pentane	0.913832753	0.853554539	1.313545944	−0.733027196	1.297622882	0.593559693
2,3,4-Trimethyl pentane	0.924157112	0.860904181	1.296867643	−0.55306026	1.196412461	0.669408195
2,2,3,3-Tetramethyl butane	0.719938743	0.700262368	1.176358882	−1.128144188	4.381479334	0.143577055
Nonane	1.04812026	1.013145813	1.427961822	0.405372413	1.165434675	0.854198537
3,3-Diethyl pentane	0.910652552	0.867821542	1.198750731	0.178462506	1.029820748	0.838080583
2,3,3-Trimethyl hexane	0.897599655	0.869087791	1.212191508	0.106204108	1.080195013	0.78748529
2,2,4-Trimethyl hexane	0.924554242	0.8986249	1.250866883	0.043463269	1.142180456	0.763248789
2,4,4-Trimethyl hexane	0.910040158	0.882787066	1.194836395	0.250914556	1.042021143	0.83894525
2,2,3,3-Tetramethyl pentane	0.853830497	0.813457607	1.206527054	−0.490086753	1.213043206	0.628096992
2,2,3,4-Tetramethyl pentane	0.954100416	0.884409969	1.388378642	−1.048668159	1.415315534	0.541949958
2,2,4,4-Tetramethyl pentane	0.906219414	0.857443799	1.261223447	−0.237753769	1.138959617	0.7187608
2,3,3,4-Tetramethyl pentane	0.87300569	0.842324297	1.133863258	0.173157949	0.99994778	0.837461859
Decane	1.09921676	1.074437917	1.479103718	0.588381262	1.191876191	0.888829309
Undecane	1.17829471	1.163155525	1.800181547	0.399214801	1.478023318	0.725725026
Dodecane	1.214440453	1.206740657	1.762651652	0.67208261	1.379250186	0.833538923
Tridecane	1.23985701	1.23584481	1.605488292	0.974155989	1.294568218	0.93848346
Tetradecane	1.321149302	1.332053536	2.117418473	0.737676827	1.609206781	0.757889506
Pentadecane	1.371403344	1.39192784	0.017807152	1.740435642	1.679071391	0.752038881

Table 4 (*Continued*)

Compounds	m_{TB}	m_{PR}	m_{TWU}	n_{TWU}	m_{mTB}	n_{mTB}
Hexadecane	1.394901657	1.420945264	2.114967851	1.073914445	1.521178229	0.882438747
Heptadecane	1.46449315	1.505258521	−0.777351953	1.82883625	2.070316255	0.62334036
Octadecane	1.464042719	1.505441548	0.225849457	1.686571293	1.611982144	0.870500382
Nonadecane	1.492518257	1.540577831	−0.126896193	1.719474058	1.690671407	0.836571252
Eicosane	1.539659748	1.59983426	0.379443476	1.659340635	1.599541349	0.945595564
Cyclopropane	0.647701146	0.59174948	0.836081998	−1.533587589	0.939762137	0.596253394
Cyclobutane	0.70157623	0.650839564	0.880623814	−0.354686292	0.815869079	0.807384029
Cyclopentane	0.746582277	0.688581783	1.007622484	−1.142461428	1.064327727	0.605189685
Methyl cyclopentane	0.843881655	0.764571867	1.169203447	−1.650375956	1.246030229	0.541281416
Ethyl cyclopentane	0.905289279	0.82629104	1.286543215	−1.388731363	1.329277809	0.541391881
Cyclohexane	0.734811991	0.699987544	0.982400328	−0.499969938	0.984442022	0.691192575
Methyl cyclohexane	0.864455055	0.78910582	1.215543887	−1.944026752	1.459319517	0.45600028
trans-1,4-Dimethlycyhclohexane	0.805310473	0.757847778	1.149799662	−1.195591132	1.398106905	0.484873492
Cycloheptane	0.793536542	0.751602413	1.08388757	−0.505592148	1.082474493	0.662816562
Cyclooctane	0.784295654	0.757827956	1.014131698	−0.123229459	0.964451395	0.776100457
1,1-Dimethyl cyclopentane	0.835324939	0.784286244	1.160849347	−0.501637075	1.128695013	0.654950288
cis-1,3-Dimethylcyclopentane	0.857948674	0.781253385	1.17302851	−0.579550682	1.045587073	0.719339361
trans-1,3-Dimethylcyclopentane	0.893428212	0.818280668	1.280501505	−1.45422168	1.418208103	0.492651694
trans-1,2-Dimethylcyclopentatne	0.872032262	0.80358252	1.236733768	−1.03172215	1.263212164	0.56974869
cis-1,2-Dimethylcyclopentatne	0.832567107	0.784237127	1.151315129	−0.496172364	1.11742014	0.664820124
1,1-Dimethyl cyclohexane	0.805841331	0.759268561	1.143435323	−1.068684418	1.326325072	0.518417964
cis-1,3-Dimethylcyclohexane	0.842643293	0.784713506	1.190106091	−1.323801705	1.355529889	0.513208644
1-Methyl-1-ethyl cyclopentane	0.927389716	0.848145852	1.297117082	−0.356993218	1.105652951	0.736457953
trans-1,2-Dimethylcylcohexne	0.844157843	0.781187321	1.18268801	−1.282259039	1.278430945	0.546808072
cis-1,4-Dimethylcyclohexane	0.852117852	0.789570061	1.197500787	−1.566342556	1.384007361	0.49939552
trans-1,3-Dimethylcyclohexane	0.859368845	0.796191171	1.21021022	−1.590075858	1.402180458	0.495005521
cis-1,2-Dimethylcyclohexane	0.829556128	0.777570166	1.178255268	−1.32171949	1.41797077	0.48541142
Propylcyclopentane	0.925969416	0.854651202	1.314154143	−1.347704672	1.361947342	0.549106089
Ethyl cyclohexane	0.886013708	0.814257563	1.24322752	−1.569385349	1.342507845	0.530258771
Isopropylcyclohexane	0.947010128	0.886349801	1.366974116	−0.547515964	1.281551242	0.629881754
Propylcyclohexane	0.919946482	0.853747389	1.307402536	−1.550797441	1.451428262	0.507088524
Butylcyclohexane	0.951241256	0.891943373	1.370005217	−1.49268178	1.565308236	0.486311848
Decyl cyclohexane	1.325956442	1.332580618	2.166650474	0.674827038	1.648481019	0.728062491
Ethylene	0.570351651	0.516020097	0.361275622	1.983454593	0.770638759	0.655185621
Propylene	0.699278695	0.61772955	0.904632738	−2.513419644	1.016115486	0.55370443
1-Butene	0.788838919	0.717231534	1.065004742	−1.808265947	1.169751624	0.551738754
cis-2-Butene	0.775751947	0.709958403	1.062364774	−1.44871236	1.177774166	0.544650233
trans-2-Butene	0.750249089	0.699493171	0.981971622	−0.43203353	0.922276684	0.747714294
1-Pentene	0.860833262	0.779718001	1.203812247	−2.02569923	1.402234878	0.469899411
cis-2-Pentene	0.860193606	0.784487179	1.205347053	−1.592093594	1.313793922	0.52082521
trans-2-Pentene	0.834423417	0.763795012	1.156783657	−1.218752809	1.181351284	0.587518398
2-Methyl-1-butene	0.831220106	0.763387471	1.154505334	−1.37822037	1.226039275	0.559865273
2-Methyl-2-butene	0.858632465	0.793033298	1.199886378	−0.672065387	1.136129691	0.651366374
1-Hexene	0.893572361	0.821924923	1.263520196	−0.947967622	1.226933298	0.607230099
1-Heptene	0.955385577	0.89388744	1.38434938	−0.602909178	1.308341649	0.61743526
1-Octene	1.011125606	0.958446409	1.496962881	−0.395561504	1.391110863	0.618498121
1-Nonene	1.060244219	1.017570853	1.591092796	−0.167113979	1.43357318	0.639844993
1-Decene	1.105123962	1.070559599	1.623779146	0.212054058	1.343749674	0.745131078
1-Undecene	1.17618249	1.154629063	1.840180919	0.193650662	1.5803937	0.653009273
1-Dodecene	1.214554429	1.201101389	1.829115628	0.533785462	1.442208762	0.776490245
1-Tridecene	1.232796622	1.223950184	1.498538679	1.041714771	1.255890901	0.972057346
1-Tetradecene	1.310225787	1.315801715	2.10823447	0.66633603	1.61649223	0.739211424
1-Pentadecene	1.351829313	1.366163308	2.239685041	0.731814693	1.689497066	0.727236037
1-Hexadecene	1.354369433	1.370273508	1.353076817	1.354833232	1.320706226	1.039143321
1-Octadecene	1.505640053	1.555367224	−1.277418434	1.85750501	2.24908821	0.577656615
1-Nonadecene	1.516992122	1.570323117	−0.546191954	1.740485639	1.784583137	0.791622923
1-Eicosene	1.552843789	1.615614346	−0.989824697	1.739569186	1.831233103	0.789105124
Propadiene	0.696891051	0.638010204	0.94705075	−2.062139596	1.590183316	0.340007924
1,2-Butadiene	0.773652689	0.707652682	0.91408784	0.265892686	0.803801481	0.939444971
1,3-Butadiene	0.730012605	0.678039296	0.977997183	−0.923670884	1.01311633	0.636592483
1,2-Pentadiene	0.797904582	0.724244805	1.050699905	−4.020872847	1.489177578	0.406842953
1,4-Pentadiene	0.737770129	0.660539336	0.875988724	−12.3789783	1.773680415	0.295999272
2,3-Pentadiene	0.841223423	0.775045389	1.167737749	−1.738485458	1.334959221	0.5099499
1,3-cis-Pentadiene	0.795543734	0.720187352	1.037183569	−4.587173786	1.521682817	0.392250438
trans-1,3-Pentadiene	0.712525327	0.657856398	0.937398702	−5.463888096	2.697902883	0.196477659
Acetanilide	1.181418436	1.176808805	1.513785675	0.885075398	1.240403417	0.935771401
Acetylene	0.689178272	0.6649115	0.783848099	0.241400531	0.730282923	0.932399498
1-Pentyne	0.845005077	0.789926164	1.131985256	−0.15213722	1.001798212	0.776244228
2-Pentyne	0.724199738	0.683325869	1.057249966	−2.006123142	2.327933992	0.250235732
Benzene	0.736702578	0.700741612	1.010805086	−0.712358568	1.087597412	0.613337972
Toluene	0.857384503	0.792935869	1.203121436	−0.885243115	1.193319444	0.608945667
Ethyl benzene	0.914737971	0.850626362	1.305818625	−0.691311384	1.244623076	0.62373593
o-Xylene	0.887854921	0.843463214	1.230625316	−0.187208197	1.118071442	0.724103558
m-Xylene	0.906695082	0.858492178	1.252309286	−0.12276649	1.106269083	0.749248115
p-Xylene	0.881531923	0.847616756	1.082652733	0.396781043	0.94805747	0.906091221
Propyl benzene	0.976383063	0.912733437	1.421509677	−0.554125529	1.317018881	0.625185651
1,2,3-Trimethyl benzene	0.938767316	0.894336014	1.166622482	0.462047786	0.988892882	0.924963905

Table 4 (*Continued*)

Compounds	m_{TB}	m_{PR}	m_{TWU}	n_{TWU}	m_{mTB}	n_{mTB}
1,2,4-Trimethyl benzene	0.95310172	0.90613423	1.185181561	0.492088654	1.001357334	0.926895663
Butyl benzene	1.048911548	0.994761173	1.588132307	−0.531548199	1.535282216	0.560728077
Isobutylbenzne	0.972491864	0.924719595	1.335886074	0.148840869	1.127663952	0.799369389
sec-Butyl benzene	0.956757345	0.897961854	1.402420794	−1.881378879	2.020722587	0.356687337
tert-Butylbenzene	0.925471407	0.87075857	1.351735894	−1.668988016	1.863179901	0.386790828
1,2-Diethyl benzene (ortho)	0.966431064	0.92217973	1.411140289	−0.43985413	1.358176721	0.619088815
1,3-Diethyl benzene (meta)	1.008107	0.950870164	1.475800644	−0.59593651	1.38661977	0.612836104
1,4-Diethyl benzene (para)	1.010253834	0.967788836	1.41246804	0.174190714	1.184013452	0.788978673
Naphthalene	0.859736585	0.825563365	1.145645151	0.014656947	1.02541694	0.792429316
1-Methylnaphthalene	0.956013049	0.901029439	1.33149632	−0.112811181	1.140191369	0.761278697
2-Methylnaphthalene	0.949733019	0.911504981	1.397701003	−0.351973527	1.42012526	0.582790263
1,2-Dimethylnaphthalene	1.048407288	1.033553548	1.394026721	0.531672741	1.177466375	0.861236486
1,3-Dimethylnaphthalene	0.997690473	0.980974793	1.1328726	0.817235737	1.013395247	0.980184308
1,4-Dimethylnaphthalene	0.976761827	0.958193665	1.31437378	0.479427593	1.090760192	0.869526091
1,5-Dimethylnaphthalene	1.03093323	1.017144	1.312270491	0.628677463	1.110369486	0.910200883
1,6-Dimethylnaphthalene	1.017040692	1.002156597	1.016966441	1.017137712	0.940077038	1.107699369
1,7-Dimethylnaphthalene	1.092559202	1.084408261	1.092560711	1.092556783	0.955975617	1.192694053
2,3-Dimethylnaphthalene	1.029070289	1.015415224	1.31550014	0.618988988	1.11161087	0.907101723
2,6-Dimethylnaphthalene	1.000507794	0.978755023	1.264639928	0.574716483	1.067268545	0.917927323
2,7-Dimethylnaphthalene	1.00327979	0.979495306	1.289625503	0.536131549	1.079496017	0.906134704
1-Ethylnaphthalene	1.012484106	0.966943149	1.494983646	−0.429766773	1.418884757	0.61312787
2-Ethylnaphthalene	0.963177401	0.939651136	1.363092519	0.171325211	1.200553258	0.75438263
1-Propylnaphthalene	1.078093153	1.069255063	1.078041918	1.078149368	1.025727291	1.066063794
2-Propylnaphthalene	1.087636027	1.080236162	1.087621991	1.087650137	0.976576774	1.149136702
2-Ethyl-3-methylnaphthalene	1.078255965	1.072828265	1.078244998	1.078267559	0.915242899	1.22865587
2-Ethyl-6-methylnaphthalene	1.085149887	1.080374482	1.085136354	1.085164617	1.006763606	1.097150347
2-Ethyl-7-methylnaphthalene	1.085149887	1.080374482	1.085136354	1.085164617	1.006763606	1.097150347
1-Pentylnaphthalene	1.146477254	1.145391612	1.907839267	0.41482038	1.635364364	0.652614442
2-Pentylnaphthalene	1.163804119	1.165032604	1.245856067	1.101887292	1.160763216	1.003277068
1-n-Nonylnaphthalene	1.258256696	1.247707272	1.772988547	0.837565335	1.353905679	0.891394023
1-n-Decylnaphthalene	1.283579123	1.277938758	1.802462349	0.906871836	1.36942082	0.903185302
Biphenyl	0.967400017	0.935107446	1.411922206	−0.141447533	1.350101974	0.642565373
Anthracene	1.066433759	1.057406948	1.066434461	1.066433177	0.707135312	1.761764842
Indane	0.903712602	0.847007569	1.278452503	−0.46022687	1.191103766	0.663441067
Cumene	0.976812311	0.915490546	1.445262308	−0.804968845	1.480995139	0.535039709
Chlorotrifluoromethane	0.709460513	0.64191635	0.895450418	−0.582004934	0.813330956	0.805822904
Difluorodichloromethane	0.770683939	0.702906807	1.05903084	−2.602712014	1.676036152	0.345664363
Bromochlorodifluoromethane	0.755097434	0.679466802	1.012945521	−1.618542383	1.068747058	0.583655156
Trichlorofluoromethane	0.750221054	0.691130623	1.027387808	−1.705973455	1.279267422	0.480230625
Carbon tetrachloride	0.722282783	0.679864835	0.961181307	−0.727085535	0.996457216	0.656115371
Carbon tetrafluoride	0.704267564	0.653092689	0.901561686	−0.52249318	0.872152378	0.741074109
Monochlorodifluoromethane	0.818286225	0.755002751	1.155693579	−1.825783077	1.579622596	0.403514266
Dichlorofluoromethane	0.760690415	0.693930417	0.992369594	−0.657511254	0.90675214	0.7603994
Chloroform	0.77370938	0.723590843	1.081331275	−1.192033173	1.289225285	0.507208494
Trifluoromethane	0.825096328	0.777570246	1.081331275	−0.349474143	1.054920807	0.710177321
Dichloromethane	0.773993534	0.716454849	1.071925042	−1.794608525	1.383193195	0.454519108
Chloromethane	0.661965177	0.614679953	0.846414553	−0.848401327	0.854846405	0.707205363
Fluoromethane	0.718475586	0.670762574	0.847965733	0.11420264	0.775982215	0.896547694
1,1-Dichloroethane	0.806675993	0.747772737	1.1073628	−0.718518646	1.081357676	0.652473164
1,2-Dichloroethane	0.82927754	0.786574937	1.026279825	0.240522775	0.900928744	0.890037526
Ethyl bromide	0.777260167	0.711122733	0.976427709	−0.621364353	0.935015535	0.750471577
Ethyl chloride	0.753268804	0.684531467	1.027767943	−1.288923236	1.061201825	0.598080378
Fluoroethane	0.753268804	0.682995774	0.866124237	0.172821519	0.77449583	0.935734041
Octofluoro-cyclobutane	0.917969706	0.900758007	1.085398795	0.589447052	0.966895214	0.938473595
Tetrafluoroethylene	0.770008135	0.730725973	1.052329874	−0.616517899	1.087868579	0.639803624
Trifluorochloroethylene	0.862954021	0.799484098	1.219077467	−2.00364413	2.067806818	0.309138138
Chlorobenzene	0.80953475	0.75524523	1.061188331	−0.255193743	0.939992836	0.802154366
Fluorobenzene	0.800105457	0.754389753	1.068272243	−0.350422679	0.992648734	0.742780151
Iodobenzene	0.829681153	0.771378946	1.154756519	−0.88344012	1.167094966	0.611157837
Hexafluorobenzene	0.97207122	0.952829144	1.178273796	0.6206292	1.026318564	0.932903039
1-Bromonaphthalene	0.980336803	0.93279185	1.376209552	−0.019601145	1.178134452	0.758951458
1-Chloronaphthalene	1.008610806	0.964507192	1.541152579	−0.480356385	1.644003233	0.506693487
Methanol	1.130151478	1.100669705	1.130201684	1.130113199	1.064837651	1.101926227
Ethanol	1.214804367	1.191388785	1.214810832	1.214801376	1.121426621	1.149554546
1-Propanol	1.289810995	1.269071073	1.723671535	0.957973626	1.335882846	0.939211452
Isopropanol	1.314061292	1.319058693	1.796854544	1.016710112	1.376848964	0.931244612
1-Butanol	1.301186221	1.297052684	2.023539227	0.537276161	1.559953855	0.757527717
sec-Butanol	1.338296528	1.335413634	2.158394	0.218278483	1.792102432	0.638414772
tert-Butanol	1.257950495	1.269285207	2.421431084	0.197504122	3.367303704	0.32626921
1-Pentanol	1.344127228	1.34966327	2.281787331	0.157134564	2.1144138	0.52585516
2-Pentanol	1.383107051	1.401707596	2.289272773	0.698962994	1.729341721	0.72239092
3-Pentanol	1.323839444	1.3319606	1.833432876	1.016255484	1.395353994	0.923750235
1-Hexanol	1.292953245	1.29462909	2.130158104	0.295668652	1.846452515	0.608337862
2-Hexanol	1.283927417	1.284757091	2.133101224	0.190074951	1.946051537	0.565541049
1-Heptanol	1.368772299	1.385432996	2.414581802	−0.052291376	2.941117905	0.370038102
2-Heptanol	1.351804025	1.370488607	1.351806058	1.351803773	1.207661532	1.186238797
1-Octanol	1.355145896	1.370955275	2.387895995	0.061791573	2.795008213	0.392491339

Table 4 (*Continued*)

Compounds	m_{TB}	m_{PR}	m_{TWU}	n_{TWU}	m_{mTB}	n_{mTB}
Octan-2-ol	1.305922442	1.309969072	2.247225434	−0.621726699	4.388347184	0.223818298
2-Ethylhexan-1-ol	1.459555682	1.488167211	2.560678886	−1.010567024	8.218406086	0.121150799
Benzyl alcohol	1.305696384	1.311539481	1.497985613	1.212837649	1.32459913	0.978520089
1-Nonanol	1.371890368	1.391105214	2.492904687	−0.134142972	3.997844114	0.26570975
2-Nonanol	1.520484703	1.574982296	1.351526335	1.540702879	1.489927548	1.031564183
1-Decanol	1.375542283	1.396359666	2.49954215	0.046146482	3.309961672	0.330879552
1-Undecanol	1.375797873	1.396680774	2.538716417	−0.281392037	5.726461309	0.181807937
1-Dodecanol	1.413361806	1.442422624	2.630194342	0.106229145	3.829756968	0.290748647
1-Tridecanol	1.409759954	1.438188876	2.630906358	0.00173052	4.514647205	0.242356894
1-Tetradecanol	1.463794136	1.504223135	2.821356087	0.206987668	4.124203763	0.279631997
1-Pentadecanol	1.57107615	1.617963569	1.566486948	1.571002779	2.053375077	0.737818699
1-Hexadecanol	1.525854898	1.581086303	3.098523853	0.49094146	3.788436301	0.322751905
1-Heptadecanol	1.584698131	1.655082455	−2.566184164	1.994806892	3.009394689	0.439292362
1-Octadecanol	1.623181597	1.704386752	−3.509677221	1.900317295	2.426491479	0.586298206
1-Nonadecanol	1.60217302	1.652677458	1.603323391	1.602142668	1.320324359	1.254443989
1-Eicosanol	1.717569786	1.825644338	−14.24225899	1.852044017	2.868430061	0.512183983
Cyclohexanol	1.203419388	1.201413312	2.115120807	−0.241987559	3.172910483	0.312151228
Dimethyl ether	0.740059218	0.677745905	0.949736091	−0.471637971	0.860098757	0.794846355
Ethyl methyl ether	1.017409864	0.977976633	1.468100764	−6.180999183	37.44686707	0.018715643
Diethyl ether	0.891048748	0.83615934	1.290210686	−0.921538662	1.417205099	0.521059544
Methyl propyl ether	0.817134079	0.792598471	0.817097263	0.817227175	0.78411399	1.053313095
Dipropyl ether	0.998034838	0.939162511	1.47552808	−0.451636543	1.371866878	0.612473156
di-Isopropyl ether	0.897545852	0.850601319	0.979003103	0.726831334	0.900855321	0.994431403
di-tert-Butyl ether	0.941389408	0.89370772	1.309653215	−0.070903177	1.145515067	0.749520709
Diphenyl ether	1.018944271	0.985388276	1.018936123	1.018953971	0.91061599	1.189741543
Formaldehyde	0.80189736	0.761103048	0.801756419	0.802253556	0.758098969	1.083263446
Acetaldehyde	0.894378367	0.837575984	1.323005527	−0.735368627	1.490394968	0.488043245
Acetone	0.873356017	0.820392097	1.157468561	−0.013720504	1.000439414	0.815842456
Pentan-2-one	0.90428376	0.852973467	0.925540227	0.863766569	0.895590456	1.015330461
Hexan-2-one	1.006401929	0.967366425	1.404677673	0.163702654	1.182796698	0.790016582
Hexan-3-one	0.986333378	0.945918593	1.426078766	−0.105038842	1.281104083	0.689944167
Heptan-2-one	1.035375712	1.002565939	1.512382691	0.046696001	1.334791812	0.700590955
Cyclopentanone	0.906020244	0.85583675	0.906018929	0.906022847	0.885626731	1.036443666
Cyclohexanone	0.976734103	0.937690914	0.976722966	0.976748364	0.878970027	1.178681761
Methyl ethyl ketone	0.8934	0.841089924	1.213930908	−0.05301688	1.054390514	0.78115194
Oxalic acid	1.558484119	1.617915615	1.558681353	1.558469778	1.319644247	1.240191929
Acetic acid	1.012118235	0.991197341	1.012108718	1.012129056	0.789896457	1.426253177
Methyl formate	0.833028844	0.779205289	1.155143735	−0.7052349	1.136645109	0.642768614
Ethyl formate	0.859733372	0.81149486	1.184005089	−0.341766301	1.09247333	0.712663369
Vinyl acetate	0.916934567	0.865360029	1.165897512	0.29465419	0.981708471	0.899963234
Phenol	1.037827355	1.014408289	1.533912567	0.111869068	1.336138694	0.715196686
m-Cresols	1.11507541	1.093531144	1.794055306	−0.280776919	2.061385273	0.449799062
o-Cresol	1.046964165	1.022358273	1.550670169	0.126502375	1.38733263	0.686232267
p-Cresol	1.136067284	1.121915232	1.675884252	0.448108965	1.404292306	0.750288855
Ethylene oxide	0.752425492	0.693093751	1.02175055	−1.188777954	1.08666406	0.592782916
Tetrahydrofuran	0.814616847	0.749248131	1.134523132	−1.355144336	1.257722035	0.531495274
Furfural	1.002672536	0.96155296	1.002600974	1.002759645	0.969021778	1.055047815
Piperidine	0.801419192	0.760255695	1.111124763	−0.625428977	1.123030335	0.641611557
Pyridine	0.813493568	0.761771966	1.136156702	−0.903999819	1.20248922	0.583611788
2-Methylpyridine	0.886123316	0.830135419	1.263728457	−0.852701403	1.291041579	0.582382165
Methylamine	0.866563616	0.830236573	1.261964029	−0.836539739	1.284272614	0.586499353
1-Propylamine	0.903061377	0.854635664	1.33386141	−1.227505245	1.706392837	0.42877945
Dimethylamine	0.895005773	0.854306386	1.312439613	−0.734369687	1.479382753	0.517599973
Diethylamine	0.88273086	0.846782418	1.11046186	0.247113449	0.969580052	0.879486362
Trimethylamine	0.766799621	0.711173609	1.065934757	−1.280120271	1.291344662	0.492412565
Triethylamine	0.908658407	0.845912724	1.23088078	−0.139647902	1.053353623	0.789589146
Acetonitrile	0.852693647	0.810730529	0.852666069	0.852745007	0.727362958	1.271686664
Propionitrile	0.885275642	0.826456019	1.179744454	0.033855839	1.00849295	0.816092127
Butyronitrile	0.960162079	0.896417467	1.318327655	0.064161707	1.096504584	0.802937018
Aniline	1.012428254	0.976052718	1.544454218	−0.22765462	1.600206269	0.537942168
o-Toluinide	1.081829315	1.048949324	1.678315428	−0.153080419	1.634064039	0.562912112
m-Toluinide	1.014846057	0.971331435	1.355036959	0.377472511	1.112868561	0.867788288
N-Methylaniline	1.02948556	0.980159565	1.029566669	1.029397527	1.020290433	1.015154551
N,N-Dimethylaniline	0.975870877	0.93939321	1.019224723	0.910062687	0.972880072	1.004539214
Dimethylsulfide	0.734081738	0.675342466	0.978657876	−1.042491996	1.004432772	0.638078819
Diethylsulfide	0.877554857	0.814739215	1.203009005	−0.349518285	1.07030568	0.73431091
Methyl mercaptane	0.739600856	0.675609465	0.98646102	−3.324455993	1.707735994	0.327657191
Ethyl mercaptane	0.769162752	0.689484529	1.036843629	−1.763392169	1.106300067	0.564188405
Ethylene glycol	1.665311097	1.765653116	4.557212386	2.348691826	1.076635435	2.21794168
Dimethylethanolamine	1.353854255	1.368238956	1.911650154	1.06737584	1.430883679	0.920115585
Diethanolamine	1.618181447	1.700851581	4.077391539	1.822852367	1.389183876	1.262192841
Tetraethylene glycol	2.030717922	2.270899093	−0.093667649	1.502662665	1.733868888	1.298789824
cis-Decahydronanphthalene	0.902895051	0.847016487	1.313199956	−0.894882799	1.430687966	0.520909332
trans-Decahydronaphthalene	0.87506136	0.822669978	1.287203175	−1.664833284	2.176991403	0.308525727
Cyclohexaylbenzene	1.047193841	1.013268314	1.620756346	−0.621546176	1.905685315	0.451281703
n-Hexylbenzene	1.111544681	1.070960645	1.598801019	0.322699118	1.28435375	0.794717705
1-Cyclopentyloctane	1.153911903	1.152197112	1.529497877	0.762741868	1.25734996	0.897064903

Table 4 (*Continued*)

Compounds	m_{TB}	m_{PR}	m_{TWU}	n_{TWU}	m_{mTB}	n_{mTB}
1-Cyclohexylheptane	1.11498861	1.108632898	1.531372721	0.614915789	1.263468808	0.853732349
1-Cyclopentylnonane	1.203561666	1.207988768	1.610162723	0.844116319	1.3064863	0.901832123
1-Cyclohexyloctane	1.168689894	1.168810891	1.542028551	0.800217882	1.264580103	0.90513683
1-Cyclopentyldodecane	1.348172773	1.372059405	1.774526078	1.111321817	1.420082264	0.937591952
1-Cyclohexylundecane	1.31255	1.331537948	1.634762404	1.119101662	1.359637392	0.956830641
Ascorbic acid	2.741792566	3.177448432	−0.48350638	1.306097933	1.556489317	2.218580575

[a] Since the acentric factor value is zero the constant is not required.

Table 5
Percent average absolute deviations (%AAD) in vapour pressure for all the cohesion factor models for various class of families with global values.

Family (N_c[a])	N_p[b]	TB	PR	TWU	*m*TB (Gasem)
Elements (10)	510	3.52	2.21	2.07	1.77
Nitrogen compounds (2)	102	4.84	6.36	4.83	2.10
Oxides (6)	306	3.89	3.87	1.64	2.04
Sulfides (2)	102	4.49	1.77	1.18	0.61
Chlorides (1)	51	1.35	0.89	0.88	0.81
Oxyhalides (1)	51	10.13	4.55	4.61	2.46
Inorganic compounds (2)	102	8.88	8.60	7.43	1.09
Alkanes (55)	2805	8.16	4.26	3.77	2.18
Cycloalkanes (28)	1428	11.95	5.92	3.72	1.79
Alkenes (22)	1122	12.35	6.24	4.95	2.66
Alkadienes (6)	306	12.84	8.57	4.26	3.18
Alkynes (3)	153	4.33	2.90	2.28	1.76
Aromatic hydrocarbons (42)	2142	6.07	3.62	2.54	1.58
Halogenated alkanes (18)	918	7.29	3.99	3.86	2.06
Halogenated cycloalkanes (1)	51	1.13	0.79	0.99	0.95
Halogenated alkenes (2)	102	11.59	7.79	7.67	4.90
Halogenated aromatic hydrocarbons (6)	306	6.39	3.05	2.60	1.87
Alcohols (27)	1377	16.04	15.39	4.34	2.96
Ethers (7)	357	10.89	9.00	5.56	3.84
Aldehydes (2)	102	7.97	7.27	6.74	5.47
Ketones (8)	408	5.45	4.38	3.31	2.76
Alkanoic acid (2)	102	4.36	4.49	4.40	1.48
Esters (3)	153	6.34	2.35	1.65	0.81
Phenols (4)	204	7.14	5.37	3.96	3.43
Heterocyclic oxygen compounds (3)	153	7.44	5.04	3.30	1.74
Heterocyclic nitrogen compounds (3)	153	7.50	3.59	1.68	0.73
Hydrocarbon nitrogen compounds (14)	714	6.87	4.94	3.90	2.81
Sulfur compounds (4)	204	10.95	4.81	4.69	2.09
Others (14)	714	11.93	7.99	5.46	5.24
Global (298)	15,198	7.26	4.98	3.54	2.20

[a] N_c, number of compounds.
[b] N_p, number of data points.

Table 6
PR type generalized expression constants.

Family	s_1	s_2	R^2	p_1	p_2	p_3	R^2
Elements	1.77	0.417	0.995	−0.411	1.723	0.421	0.995
Oxides	1.479	0.416	0.984	0.237	0.136	0.426	0.984
Alkanes	1.2	0.5	0.975	−0.353	1.538	0.459	0.98
Cycloalkanes	1.25	0.532	0.888	−1.161	2.205	370	0.91
Alkenes	1.167	0.549	0.988	−0.305	1.461	0.496	0.991
Alkadienes	0.971	0.603	0.875	1.675	−0.158	0.736	0.918
Aromatic hydrocarbon	1.001	0.599	0.883	0.324	0.724	0.654	0.884
Halogenated alkanes	1.08	0.537	0.631	−6.435	3.95	0.226	0.669
Halogenated aromatic hydrocarbons	1.277	0.497	0.956	−11.3	8.433	−0.583	0.973
Alcohols	0.791	0.854	0.635	0.008	0.778	0.858	0.635
Ethers	0.671	0.705	0.344	0.406	0.401	0.746	0.345
Ketones	0.97	0.583	0.586	−6.936	6.174	−0.378	0.647
Hydrocarbon nitrogen compounds	1.052	0.565	0.858	−0.59	1.465	0.496	0.859
Others	0.854	0.709	0.995	−0.038	0.951	0.668	0.995

Table 7
TB type generalized expression constants.

Family	s_1	s_2	R^2	p_1	p_2	p_3	R^2
Elements	1.663	0.381	0.993	−0.314	1.627	0.383	0.994
Oxides	1.516	0.379	0.979	0.455	1.292	0.4	0.98
Alkanes	1.361	0.427	0.992	−0.143	1.498	0.4	0.993
Cycloalkanes	1.353	0.447	0.936	−0.52	1.781	0.375	0.94
Alkenes	1.348	0.439	0.998	−0.093	1.437	0.423	0.994
Alkadienes	1.11	0.515	0.905	1.923	−0.185	0.668	0.951
Aromatic hydrocarbon	1.182	0.494	0.935	0.219	0.995	0.532	0.936
Halogenated alkanes	1.185	0.457	0.74	−3.433	2.716	0.291	0.75
Halogenated aromatic hydrocarbons	1.406	0.411	0.987	−4.004	3.941	0.028	0.989
Alcohols	0.958	0.763	0.627	0.092	1.097	0.712	0.627
Ethers	0.702	0.649	0.353	0.642	0.246	0.715	0.355
Ketones	1.101	0.49	0.594	−7.352	6.617	−0.53	0.648
Hydrocarbon nitrogen compounds	1.087	0.507	0.839	−0.671	1.556	0.429	0.841
Others	1.084	0.579	0.997	−0.007	1.103	0.591	0.997

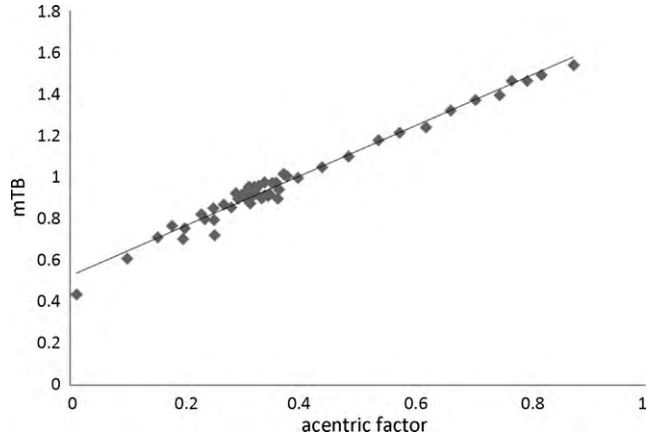

Fig. 1. Linear fit of TB model for alkanes: (■) actual data points and (—) fitted trend line.

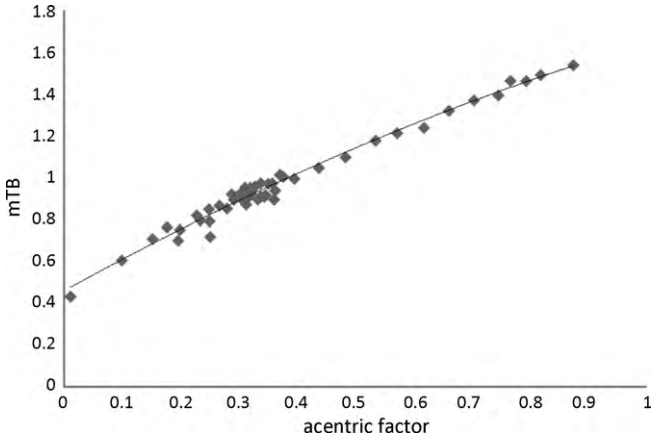

Fig. 2. Quadratic fit of TB model for alkanes: (■) actual data points and (—) fitted trend line.

Fig. 1 shows fitting of the TB model for alkane family using linear fit (Eq. (10)). Fig. 2 shows the same for quadratic fit (Eq. (11)). In similar way the constants for all the families for both the models (TB and PR) were obtained. Coefficients s_i (i = 1, 2) and p_i (i = 1–3) for both PR and TB type cohesion factor models are listed in Tables 6 and 7. These tables also list R^2 (square of the correlation coefficient) values for the trend line fitted. R^2 value indicates the goodness of fit of the model. The value must be close to unity for exact fit. As expected the families having polar compounds do not have a good fit and hence one must be careful while using them.

4. Conclusions

Saturation vapour pressures for 298 compounds in the range of temperature from freezing point to critical point were evaluated with the PR EOS. Four compound specific models were evaluated for predicting vapour pressure. For all the four models, compound specific parameters were obtained and are listed in the present work. All the models having compound specific parameter performed acceptable but, it was found that the modified Trebble–Bishnoi model (Gasem *et al.*, 2001) performed best with little over 2% AAD Twu type model followed modified TB model with 3.54% AAD. For only single parameter, original PR type model worked better compared to original TB type model. Family wise generalisation for original PR and original TB models was done for 14 (fourteen) families. It was found that both the models work parallel with original PR being marginally better. It was observed that linear generalized expression (Eq. (10)) was similar in accuracy to quadratic expression (Eq. (11)).

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