

## New Generalization of Cohesion Factor Model for Polar Compounds: Peng-Robinson Equation of State

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Predicting physical properties is one of the major requirements in process engineering. Equations of state (EoS) are widely used for predicting the physical properties. Among many EoS, cubic equations of state (cubic EoS) are being used because they are simple and applicable over a wide range of temperature and pressure. However, these cubic EoS fail to predict the properties of a compound having polarity, associating tendency as well as hydrogen bonding. In the present study, a new generalization for cohesion factor to be used with Peng-Robinson (PR) EoS is proposed. In developing the model, compound-specific parameters for nearly 300 compounds were generated. These compound-specific parameters were correlated in terms of the reduced dipole moment and critical compressibility factor. Proposed models were compared with models available in the literature. Vapor pressure, heat of vaporization, saturated liquid density and second virial coefficient of the compounds were predicted. It was observed that the models with a reduced dipole moment predicted various properties accurately for highly polar compounds without losing accuracy in predicting properties for non-polar compounds.

**Keywords:** PR EoS, Cohesion factor, Reduced dipole, Vapor pressure

### INTRODUCTION

In the last few decades, process industries encounter with an immense growth in the use of process simulators. Use of process simulators ranges from training operators to debottlenecking complex problems. Selecting a proper thermodynamic model is the most critical step for getting the accurate simulation results. Amongst various thermodynamic models available, equations of state (EoS) play a significant role in representing phase equilibrium of pure fluids and mixtures. Equations of state based on the Statistical Associating Fluid Theory (SAFT) and its different variations [1] are very accurate, however, cubic equations of state (cubic EoS) offer simplicity and wide

applicability. Most of the cubic EoS can be written as a generic form given in (1),

$$P = \frac{RT}{V-b} - \frac{a(V-k_3b)}{(V-b)(V^2+k_1bV-k_2b^2)} \quad (1)$$

where a, b,  $k_i$  ( $i = 1, 2, 3$ ) may be universal constants, fluid-specific constants or functions of temperatures. Since van der Waals proposed the first cubic EoS, there has been extensive effort in improving the predictive capabilities of cubic EoS. Redlich-Kwong (RK) [2] cubic EoS was the first equation to be successfully applied to the prediction of the vapour phase properties. Currently, the most frequently used cubic EoS in engineering practice are Soave-Redlich-Kwong (SRK) EoS [3] and Peng-Robinson (PR) EoS [4]. In the present work, PR cubic EoS was considered as it is widely used cubic EoS. PR cubic EoS can be expressed as,

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

where

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

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

$\Omega$  and  $\psi$  are the parameters for PR cubic EoS and their values are 0.07780 and 0.45724, respectively.  $\alpha(T_r)$  is the cohesion factor (popularly known as alpha function) and represents the dependency of the attraction term  $a(T)$  on temperature.

Modifications in van der Waals type EoS can be classified in the following categories,

- Modification in functional form of the pressure-volume relationship
- Modifications in attraction term of cubic EoS
- Modifications in repulsion term of cubic EoS
- Modifications in both attraction and repulsion terms

These modifications have improved the performance of cubic EoS in predicting liquid phase properties as well as other saturation properties. There have been several efforts for improving the predictions for the polar compounds by modifying the alpha expression, though a major success was not achieved. Mathias [5] considered compound-specific polar parameter  $p$  to take care of polar compounds and proposed the expression as,

$$\alpha = [1 + m(1 - \sqrt{T_r}) - p(1 - T_r)(0.7 - T_r)]^2 \quad (5)$$

however, he could not generalize the polar parameter  $p$ . By keeping the basic equation of PR as it is, Stryjek and Vera modified the dependency of alpha function as, [6]

$$\alpha = [1 + \kappa(1 - T_r^{0.5})]^2 \quad (6)$$

with

$$\kappa = \kappa_0 + \kappa_1(1 + T_r^{0.5})(0.7 - T_r) \quad (7)$$

$$\kappa_0 = 0.378893 + 1.489715\omega - 0.17131848\omega^2 + 0.0196554\omega^3 \quad (8)$$

where  $\kappa_1$ , the adjustable parameter characteristic of each pure compound, is obtained by fitting pure component vapor pressure data. Most of the cohesion function models proposed in the literature were generated either by considering non-polar or slightly polar compounds. Valderrama *et al.* [7] also proposed a cohesion factor model (to be used with SRK cubic EoS) to take care of polarity through the parameter  $\omega Z_c$ . Figueria *et al.* [8-9] proposed generalized expressions for cohesion factor model (for PR cubic EoS) based on compound-specific parameters for more than 300 compounds. They were successfully able to generalize the functional form for empirical parameter suggested by Stryjek and Vera [6] and Gibbons and Laughton [10]. Recently Forero and Velasquez [11] have developed a generalized expression for polar compounds using polar factor of Halm-Stiel. However, they changed the alpha function to Hayne type. Hosseinifar and Jamshidi [12] proposed a new attraction term containing boiling point to improve the prediction of polar compounds properties. Lately, most of the works for polar compounds were concentrated on three- or many-parameter EoS [13-17] or using Cubic plus association EoS [18-21]. Ghanbari *et al.* [22] have compiled modifications in PR cubic EoS. However, not all alpha functions can be considered, and Guennec *et al.* [23] provided the consistency test required to be followed by alpha functions. In the present work, the objective was to use a two-parameter EoS with simple alpha function model, and hence, comparison was limited to Figueria models developed to deal with polar compounds. As shown in results and discussion section, even the models proposed by Figueria *et al.* failed to predict properties for highly polar compounds. In the present study, the compounds were selected in a way that they represent different ranges of polarity. An effort was made to use dipole as one of the parameters in generalizing cohesion factor expression. It was observed that the addition of this parameter has improved the capacity of PR cubic EoS to predict the properties of highly polar compounds without losing the accuracy for non-polar and weakly polar compounds. Cohesion factor with  $\omega Z_c$  as a polar parameter used with PR cubic EoS was also developed in the present

study, though it did not show any improvement on the performance.

## DEVELOPMENT OF NEW MODELS

In our previous study, [24] ten models of cohesion factors were compared for predicting properties of nearly 300 compounds. It was observed that out of the models studied not a single model was capable of predicting the properties of the large variety of compounds accurately. For SRK cubic EoS, it was observed that cohesion function with compound-specific parameter improved the predictions of the properties [25]. Hence, cohesion factor models with compound-specific parameter(s) were developed in the present work for PR cubic EoS. Four models representing three categories (polynomial, exponential and linear relationship in acentric factors) of cohesion factor expressions were selected for which compound-specific parameters were generated. Details about the models with their mathematical expressions are given in Table 1. Characteristic constants for these models were obtained for all the compounds. Methodology for obtaining the compound-specific parameter(s) is discussed elsewhere [25,26].

### Development of Generalized Model for Cohesion Factor Parameter

It was observed that compound-specific models were able to predict the properties accurately. However, in order to use these models for a wider range of applications, generalization of the parameter(s) was required. Generalized expressions for parameter 'm' were developed for single parameter models (*i.e.*, for SRK and TB type models listed in Table 1) in the present study. For generalization, two parameters were considered,

Critical compressibility factor (Valderamma Approach) [7]

### Dipole Moment

Values of m, fitted to pure component vapor pressure data, were correlated with the product  $\omega Z_c$  as shown in Fig. 1. The resulting expression was a straight line with a correlation coefficient of 0.924. This was done for only TB type model as the linear fit for the SRK type model was

unsatisfactory. The model expression is provided in Table 2 and represented as PRNSMwzc.

In the other approach parameter, m was correlated with dipole moment. This inclusion was done in order to take care of the polarity of the compound studied in the work. Since the dipole moment is the direct measure of the compound polarity, it was considered for correlating the parameter. Different relations were tried, but, a wide range of values of dipole moment was not allowing a generalized acceptable fit. To narrow down the range of the dipole moments, reduced dipole was used. The reduced dipole moment was defined as: [30]

$$\mu_r \equiv \frac{\mu^2 P_c 10^5}{T_c^2} \quad (9)$$

where  $\mu$  is dipole in Debye,  $P_c$  is the critical pressure in atmosphere and  $T_c$  is the critical temperature in K. These values were obtained from the handbook of Yaws [31]. Compound-specific parameters were correlated with the reduced dipole moments as expressed in Eqs. (10) and (11).

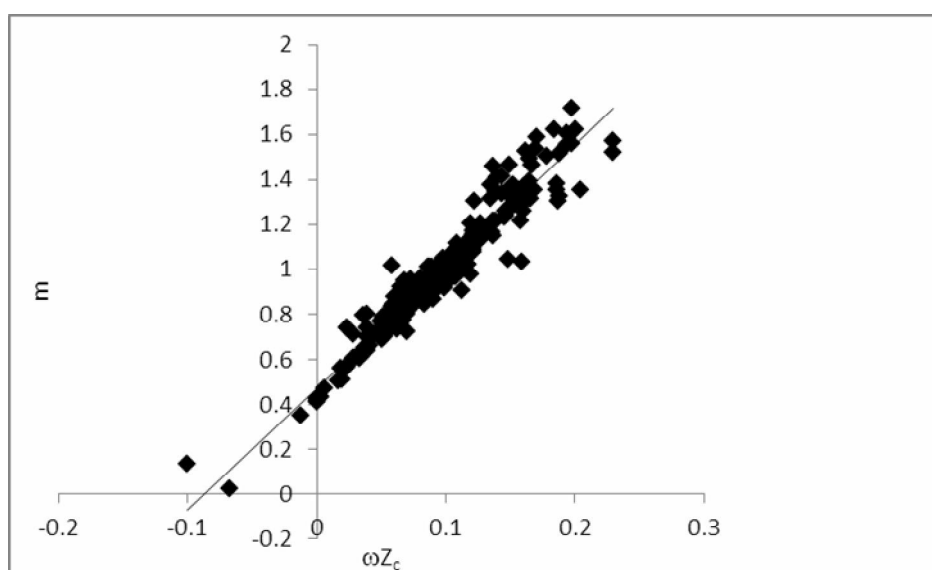
$$m = a + b\omega + c\mu_r \quad (10)$$

$$m = a + b\omega + c\omega^2 + d\mu_r \quad (11)$$

For both expressions, m parameter of the SRK type cohesion factor and the m parameter of TB type cohesion factors were correlated, resulting in four different models for PR cubic EoS. The coefficients of the models were obtained by minimizing the square of the difference between the generalized and compound-specific m values calculated. This was done using *Solver* function of Microsoft Excel®. Parameters obtained for Eqs. (10) and (11) are listed in Table 2 and represented by PRNSM1D to PRNSM4D. These models are different from previously proposed models as these models have a continuous application (*i.e.*, no discontinuity in terms of polarity, acentric factor or reduced temperature) and they are generalized in nature and hence require only critical properties and dipole moment as input for the estimation of

**Table 1.** Models Considered for Obtaining Compound-specific Cohesion Factors

Model	Expression	Remarks
SRK type [3]	$[1 + m(1 - \sqrt{T_r})]^2$	Single parameter
TB Type [27]	$\exp(m_{TB}(1 - T_r))$	Single parameter
Twu Type [28]	$\alpha = \alpha^0 + \omega(\alpha^1 - \alpha^0)$ with $\alpha^0 = \exp(m_{Twu}(1 - T_r))$ $\alpha^1 = \exp(n_{Twu}(1 - T_r))$	Two parameters
Modified TB type (mTB) (Gasem <i>et al.</i> ) [29]	$\exp(m_{mTB}(1 - T_r^{n_{mTB}}))$	Two parameters



**Fig. 1.** Parameter  $m$  as a function of  $\omega Z_c$  for PR EoS for TB type model

various properties using EoS. Table 2 also lists cohesion factor models developed by Figueria *et al.* [9] using Stryjek and Vera as well as Gibbson and Laughton cohesion function. These two models were compared in the present study with the developed models as these two models were shown to predict vapor pressure of polar compounds

accurately.

### PERFORMANCE OF ALL THE MODELS FOR THE PREDICTIONS OF PROPERTIES

The performance of the models was compared for the

**Table 2.** Cohesion Factor Models Compared in the Present Study (PR Cubic EoS)

Sr. No.	Model expression	Representation
1	$\alpha = \exp[(0.4718 + 5.4112\omega Z_c)(1 - T_r)]$	PRNSMwzc
2	$\alpha = [1 + (0.461807 + 1.288262\omega - 0.000341\mu_r)(1 - T_r^{0.5})]^2$	PRNSM1D
3	$\alpha = \exp[(0.555899 + 1.119522\omega - 0.000328\mu_r)(1 - T_r)]$	PRNSM2D
4	$\alpha = [1 + (0.406691 + 1.524095\omega - 0.158751\omega^2 - 0.00030\mu_r)(1 - T_r^{0.5})]^2$	PRNSM3D
5	$\alpha = \exp[(0.476403 + 1.459673\omega - 0.228972\omega^2 - 0.000269\mu_r)(1 - T_r)]$	PRNSM4D
6	$\alpha = 1 + (m(T_r - 1) + n(\sqrt{T_r} - 1))$ $m = 4.615548 - 14.922359Z_c + 1.874896\omega$ $n = -9.267944 + 27.407301Z_c - 6.549678\omega$	PRFGL
7	$\alpha = [1 + (m + n(1 + \sqrt{T_r})(0.7 - T_r))(1 - \sqrt{T_r})]^2$ $m = 0.379368 + 1.459994\omega - 0.125569\omega^2$ $n = 0.599529 - 1.952083Z_c + 0.080764\omega - 0.209272\omega^2$	PRFSV

**Table 3.** Details of the Properties Predicted Using Generalized Models

Sr. No.	Property	No. of compounds (Polar compounds)	Reference data type	Reference for prediction model
1	Vapour pressure	70 (52)	Pseudo-experimental	[7]
2	Heat of vaporization	70 (52)	Pseudo-experimental	[32]
3	Second virial coefficients	25 (19)	Experimental	[32]
4	Saturated liquid density	10 (07)	Pseudo-experimental	[34]

predictions of properties such as vapour pressure, heat of vaporization, second virial coefficients, saturated liquid density. Seven generalized models listed in Table 2 were compared based on %AAD (defined as  $\%AAD = 100/N_p \sum \frac{abs(M_{exp} - M_{cal})}{M_{exp}}$ , where  $N_p$  is the no. of data points,  $M_{cal}$  is the predicted property and  $M_{exp}$  is the experimental or pseudo-experimental values of property) of various properties.

Table 3 provides the details about the properties

predicted, and number/type of compounds considered in the prediction and models used for the prediction. Details of the compounds considered for predicting various properties are available in the supplementary material. All the compounds considered for the study were categorized as non-polar, weakly polar (up to 1.7 Debye) and highly polar ( $> 1.7$  Debye). Table 4 shows the overall performance of the models for non-polar, weakly polar and highly polar compounds for vapour pressure. Proposed models with a

**Table 4.** Overall Performance of the Models, %AAD, in Vapour Pressure Predictions

	PRNSMWzc	PRNSM1D	PRNSM2D	PRNSM3D	PRNSM4D	PRFGL	PRFSV
NP <sup>a</sup> (18)	26.45	8.77	13.32	8.73	14.33	4.93	5.35
WP <sup>b</sup> (38)	16.57	11.07	15.44	10.98	14.18	9.80	9.89
HP <sup>c</sup> (14)	14.67	7.16	7.86	7.41	8.43	14.08	13.69
Global	18.73	9.70	13.38	9.69	13.07	9.40	9.48

<sup>a</sup>NP: Non-polar. <sup>b</sup>WP: Weakly polar. <sup>c</sup>HP: Highly polar.

**Table 5.** Overall Performance of the Models, %AAD, in Heat of Vaporization Predictions

	PRNSMWzc	PRNSM1D	PRNSM2D	PRNSM3D	PRNSM4D	PRFGL	PRFSV
NP (18)	8.90	6.93	8.30	6.73	8.04	5.94	6.00
WP (38)	8.02	5.95	6.76	6.13	6.87	5.93	5.92
HP (14)	9.80	8.95	8.64	8.64	9.45	13.56	13.31
Global	8.60	6.80	7.53	6.79	7.69	7.46	7.42

**Table 6.** Overall Performance of the Models, %AAD, in Second Virial Coefficient Predictions

	PRNSMWzc	PRNSM1D	PRNSM2D	PRNSM3D	PRNSM4D	PRFGL	PRFSV
NP (06)	22.71	19.54	20.16	27.89	20.71	31.50	49.57
WP (13)	31.12	34.77	30.20	35.53	30.96	26.48	32.76
HP (06)	98.57	59.21	104.23	60.43	104.88	309.46	566.70
Global	45.29	36.98	45.56	39.67	46.24	95.60	164.94

**Table 7.** Overall Performance of the Models, %AAD in Saturated Liquid Density Predictions

	PRNSMWzc	PRNSM1D	PRNSM2D	PRNSM3D	PRNSM4D	PRFGL	PRFSV
NP (03)	9.13	9.42	9.49	9.26	9.22	27.46	27.46
WP (04)	12.13	12.82	13.00	12.48	12.46	51.53	51.53
HP (03)	14.24	14.16	14.20	14.13	14.17	15.48	15.48
Global	6.40	6.47	6.51	6.41	6.42	12.54	12.54

**Table 8.** Untransformed %AAD Values for all the Models Considered in the Study

Models	Vapor pressure	Second virial coefficient	Heat of vaporization	Saturated liquid density	Overall
PRNSM <sub>wzc</sub>	18.73	47.85	8.60	6.40	81.58
PRNSM1D	9.70	36.98	6.80	6.47	59.95
PRNSM2D	13.38	45.56	7.53	6.51	72.98
PRNSM3D	9.69	39.67	6.98	6.41	62.75
PRNSM4D	13.07	46.24	7.69	6.42	73.42
PRFSV	9.48	164.94	7.42	12.54	194.38
PRFGL	9.40	95.60	7.46	12.54	125

**Table 9.** Weighting Factors Given for Incorporating Importance of Properties and Data

Property	Weighting factor based on importance	Weighting factor based on the database	Remarks
Vapor pressure	4	4	Pseudo-experimental data with 70 compounds (range of temperature from $T_F$ to $T_C$ )
Second virial coefficient	4	2	Experimental data for 25 compounds
Heat of vaporization	3	4	Pseudo-experimental data with 70 compounds (Range of temperature from $T_F$ to $T_C$ )
Saturated liquid density	3	5	Pseudo-experimental data for 10 compounds

reduced dipole, as a parameter, were found to be accurate in predicting the vapour pressure compared to the other models. It was also observed that the behaviour of the proposed models having reduced dipole was drastically better for the highly polar compounds compared to other models. Moreover, these models were at par with other generalized models for non-polar and weakly polar

compounds. Tables 5 to 7 show deviation in predicting heat of vaporization, second virial coefficient and saturated liquid density, respectively. One can observe that for highly polar compounds the proposed models were much better than the others and also in parallel with others for non-polar and weakly polar compounds. For saturated liquid density, the performance of PRFGL and PRFSV models was not

**Table 10.** Transformed %AAD Values for all the Models Considered in the Study

Models	Over all transformed score
PRNSM1D	629.69
PRNSM3D	652.31
PRNSM2D	766.57
PRNSM4D	767.62
PRNSMwzc	881.68
PRFSV	1192.82
PRFGL	1748.34

proper for non polar and week polar compounds. The proposed models predicted density with a relatively good prediction. One of the possible reasons for improved performance is inclusion of polarity in the expression of parameter 'm' and also inclusion of highly polar compounds in the model developed. To see the overall performance of the models, a combined untransformed %AAD (%AAD values obtained by summing global %AAD of each individual property) value was obtained. These values are listed in Table 8. PRNSM1D and PRNSM3D have the lowest scores of 59.95% and 62.75%, respectively, for the generalized models.

Considering the fact that various properties have their own importance as well as mathematical complexity in predictions, each of the %AAD values was multiplied by a weighting factor based on the importance of the property. The factor ranges from 1 (least important) to 5 (most important) property. A weighting factor was also given based on the type of data considered for comparison and the number of compounds considered for the property prediction as they also have an effect on comparing the models. Table 9 provides the information on these weighting factors, along with the type and number of experimental data. Transformed %AAD values were obtained by multiplying untransformed %AAD with weighting factors. Transformed %AAD values of all the models are listed in Table 10 in order of their performance. PRNSM1D model showed the least score with PRNSM3D

model following it closely.

## CONCLUSIONS

In the present work, five generalizations of cohesion factor models of PR cubic EoS were proposed based on 300 compounds covering 25 families and a wide range of polarity. Out of these five models, one model (PRNSMwzc) involves the addition of critical compressibility factor and four models (PRNSM1D to PRNSM4D) involve reduced dipole moment as one of the parameters in cohesion factor generalization. These five models were compared with two models shown to be accurate for polar compounds. Comparison of the performance was done based on the prediction of various properties. The models were developed by minimizing the error in vapor pressure predictions and hence, definitely proved to be better compared to others for vapor pressure predictions. However, to examine the robustness of the models, other saturation properties were also predicted. Moreover, various properties were given different weighting factor based on the importance and the type of reference data used to provide a holistic approach in comparing the models. The general findings are listed below,

- Addition of critical compressibility factor did not improve the performance of the PR cubic EoS in predicting the properties of polar compounds



- Models involving reduced dipole moment as a parameter performed much better for highly polar compounds and they were in parallel with the other models for predicting the properties of non-polar and weakly polar compounds
- Models having generalized expression as Eq. (10) performed better for predicting the properties compared to the models having generalized expression as Eq. (11). Since the later type of the models were having second power dependency on acentric factor they failed in predicting vapor pressure and second virial coefficients of high acentric factor compounds which was reflected by high %AAD values in the respective properties
- SRK type cohesion factor expressions (*i.e.*, PRNSM1D and PRNSM3D) performed better compared to exponential form of TB type.
- Based on the performance of transformed %AAD, PRNSM1D and PRNSM3D should be the choices for predicting the properties using PR EoS for highly polar compounds and mixtures having such compounds

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