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CONSTRUCTION AND TUNING OF A FLUID MODEL USING PVTi SOFTWARE: A COMPARATIVE STUDY OF EOS REGRESSION TECHNIQUES

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ABSTRACT

PVTi software is widely used in the petroleum industries. It helps to estimate the fluid property of the reservoir, simulation experiments, regression and create a fluid system. In order to estimate the fluid behaviour, regression was conducted to the equation of state (EOS) to obtain a close-fit to the experimental data of the fluid. The EOSs that were investigated are Soave-Redlich-Kwong and Peng-Robinson for two and three parameters. The parameters to be regressed were selected by using Successive Lumping Algorithm method. The result obtained by PVTi software were compared by using root mean square (RMS) method while the result obtained between the EOSs were compared using percentage deviation (%Dev). It was proven that the regression values manage to obtain a close fit compare to the first predicted value that the EOS calculated. From the oil sample given, Soave-Redlich-Kwong 3 (SRK3) was able to be regress to have a close-fit to the experimental data.

Keywords: PVTi software, regression, EOS, SRK, PR

1.0 INTRODUCTION

PVT properties are the general term used to express the volumetric behaviour of a reservoir fluid as a function of pressure and temperature. PVT experiments was conducted in order to have extensive knowledge of the volumetric and phase changes the reservoir fluid is likely to experience during the transportation from petroleum reservoir to oil refinery. From the knowledge, the production can be optimized for oil or a gas field.

Therefore, the aim of this study is to construct and tune a fluid model using PVTi software and assess performance of different EOS regression techniques.

To achieve this aim, the study focuses on the following objectives:

1. To develop a fluid model using available PVT data.
2. To apply EOS regression techniques to tune the model.
3. To compare the models to identify the most accurate method for predicting fluid behaviour.

1.1 TURNING OF EOS

The compositional analysis of the reservoir fluids is not always very reliable because it composed of thousands of compounds which are described by a limited number of pure substances and the carbon groups are not fully defined. To estimate the critical properties of the carbon groups required for EOS calculations, the correlations of the compositional analysis were generalized. The generalized correlations often have a diverged result among themselves. Thus making the prediction of EOS inaccurate for real reservoir fluids.

In order to improve the prediction, industries calibrate or tune an EOS model against experimental data generated at appropriate conditions for specific field studies. The tuning was done by adjusting the values of input data to the phase behaviour model to minimize the difference between the predicted and measured values.

According to Abolfazli and Jamshidi (2021), the deviation between the predicted and experimental data is not due to the EOS accuracy but it is mostly due to the input data. Therefore, instead of modifying EOS parameters indiscriminately to match the experimental data, the tuning process (non-linear regression) should be conducted first to evaluate and improve the input data. The tuning parameter is not a straightforward process, therefore appropriate parameters need to be selected (Bennett and Yang, 2022).

According to Chen and Liu (2023), regression analysis is a statistical tool for the investigation of relationships between variables. Regression is a non-linear programming calculation that places global upper and lower limits on each regression variable. Regression is used to match the experimental PVT data with the EOS. This is because the predictive capability of EOS may be

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poor due to each reservoir's fluids having their own properties. According to Ghareb and Khalaf (2024), with regression, the EOS will be able to predict the observed reservoir fluid PVT behaviour.

1.2 *Root-Mean-Square (RMS) Error*

According to Rahman and Pederson (2020), in the regression line application, the RMS error is used to predict the average value of y (dependent) associated with a given x (independent) value. To determine the RMS error, the residuals need to be calculated first. Residuals are the difference between the experimental values and the calculated values. The RMS value can be either positive or negative depending on the predicted value of it is under or overestimates the actual value. The RMS error is then used as a measure of the spread of the y value on the calculated y value. Equation (I) shows the RMS error equation.

$$RMS_{error} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}} \quad \ldots\ldots (1)$$

In the PVTi software normalize RMS error (NRMSE) is used where the RMSE is normalized to the range of the observed data shown by equation (2) (Rahman and Pederson, 2020). The NRMSE value is always between 0 and 1. The summarized equation used for NRMSE in the PVTi software is shown in equation (3) (Schumberger, 2021). According to Rahman and Pederson (2020), lower value of RMS indicates better fit.

$$NRMSE = \frac{RMSE}{y_i} \quad \ldots\ldots (2)$$

$$RMS = \sqrt{\frac{\sum_{1}^{n_{obs}} \left(\frac{obs-calc}{obs}\right)^2}{n_{obs}}} \quad \ldots\ldots (3)$$

1.3 *Cubic Equation of State*

Cubic EOS is widely used on PVT calculations for oil and gas mixtures. The most famous EOS developed 100 years ago, was van der waals equation (1873). Later Redlich and Kwong (RK) (1949) developed EOS that can be used extensively. In 1972, Soave improved (RK) the equation to obtain a new EOS. After a few years, Peng-Robinson (1976 and 1978) developed a new EOS. Next, Abolfazli and Jamshidi, (2021) improve the liquid density production by presenting a volume-shift concept to the present EOS (three parameter) (Abolfazli, S., & Jamshidi, 2021). In this report, Saove-Redlich-Kwong (SRK) and Peng Robinson (PR) were investigated.

1.4 *Soave-Redlick-Kwong (SRK) Equation*

The original equation (4) of SRK was developed by Redlick-Kwong (RK) (1949). The term ($a / T^{0.5}$) in RK equation was replaced with a more general temperature-dependent term denoted by $a_c\alpha$ (T) by Soave (1972) as shown by equation (5). Soave introduced this general term because he discovered that there is a linear dependency of square root of the a-parameter ratio vs the square root of the reduced temperature ($T_r = T/T_c$).

$$P = \frac{RT}{V-b} - \frac{a}{\sqrt{T}\,V(V+b)} \quad \ldots\ldots (4)$$

$$P = \frac{RT}{V-b} - \frac{a\,\alpha\,(T)}{V(V+b)} \quad \ldots\ldots (5)$$

$$a = \frac{0.42747R^2T_c^2}{P_c} \quad \ldots\ldots (6)$$

$$b = \frac{0.08664RT_c}{P_c} \quad \ldots\ldots (7)$$

$$\alpha\,(T) = 1 + m\,(1 - T_r^{0.5})^2 \quad \ldots\ldots (8)$$

$$m = 0.480 + 1.574\,\omega - 0.176\,\omega^2 \quad \ldots\ldots (9)$$

1.5 *Peng-Robinson (PR)*

According to Abolfazli, S., & Jamshidi (2021), by using the SRK equation, the predicted liquid densities are in general too low, Peng and Robinson (1976), noticed this weakness of SRK equation, where the

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predicted critical compressibility factor for the pure-component are generally lower than the experimental data. Therefore, Peng and Robinson suggested the equation below:

$$P = \frac{RT}{V-b} - \frac{a\,\alpha}{V^2 + 2bV - b^2} \quad \text{(10)}$$

$$a = 0.45724\,\frac{R^2 T_c^2}{P_c} \quad \text{(11)}$$

$$b = 0.07780\,\frac{RT_c}{P_c} \quad \text{(12)}$$

$$\alpha = [1 + k\,(1 - T_r^{0.5})]^2 \quad \text{(13)}$$

$$k = 0.37464 + 1.5422\omega - 0.26992\omega^2 \quad \text{(14)}$$

1.6 *Parameter*

In the EOS equation, it is divided into two-parameter and three-parameter. Cubic EOS was originally a two-parameter. Later, the three parameter EOS was introduced by Jhaveri and Youngren. (1988) to improve the volumetric predictions into a two-parameter cubic EOS. According to Jhaveri and Youngren (1988), the third parameter alters certain translations along the volume axis when the phase volume axis was modified. Thus the third parameter does not change the vapour liquid equilibrium and will not affect the result obtained from the two-parameter EOS.

For the two-parameter EOS, it has two mixture parameters a and b which are related to the component's critical temperature, T_c, critical pressure, P_c, acentric facto,Ш, and z_i is the mole fraction of component i. The two parameter EOS can be written as below:

$$E^2(T,P,V,z_i\ a, b) = 0 \quad \text{(15)}$$

For the three-parameter EOS, the third parameter c. was introduced into the two-parameter where:

$$\tilde{V} = V - c \quad \text{(16)}$$

Giving the three –parameter EOS

$$E^3(T, p\ \tilde{v}, z_i\ a, b, c) = 0 \quad \text{(17)}$$

2.0 METHODOLOGY

2.1 *Input the data in PVTi simulation software*

First, the oil sample compositions (Table 2.1-1) were defined by inputting the mole fraction given. Then the SRK3 EOS was selected for the first simulation followed by PR3 SRK2 and PR2 for the next simulation. After that the experiments were defined for the simulation by setting the experimental properties (constant composition expansion (CCE) and differential liberation (DL) as shown in Table 2.1-2 and Table 2.1-3 Next, all the experiments were simulated and the observation for the experiments were plotted. Since the EOS plotted was not close-fit to the observation data a regression needs to be done to improve the EOS model of a regression. In order to determine the quality of the turned fluid model, the selection of regression parameters is important. The method of selecting the regression parameters was explained in Section 2.2.

Table 2.1-1 Fluid Composition (%) and

Table 2.1-2 CCE at 234 T

P(paig)	V/Vs	P(psig)	V/Vs
	5000	0.9581	2692
			1.0090
	4500	0.9655	2605
			1.0218
	4000	0.9738	2500
			1.0410
	3500	0.9829	2362
			1.0697
	3200	0.9892	2203
			1.1082

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Properties at reservoir conditions	
CO_2	1.03
N_2	0.55
C_1	0.55
C_2	36.47
C_3	9.33
C_4	8.85
C_5	6.00
C_6	3.78
C_{7+}	3043
M+	200
	0.8366

Table 2.1-3 DL at 234 °F

P(psig)	Relative oil volume	Solution GOR (scf/bbl)	Oil Density (lb/ ft^3)	Gas gravity
2746	1.866	1230	38.019	-
2598	1.821	1151	38.468	0.848
2400	1.771	1059	38.955	0.849
2200	1.725	972	39.417	0.941
1897	1.658	849	40.160	0.836
1600	1.599	737	40.847	0.837
1300	1.543	631	41.546	0.846
1000	10488	529	42.245	0.872
700	1.433	428	43.000	0.920
394	1.371	321	43.874	1.038
195	1.313	231	44.605	1.248
112	1.274	178	45.142	1.458
0	1.086	0	47.988	2.245

2.2 *Selection of Regression Parameter*

Table 2.2-1 Selected EOS parameters for regression Component based regression variables

Mnen	Omega_A	Omega_B	P_{crit}	T_{crit}	$V_{crit}V$	$Z_{crit}V$	$A_{cen}F_{ac}$	S_{shft}
CO_2	1							
N_2								
C_1								
C_2	1							
C_3	2		1	1				
C_4	2		1	1				
C_5	2			2				
C_6				2				
C_{7+}	3		2					

Table 2.2-1 shows the parameter chosen after trial and error method were conducted to obtain the smallest value of RMS for SRK3. Then, the parameters were kept constant for each different EOS simulation to determine which EOS most closely matches the available experimental data.

In successive Lumping theories, it is impossible if C_3 is left as a single component when C_2 and C_4 was lump together as the parameter. The method chosen for the selection of parameter for regression follows the Successive Lumping Algorithm method. This method was said to be

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definitely faster because fewer objective function values are calculated compared to Full Search Algorithm and Fast Stepwise Search Algorithm (Chen and Liu, 2023). The downside of this method is that it may miss the best choice of parameters. The same number shown in the regression variables indicate that they were lumped together to make one variable.

The trial and error method were conducted by first grouping C_1 to C_6 and make C_{7+} to be the second variable. Then based on the regression result obtained, different compound grouping was created. The parameter that have the largest value in the covariance table was removed as it was the least determined by the regression and the two parameters which has value which was closed to 1 or – 1 were either removed or grouped together.

In this simulation, only Ω_a, P_{crit}, and T_{crit} were tuned for the regression. Even though according to Chen and Liu (2023), the parameters which may be tuned are Ω_a, Ω_b, T_{crit}, P_{crit}, acentric factor, A_c and volume correction parameter V_{crit} the only parameters that manage to show a close match are the parameters shown in Figure 3.2-1.

3.0 RESULT AND DISCUSSION

To see a much clearer results, percentage deviation (18) was used to compare the experimental value and the calculated value. The closer the value to 0, the closer the value matches the available experimental data. In order to make the comparison much simpler, only reading from 2746 psig were taken for all the properties for each EOS.

$$\%Dev = \frac{CalculatedResult - ExperimentalResult}{EzperimentalResult} \times 100\% \quad (18)$$

3.1. *Soave-Redlick – Kwong 3 (SRK3)*

Table 3.1-1 shows the experimental and calculated fluid sample properties for SRK3 EOS. From the % Dev calculated, it can be seen that the predicted value for the EOS is beggar than the regressed EOS value. This shows that the regressed parameter chosen was able to produce a close match compared to the original EOS value. The RMS value obtained after the regression was 0.01413.

Table 3.1-1 Experimental and calculated fluid sample properties for SRK3 EOS

Property	Experimental	Predicted	%Dev.	Regressed	%Dev.
Relative Volume	0.9581	0.9376	-2.14	0.9499	-0.86
Oil density (1b/ ft^3)	38.019	38.664	1.70	38.102	0.22
GOR (Mscf / stb)	1.230	1.168	-5.04	1.2396	0.78
Oil relative volume	1.866	1.772	-5.04	1.8745	0.46
Gas gravity	0.848	0.790	-684	0.8478	-0.02
Sat pressure (psig)	2746	2508	-867	2755.501	0.35
Oil density (lb/ ft^3)	38.019	38.3596	0.90	38.1022	0.22

3.2 *Peng-Robinson 3(PR3)*

Table 3.2-1 shows the experimental and calculated fluid sample properties for PR3 EPS. From the %Dev calculated, it can be seen that the predicted value for the EOS is bigger than the regressed EOS value. This shows that the regressed parameter chosen was able to produce a close match compared to the original EOS value. The RMS value obtained after the regression was 0.013235.

Table 3.2-1 Experimental and Calculated fluid sample properties for PR3 EOS

Property	Experimental	Predicted	%Dev.	Regressed	%Dev
Relative Volume	0.9581	0.9576	-0.64	0.9534	-0.49
Oil density (1b/ ft^3)	38.019	38.867	2.23	37.929	-0.24
GOR (Mscf/ stb)	1.230	1.1597	-5.72	1.2389	0.72
Oil relative volume	1.866	1.7545	-5.98	1.8826	0.89
Gas gravity	0.848	0.798	-5.90	0.8452	-0.33
Sat pressure (psig)	2746	2705.281	-1.48	2750.326	0.16
Oil density (lb/ ft^3)	38.019	38.8234	2.12	37.9296	-0.24

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3.3 *Soave-Redlick-Kwong 2 (SRK2)*

Table 3.3-1 shows the experimental and calculated fluid sample properties for SRK2 EOS. From the % Dev calculated it can be seen that the predicted value for the EOS is bigger than the regressed EOS value. This shows that the regressed parameter chosen was able to produce a close match compared to the original EOS value. The RMS value obtained after the regression was 0.014331.

Table 3.3-1 Experimental and calculated fluid sample properties for SRK2 EOS

Property	Experimental	Predicted	%Dev.	Regressed	%Dev.
Relative Volume	0.9581	0.9468	-1.18	0.9473	-1.13
Oil density (1b /ft^3)	38.019	32.944	-13.35	38.608	-1.08
GOR (Mscf /stb)	1.230	0.9199	-25.21	1.2304	0.06
Oil relative volume	1.866	1.6377	-12.23	1.8819	0.85
Gas gravity	0.848	0.7901	-6.83	0.8438	-0.50
Sat pressure (psig)	2746	2507.997	-8.67	2719.712	-0.96
Oil density (lb /ft^3)	38.019	32.7229	-13.93	37.5777	-1.16

3.4 *Peng Robinson 2 (PR2)*

Table 3.4-1 shows the experimental and calculated fluid sample properties fro PR2 EOS. From the % Dev calculated it can be seen that the predicted value for the EOS is bigger than the regressed EOS value. This shows that the regressed parameter chosen was able to produce a close match compared to the original EOS value. The RMS value obtained after the regression was 0.017035.

Table 3.4-1 Experimental and calculated fluid sample properties for PR2 EOS

Property	Experimental	Predicted	%Dev.	Regressed	%Dev.
Relative Volume	0.9581	0.9545	-0.38	0.9504	-0.80
Oil density (1b / ft^3)	38.019	36.818	-3.16	38.162	0.38
GOR (Mscf / stb)	1.230	1.026	-16.59	1.2253	-0.38
Oil relative volume	1.866	1.6385	-12.19	1.8469	-1.02
Gas gravity	0.848	08004	-5.61	0.8709	2.70
Sat. pressure (psig)	2746	2705.281	-1.48	2697.467	-1.77
Oil density (lb / ft^3)	38.019	36.779	-3.26	38,1085	0.24

3.5 *Predicted and Regression Value*

To compare which EOS able to predict the behaviour close to the experimental data, the average value of all the %Dev property were calculated using equation (19). Table 4.5-1 shows the average value of calculated %Dev. From table 4.5-1, the higher error was shown by SRK2 followed by PR2, SRK3 and PR3. This shows that three parameter was able to predict the fluid behaviour better than the two-parameter as said by Jhaveri and Youngren (1988). The table also shows that the lowest value of % Dev or the closest match to the experimental data was predicted by SRK3 with 0.42% after regression.

Average %Dev = $\frac{\sum_{i=1}^{n}[\%Dev.]}{n}$ ..... (19)

Table 3.5-1 Average Value of % Dev for each EOS

EOS	Predicted	Regressed
SRK3	**4.33**	**0.42**
PR 3	**3.44**	**0.44**
SRK2	**11.6**	**082**
PR2	**6.10**	**1.04**

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3.6 *Comparing the EOS regression result*.

Table 3.6-1 shows the summary of all % Dev calculated for all the EOS. The highlighted box shows the value that is close to zero or in other word, that showing a close match towards the experimental data. The yellow box shows a better % Dev between the three-parameter EOS while the blue box is for two-parameter EOS. From table 4.5-1, between the three parameter EOS, PR3 shows a much closer match for the relative volume. GOR and saturation pressure while SRK3 shows a closer match for the oil density, oil relative volume gas gravity and oil density. This shows that for the three-parameter, SRK3 managed to predict most of the fluid behaviour in the reservoir. For the two-parameter, PR2 managed to display a closer match for the relative volume and oil density while for SRK2 a closer match was obtained in the GOR, oil relative volume gas gravity and the saturation pressure. This shows that for the two-parameter SRK2 manage to predict most of the fluid behaviour in the reservoir.

Table 3.6-1 Comparison of regression %Dev between all the conducted EOS

Property	SRK3	PR3	SRK2	PR2
Relative Volume	-0.86	-0.49	-1.13	-0.80
Oil density (1b /ft^3)	0.22	-0.24	-1.08	0.38
GOR (Mscf /stb)	0.78	0.72	0.06	-0.38
Oil relative volume	0.46	0.89	0.85	-1.02
Gas gravity	-0.02	-.033	-0.50	2.70
Sat pressure (psig)	0.35	0.16	-0.96	-1.77
Oil density (lb/ ft^3)	0.22	-0.24	-1.16	0.24

From table 3.6-2 it can be seen that SRK3 shows a much better result compare to SRK 2. This concludes that SRK3 EOS with variable parameter chosen was able to obtain a close match with the experimental result. Figure 3.6-1, 3.6-2, 3.6-3 and 3.6-4 show the graph produce from the PVTi after regression. Red dot represents the experimental value, blue line represents the predicted value from EOS and the green line represents the regression value.

Table 3.6-2 Comparison of %Dev between SRK3 and SRK2

Property	SRK3	SRK2
Relative Volume	-0.86	-1.13
Oil density (1b/ ft^3)	0.22	1.08
GOR (Mscf/ stb)	0.78	0.06
Oil relative volume	0.46	0.85
Gas gravity	-0.02	-0.50
Sat pressure (psig)	0.35	-0.96
Oil density (lb /ft^3)	0.22	-1.16

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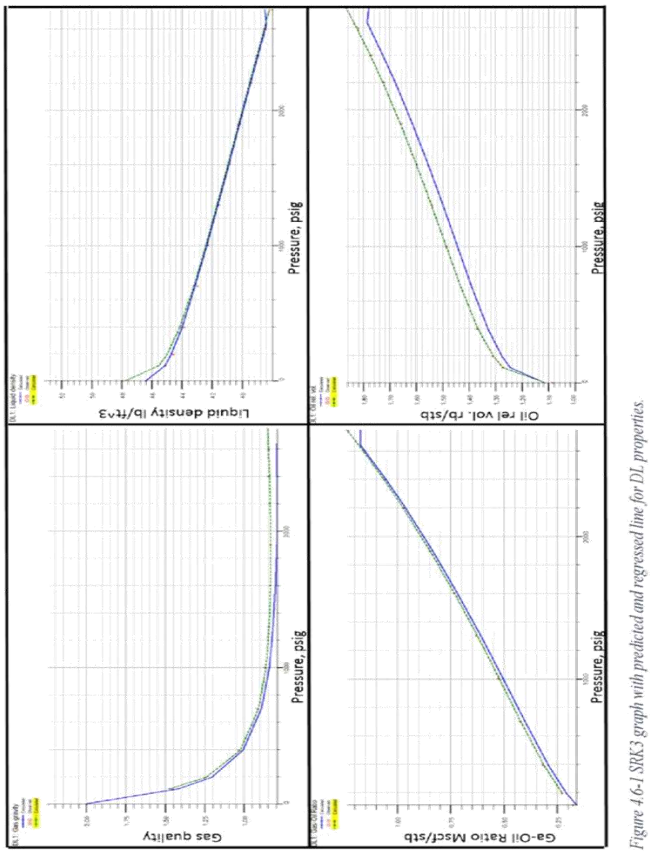

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Figure 4.6-1 SRK3 graph with predicted and regressed line for DL properties.

Figure 3.6-1 SRK3 graph with predicted and regressed line for DL properties

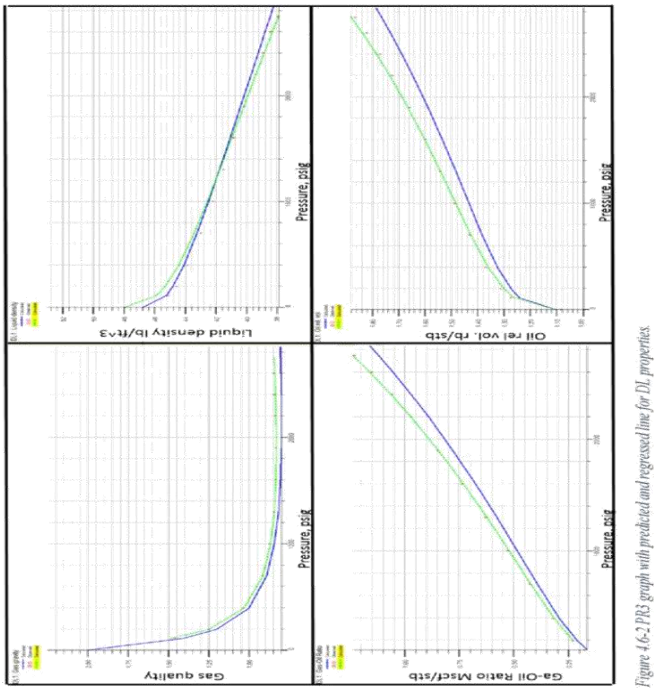

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Figure 4.6-2 PR3 graph with predicted and regressed line for DL properties.

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Figure 3.6-2 PR3 graph with predicted and regressed line for DL properties

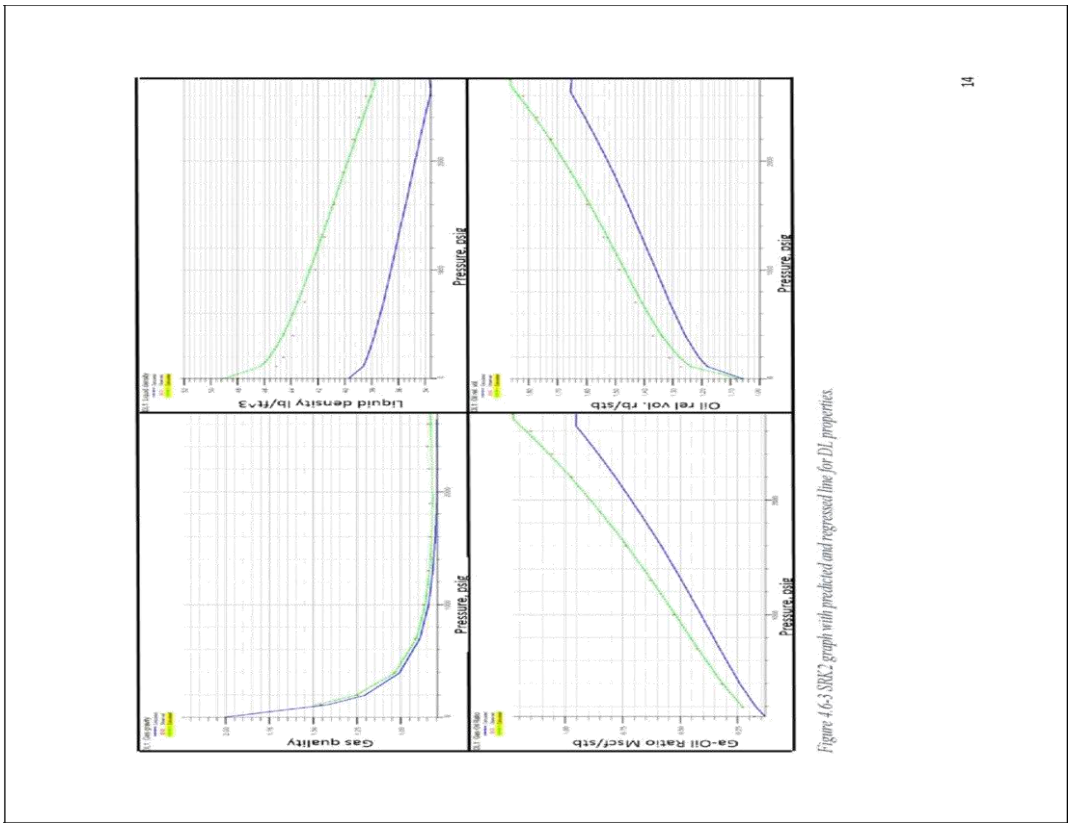

Figure 3.6-3 SRK2 graph with predicted and regressed line for DL properties

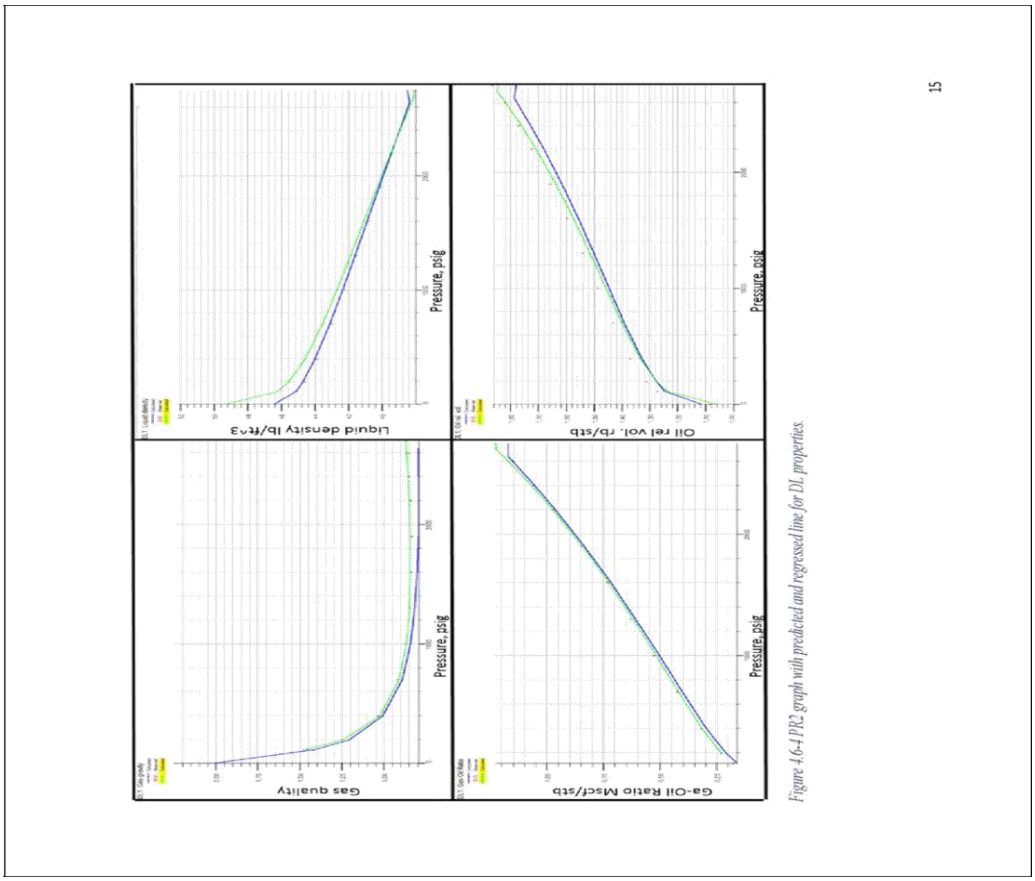

Figure 3.6-4 PR2 graph with predicted and regressed line for DL properties

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4.0 CONCLUSION

In conclusion, regression is necessary to be conducted to the EOS in order to predict the fluid behaviour in the reservoir. From this report, it is proven that by using regression, the RMS value for each of EOS was improved by adjusting the variable parameter. From the comparison made, based on the variable parameter chosen. SRK3 shows the closest match towards the experimental data compared to the other EOS.

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