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A Method for Predicting the Phase Behaviour of Trinidad Gas Condensates

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Abstract: *Gas condensate compositional simulation studies are conducted to evaluate gas and condensate reserves. This is carried out when making comparisons of production methods for the economic development of a reservoir. The experimental data needed for the evaluation are dew point pressure, gas compressibility factor (z factor)), liquid volume and produced gas (Constant Volume Depletion, CVD data) and are nowadays determined from a tuned Equation of State (EOS). However the open literature has shown that there is no consistency in the number of Single Carbon Number (SCN) groups, EOS tuning parameters, lumping schemes and weight factors applied to the experimental when tuning an EOS for use in compositional simulation studies, particularly for gas condensate fluids. Publications have shown that the two most widely used sets of parameters from the EOS that are tuned are the Binary Interaction Coefficient (BIC) with the critical properties and acentric factor or BIC and the EOS coefficients called the omegas (Ωs). The number of SCN groups used for tuning varies from ten to more than forty. However, there are currently no criteria for selecting the most reliable lumping scheme that will give similar accuracy to using the many SCN groups except by trial and error or by algorithms designed to test a number of schemes and from which the best one is selected. In this paper, the Peng-Robinson EOS has been tuned and tested to predict CVD data for six Trinidad gas condensate samples. Compositional analysis greater than Single Carbon Number 24 (SCN24) is required for the SCN route. The two sets of tuning parameters were used with and without the volume shift parameter (VSP). Our parametric study demonstrated that the VSP should not be applied with the Ωs when tuning the Peng-Robinson EOS. With weight factors of 1 for liquid volume, 10 for gas compressibility factor and without the VSP, the Ωs give better prediction of CVD data than the critical properties and acentric factor even with the VSP included. The SCN groups for one sample were lumped into six Multiple Carbon Number (MCN) groups using the simple Whitson's lumping scheme. Our tuning technique with the Ωs and with our new weight factors for the experimental data, gave differences of less than ±4.0 % from the tuned EOS predictions before and after lumping of the SCN group so that complex algorithms are not necessary to select an appropriate lumping scheme to reduce cost and computer time when performing simulation studies. The tuning technique with only one regression step, showed consistency in tuning the Peng-Robinson EOS with the Ωs and could be used for simulation studies of Trinidad gas condensate systems.*

Keywords: *Gas Condensate, Equation of State, tuning parameters, weight factors, Trinidad*

1. Introduction

Gas condensate field development planning requires compositional simulation studies using a tuned Equation of State (EOS) for the evaluation of gas and condensate reserves, production methods, facilities design as well as economic development (Coats et al., 1986; Pedersen et al., 1989; Danesh, 1998). The physical property data needed for such evaluation are dew point pressure, gas compressibility factor, liquid volume and produced gas (Constant Volume Depletion, CVD data).

Tuning involves adjustment of groups or sets of the most difficult to measure EOS parameters so as to minimise the difference between predicted and measured PVT data (Agarwal and Nghiem, 1990). Al-Sadoon and Almarry (1985) demonstrated the success of tuning by regression with binary interaction coefficient (BIC), between methane and the heavy fractions (greater than hexanes and including the plus fraction) and the critical pressure, P_c, critical temperature, T_c and acentric factor, ω, for the plus fraction. Demonstrations by Coats et al (1986) were with BIC between methane and the heavy fractions and the Ωs (omegas of methane and omegas of the plus fraction) for various reservoir fluids. Unicamp and Rodriguez (1992) tuned the Peng Robinson (1976)

EOS first with the tuning parameters selected by Al-Sadoon and Almarry (1985) and then with the parameters selected by Coats et al. (1986) to predict dew point pressure, produced gas and gas compressibility factor with errors of less than 10 %. The prediction of liquid volume was not included in their demonstration.

Danesh (1998) pointed out that the volume shift parameter (VSP) (Jhaveri and Youngren, 1984) should also be included as a tuning parameter to improve the accuracy in the prediction of liquid volume and to assign a weight factor of 40 to dew point pressure and 10 to liquid volume. However the open literature did not demonstrate if the VSP and suggested weight factors should be used with BIC, P_c, T_c and ω or with BIC and the Ωs.

The data required for the physical property prediction by any EOS are pressure, temperature and composition. The composition of a sample is experimentally determined by gas chromatography and components heavier than pentanes are lumped into Single Carbon Number (SCN) groups (Katz and Firoozabadi, 1978; Pedersen et al., 1989; Hosein, 2004; Hosein and Dawe, 2011). The last group is known as the plus (C_+) or last fraction. Prior to tuning, the number of SCN (Single Carbon Number) groups required to converge the EOS predicted values to the experimentally measured values is determined (Pedersen et al., 1989; Danesh, 1998). Often extended analysis of the plus fraction (Pedersen et al., 1989; Hosein and McCain 2009) from as low as SCN10 (Coats et al., 1986) to as high as SCN45 (Al-Meshari and McCain, 2007) has been reported as needed for this step. Studies have shown that after performing this step, minimal tuning of the EOS parameters is required (Pedersen et al., 1989; Danesh 1998; Hosein 2004).

However, in order to reduce simulation costs and computing time, lumping schemes (Whitson, 1980, Behrens and Sandler 1986; Ahmed 1989; Pedersen et al 1989; Danesh, 1998) to reduce the number of SCN groups into three to five Multiple Carbon Number (MCN) groups (pseudo-components) are used.

The number of MCN groups required and the distribution of SCN groups within each MCN group can be calculated by a simple form (e.g. Whitson (1980)) or more complex lumping forms (e.g. Behrens and Sandler (1986)). Currently, there are no standard criteria for selecting the best lumping scheme to give similar accuracy as can be calculated by the many SCN groups, except by trial and error or by algorithms (Danesh, 1998; Kai, 2001) designed to test a number of schemes. The best one is then selected.

All cubic EOS have a theoretical inherent deficiency in predicting liquid volume away from the critical point and require some degree of tuning especially for gas condensate systems (Pedersen et al., 1989). In the Petroleum Industry, the Soave Redlich Kwong (SRK) (Soave, 1972) and the Peng Robinson (1976) are the two most widely used (Danesh, 1998). Although the selection between the two is a matter of user preference, the Peng Robinson (1976) EOS was developed to improve the prediction of liquid volume (see Appendix for details) in comparison to the SRK and the degree of tuning required should also be less than the SRK (Ahmed, 1986; Danesh 1998).

In this paper a parametric method for tuning the Peng-Robinson (1976) EOS to accurately predict CVD data without the VSP is presented, using a range of components, tuning parameters and weight factors for the experimental data that gave acceptable predictions of CVD data for six Trinidad gas condensate samples. We use the Whitson (1980) lumping scheme to demonstrate that our tuning technique gives minimal differences before and after lumping (Hosein, 2004). Hence complex algorithms are not necessary to select an appropriate lumping scheme.

2. Thermodynamic Model and Fluid System

Trinidad gas (condensate) reservoirs are located offshore the Southeast coast and the North coast. Our tuning technique was demonstrated using six samples which were taken from each of the gas condensate fields and were analysed by Hosein (2004) as follows:

2.1 Sample Composition and Properties of the SCN Groups and the Plus Fractions

The compositions of the samples were obtained by gas chromatography and are shown in Appendix 1, Table A1. These are lean gas condensates with mole % of the $C_{7+} \leq 4$ % (McCain, 1990). The Specific gravity and molecular weight of the SCN groups (see Table A1) were taken from charts published by Katz and Firoozabadi, (1978), as suggested by Hosein and Dawe (2011). Similar properties for the plus fractions were determined experimentally after performing True Boiling Point (TBP) analysis (Hosein, 2004, Hosein and Dawe, 2011). The EOS parameters P_c, T_c and ω for the SCN groups and the plus fractions were determined from correlations published by Kesler and Lee (1976) and Lee and Kesler (1980). The splitting of the C_{20+} fraction was performed using the gamma distribution function (Whitson, 1983) as described by Al Mesharri and McCain (2007) for gas condensate systems.

2.2 PVT Data (see Appendix 2)

Gas condensate PVT studies were conducted using the PVT facilities at The University of the West Indies (UWI) (Hosein, 2004). These data are shown in Table A2. The sample validity and accuracy of the sample compositions and PVT data were evaluated in the same study by Hosein (2004).

2.3 The Peng-Robinson (1976) EOS and Tuning Parameters (see Appendix 1)

The Peng-Robinson (1976) EOS was separately tuned using the sets of tuning parameters studied by Al-Sadoon

and Almarry (1985) and by Coats et al. (1986) and then repeated by including the VSP as suggested by Danesh (1998). The default values for Ω_a and Ω_b were 0.4572 and 0.0778, respectively (WINPROP, 2002). The correlation published by Oellrich et al. (1981) was used for obtaining BIC between methane and the heavy fractions as follows:

$$BIC = 1- [(2\ Vc_i^{1/3}\ Vc_j^{1/3}\ )^{1/2}\ /\ (Vc_i^{1/3} + Vc_j^{1/3})]^n \qquad (1)$$

where Vc_i and Vc_j are the critical volumes of component i and component j. BIC was evaluated by tuning the Hydrocarbon Interaction Coefficient Exponent (HICE), n. An exponent value of 1.2 was used as a starting value (WINPROP, 2011). The upper and lower bounds for the tuning parameter were set to allow a change of ±20 % of the test values so as to ensure that they remain physically reasonable (WINPROP, 2011). For HICE the bounds were set (between 0.0 and 1.8) which are the limits appropriate for typical petroleum fluids (WINPROP 2011).

2.4 Tuning by Regression

Experimental PVT data (Appendix 1, Table A2) were used together with a multi-variable regression scheme (WINPROP 2011) whereby the selected set of EOS parameters was adjusted until a minimum difference between predicted and experimental values was attained (Agarwal and Nghiem, 1990). Each regression was performed in a single step by minimising the objective function F (Dennis et al., 1981), as follows:

$$F = \sum_i^N [\ w_i\ (y_{i,\ pred.} - y_{i,\ expt.})\ /\ y_{i,\ expt.}\ ]^2 \qquad (2)$$

where $y_{i,pred.}$ and $y_{i,expt.}$ correspond to the predicted and experimental CVD values respectively. The weight factors, w_i, assigned to the experimental data for testing are shown in Table 1. The weight factor of 10 for liquid volume was suggested by Danesh (1998). The weight factors of 1 for liquid volume and 10 for gas compressibility factor were determined in this study by trial and error for tuning with the Ωs.

Table 1. Average Absolute Deviation between Pang- Robinson (1976) EOS Pred. and Expt. Liquid Volume and Gas Compressibility Factor with and without the Volume Shift Parameter for published and tested Weight Factors and with analyses greater than SCN24

	Options and Tests	AAD (%) in Liquid Vol.	AAD (%) in Z Factors
Published Weight Factor		10 (Danesh 1998)	0
After Tuning Set A, with VSP	***Option A***	***< 12***	***<3***
After Tuning Set A, without VSP	Test A I	<25	***<3***
After Tuning Set B, with VSP	Test B2	<12	<10
After Tuning Set B, without VSP	Test B3	<10	<15
Tested Weight Factor		1	10
After Tuning Set B, without VSP	***Option B***	***< 10***	***<3***
After Tuning Set B, with VSP	Test B I	<15	***<3***
After Tuning Set A, without VSP	Test A2	<30	<3
After Tuning Set A, with VSP	Test A3	<20	<3

Legends:
ADD = Average Absolute Deviation; DPP = Dew Point Pressure; Z factor= Gas Compressibility Factor; LDO = Liquid Volume
PG = Produced Gas; VSP =Volume Shift Parameter;
Set A = BIC and Pc, Tc and to for the plus fraction
Set B = BIC , Ωa and Ωb for methane and Ωa and Ωb for the plus fraction

3. Simulation of Constant Volume Depletion (CVD) Data

3.1 EOS Predictions

Figure 1 shows the average absolute deviations (see Eq. 3) between Peng-Robinson (1976) EOS predicted and experimental CVD data for all samples, with increasing analysis to C_{7+}, C_{11+}, C_{15+}, C_{20+}, C_{25+}, and C_{30+}. The deviations (as defined below) were in the range 10 to 30 % for dew point pressures (DPP), 50 to 100 % for liquid volume (LDO) and 20 to 40 % for produced gas (PG).

Average Absolute Deviation (AAD in %)

$$= \frac{1}{n} \times \sum_{i=1}^{n} \left| \frac{y_{pred.} - y_{expt.}}{y_{expt.}} \right| \times 100\ (\%) \qquad (3)$$

These results show that the EOS has limitations and cannot produce a set of minimum deviations for any of the plus fraction range studied. It is showed that the gas compressibility (Z) factor was accurately predicted with a deviation of less than 4 %.

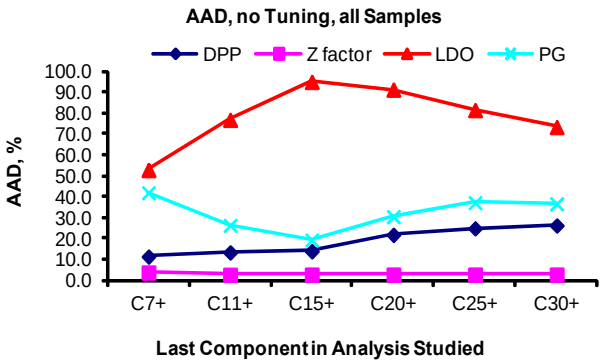

Figure 1. Average Absolute Deviation between Expt. and EOS Pred. CVD Data before Tuning for all Samples

The challenge faced was how to improve the predictions of dew point pressure, liquid volume and produced gas after tuning the Peng-Robinson (1976) EOS with a defined range of components, tuning parameters and weight factors for best possible accuracy.

3.2 Peng-Robinson (1976) EOS Predictions after Tuning BIC and the heavy fractions and Pc, Tc and ω for the plus fraction (Al-Sadoon and Almarry 1985).

3.2.1 Tuning with the VSP and a weight factor of 10 for liquid volume (Option A)

Figure 2 shows the average absolute deviations (see Eq. 3) between Peng-Robinson (1976) EOS predicted and experimental CVD data for all samples, with increasing analyses as described above (see also Table 1). For analyses up to C_{25+}, and up to C_{30+}, predictions of CVD data were obtained, with deviations lower than 5% for dew point pressure (DPP), lower than 12 % for liquid volume (LDO), lower than 10 % for produced gas (PG) and lower than 2 % for gas compressibility (Z) factor.

These results were obtained with the VSP and by applying a weight factor of 10 for liquid volume as suggested by Danesh (1998) and 40 for dew point pressure as suggested by Coats et al. (1986). These results were obtained for the six samples studied which demonstrate consistency in tuning the Peng-Robinson (1976) EOS.

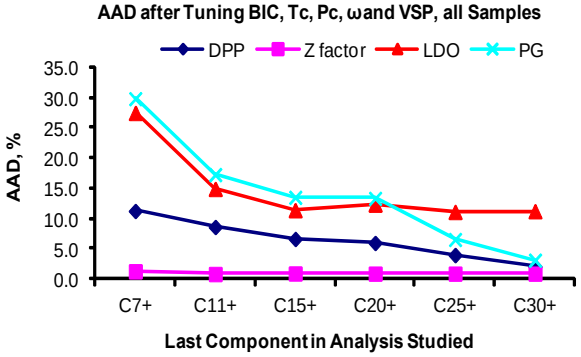

Figure 2. Average Absolute Deviation between Expt. and EOS Pred. CVD Data after Tuning Set A for all Samples

3.2.2 Tuning without the VSP and a weight factor of 10 for liquid volume (Test A1)

Without the VSP the prediction of liquid volume is less accurate than option A with deviations higher than 12 % but lower than 25 % (see Table 1).

3.2.3 Tuning without the VSP and a weight factor of 1 for liquid volume and 10 for Z factor (Test A2)

Without the VSP and with a weight factor of 1 for liquid volume and 10 for gas compressibility factor, the prediction of liquid volume is less accurate than option A with deviations higher than 12 % but lower than 30 % (see Table 1).

3.2.4 Tuning with the VSP and a weight factor of 1 for liquid volume and 10 for Z factor (Test A3)

With the VSP and with a weight factor of 1 for liquid volume and 10 for gas compressibility factor the prediction of liquid volume is less accurate than option A with deviations higher than 12 % but lower than 20 % (see Table 1).

3.3 EOS Predictions after Tuning Parameter BIC for the heavy fractions, Ω_a and Ω_b for methane and Ω_a and Ω_b for the Plus Fraction (Coats et al 1986).

3.3.1 Tuning without the VSP and a weight factor of 1 for liquid volume and 10 for Z factor (Option B)

Figure 3 shows the average absolute deviations between Peng-Robinson (1976) EOS predicted and experimental CVD data for all samples with increasing analyses as described earlier (see also Table 1). For analyses up to C_{25+}, and up to C_{30+}, predictions of CVD data were obtained, with deviations lower than 3 % for dew point pressures (DPP), lower than 10 % for liquid volume (LDO), lower than 5 % for produced gas (PG) and lower than 3 % for gas compressibility (Z) factor.

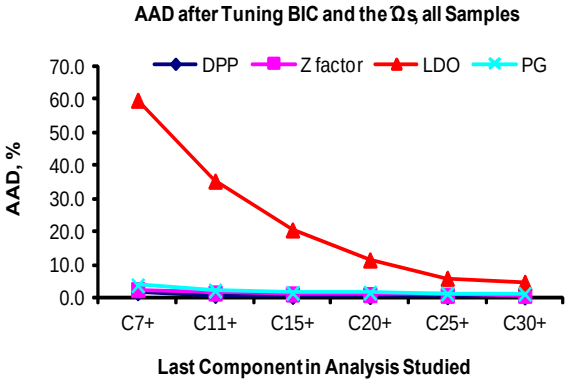

Figure 3. Average Absolute Deviation between Expt. And EOS Pred. CVD Data after Tuning Set B for all Samples

These results were obtained without the VSP and by applying a weight factor of 1 for liquid volume and 10 for gas compressibility factor. These new weight factors were determined by trial and error and are applicable for the Ωs only. The published weight factor of 40 was used for dew point pressure as suggested by Coats et al. (1986).

This new information on tuning the EOS with the Ωs was not found in the open literature. This new information when applied, shows consistency in tuning the EOS with the Ωs and gives more accurate predictions

than option A (BIC, Pc, Tc and ω, with VSP included).

3.3.2 Tuning with the VSP and a weight factor of 1 for liquid volume and 10 for Z factor (Test B1)

With the VSP and with a weight factor of 1 for liquid volume and 10 for gas compressibility factor, the prediction of liquid volume although acceptable was less accurate than option B with deviations higher than 10 % but lower than 15 % (see Table 1).

3.3.3 Tuning with the VSP and a weight factor of 10 for liquid volume (Test B2)

With the VSP and with a weight factor of 10 for liquid volume the prediction of gas compressibility factor was less acceptable than option B with deviations higher than 3 % but lower than 10 % (see Table 1). The prediction of liquid volume, although being acceptable, was less accurate than option B with deviations higher than 10 % but lower than 12 %.

3.3.4 Tuning without the VSP and a weight factor of 10 for liquid volume (Test B3)

Without the VSP and with a weight factor of 10 for liquid volume, the prediction of gas compressibility factor was less acceptable than option B with deviations higher than 3 % but lower than 15 % (see Table 1).

4. Tuning of the Peng-Robinson (1976) EOS before and after Lumping

Our tuning technique with the Tuning Parameters BIC for the heavy fractions, Ω_a and Ω_b for methane and Ω_a and Ω_b for the plus fraction, weight factors of 40 for dew point pressure 1 for liquid volume and 10 for Z factor was applied to all samples. This is to compare predictions before and after lumping as follows:

The compositions of the gas condensate samples PL1 to PL6 (taken from Hosein 2004) were lumped using Whitson (1980) lumping scheme (see Table 2) and were tuned to predict dew point pressure, gas compressibility factor, liquid volume and produced gas.

The Average Absolute Deviations between the tuned EOS (Peng-Robinson, 1976) predicted data before and after lumping were less than 2.0 % for all samples studied as shown in Table 3. These results indicate that the Whitson's (1980) lumping scheme when applied with our tuning technique can give accurate, and similar, predictions to those obtained before lumping.

5. Tuning Procedures

A set of step-by-step tuning procedures is derived from this study. These are:

1. Analyse experimentally the well-stream compositional data range to between C_{25+} and C_{30+} and input into the software (e.g., WINPROP, PVTi, etc.).
2. If the available experimental compositional is lower than this range, then extend the plus fraction using the gamma distribution function (Whitson, 1983). (This option is available in the software).

Table 2. Compositions and Properties for Trinidad Samples PL1 to PL6 after Lumping with Whitson's (1980) Lumping Scheme

MCN Groups	Symbol	PL1 Mole %	Specific Gravity	Molecular Wt., g/mol	MCN Groups	Symbol	PL2 Mole %	Specific Gravity	Molecular Wt., g/mol
SCN7 to SCN9	MCN1	1.841	0.748	107	SCN7 to SCN9	MCN1	1.360	0.747	106
SCN10 to SCN12	MCN2	0.797	0.791	144	SCN10 to SCN12	MCN2	0.568	0.791	144
SCN13 to SCN15	MCN3	0.511	0.825	189	SCN13 to SCN16	MCN3	0.420	0.828	194
SCN16 to SCN20	MCN4	0.530	0.856	251	SCN17 to SCN22	MCN4	0.266	0.862	263
SCN21 to C25+	MCN5	0.245	0.890	346	SCN23 to C25+	MCN5	0.139	0.895	384

MCN Groups	Symbol	PL3 Mole %	Specific Gravity	Molecular Wt., g/mol	MCN Groups	Symbol	PL4 Mole %	Specific Gravity	Molecular Wt., g/mol
SCN7 to SCN9	MCN1	1.513	0.747	106	SCN7 to SCN9	MCN1	1.098	0.748	107
SCN10 to SCN12	MCN2	0.614	0.791	144	SCN10 to SCN12	MCN2	0.504	0.791	144
SCN13 to SCN16	MCN3	0.447	0.828	194	SCN13 to SCN15	MCN3	0.303	0.825	188
SCN17 to SCN21	MCN4	0.223	0.859	258	SCN16 to SCN20	MCN4	0.273	0.865	248
SCN22 to C25+	MCN5	0.122	0.888	356	SCN21 to C25+	MCN5	0.090	0.888	345

MCN Groups	Symbol	PL5 Mole %	Specific Gravity	Molecular Wt., g/mol	MCN Groups	Symbol	PL6 Mole %	Specific Gravity	Molecular Wt., g/mol
SCN7 to SCN9	MCN1	1.136	0.743	107	SCN7 to SCN9	MCN1	0.892	0.741	106
SCN10 to SCN12	MCN2	0.438	0.786	144	SCN10 to SCN12	MCN2	0.341	0.786	144
SCN13 to SCN15	MCN3	0.249	0.820	188	SCN13 to SCN15	MCN3	0.194	0.820	188
SCN16 to SCN20	MCN4	0.193	0.850	245	SCN16 to SCN20	MCN4	0.136	0.850	244
SCN21 to C25+	MCN5	0.106	0.879	330	SCN21 to C25+	MCN5	0.053	0.883	326

Table 3. AAD in % between DPP, Z Factor, LDO and PG before and after Lumping, for Trinidad Samples PL1 to PL6

Sample	AAD in % DPP	AAD in % Z Factor	AAD in % LDO	AAD in % PG
PL1	0.04	0.12	0.53	0.27
PL2	0.04	0.02	0.19	0.03
PL3	0.03	0.02	1.72	0.03
PL4	0.04	0.04	1.27	0.04
PL5	0.00	0.05	0.19	0.01
PL6	0.03	0.00	1.67	0.02

3. Analyse experimentally the wellstream compositional data range to between C_{25+} and C_{30+} and input into the software (e.g., WINPROP, PVTi, etc.).
4. If the available experimental compositional is lower than this range, then extend the plus fraction using the gamma distribution function (Whitson, 1983). (This option is available in the software).
5. If experimental specific gravity and molecular weight of the SCN groups (obtained by True Boiling Point analysis) are not available then select this data from charts published by Katz and Firoozabadi (1978). (This option is available in the software).
6. Lump from C_7 to the last fraction into MCN groups by selecting the Whitson (1980) lumping scheme.
7. Determine the EOS parameters P_c, T_c and ω for the MCN groups and the plus fractions by selecting the correlations published by Kesler and Lee (1976) and Lee and Kesler (1980).
8. Select the default values for Ω_a (0.4572) and Ω_b (0.0778) (taken from WINPROP, 2011).
9. Select the correlation published by Oellrich et al (1981) for obtaining BIC between methane and the heavy fractions. Select an exponent value of 1.2 as a starting value for tuning the Hydrocarbon Interaction Coefficient Exponent (HICE), n (WINPROP, 2011).
10. Select the tuning parameters BIC between methane and the heavy fractions, Ω_a and Ω_b for methane and Ω_a and Ω_b for the plus fraction.
11. Set weight factors of 40 for dew point pressure 1 for liquid volume and 10 for Z factor.
12. Set the upper and lower bounds for the tuning parameters to allow a change of ±20 % of the test values so as to ensure that they remain physically reasonable (WINPROP, 2011). For HICE, set the bounds (between 0.0 and 1.8) which are the limits appropriate for typical petroleum fluids (WINPROP, 2011).

5. Conclusions

From the study, the following conclusions are made:

1. Compositions beyond SCN24 give best prediction of CVD data by the tuned EOS studied.
2. The volume shift parameter should be included with the parameters BIC, Pc, Tc and ω when tuning the Peng-Robinson (1976) EOS. A weight factor of 10 as suggested by (Danesh, 1998) should be applied to liquid volume.
3. The volume shift parameter (VSP) should not be included with the parameters BIC and the Ωs when tuning the Peng-Robinson (1976) EOS. A weight factor of 1 should be applied to liquid volume and 10 to gas compressibility factor.
4. Peng-Robinson (1976) EOS predictions of CVD data with the tuning parameters BIC and the Ωs were more accurate than with the tuning parameters BIC, Pc, Tc, ω and VSP.
5. The accuracy obtained with Whitson's (1980) lumping scheme shows that it can be applied in compositional simulation studies and complex forms of lumping and algorithms to select the best lumping schemes that are not required.
6. This study demonstrated the consistency in tuning the Peng-Robinson (1976) EOS with one regression step which avoids wastage of time spent in trial and error when tuning.

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Appendix 1: Peng-Robinson (1976) EOS

The Peng-Robinson (1976) EOS, which when expressed in terms of molar volume has the form:

$$P = (RT/(V-b)) - a\alpha / [V(V+b)+b(V-b)] \quad (A1)$$

where P and T are the pressure and temperature of the system, R is the molar gas constant, a and b are constants characterising the molecular properties of the individual components in a mixture. Parameter b corrects for the volume of the molecules which is considered negligible for an ideal gas. Parameter a, corrects for attractive forces between molecules and the walls of the containing vessel (Peng-Robinson, 1976; Ahmed, 1989) and parameter α (Soave, 1972) was included to make parameter a temperature dependent.

By imposing the classical Van der Waals' (1967) critical point constraints on Equation A1, (Peng-Robinson, 1976) expressions for a and b can be obtained as follows:

$$a = \Omega_a R^2 T_c^2 / P_c \quad \text{and} \quad b = \Omega_b RT_c / P_c \quad (A2)$$

where P_c and T_c are the critical pressure and temperature of the component. Expressing equation1 (Peng-Robinson, 1976) in terms of the gas compressibility factor z_c (Soave, 1972; Martin, 1979), the coefficients Ω_a and Ω_b take the values of 0.45724 and 0.07780 at the critical point.

Peng-Robinson (1976) adopted Soave's (1972) approach for calculating the parameter α, where the acentric factor ω was introduced to characterise the non-sphericity of component molecules for improved predictions by:

$$\alpha = (1+(0.480+1.574\omega-0.176\omega^2)(1-T_r^{0.5}))^2 \quad (A3)$$

where $(T_r = T/T_c)$

Peng-Robinson (1976) extended their equation to mixtures

and included a binary interaction coefficient (BIC) $k_{ij,}$ (Soave, 1972) into the attractive pressure term, to model intermolecular interaction in a mixture by empirical adjustment, as follows:

$$(a\alpha)_m = \sum_i \sum_j [x_i x_j (a_i a_j \alpha_i \alpha_j)^{0.5} (k_{ij} - 1)] \quad \text{(A4)}$$

$$b_m = \sum_i [x_i b_i] \quad \text{(A5)}$$

where x_i and x_j represent the mole fractions of components i and j in a liquid mixture. These are replaced by y_i and y_j a for a gas mixture. BICs are dependent on differences in molecular sizes in a mixture and are determined from correlations or by minimising the difference between predicted and experimental saturation pressure for binary systems (Danesh, 1998).

Theoretically, EOS has an inherent deficiency in predicting liquid density away from the critical point. A correction parameter c (Jhaveri and Youngren, 1984) can be applied to the Peng-Robinson (1976) EOS to correct for liquid and vapor volumes as follows:

$$V_{L\,corr.} = V_L - \sum_i (x_i\ c_i) \quad \text{(A6)}$$

$$V_{V\,corr} = V_V - \sum_i (y_i\ c_i) \quad \text{(A7)}$$

where x_i and y_i are the mole fractions of component i in the liquid and gas phase, V_L and V_V are the volumes of the liquid and gas phase as calculated by the Peng-Robinson (1976) EOS, $V_{L\ corr.}$ and $V_{V\ corr.}$ are the corrected volumes of the liquid and gas phase and c_i is the volume correction parameter defined by:

$$c_i = VSP_i\ b_i \quad \text{(A8)}$$

where $VSP_i = 1 - d / (M)_i^e$

In Equation A8, b_i is the Peng-Robinson (1976) molecular parameter for component i, defined in Equation A2. VSP_i is a dimensionless parameter of component i, called the volume shift parameter. Values of VSP for the components methane to pentane have been documented by Ahmed (1989). For the Single Carbon Number (SCN) groups (greater than pentanes) and the plus fraction, VSP_i is determined from the molecular weight M_i of each component (Table A1) and the positive correlation coefficients d and e (Jhaveri and Youngren, 1984). Where no experimental data is available for calculating d and e, Jhaveri and Youngren (1984) recommended adjusting coefficient d to match the C_{7+} density and to use a value of 0.2051 for the power coefficient e.

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Table A1: Compositions and Properties for Trinidad Samples PL1 to PL6

Component	**Symbol**	**PL1 Mole %**	**PL2 Mole %**	**PL3 Mole %**	**PL4 Mole %**	**PL5 Mole %**	**PL6 Mole %**	**Specific Gravity**	**Molecular Wt., g/mol**
Carbon dioxide	CO2	0.241	0.874	0.350	0.323	0.284	0.585	0.817	44
Nitrogen	N2	0.115	0.058	0.077	0.088	0.077	0.088	0.809	28
Methane	C1	88.040	89.220	91.890	91.650	92.99	91.640	0.300	16
Ethane	C2	4.609	3.553	1.826	3.333	1.83	3.521	0.356	30
Propane	C3	1.536	1.678	1.212	1.222	1.169	1.313	0.507	44
iso-Butane	i-C4	0.385	0.471	0.383	0.316	0.346	0.298	0.563	58
n-Butane	n-C4	0.428	0.559	0.500	0.335	0.447	0.392	0.584	58
iso-Pentane	i-C5	0.224	0.236	0.241	0.152	0.206	0.160	0.624	72
n-Pentane	n-C5	0.186	0.225	0.216	0.125	0.203	0.162	0.631	72
Hexanes	C6	0.312	0.373	0.386	0.188	0.326	0.225	0.685	84
Heptanes	C7	0.561	0.458	0.508	0.346	0.368	0.307	0.722	96
Octanes	C8	0.789	0.583	0.652	0.444	0.471	0.380	0.745	107
Nonanes	C9	0.491	0.319	0.353	0.308	0.297	0.205	0.764	121
Decanes	C10	0.354	0.245	0.286	0.231	0.208	0.157	0.778	134
Undecanes	C11	0.267	0.196	0.194	0.165	0.141	0.113	0.789	147
Dodecanes	C12	0.176	0.127	0.134	0.108	0.089	0.071	0.800	161
Tridecanes	C13	0.197	0.148	0.146	0.122	0.101	0.079	0.811	175
Tetradecanes	C14	0.170	0.105	0.121	0.095	0.079	0.062	0.822	190
Pentadecanes	C15	0.144	0.093	0.103	0.084	0.069	0.053	0.832	206
Hexadecanes	C16	0.119	0.074	0.077	0.068	0.052	0.039	0.839	222
Heptadecanes	C17	0.104	0.066	0.065	0.059	0.045	0.032	0.847	237
Octadecanes	C18	0.099	0.054	0.052	0.049	0.037	0.028	0.852	251
Nonadecanes	C19	0.080	0.045	0.041	0.040	0.031	0.021	0.857	263
Sample		**PL1**	**PL2**	**PL3**	**PL4**	**PL5**	**PL6**		
Mole %	C_{7+}	3.924	2.753	2.919	2.268	2.122	1.616		
Specific Gravity	γ_{7+}	0.8031	0.8004	0.7939	0.7967	0.7918	0.7869		
Molecular Wt.	M_{7+}	160	157	150	153	148	143		
Mole %	C_{11+}	1.729	1.148	1.12	0.939	0.778	0.567		
Specific Gravity	γ_{11+}	0.8409	0.8407	0.8356	0.8349	0.8343	0.8296		
Molecular Wt.	M_{11+}	221	222	213	211	211	203		
Mole %	C_{15+}	0.919	0.572	0.525	0.449	0.368	0.241		
Specific Gravity	γ_{15+}	0.8619	0.8642	0.8590	0.8576	0.8568	0.8532		
Molecular Wt.	M_{15+}	270	278	266	261	263	254		
Mole %	C_{20+}	0.373	0.240	0.187	0.149	0.134	0.069		
Specific Gravity	γ_{20+}	0.8809	0.8839	0.8794	0.8783	0.8739	0.8718		
Molecular Wt.	M_{20+}	326	345	332	321	320	315		

Sources: Data taken from Hosein (2004), Katz and Firoozabadi (1978)

Table A2: Constant Volume Depletion Data (CVD) for Trinidad Gas Condensate Samples PL1 to PL6 measured at Reservoir Temperature

Pressure psia	Prod. Gas (Cum.), %	Liquid Vol. (Cum.), %	Gas Comp. Factor, Z
Sample PL1 (reservoir temperature = 186 °F)			
6544.7	0.00	0.00	0.000
5814.7	6.14	2.34	1.062
5114.7	13.02	4.92	1.003
4414.7	21.09	6.53	0.953
3614.7	32.01	7.54	0.911
2814.7	44.89	8.02	0.886
2014.7	59.46	8.15	0.885
1314.7	72.95	8.04	0.905
714.7	84.44	7.81	0.938
Sample PL3 (reservoir temperature = 184 °F)			
5159.7	0.00	0.00	0.000
4414.7	9.71	1.30	0.957
3614.7	22.50	2.50	0.918
2814.7	37.90	3.50	0.902
2014.7	55.25	4.00	0.908
1314.7	70.98	4.00	0.928
714.7	84.16	3.80	0.956
Sample PL5 (reservoir temperature = 180 °F)			
4844.7	0.00	0.00	0.000
4114.7	10.80	1.00	0.952
3414.7	23.06	1.80	0.923
2714.7	37.42	2.50	0.910
2014.7	53.47	3.00	0.912
1314.7	69.81	3.20	0.929
714.7	83.58	3.20	0.956

Pressure psia	Prod. Gas (Cum.), %	Liquid Vol. (Cum.), %	Gas Comp. Factor, Z
Sample PL2 (reservoir temperature = 221 °F)			
7824.7	0.00	0.00	0.000
6714.7	6.93	0.70	1.164
5614.7	15.70	1.70	1.073
4414.7	28.17	3.60	0.983
3214.7	44.49	4.90	0.928
2214.7	60.77	5.30	0.925
1314.7	76.45	5.30	0.945
714.7	86.93	5.20	0.968
Sample PL4 (reservoir temperature = 197 °F)			
6404.7	0.00	0.00	0.000
5799.7	6.56	0.33	1.079
5099.7	13.90	0.92	1.018
4399.7	21.40	1.66	0.974
3599.7	32.74	2.56	0.932
2799.7	45.92	3.30	0.909
1999.7	60.67	3.73	0.904
1200.7	74.70	3.86	0.919
699.7	86.08	3.84	0.949
Sample PL6 (reservoir temperature = 202 °F)			
5922.7	0.00	0.00	0.000
5014.7	9.76	0.50	1.002
4014.7	22.90	0.90	0.944
3014.7	39.78	1.30	0.911
2114.7	57.38	1.60	0.906
1314.7	73.73	1.80	0.926
714.7	85.28	1.90	0.954

Source: Data taken from Hosein (2004)

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