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Research Article

An Alternative Method for Correlation and Prediction of Thermo Physical Properties of Fluids-Critical Pressures

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ABSTRACT

Based on the linear free energy relationships (LFERs) theory and thermodynamics formulas, an alternative method predicting the critical pressure (Pc) of pure fluids is proposed for the first time. According to the regression result of 15 homologues, 516 substances, correlation equations between Pc and molecular descriptors were obtained. The mean relative deviations (MD) of the 15 equations are from 1.68% to 3.76%. In addition, the squared correlation coefficients (R2) of the most of equations are larger than 0.91. The results reveal that the equations exhibit better effects with a simple form of the equation, high prediction accuracy, definition theory meaning, and wide applicability. This study successfully combines the macroscopic physical properties with the characteristics of molecules and breaks through the experimental or theoretical application scope, while perfecting the calculation of Pc for pure fluids.

Keywords: Critical pressure; Linear free energy relationships (LFERs) theory; Regression; Organic compounds

INTRODUCTION

Critical temperature, pressure, volume, density, compressibility factor are the most important physical parameters. As the basic physical properties of substances, they are necessary variables not only in calculating or estimating physical and chemical properties but also in many chemical engineering and process designs. However, the quantity of experimental data is very finite until now because of extensive difficulty in measuring the critical state. Therefore, the existing critical parameters do not meet the current requirements for chemical production, process design, and scientific research. This predicament causes some methods for evaluating the critical parameters of unknown compounds by combining known data with modern prediction method to emerge as times require.

Group contribution method is the most widely used and studied [1-15]. Although the early group contribution methods bare the advantages of a simple form and convenient calculation, they could not distinguish isomers and ignored interactions between bonds. There was a significant improvement in accuracy when these defects were resolved [2-4]. In addition Valderrama et al. [10], Skander et al. [11] and Lymperiadis et al. [12] successively proposed some new methods based on the group contribution method. It should be emphasized that Wang et al. and Ma et al. [13-15] have successfully applied a position group contribution method in calculating critical properties, which solves the difficult problem of failing to distinguish isomers. For the prediction of the critical properties of isomers, the topology method [16,17] was also a good option, due to its excellent capability of distinguishing isomers.

The association equation method [18-20] was also commonly used. In this method, the characteristic groups were first divided into various types and then the basic physical properties of molecular weight M, boiling temperature Tb, and number of carbon atoms were selected and related with the critical parameters. For example, Klincewicz et al. [18] predicted 199 compounds by dint of Tb and M. Ma et al. [19] calculated the Pc of 221 compounds by using Tb, d20 4 and M. Lu et al. [20] and Vejahati et al. [21] also put forward a set of similar equations using simple physical properties as variables to predict critical parameters. These equations are simple, understandable and accurate.

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The artificial neural network method is very applicable in the physical prediction field. Kuang et al. [22] and Gharagheizi et al. [23,24] predicted the critical properties of pure substances by combining an artificial neural network with the group contribution method and obtained a result with high accuracy. In addition, critical properties could also be predicted on the basis of the liquid state equation and semi-empirical model for describing other physical properties [25]. Quantitative structure property relationship (QSPR) methods [26,27] and the cubic equation of state [28-30] have been used to predict the critical parameters of pure substances. In summary, great progress has been made in predicting critical parameters, but not every method is suitable for all substances. Some methods are aimed at specific points and have their limitations. Therefore, scientific researchers should select simple, accurate methods according to an actual need. In this paper, we proposed a new method primarily based on the linear free energy relationships (LFERs) theory [31,32] to predict the Pc of pure fluids. The LFERs theory posits that the molecular basic property can be expressed by five molecular descriptors as described in Equation (1).

$SP=c+eE+sS+aA+bB+vV$ (1)

Where, the dependent variable SP is some property of a series of solutes in a fixed phase. The independent variables or descriptors are solute properties as follows: E is an excess molar refraction, denoting the solute excess molar refraction that reflects the solute's ability to interact with the surrounding solvent molecules through π- and lone electron pairs; S is the dipolarity/polarizability; A is the overall hydrogen bond acidity; B is the overall hydrogen bond basicity and V is the characteristic McGowan volume. The molecular descriptors may be of either experimental origin or calculated based solely on molecular structure considerations. The set of coefficients, i.e., c, e, s, a, b and v can be obtained by using a multiple linear regression analysis. According to the LFERs model, many properties for substances can be researched with the known molecular descriptors and the set of molecular descriptors has the advantage of distinct significance, wide substance range, simple calculation, and high precision, as stated in the research [31-82].

By the enlightenment of the LFERs model, we hold that the characteristics of the molecular descriptors factually reflect the intermolecular interaction and the macroscopic property are decidedby the substance structure and reciprocity of the molecules. This indicates that the set of molecular descriptors should be widely applicable in estimating the physicochemical properties of substances.Therefore we suggest that the Pc can be denoted as an equation using five molecular descriptors of the LFERs theory. This paper aims at obtaining correlation equations between the Pc of various compounds and the five molecular descriptors. To our best knowledge, although the LFERs theory has been widely used, the research of Pc using the LFERs theory has never been published. The detailed process will be introduced in the latter paragraphs.

MATERIALS AND METHODS

There are intermolecular interactions, mutual attraction and mutual repellence in a molecular system. When the mutual repellence is larger than the mutual attraction the substance is in a gaseous state. When the mutual attraction is larger than or at least equal to the mutual repellence, the gas will likely be transformed into liquid. The intermolecular mutual attraction can be considered independent of the temperature. Contrastingly, the mutual repellence resulting from an intermolecular collision depends intensively on temperature. Therefore, only the gas temperature that has decreased to some extent can have a mutual attraction being greater than or equal to the mutual repellence. Furthermore, the gas could be converted into liquid. The allowable maximum temperature when the mutual attraction is equal to the mutual repellence is the critical temperature. When the temperature is greater than the critical temperature, the gas cannot be liquefied no matter how much pressure is applied. The minimum pressure required at the critical temperature is the Pc. Therefore, it can be considered that when the critical temperature remains constant, the mutual repellence that resulted from molecular collision is also determinate. To force gas into a liquid state, the intermolecular attraction must be equal to the intermolecular repellence, and the applied pressure is definite. Therefore, the Pc can be expressed by the intermolecular force.

In this paper, using five molecular descriptors, the Pc is expressed as:

$Pc=F(E, S, A, B, V)$ (2)

Furthermore, the Pc could be denoted as the following formula according to the LFERs model.

$Pc=c+eE+sS+aA+bB+vV$ (3)

The c, e, s, a, b and v are the undetermined coefficients of the equation, which are determined by multiple linear regression analyses of the experimental Pc data for a series of organic compounds considered in this paper. E, S, A, B, and V are the molecular descriptors of the substance. The molecular descriptors for all of the compounds considered in the present study are taken from thepublished literature [31-76].

The five molecular descriptors were directly used in the regression for most of the compounds. However, for some compounds, if the five molecular descriptors were used directly to regress, such as alkene, alcohol, aldehyde, acid, and amine, then the errors were large.

Therefore, we corrected the equations for these compounds as follows:

$Pc=2(E,S,A,B,V)$ (4)

The reason for this correction was that the correlation between the Pc and the normal boiling point was apparent in many estimating methods. 3, 83-85 Therefore, the equation of Pc can be transformed into

$Pc=Tb(E, S, A, B, V)$ (5)

On the process of regressing, no data on boiling point were used since the boiling point was closely related to the five molecular descriptors, which can be revealed by our ongoing research. Therefore, the boiling point can be expressed by the molecular descriptors as

Tb=F (E, S, A, B, V) (6)

Therefore, the Pc can be formulated as Equation (4).

In other words, there are two equations, Equation (2) and (4), for researching the Pc. Not all homologues adopt the same mode. There is no obvious difference between the two equations for these types of compounds except alkene, alcohol, aldehyde, acid, and amine. Therefore, for the sake of simplicity, we adopt the original method expressed as in Equation (2) and (3).

The data of Pc for the pure substances were collected from the Lange's Handbook of Chemistry (the 15th edition), Handbook of Chemistry and Physics printed by the CRC, Chemical Properties Handbook published by World Publishing Corporation and McGraw-Hill Book, Co., and Physical Properties Data book of Chemical and Chemical Industry published by Chemical Industry Press of China. The 516 collected compounds are first classified into 15 genera and then the 15 homologues are regressed by a step wise regression analysis. Fifteen equations are established and evaluated using the squared correlation coefficient (R2), the F test and the mean relative deviation (MD). All the Pc and molecular descriptors used for model validation are presented in the supplementary material.

Table 1: Regression equations for Pc.

S.no	Compound types	Number	Regression equations	R2	F	MD%
1	Halogenated benzene	16	pc=(71.70 ± 8.70)+(18.20 ± 5.28)E+(-47.00 ± 11.69)V	0.86	38.92	3.47
2	Alkane	145	pc=(45.16 ± 1.25)+(21.11 ± 3.35)E+(-14.00 ± 0.90)V	0.92	852.32	3.65
3	Alkene	55	pc=(58.46 ± 2.29)+(13.22 ± 2.85)E+(-37.09 ± 3.42)V+(7.49 ± 1.10)VV	0.98	792.11	3.25
4	Alkyne	17	pc=(76.80 ± 3.90)+(-46.80 ± 5.50)V	0.96	329.01	2.78
5	Arenes	37	pc=(51.48 ± 3.00)+(16.08 ± 3.16)E+(-46.83 ± 20.10)B+(-19.14 ± 2.37)V	0.91	112.53	3.57
6	Phenol	15	pc=(86.89 ± 22.44)+(-27.75 ± 25.77)S+(37.74 ± 10.53)A+(55.03 ± 31.66)B+(-53.91 ± 13.12)V	0.98	105.01	3.39
7	Alcohol	39	pc=(37.03 ± 11.44)+(193.62 ± 38.25)S+(-40.07 ± 14.98)V+(13.37 ± 2.31)V2+(32.30 ± 23.07)BV+(-84.94 ± 21.82)SV+(-65.42 ± 33.84)SB	0.98	276.6	3.89
8	ether	28	pc=(54.35 ± 2.11)+(11.64 ± 2.31)S+(-25.64 ± 2.31)V	0.95	260.46	3.52
9	Aldehyde	25	pc=(89.80 ± 4.43)+(-95.61 ± 15.31)B+(48.54 ± 15.79)E 2+(31.97 ± 12.21)ES+(-55.17 ± 9.33)EV+(75.18 ± 20.51)SB+(-75.09 ± 6.89)SV+(14.80 ± 2.18)V 2	0.99	708.95	1.84
10	Ketone	15	pc=(50.90 ± 3.28)+(14.24 ± 3.96)S+(-27.53 ± 2.55)V	0.98	280.28	1.82
11	Acid	22	pc=(36.73 ± 16.32)+(81.58 ± 30.13)E+(63.90 ± 22.51)A+(-50.19 ± 8.68)V+(10.45 ± 2.90)V2+(-178.01 ± 63.61)EB	0.99	317.23	3.18
12	Ester	48	pc=(50.76 ± 2.19)+(10.71 ± 5.00)E+(3.36 ± 2.74)S+(-21.12 ± 1.56)V	0.95	269.89	3.35
13	Amine	26	pc=(131.71 ± 25.09)+(-103.35 ± 18.32)V+(-96.43 ± 29.91)EV+(473.51 ± 233.13)SA+(-517.72 ± 194.44)SB+(204.34 ± 71.60)SV+(-1367.72 ± 775.90)A2 +(603.41 ± 195.19)AB+(-272.64 ± 78.25)AV+ (32.17±5.25)V2+(143.36 ± 76.67)ES+(106.29 ± 25.26)EB	0.99	121.1	2.11
14	Nitrile	16	pc=(58.43 ± 3.08)+(63.26 ± 34.40)A+(-22.86 ± 7.23)B+(-18.08 ± 3.71)V	0.97	145.04	1.68
15	Nitro	22	pc=(70.98 ± 3.38)+(12.04 ± 2.43)E+(-42.21 ± 4.94)V	0.96	205.71	2.07

RESULTS AND DISCUSSION

In the researching of the Pc, a regression analysis of 516 substance from 15 categories was carried out (including saturated, unsaturated, chain, branched chain, cyclic, benzene ring, carbonyl compounds, hydroxyl compounds, and compounds containing N, O and halogen). The fitting equations of the Pc are listed in Table 1. The mean relative deviations (MD) of the obtained equations are from 1.68% to 3.76%. It is undeniable that when compared with other published methods [3,4,18,25,26,83-91]. Our equations have no remarkable increase in precision and even decrease a little as listed in Table 2. However, considering the difficulty of the measurement and estimation of Pc, the accuracy was reasonably high. In addition, our method has the advantages of simple form and easy calculation. The molecular descriptors are available for several thousand compounds in the published research [31-76] or can be estimated based on the existing methods [32,35,69]. Additionally, we can obtain the molecular descriptors using ADME software [92].

Table 2: Number of compounds and mean relative deviations (MD%) of some studies.

S.no	Reference	Number of compounds	Mean relative deviation (%)
1	1	275	2.72
2	2	269	2.89
3	3	286	2.98
4	4	445	5.3
5	18	199	5.1
6	22	1230	1.5
7	86	501	2.09
8	87	112	2.61
9	88	201	2.33
10	89	501	2.15
11	90	1696	1.1
12	91	408	2.47
13	This work	516	1.68~3.76(total 2.88)

For the halo hydrocarbon, only halogenated benzene was fitted. This was because the fitting effects of other similar compounds were very poor. For nitrogen compounds, we did not select the amides and aniline for the study because of the lack of data for them.

We adopted the following five figures to represent the predictive effect of estimating the Pc (Figures 1-5).

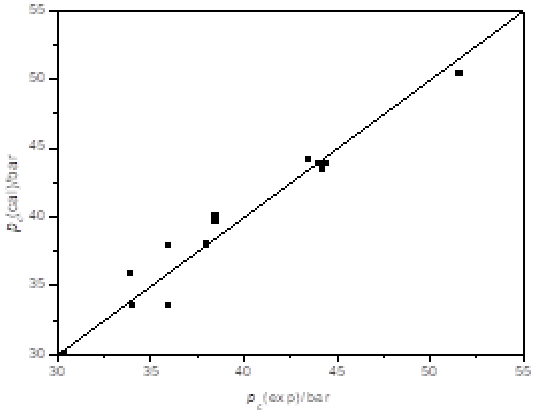

Figure 1: Comparison of experimental and calculated pc values for 22 nitryl compounds, MD = 2.07% (by uncorrected equation).

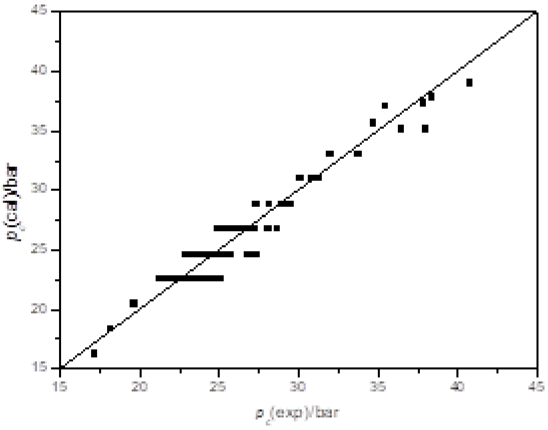

Figure 2: Comparison of experimental and calculated pc values for 145 alkanes, MD = 3.65% (by uncorrected equation).

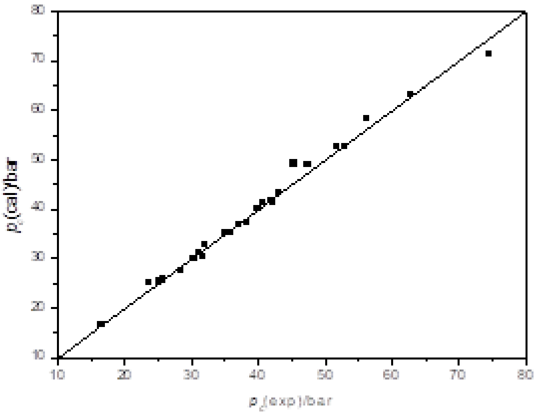

Figure 3: Comparison of experimental and calculated pc values for 25 aldehydes, MD = 1.84% (by corrected equation).

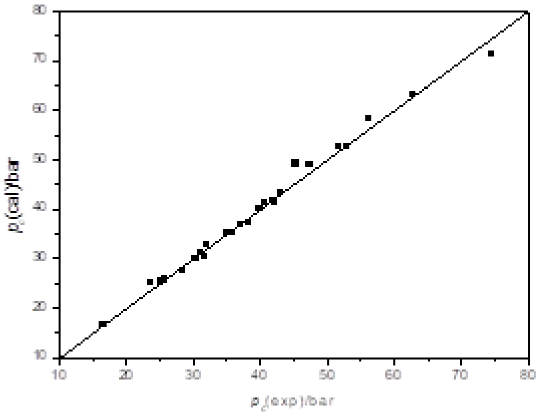

Figure 4: Comparison of experimental and calculated pc values for 26 amines, MD=2.11% (by corrected equation).

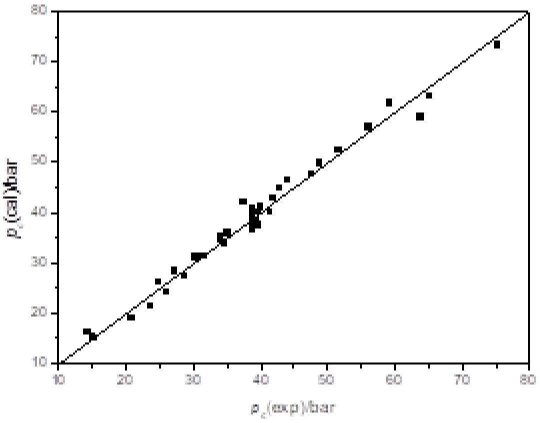

Figure 5: Comparison of experimental and calculated Pc values for 39 alcohols, MD=3.89% (by corrected equation).

To confirm the service ability of our equations for Pc, the other 9 categories of 51 compounds beyond the regression were selected to predict the Pc. The calculated values and the corresponding experimental data are listed in Table 3. As seen from Table 3, most of the calculated results correlate with that of the experiment. However, there is serious departure for some compounds. This situation can be explained by the following reasons. First, the intermolecular interaction was very complicated. The five arguments of the equations cannot integrally describe the interaction and molecular structure. The second reason is the defection of the molecular descriptors, for instance, the isomers have identical V values, which is always unconformable with the real case. In addition, there is not hydrogen bond for some systems. Therefore, some factors related with molecular structure and interaction affecting Pc may be absent from the obtained equations, resulting in large error. These aspects may be the main deficiencies of our method. Considering the difficulty of measuring Pc, the prediction effect is favorable.

Table 3: Comparison of experimental and calculated Pc values (in bar).

S.no	Formulae	Name	Pc(exp)	Pc(cal)	Error/%
1	C7H8O	3-Methylphenol(m-Cresol)	45.6	53.31	
2	C8H10O	3,5-dimethylphenol	36.48	47.93	
3	C10H14O2	p-tert-butyl catechol	37.7	48.86	
4	C6H6	benzene	48.98	41.02	16.25
5	C8H6	phenyl ethyne	44.03	33.7	23.45
6	C16H26	n-decyl benzene	17.7	13.09	26.03
7	CH4O	methanol	80.96	67.16	
8	C12H26O	1-dodecanol	19.3	16.84	
9	C13H28O	1-tridecanol	18.1	15.62	
10	C14H30O	1-tetradecanol	17	14.93	
11	C5H10O	3-pentanone	37.39	37.48	
12	C5H8O	Cyclo pentanone	58.5	43.32	25.94
13	C9H18O	di-isobutyl ketone	24.8	20.55	17.13
14	CH4	methane	46.04	41.44	10
15	C2H6	ethane	48.8	39.34	19.4
16	C3H6	Cyclo propane	55.75	47.47	14.86
17	C3H8	propane	42.49	37.23	12.37
18	C5H10	Cyclo pentane	45.02	40.2	10.7
19	C7H16	2,2-dimethylpentane	37.73	28.82	23.61
20	C8H16	cis-1,2-dimethylcyclohexane	29.38	34.28	
21	C8H16	trans-1,4-dimethylcyclohexane	29.38	32.38	
22	C8H17	Ethyl cyclohexane	30.4	33.89	
23	C10H20	1-cyclopentylpentane	25.05	28.78	
24	C10H22	2,7-dimethyloctane	20.97	22.51	
25	C10H22	3-ethyl-2,3,4-trimethylpentane	25.43	22.51	11.48
26	C10H22	2,2,3,3,4-pentamethylpentane	25.84	22.51	12.88

27	C10H22	3,3,4,4-tetramethylhexane	25.74	22.51	12.54
28	C10H22	3,3-diethyl-2-methylpentane	25.33	22.51	11.13
29	C10H22	3-ethyl-2,2,3-trimethylpentane	25.74	22.51	12.54
30	C14H30	n-tetradecane	16.21	14.11	12.95
31	C15H32	n-pentadecane	15.2	12.01	21
32	C16H34	n-hexadecane	14.19	9.9	30.2
33	C2H6O	dimethyl ether	53.7	45.98	14.38
34	C10H22O	di-n-pentyl ether	20.9	17.31	17.18
35	C3H4	propadiene	54.7	47.79	12.63
36	C5H6	Cyclo pentadiene	51.5	43.9	14.76
37	C5H8	Cyclo pentene	47.9	41.66	13.03
38	C6H10	cyclohexene	43.5	38.74	10.93
39	C6H8	cyclohexa-1,3-diene	47.3	41.43	12.41
40	C8H16	2-ethyl-1-hexene	30.7	26.71	13
41	C20H40	1-eicosene	12.2	15.11	-23.85
42	C2H4O2	methyl formate	59.98	45.28	24.5
43	C3H4O2	vinyl formate	50.2	44.29	11.78
44	C3H6O2	ethyl formate	47.42	41.74	11.97
45	C3H6O2	methyl acetate	46.9	41.63	11.23
46	C7H12O2	n-butyl acrylate	26.3	30.96	
47	C10H12O4	diallyl maleate	23.3	28.69	
48	C10H20O2	Iso-pentyl isovalerate	22	18.98	13.7
49	C12H14O4	diethyl phthalate	23.3	27.14	
50	CH3NO2	Nitro methane	63.13	56.86	9.93
51	C3H5N3O9	nitroglycerine	30	26.1	12.98

CONCLUSION

Based on the thermodynamics theory and the LFERs model, a novel method of calculating the Pc of pure fluids was proposed for the first time. This method not only correctly describes and predicts Pc quantitatively but also expands the range of available applications for the LFERs theory. This method breaks through the application scope of the empirical equation or theoretical equation. Furthermore, the proposed method consummates the computation of the critical properties of pure fluids in the engineering design, which exhibits better prediction accuracy and wide applicability.

It should be admitted that our method has some drawbacks. The five molecular descriptors of the equations cannot integrally describe the interaction and molecular structure, and therefore, some factors affecting Pc may be absent from the obtained equations. For the molecular descriptors, the isomers have identical V values, which is always unconformable with the real case. In addition, there is not hydrogen bond for some systems. These deficiencies resulted in large error for some compounds. However, considering the difficulty of measuring Pc, the prediction effect is favorable.

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