Assignment 1 Report

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The code is well-commented and self-explanatory at most points however a few paragraphs are necessary for further clarification.

1 METHODOLOGY

At first, some initial parameters have been introduced including the given temperature (T, K), pressures (P, bar), experimental Z-factors, and universal gas constant (R, L.bar/k/mol). Then the critical properties of CO_2 including critical pressure and temperature which are available in the literature are entered as Pc and Tc respectively. [1] The acentric factor for CO_2 is also assumed to be equal to 0.225 and notated as 'omega' in the code. [2]

Table 1 - Acentric factor and critical properties of CO_2 [2]

component	T_c/K	P_c/bar	ω
carbon dioxide	304.12	73.74	0.225
octane	568.70	24.90	0.399
hexadecane	723.00	14.00	0.718
methylcyclohexane	572.19	34.71	0.235
cis-decalin	703.60	32.00	0.276
methylbenzene	591.75	41.08	0.264

As the first task, SRK equation of state is solved for molar volume of CO_2 using MATLAB solve function. The equation of state is re-arranged to form a cubic equation with the molar volume, v, as the unknown:

$$Pv^3 - RTv^2 - v(RTB + Pb^2 - a) - ab = 0 \quad \text{Eq. 1}$$

Where a and b are defined in the problem sheet. Then Z-factor is solved using the ideal gas equation of state:

$$Z = \frac{PV}{RT} \quad \text{Eq. 2}$$

In this case Z-factor is notated as Z_SRK in the code. Same process has been carried out to also calculate Z-factor by the Peng-Robinson EOS. Here the final equation to be solved is arranged as the following term:

$$-Pv^3 + (RT - Pb)v^2 + (2bRT - a + 3Pb^2)v - b(Pb^2 + RTb - a) = 0 \quad \text{Eq. 3}$$

And then again Z-factor is obtained via Eq. 2 and saved in Z_PR. In the code, however, for this second case, some parameters are renamed to avoid any errors; e.g. molar volume is denoted as x.

2 Results and Discussion

In the final section of the code plots are generated to compare the results. After running the code, 5 figures should be generated in total which will be explained in detail.

The first plot, Figure 1, shows the variation of Z-factor obtained via SRK EOS by pressure, also comparing it with the experimental Z-factor given in the problem sheet. It is evident from the plot that a good match has been obtained in low to medium pressures, however, in high pressure the SRK method was a relatively poor fit to experimental data.

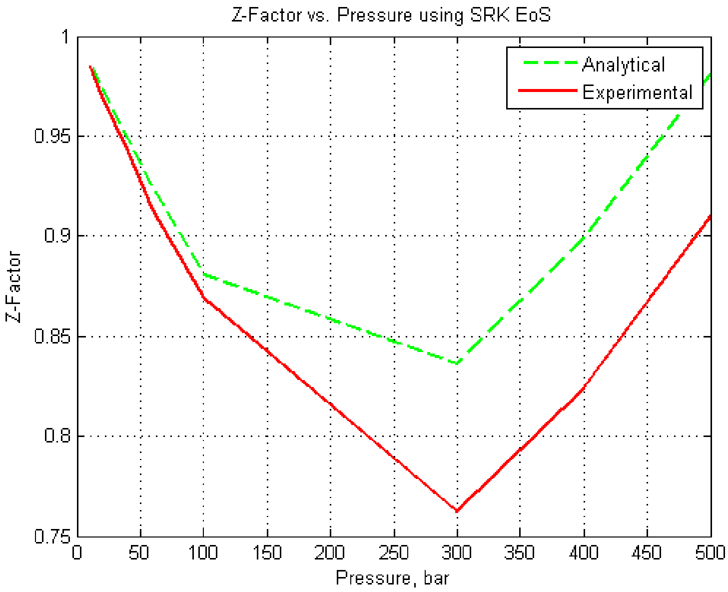

Figure 1 - Variation of SRK Z-factor and Experimental Z-factor with pressure

A better demonstration is given by the second plot, Figure 2, in which the experimental Z-Factor is compared directly with the analytical one. Here the match represented by R^2 is a relatively good match of 0.83.

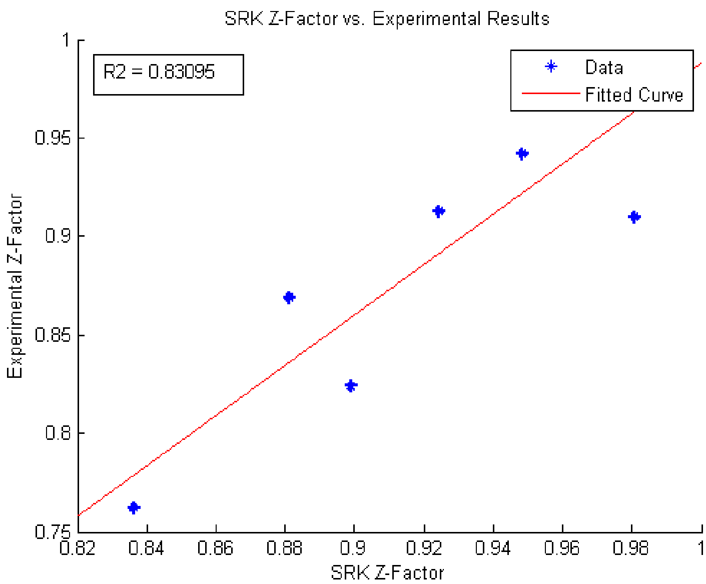

Figure 2 - Comparison of analytical SRK Z-factor with the experimental data

The above-mentioned plots have also been generated for the case of Peng-Robinson EOS. The results are shown in Figures 3, and 4. The first plot shows a better match with experimental data compared to the case of SRK equation of state. The plot has some deviation in middle pressure ranges, however, nothing solid can be stated given the fairly low amount of data investigated.

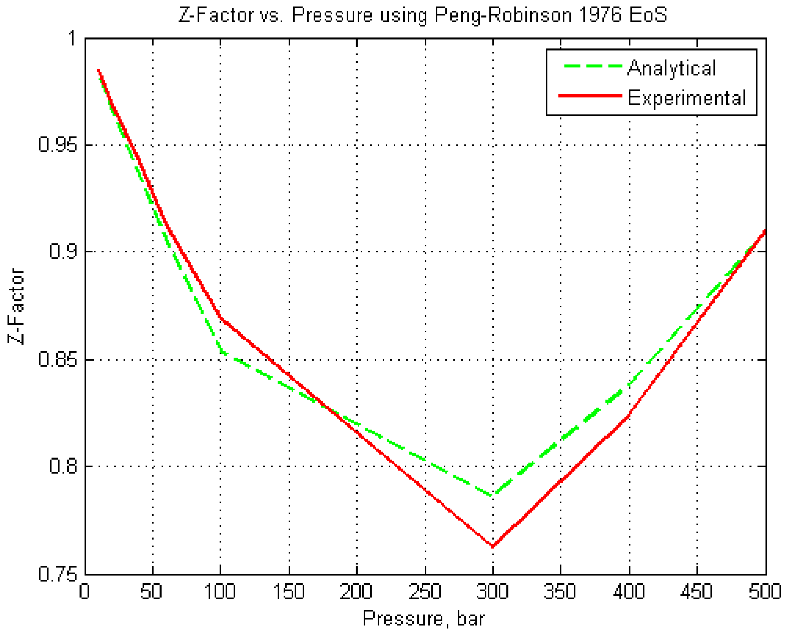

Figure 3 - Variation of Peng-Robinson Z-factor and Experimental Z-factor with pressure

Again, the comparison plot of Z-factors is generated to compare the analytically obtained Z-factors using Peng-Robinson EOS to the experimental data. Figure 4 shows an excellent fit of R^2 equal to 0.98 which demonstrates that the experimental data are better matched with the Peng-Robinson method rather than SRK EOS.

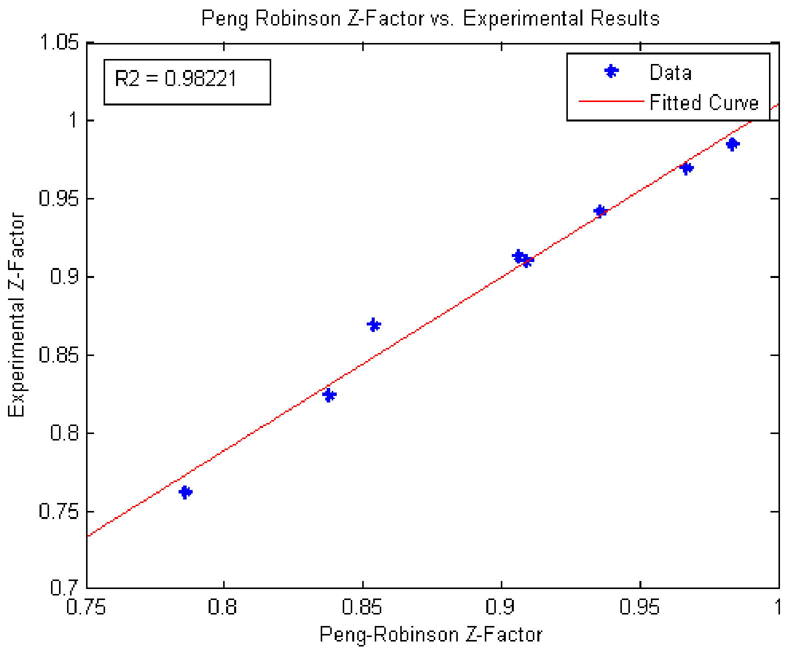

Figure 4 - Comparison of analytical Peng-Robinson Z-factor with the experimental data

Finally, a plot has been generated to compare the molar volume obtained using each equation of state. Figure 5 shows the comparison between molar volumes the three different cases. The variation is fairly small and has to be investigated with a larger dataset.

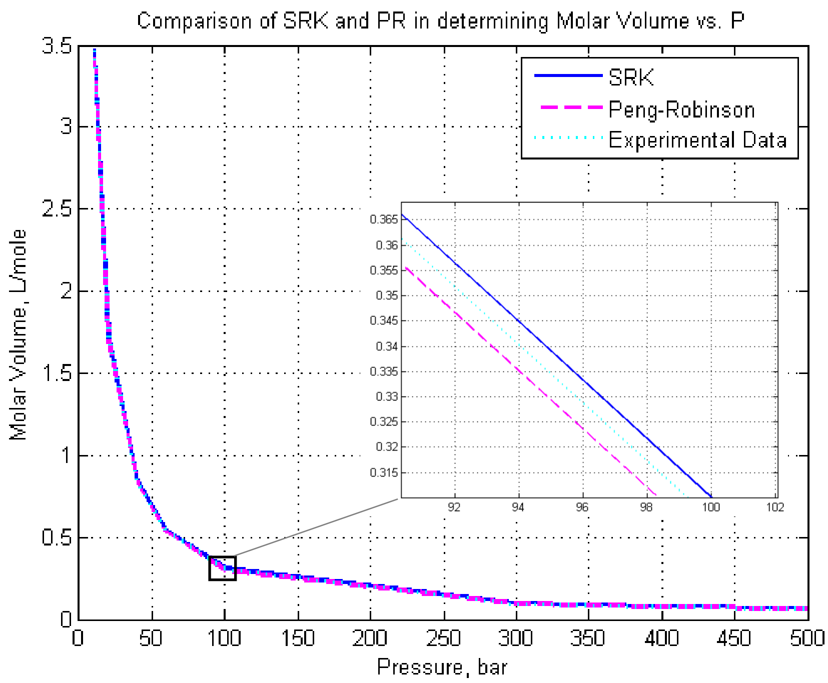

Figure 5 - Comparison between the two models and the experimental molar volumes.

3 CONCLUSION

As a brief conclusion, it can be inferred from the generated plots that and matches between experimental data and the two equations of state that the second case (Peng-Robinson EOS) was more successful at fitting the experimental data.

4 REFERENCES

1. Engineering ToolBox, (2018). *Carbon Dioxide - Thermophysical Properties.* [online] Available at: https://www.engineeringtoolbox.com/CO2-carbon-dioxide-properties-d_2017.html [accessed 10 Apr, 2020]
2. *Bubble and Dew Points of Carbon Dioxide + a Five-Component Synthetic Mixture: Experimental Data and Modeling with the PPR78 Model* - Scientific Figure on ResearchGate. Available from: https://www.researchgate.net/figure/Critical-Temperature-Tc-Critical-Pressure-Pc-and-Acentric-Factor-o-of-the-Pure_tbl2_231540860 [accessed 10 Apr, 2020]