Prediction of Vapor-Liquid Equilibrium Properties for the Mixture of Propylene+Propane from the Combined Use of Peng-Robinson Equation of State and COSMO-RS model

Xinyun Pu, Lehuan Wu, and Yansheng Liu

Abstract—In this research, the prediction of vapor-liquid equilibrium (VLE) of the binary mixture of propylene+propane from the combined use of the Peng-Robinson equation of state (PR-EOS) and the COSMO-RS model is examined. Following the Van der Waals mixing rule (VdW), the average deviations in both the pressure and vapor phase composition from the method are no more than 0.32% and 0.57%, respectively. Based on the results, it has been shown that PR-EOS+VdW+COSMO-RS is a promising approach for propylene+propane VLE predictions over a wide range of temperatures. This method introduces only one adjustable parameter. Assuming the adjustable parameter as a function of temperature, this method is used as a straight forward process without any iteration to estimate VLE data.

Index Terms—COSMO-RS, Peng-Robinson equation of state, propane, propylene, vapor-liquid equilibrium.

I. INTRODUCTION

The separation of propylene-propane plays an important role in the petrochemical sector. Due to the close boiling point and lower relative volatiles of propylene and propane, the obtaining of high purity propylene (>99.5mole%) by traditional rectification process is quite difficult. Much effort has been made to find the suitable correlation for their vapor-liquid equilibrium data [1]-[6]. However, when using simulation software to predict the two phase equilibrium of propylene and propane, neither Soave-Redlich-Kwong (SRK) nor Peng-Robinson (PR) equation of state can lead to the high-precision solutions [7]. The prediction deviations of the common used methods are presented in Table I.

What's more, the errors come from the equilibrium prediction can directly affect the design process of distillation. Kister [9] has pointed out that errors in relative volatility are the most underrated factor that affects both tray and packing efficiency. As in Fig. 1, at very low relative volatilities ($\alpha < 1.2$), small errors in VLE have a huge impact on tray efficiency. For instance, at a relative volatility of 1.1, a -4% error in relative volatility gives a tray efficiency 40%-50% higher than its true value. Since the relative volatility of propylene+propane system ranges from 1.05-1.21, the effect of VLE errors on column design will be greatly magnified. The purpose of this work is to develop an improved method to predit the VLE properties for the binary mixture of

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propylene+propane.

| TABLE I: THE PREDICTION DEVIATIONS FOR THE BINARY MIXTURE OF | |
|--|---|
| PROPYLENE(1)+PROPANE(2) USED BY MODELS IN ASPEN V8.6 PROGRAM | Л |

| Equation | $T(\mathbf{K})$ | $AAD\%-P^a$ | $AAD\%-y_1^b$ | AAD%- α^{c} |
|------------|-----------------|-------------|---------------|--------------------|
| SRK | 230-350 | 1.02 | 0.34 | 0.83 |
| PR | 230-350 | 0.42 | 0.36 | 0.86 |
| PRWS | 230-350 | 0.41 | 0.40 | 1.04 |
| UNIFAC | 230-350 | 1.58 | 1.46 | 2.66 |
| UNIFAC-DMD | 230-350 | 1.27 | 1.18 | 2.07 |
| UNIQUAC | 230-350 | 1.01 | 2.43 | 6.55 |
| UNIQUAC-RK | 230-350 | 1.10 | 1.26 | 3.23 |
| BWR-Le | 230-350 | 1.38 | 1.50 | 3.15 |

$$\begin{bmatrix} AAD\% - P = \frac{1}{N} \sum_{i=1}^{N} 100 \left| \frac{v_{i,REF} - v_{i,cal}}{p_{i,REF}} \right|$$

$$\stackrel{b}{=} AAD\% - y_i = \frac{1}{N} \sum_{i=1}^{N} 100 \left| \frac{y_{i,REF} - y_{i,cal}}{y_{i,REF}} \right|$$

ln

-n

^c AAD% -
$$\alpha = \frac{1}{N} \sum_{i=1}^{N} 100 \left| \frac{\alpha_{i,REF} - \alpha_{i,cal}}{\alpha_{i,REF}} \right|$$

Reference Data: [8]



Fig. 1. Direct effect of errors in relative volatility on error in tray efficiency.

Since its first publication in 1995, the quantum chemically based conductor-like screening model for realistic solvation (COSMO-RS) has developed a widely accepted and independent method for the fluid phase equilibrium simulation [10]-[12]. Numerous studies [13]-[17] have been carried out with the computation of activity coefficients in the liquid phase for VLE calculations. For the mixture of propylene+propane, VLE data at various temperatures are previously reported by some athors [1]-[6], [8], [18]-[20]. In the design of the C_3 distillation column, the operating temperature ranges from 300-330 K, and the pressure is above 3 MPa. The VLE data are usually estimated by thermodynamic models based on the fundamental phase equilibrium criterion of equality of chemical potential in both phases [21]. This process is based on the gamma(γ)-phi(ϕ) calculation method. In this work, the Peng-Robinson equation of state (PR-EOS) with the Van der Waals (VdW) mixing rule and COSMO-RS model are applied for prediction of VLE of the propylene+propane system which can be considered as moderately non-ideal mixtures. Meanwhile the average deviations in pressures and vapor phase compositions obtained from this correlation are presented.

II. THEORY

The toal pressure P^{tot} has been calculated from

$$P^{tot} = P_1^{sat} \gamma_1 x_1 + P_2^{sat} \gamma_2 x_2 \tag{1}$$

 P^{tot} means the total pressure of the system, P_1^{sat} (propylene), P_2^{sat} (propane) the pure compound saturation vapor pressure, x_1 , x_2 the mole fraction of compound in the liquid phase, and γ_1 , γ_2 the activity coefficient. Both the activity coefficients are computed by COSMOtherm program [22], which provides an efficient and flexible implementation of the COSMO-RS method.

For the system, the pure compound saturation vapor pressure has been obtained from Wanger equqation. The coefficients for (2) are given in Table II.

$$\ln\left(P_{i}^{sat}\right) = \ln\left(A\right) + \frac{1}{1-\tau} \left(C\tau + D\tau^{1.5} + E\tau^{3} + F\tau^{6}\right)$$

$$\tau = 1 - \frac{T}{B}$$
(2)

TABLE II: WANGER EQUATION COEFFICIENTS IN [kPa]/[K]

| | Propane | Propylene |
|-----------------------|----------|-----------|
| А | 4248 | 4600 |
| В | 369.83 | 364.90 |
| С | -6.72219 | -6.64231 |
| D | 1.33236 | 1.21857 |
| E | -2.13868 | -1.81005 |
| F | -1.38551 | -2.48212 |
| Temperature range (K) | 145-370 | 140-365 |

In this work, the vapor fugacity coefficients ϕ_1 , ϕ_2 of propylene and propane have been calculated by PR-EOS [23].

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)}$$
(3)

$$a(T) = \left(0.45724 \frac{R^2 T_c^2}{P_c}\right) \alpha(T)$$
(4)

$$b = 0.07780 \frac{RT_c}{P_c} \tag{5}$$

$$\alpha(T) = \left[1 + k\left(1 - T_r^{0.5}\right)\right]^2$$

$$k = 0.37464 + 1.54226\omega - 0.26992\omega^2$$
(6)

The parameter a(T) is a function of temperature, b the constant, k a constant characteristic of both components, ω the acentric factor, P and P_c the absolute and critical pressures, T and T_c the absolute and critical temperatures, T_r

the reduced temperature and v is the molar volume. The parameters of propylene and propane used to calculate are summarized in Table III.

| TABLE III: CHARACTERISTIC PROPERTIES OF PROPYLENE AND PROPANE |
|---|
|---|

| Characteristic property | Propane | Propylene |
|--------------------------------|---|-----------------------------------|
| Chemical formula | CH ₃ CH ₂ CH ₃ | CH ₂ CHCH ₃ |
| Molar mass (g/mol) | 44.10 | 42.08 |
| Boiling point, $T_b(K)$ | 231.06 | 225.46 |
| Critical temperature, $T_c(K)$ | 369.85 | 365.57 |
| Critical pressure, $P_c(MPa)$ | 4.248 | 4.665 |
| Acentric factor, ω | 0.1524 | 0.1408 |

According to Klamt [24], it is possible to adjust the COSMO-RS method to achieve better predictions for a specific system. From the viewpoint of the molecule or compound, it is possible to modify the COSMO charge surface of a molecule, thus accounting for the deficits of the quantum chemical DFT-COSMO calculations for the specific molecule used. The electrostatic misfit energy contribution in COSMO-RS is given in (7).

$$E_{MF}\left(\sigma,\sigma'\right) = a_{eff} \frac{a}{2} \left(\sigma + \sigma'\right) \tag{7}$$

The parameters σ and σ are surface charge values, a_{eff} is the effective contact area, a' is the misfit prefactor, an adjustable parameter. The electrostaic misfit term can be modified through the global C_{MF} factor command. This will scale the a' coefficient in the COSMOtherm parameter set by the given value of factor. The parameter C_{MF} in this work is obtained by minimizing the following objective function (8), where N is the number of experimental points, P_{REF} and P_{cal} (P^{tot}) are reference and calculated pressures.

$$Objection \ function = \frac{1}{N} \sum_{i}^{N} \left(\frac{\left| P_{i,REF} - P_{i,cal} \right|}{P_{i,REF}} \times 100 \right)^{2}$$
(8)

$$y_i = \frac{P_i^{sat} x_i \gamma_i}{P^{iot} \phi_i} \tag{9}$$

Eventually, the vapor pressure P^{tot} and activity coefficient γ_i are predicted by COSMOtherm program. The vapor fugacity coefficient ϕ_i is predicted by PR-EOS and the vapor mole fraction y_i is calculated by (9).

III. RESULTS AND DISCUSSIONS

A. Saturated Vapor Pressure of Propylene and Propane

The deviations in saturation vapor pressure P_i^{sat} between the calculated values and literature data at various temperatures are presented in Table IV. For the saturation vapor pressure data reported by Harmens [8], the average deviations are 0.39% for propylene and 0.11% for propane. In case of the published values introduced by Horwat and Swift [4], the average deviations are 0.22% and 0.21%. The average deviations are 0.50% and 0.21%, respectively for Hirata's [5] data at low temperatures. Generally, all deviation values are low and acceptable.

B. Vapor-Liquid Equilibrium of Propylene and Propane

The deviations in pressure and in vapor phase compositions at various temperatures are presented in Table V. From the results, it is found that for the temperature ranging from 230 to 350 K, the values of AAD% - P vary within 0.07%-0.56%, meanwhile, the values of $AAD\% - y_1$ vary within 0.11%-0.75%. These values for Horwat and Swift's data vary within 0.11-0.32% and 0.27%-0.57%. Generally, all values are relatively small and acceptable. For the parameter C_{MF} , it decreases linearly as the temperature increases. As we have mentioned above, C_{MF} is set to modify the misfit prefector a', which is related to the effective contact area $a_{\rm eff}$ in DFT-COSMO calculations. When the temperature rises, the effective charge surface of propylene-propane system will reduce, which leads to the weakening of the electrostatic misfit energy contribution.

A plot of relative volatility dependent on temperature is shown on Fig. 2, illustrating the typical behavior of increasing relative volatilities with decreasing temperatures, with the exception of propylene rich mixtures at low temperatures.

Below 270 K, for rich propylene mixtures ($x_1 = 0.9$), the relative volatility decreases as the temperature decreases, previously pointed out by Funk and Prausnitz [25].

The relative volatility of propylene-propane system is calculated by (10). With the increasing temperatures, P_1^{sat} / P_2^{sat} decreases (Fig. 3), ϕ_1 increases and ϕ_2 decreases (ϕ_2 / ϕ_1 decreases), both γ_1 and γ_2 decreases. A plot of γ_1 / γ_2 dependent on temperature is shown on Fig. 4. For rich propylene mixtures ($x_1 > 0.53$), γ_1 / γ_2 increases with temperatures, which makes the relative volatility of propylene-propane system unpredictable.

This interesting phenomenon occurs because the activity coefficient of propane (γ_2), the less volatile component, is rising with decreasing temperature. It may explain why the relative volatility of propylene-propane system is not only related to the temperature and pressure, in some cases it is also related to the concentration of propylene.

$$\alpha = \frac{y_1 / x_1}{y_2 / x_2} = \frac{P_1^{sat}}{P_2^{sat}} \times \frac{\gamma_1}{\gamma_2} \times \frac{\phi_2}{\phi_1}$$
(10)

0.21^e

| | TABLE IV | COMPARISONS OF VAPOR PRESS | URE AT VARIOUS TEMPERATU | JRES | | |
|---------------------|-----------------------|---------------------------------|--------------------------|---------------------------------|--|--|
| T (K) | | Propylene | | Propane | | |
| | $ \triangle P ^{a}$ | $ \Delta P $ (0() | $ \vartriangle P ^{a}$ | $ \Delta P $ (96) | | |
| | (MPa) | $\overline{P_{REF}^{sat}}$ (70) | (MPa) | $\overline{P_{REF}^{sat}}$ (70) | | |
| 230 ^b | 0.0004 | 0.32 | 0.0002 | 0.21 | | |
| 240 ^b | 0.0009 | 0.48 | 0.0002 | 0.14 | | |
| 250 ^b | 0.0011 | 0.40 | 0.0003 | 0.14 | | |
| 260 ^b | 0.0012 | 0.31 | 0.0002 | 0.06 | | |
| 270 ^b | 0.0027 | 0.51 | 0.0001 | 0.02 | | |
| 280 ^b | 0.0032 | 0.45 | 0.0005 | 0.09 | | |
| 290 ^b | 0.0036 | 0.38 | 0.0001 | 0.01 | | |
| 300 ^b | 0.0044 | 0.36 | 0.0003 | 0.03 | | |
| 310 ^b | 0.0067 | 0.44 | 0.0016 | 0.13 | | |
| 320 ^b | 0.0081 | 0.42 | 0.0024 | 0.15 | | |
| 330 ^b | 0.0099 | 0.42 | 0.0035 | 0.18 | | |
| 340 ^b | 0.0100 | 0.34 | 0.0041 | 0.17 | | |
| 350 ^b | 0.0069 | 0.20 | 0.0033 | 0.11 | | |
| | | 0.39 ^e | | 0.11 ^e | | |
| 227.59 ^c | 0.0000 | 0.00 | 0.0004 | 0.46 | | |
| 244.26 ^c | 0.0004 | 0.18 | 0.0004 | 0.23 | | |
| 260.93 ^c | 0.0011 | 0.28 | 0.0007 | 0.22 | | |
| 227.59 ^c | 0.0020 | 0.30 | 0.0012 | 0.22 | | |
| 294.26 ^c | 0.0023 | 0.22 | 0.0021 | 0.24 | | |
| 310.93 ^c | 0.0037 | 0.24 | 0.0030 | 0.23 | | |
| 327.59 ^c | 0.0055 | 0.24 | 0.0029 | 0.15 | | |
| 344.26 ^c | 0.0095 | 0.30 | 0.0003 | 0.01 | | |
| 360.93° | 0.0111 | 0.26 | 0.0032 | 0.09 | | |
| | | 0.22 ^e | | 0.21 ^e | | |
| 223.75 ^d | 0.0005 | 0.53 | 0.0002 | 0.28 | | |
| 228.65 ^d | 0.0005 | 0.43 | 0.0002 | 0.22 | | |
| 233.45 ^d | 0.0007 | 0.49 | 0.0002 | 0.18 | | |
| 239.35 ^d | 0.0010 | 0.55 | 0.0002 | 0.14 | | |
| | | | | | | |

^a $\Delta P = P_{ref}^{sat} - P_{cal}^{sat}$ ^bReference [8] ^cReference [4] ^dReference [5] ^eAverage

0.50^e

| T(K) | $C_{_{MF}}$ | AAD% - P | $AAD\% - y_1$ | |
|--|---|---------------------------------------|---------------|--|
| 230 ^a | 1.25 | 0.56 | 0.74 | |
| 240 ^a | 1.20 | 0.38 | 0.74 | |
| 250 ^a | 1.15 | 0.34 | 0.75 | |
| 260^{a} | 1.10 | 0.31 | 0.73 | |
| 270 ^a | 1.05 | 0.28 | 0.70 | |
| 280^{a} | 1.00 | 0.26 | 0.65 | |
| 290 ^a | 0.95 | 0.23 | 0.60 | |
| 300 ^a | 0.90 | 0.17 | 0.54 | |
| 310 ^a | 0.85 | 0.17 | 0.48 | |
| 320 ^a | 0.80 | 0.14 | 0.42 | |
| 330 ^a | 0.75 | 0.14 | 0.35 | |
| 340^{a} | 0.70 | 0.12 | 0.26 | |
| 350 ^a | 0.65 | 0.07 | 0.11 | |
| | | $C_{MF} = 1.25 - \frac{T - 230}{200}$ | | |
| 227.59 ^b (-50°F) | 1.1000 | 0.32 | 0.39 | |
| 244.26 ^b (-20 ^o F) | 1.0625 | 0.11 | 0.31 | |
| 260.93 ^b (10°F) | 1.0250 | 0.12 | 0.28 | |
| 277.59 ^b (40°F) | 0.9875 | 0.13 | 0.27 | |
| 294.26 ^b (70°F) | 0.9500 | 0.14 | 0.29 | |
| 310.93 ^b (100°F) | 0.9125 | 0.17 | 0.35 | |
| 327.59 ^b (130°F) | 0.8750 | 0.18 | 0.39 | |
| 344.26 ^b (160°F) | 0.8375 | 0.18 | 0.40 | |
| 360.93 ^b (190°F) | 0.8000 | 0.23 | 0.57 | |
| | $C_{MF} = 1.1 - \frac{T(^{0}\mathrm{F}) + 50}{800}$ | | | |

TABLE V: Parameter $\,C_{_{M\!F}}$, Average Deviations in Pressures and Vapor Phase Composition

^aReference [8] ^bReference [4]



Fig. 2. Relative volatilities of propylene and propane mixtures.







Fig. 4. γ_1 / γ_2 at various temperatures.

IV. CONCLUSION

The published VLE data for the binary mixture of propylene+propane are correlated with COSMO-RS model combined with PR-EOS. Good agreements between calculated and reference data are confirmed. It is concluded that the prediction of vapor-liquid equilibrium properties for the propylene+propane mixture with the method in this study is reasonable. While conventional methods based on the state of equations usually require binary interaction parameters or the mixing rules with iteration. Once the method in this study is trained, estimation of the VLE data becomes a straight forward process requiring only one parameter (C_{MF}), which saves computational time considerably. In addition this method does not require the binary interaction parameters. If

developed efficiently, due to the linear relationship between the temperature and the parameter $C_{\rm MF}$, the prediction for other ranges can be extrapolated.

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