# A GENERALIZED PATEL-TEJA EQUATION OF STATE FOR POLAR AND NONPOLAR FLUIDS AND THEIR MIXTURES

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## Introduction

Patel and Teja[1,2] proposed a three-parameter cubic equation of state (EOS) which has proved to provide good representation of vapor-liquid equilibrium (VLE) for several mixtures.

The Patel-Teja (PT) equation contains two adjustable empirical parameters which can be calculated using vapor pressure data for pure components. Patel and Teja[2] reported values of these parameters for 34 substances. More recently, Georgeton et al.[3] have recalculated these parameters and have also provided the values for 29 more substances.

Patel and Teja[1,2] were able to correlate the two empirical parameters in terms of the acentric factor. However, the correlations are valid for nonpolar fluids only. Valderrama and Cisternas[4] correlated the

parmeters in the PT equation in terms of the critical compressibility factor. The correlations, however, are not of general applicability.[5] Therefore, the two parameters in the PT equations should, in principle, be calculated from vapor pressure data. Another problem with the PT equation is the introduction of an additional mathematical complexity which is not present in other common cubic EOS such as the Soave-Redlich-Kwong[6] or the Peng-Robinson[7] equations. This problem is the solving of an additional cubic equation for one of the three parameters of the EOS. **Table 1** gives details.

In this note I propose new generalized correlations for the parameters in the PT equation. These correlations solve the problems mentioned above by transforming the equation into a generalized EOS and by eliminating the necessity of solving any additional equation. Therefore, the generalized proposed equation of state regains the form of the standard

**Table 1.** Patel-Teja equation of state

Equation of state

$P = RT/(V-b) - a_c\alpha(T_R)/[V(V+b)+c(V-b)]$

$a_c = \Omega_a RT_c^2/P_c$

$b = \Omega_b RT_c/P_c$

$c = \Omega_c RT_c/P_c$

$\alpha(T_R) = [1 + F(1-\sqrt{T_R})]^2$

$\Omega_c = 1 - 3\gamma_c$

$\Omega_a = 3\gamma_c^3 + 3(1-2\gamma_c)\cdot\Omega_b + \Omega_b^2 + 1 - 3\gamma_c$

$\Omega_b$ is the smallest positive root of the cubic:

$\Omega_b^3 + (2-3\gamma_c)\cdot\Omega_b^2 + 3\gamma_c^2\Omega_b - \gamma_c^3 = 0$

F and $\gamma_c$ are adjustable empirical parameters

Values of F and $\gamma_c$ for 63 substances are given by Georgeton et al.[3]

For nonpolar fluids only, the following correlations in terms of the acentric factor $\omega$ can be used[2]

$F = 0.45213 + 1.3098\omega - 0.295937\omega^2$

$\gamma_c = 0.329032 - 0.076799\omega + 0.0211947\omega^2$

For mixtures

$a_m = \sum_i \sum_j x_i x_j a_{ij}, \quad a_{ij} = (a_i a_j)^{1/2}(1-k_{ij})$

$b_m = \sum_i x_i b_i \quad \text{and} \quad c_m = \sum_i x_i c_i$

two-parameter EOS (such as Soave or Peng-Robinson) with the advantage of having an extra generalizing parameter.

## 1. Development of Equations

The cubic equation under study is:

$$P = \frac{RT}{V-b} - \frac{a_c\alpha(T_R)}{V(V+b)+c(V-b)} \qquad (1)$$

where

$$a_c = \Omega_a R^2 T_c^2/P_c$$
$$b = \Omega_b RT_c/P_c \qquad (2)$$
$$c = \Omega_c RT_c/P_c$$

$$\alpha(T_R) = [1 + F(1-\sqrt{T_R})]^2 \qquad (3)$$

In the original PT equation, the coefficients $\Omega_a$, $\Omega_b$ and $\Omega_c$ are calculated, using an empirical critical parameter $\gamma_c$ as shown in Table 1. The coefficient F is the second adjustable parameter in the PT equation. Since the work of Georgeton et al.[3], values of $\gamma_c$ (and therefore of $\Omega_a$, $\Omega_b$, and $\Omega_c$) and F for 63 substances are available.

Several pure-component properties were considered to generalize F and the $\Omega$'s. The best correlations have been found with the use of the critical compressibility factor for the $\Omega$'s and with the product [acentric
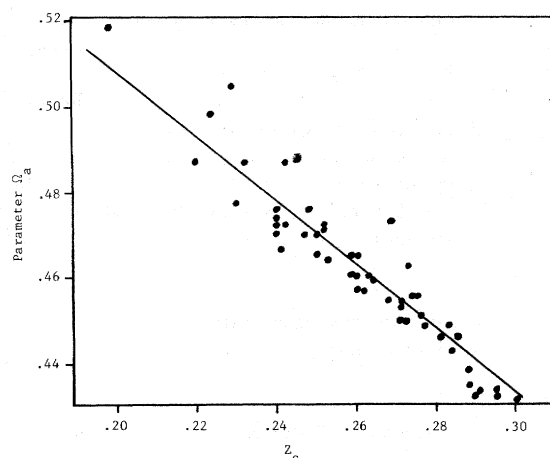


**Fig. 1.** Correlation for the parameter $\Omega_a$ as a function of the critical compressibility factor
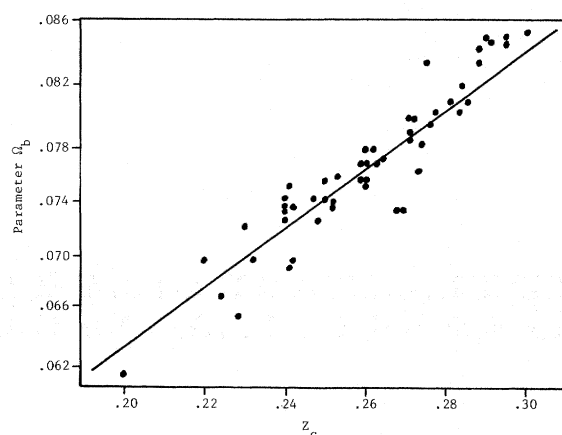


**Fig. 2.** Correlation for the parameter $\Omega_b$ as a function of the critical compressibility factor
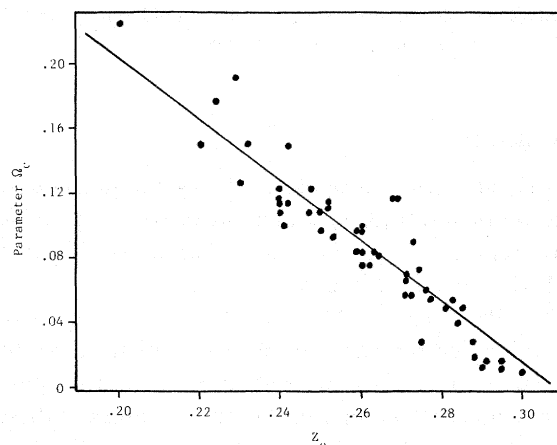


**Fig. 3.** Correlation for the parameter $\Omega_c$ as a function of the critical compressibility factor

factor] × [critical compressibility factor] for the coefficient F. **Figures 1** to **4** show the correlations. These findings corroborate other results presented in the literature in which these two properties (acentric factor and critical compressibility factor) are used to
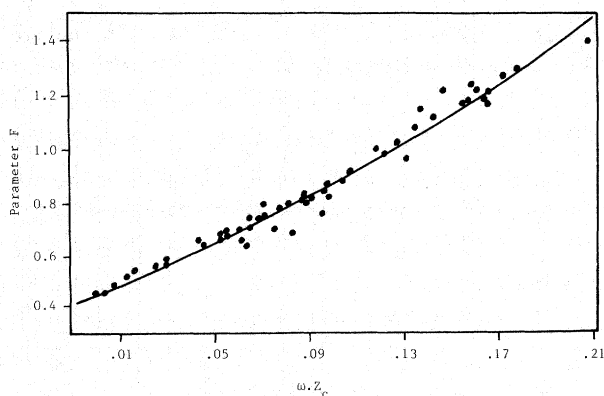
**Fig. 4.** Correlation for the parameter $F$ as a function of the group [acentric factor] × [critical compressibility factor]

**Table 2.** Proposed generalized PTV equation of state

Equation of state

$$P = RT/(V-b) - a_c\alpha(T_R)[V(V+6) + c(V-b)]$$

$$a_c = \Omega_a RT_c^2/P_c$$

$$b = \Omega_b RT_c/P_c$$

$$c = \Omega_c RT_c/P_c$$

$$\alpha(T_R) = [1 + F(1 - \sqrt{T_R})]^2$$

$$\Omega_a = 0.66121 - 0.76105.Z_c$$

$$\Omega_b = 0.02207 + 0.20868.Z_c$$

$$\Omega_c = 0.57765 - 1.87080.Z_c$$

$$F = 0.46283 + 3.58230(\omega \cdot Z_c) + 8.19417(\omega \cdot Z_c)^2$$

For mixtures

$$a_m = \sum_i \sum_j x_i x_j a_{ij}, \quad a_{ij} = (a_i a_j)^{1/2}(1 - k_{ij})$$

$$b_m = \sum_i x_i b_i \quad \text{and} \quad c_m = \sum_i x_i c_i$$

Expressions for the pure-component fugacity and for the fugacity of a component in a mixture can be obtained from references (1) or (2).

generalize equations of state.[5,8-11] The advantages and disadvantages of using $Z_c$ as a generalizing parameter have been discussed elsewhere.[12,13] The proposed correlations are:

$$\Omega_a = 0.66121 - 0.76105 \cdot Z_c$$

$$\Omega_b = 0.02207 + 0.20868 \cdot Z_c \qquad (4)$$

$$\Omega_c = 0.57765 - 1.87080 \cdot Z_c$$

$$F = 0.46283 + 3.58230(\omega \cdot Z_c) + 8.19417(\omega \cdot Z_c)^2 \qquad (5)$$

Values of $F$ and the $\Omega$'s using these correlations are represented by the solid line in Figs. 1 to 4. The proposed generalized EOS is summarized in **Table 2**.
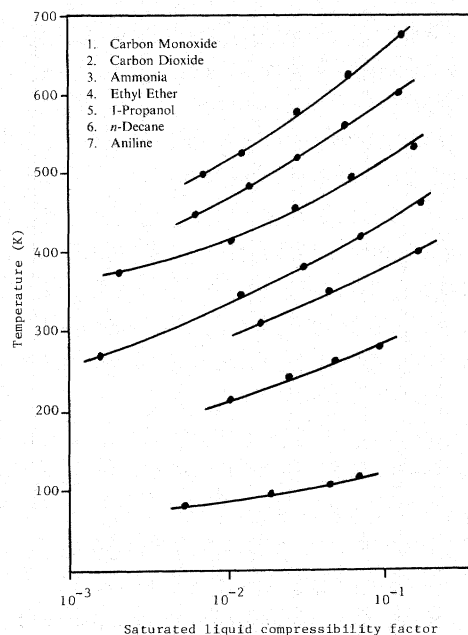


Saturated liquid compressibility factor

**Fig. 5.** Prediction of compressibility factor of several substances using the generalized Patel-Teja equation of state. Literature data (●) are from Schlunder[14]
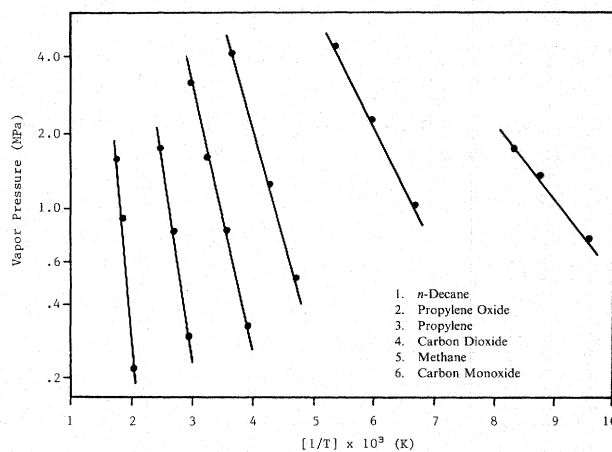


**Fig. 6.** Preduction of vapor pressure of several substances using the generalized Patel-Teja equation of state. Literature data (●) are from Schlunder[14]

## 2. Application of the Generalized EOS

Vapor pressure, liquid- and vapor-phase compressibility factors, and vapor-liquid equilibrium in mixtures have been predicted using the proposed correlations. Some results are shown in **Figs. 5** to **8**. A more extensive study of the application of the proposed equation is in progress.

### Conclusions

The empirical parameters of the Patel-Teja equation of state have been correlated in terms of the acentric factor and of the critical compressibility factor. The new PTV equation of state is a generalized equation in which no adjustable parameters are needed. The
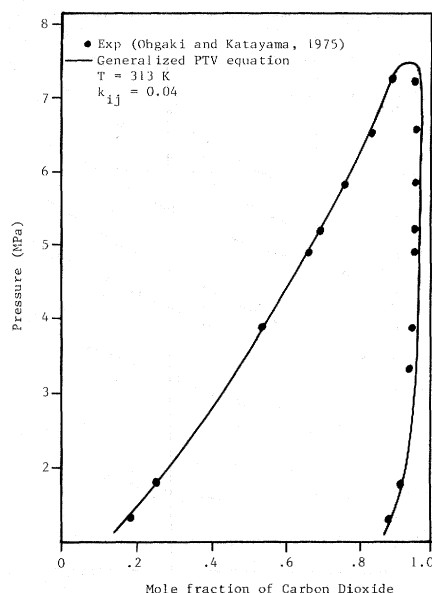
**Fig. 7.** Prediction and correlation of bubble pressure for the $CO_2$-ethyl acetate system at 313 K Experimental data are from Ohgaki and Katayama[15]
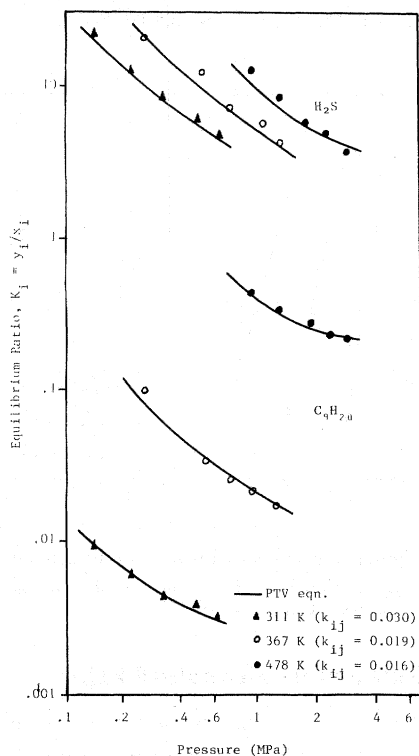


**Fig. 8.** Equilibrium ratios at three temperatures for $H_2S$ and nonane using the generalized Patel-Teja equation of state. The full lines are calculated values and the points are experimental values from Eakin and de Vaney[16]

equation has given good results for pure polar and nonpolar fluid properties and VLE in mixtures containing polar and nonpolar substances.

**Note**

A computer program to perform VLE calculations using the proposed EOS is available from the author. Hard printed copies or diskettes can be obtained upon request.

**Nomenclature**

| | | |
|---|---|---|
| $a_c$ | = | force constant at the critical point |
| $a_i, a_j$ | = | force constants for components $i$ and $j$ in the mixture |
| $a_{ij}$ | = | cross-force constant in the mixture |
| $a_m$ | = | force constant for the mixture |
| $b, c$ | = | volume constants |
| $b_i, c_i$ | = | volume constants for components $i$ and $j$ in the mixture |
| $b_m, c_m$ | = | volume constants for the mixture |
| EOS | = | equation of state |
| $F$ | = | adjustable empirical parameter |
| $k_{ij}$ | = | binary interaction parameter |
| $P$ | = | pressure |
| $P_c$ | = | critical pressure |
| $PT$ | = | Patel-Teja equation of state |
| $R$ | = | ideal-gas constant |
| $T$ | = | temperature |
| $T_c$ | = | critical temperature |
| $T_R$ | = | reduced temperature |
| $V$ | = | molar volume |
| VLE | = | vapor-liquid equilibrium |
| $x_i, x_j$ | = | mole fractions of components $i$ and $j$ in the mixture |
| $Z$ | = | compressibility factor |
| $Z_c$ | = | critical compressibility factor |
| | | |
| $\alpha$ | = | temperature function |
| $\gamma_c$ | = | adjustable critical parameter |
| $\Omega_a$ | = | force constant coefficient |
| $\Omega_b, \Omega_c$ | = | volume constant coefficients |
| $\omega$ | = | acentric factor |

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