Energy 251 Project Report Part A

Youssef Aitousarrah

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1 Introduction

The aim of this report is to treat the case of a reservoir production using EOR operations based on gas injection. We are interested in exploring the different mixtures than can be used for this purpose (mixtures of Liquified Petroleum Gas and CO_2). The first part of the project explains the pseudoization and lumping of the reservoirs components before using these results in determining the saturation pressure (via a CCE PVT experiment) of the oil and plotting the reservoirs fluid relative volume (relative to the saturation volume) in function of pressure, the result will be confronted to the experimental data. Additionally, the part A of this project also explores the coding and testing of a mixing cell algorithm to estimate the MMP (Minimal Miscibility Pressure) of the injectant. The results of the SPE 116823 article will be reproduced to verify the routine's accuracy.
The part B develops the use of the mixing cell routine to find MMP for mixtures of CO_2 and LPG with different proportions and also the determination of viscosity using LBC correlation and corresponding states method.

2 Methodology and Implementation

This section of the report explains the methodology that has been followed to develop the various algorithms for part A and B.
The first one does the plus fraction expansion and computes the different critical parameters of the pseudo-components that are going to be used as an input for the EOS. The steps performed for this matter are the following:

- First, I decided to compare two possible expansion and lumping. In the first one I started the expansion from C_7 component, see Table 1 and in the second one I started from C_{11}, see Table 2, and expand it using Pedersen et al procedure. The ABCD-Routine is used to determine the A, B, C and D values. I also incorporated the additional information about Heptane plus fraction density and use it to compute the A, B, C and D and compare the results with the previous calculations, the most obvious differences are in temperatures, but the values still close to each other.

- The critical parameters (critical pressure, critical temperature and the

accentric factor) are then computed using correlations from the reader (page 160/161).

- Next, these parameters are used to compute the critical parameters of each pseudo-components. The weights of the pseudo-components has to be fairly equal, this was the criteria used to define the lumped hydro-carbons for each PS, the five lumped pseudo-components for the SRK trial (C_{7-12} , C_{13-18}, C_{19-26}, C_{27-37} and C_{38+}) have respectively the following mass fraction of the overall plus fraction mass: 0.2044, 0.1992, 0.2131, 0.1867 and 0.1965. And for the PR trial I chose to expand the plus fraction and use all the defined component such as they are, the mass fractions of the lumped pseudo-component (C_{11-13}, C_{14-16}, C_{17-20}, C_{21-27} and C_{28+}) are: 0.2228, 0.1853, 0.1895, 0.2059 and 0.1965.

- Then, the values found in the previous step (molar fraction, T_c, P_c and ω of each PS) are used, in addition to the ones from the components that are not included in the expanded fraction, to perform the CCE routine.

- The CCE routine is performed by starting with a high pressure exceeding the saturation pressure and repeatedly reducing this pressure after flashing the oil (keeping the temperature and the composition constant). We also save the volume $V = vV^v + lV^l$ where v and l are the liquid and vapor fractions obtained from the flash, and V^v and V^l are the liquid molar volume and vapor molar volume. The saturation point can be determined using a bisection method that explores the values between a max and a min pressure to yield the saturation pressure to a certain tolerance. The saved values are then used to plot the relative volume (dividing the volume by the saturation volume) against the pressure. A particular point that we should pay attention to is how to choose the volume, when the liquid fraction from the flash is greater than 1 we have $V = V^l$, and if it is smaller than zero we have $V = V^v$.

- One important point that needs to be stressed is to choose the Z root of the EOS based on the minimization of Gibbs Free Energy.

- Finally, the plot is confronted to the experimental one. And some changes are made on the heavy components to see the effects on the results.

The second part handles implementation of the mixing-cell algorithm to determine the MMP pressure. The steps performed for this matter are the following:

- The general idea of the algorithm is to increase the pressure progressively until the MMP pressure is attained. For each pressure step, we compute the contacts by continually mixing neighboring cells until the key tie line lengths converge. The convergence is verified by checking if the tie-length evolution between successive contacts for three successive cells is smaller than a tolerance factor.

- The first pressure increment is obtained by adding a constant value (200 psia in this case) to the initial pressure of 500 psia. The second increment is obtained by doing an extrapolation of the eq: $TL_{min} = aP + b$, where TL_{min} is the minimum key tie-line length and P is the pressure, we use to the two previous pressure to obtain a first estimation of the MMP and the pressure increment is set to be the difference between P and MMP divided by 3 or any other number depending on the desired precision. For subsequent pressures, we can use the relationship $TL_{min}^n = aP + b$ where a regression must be done to determine the three constants n, a and b, the MMP is then estimated by setting TL equal to zero.

- We repeat this until the difference between the estimated MMP and the previous one is smaller than a tolerance pressure (set equal to 20 psia in this case). Another convergence criteria could be the TL_{min} close to zero to a certain tolerance factor.

- To reproduce the fig.2 in the SPE 116823 paper, we fix the pressure at 1.34×10^7 Pa (2000 psi) and the temperature at 344.26 K (160 °F). Then, we mix the cells increasing the contact number successively until exceeding 125 contact which is the biggest one in the fig. We finally plot the key tie-line length versus the cell number for 4 different contact number: 25, 50, 100, 125. The results can be seen in the next section.

- fig.4 is reproduced by computing the MMP using the routine described in the previous points. We start by an initial pressure of 500 psia and keep increasing it until the MMP converges (TL_{min} approaches zero). During the mixing procedure for each pressure, we save the key tie-line

Lengths (oil, gas and crossover) after convergence. At the end, we plot these key tie-line lenghts versus pressure.

The third routine uses the previous one to compute the MMP for different combination of LPG and CO_2. Then, a plot containing the evolution of this pressure in respect to the mole fraction of LPG is produced.

The fourth algorithm development treated the viscosity determination. And it is composed of the following:

- For the LBC correlation, I implemented the eq 8.10 from the reader. There are several critical points regarding units, volume determination,...and they will be discussed in the discussion part.

- The corresponding states algorithm was developed using the eq 8.23 from the reader which gives a relationship between the mixture's viscosity and a reference viscosity of methane. There are also a few points that need to be discussed about how to avoid some errors during this implementation.

3   Results

Results that are related to Part A and are not required in this report will not be shown because I have already included them in the report for Part A. Only parts that are required or where there are differences between part A and B will be mentioned in this present report.

- Table of the EOS input for the pseudoized reservoir fluid:

Component	Mole %	Tc (K)	Pc (atm)	ω	MW (g/mol)
Hydrogen Sulfide	0				34.08
Carbon Dioxide	0.44	304.2	72.9	0.228	44.01
Nitrogen	0.17	126.2	33.6	0.04	28.013
Methane	34.63	190.6	45.4	0.008	16.043
Ethane	2.63	305.4	48.2	0.098	30.07
Propane	3.35	369.8	41.9	0.152	44.097
iso-Butane	0.92	408.1	36	0.176	58.123
n-Butane	1.75	425.2	37.5	0.193	58.123
iso-Pentane	0.89	460.4	33.4	0.251	72.15
n-Pentane	1.01	469.6	33.3	0.251	72.15
Hexanes	1.52	507.4	29.3	0.296	84
C_{7-12}	21.23	580.5	25.6	0.44	130
C_{13-18}	12.68	666.9	20.6	0.667	212.2
C_{19-26}	9.34	759.4	17.8	0.876	308
C_{27-37}	5.78	875.1	14.2	1.0465	436.5
C_{38+}	3.67	1114.1	12	0.8191	722.8

Table 1: EOS (SRK) input for the pseudoized reservoir fluid

Component	Mole %	Tc (K)	Pc (atm)	ω	MW (g/mol)
Hydrogen Sulfide	0				34.08
Carbon Dioxide	0.44	304.2	72.9	0.228	44.01
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iso-Pentane	0.89	460.4	33.4	0.251	72.15
n-Pentane	1.01	469.6	33.3	0.251	72.15
Hexanes	1.52	507.4	29.3	0.296	84
Heptanes	5.00	548.0	30.7	0.28	96
Octanes	6.02	575.0	28.4	0.312	107
Nonanes	3.99	603.0	26.0	0.348	121
Decanes	3.55	626.0	23.9	0.385	134
C_{11-13}	11.53	633.2	21.7	0.6254	163.5
C_{14-16}	7.64	675.9	19.0	0.7964	205.4
C_{17-20}	6.33	721.3	17.0	0.9805	253.6
C_{21-27}	5.33	785.1	15.0	1.2222	326.7
C_{28+}	3.3	923.8	12.7	1.4	504.4

Table 2: EOS (PR) input for the pseudoized reservoir fluid

Component	Mole %	Tc (K)	Pc (atm)	w	MW (g/mol)
Hydrogen Sulfide	0				34.08
Carbon Dioxide	0.44	304.2	72.9	0.228	44.01
Nitrogen	0.17	126.2	33.6	0.04	28.013
Methane	34.63	190.6	45.4	0.008	16.043
Ethane	2.63	305.4	48.2	0.098	30.07
Propane	3.35	369.8	41.9	0.152	44.097
iso-Butane	0.92	408.1	36	0.176	58.123
n-Butane	1.75	425.2	37.5	0.193	58.123
iso-Pentane	0.89	460.4	33.4	0.251	72.15
n-Pentane	1.01	469.6	33.3	0.251	72.15
Hexanes	1.52	507.4	29.3	0.296	84
Heptanes	5	548	30.7	0.28	96
Octanes	6.02	575	28.4	0.312	107
Nonanes	3.99	603	26	0.348	121
Decanes	3.55	626	23.9	0.385	134
C_{11-13}	11.53	635.6	21.6	0.6256	163.5
C_{14-16}	7.64	677.1	19.0	0.7965	205.4
C_{17-20}	6.33	721.3	16.9	0.9805	253.6
C_{21-27}	5.33	783.6	14.9	1.222	326.7
C_{28+}	3.3	920.1	12.7	1.3996	504.4

Table 3: EOS (PR) input for the pseudoized reservoir fluid using the additional information about Heptane Plus fraction density.

- Comparison between the prediction from CCE and experimental data for PR EOS. For the saturation pressure, I found $P_{sat} = 1.37 \times 10^7$ Pa:
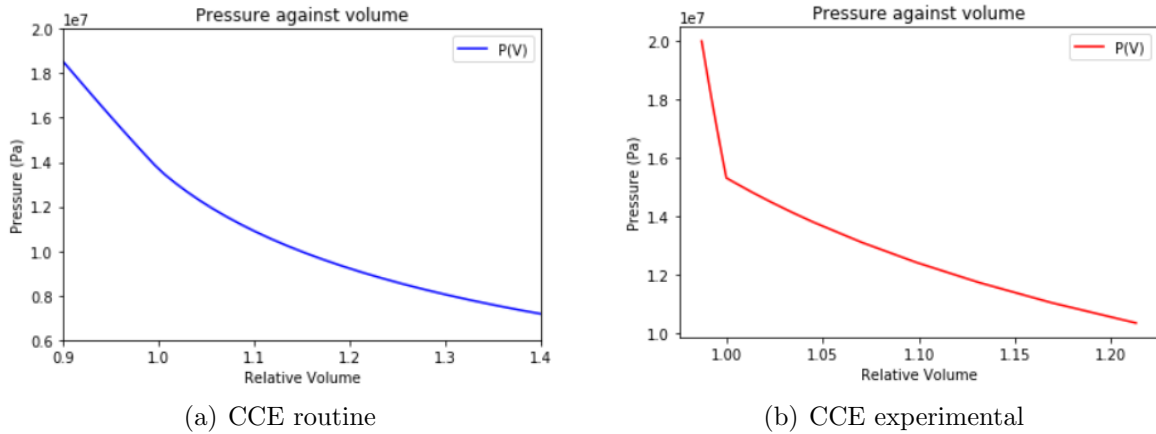

(a) CCE routine

(b) CCE experimental

Figure 1: CCE routine (PR) comparison with experimental results

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- Comparison between the prediction from CCE and experimental data for SRK EOS. For the saturation pressure, I found $P_{sat} = 1.39 \times 10^7$ Pa:

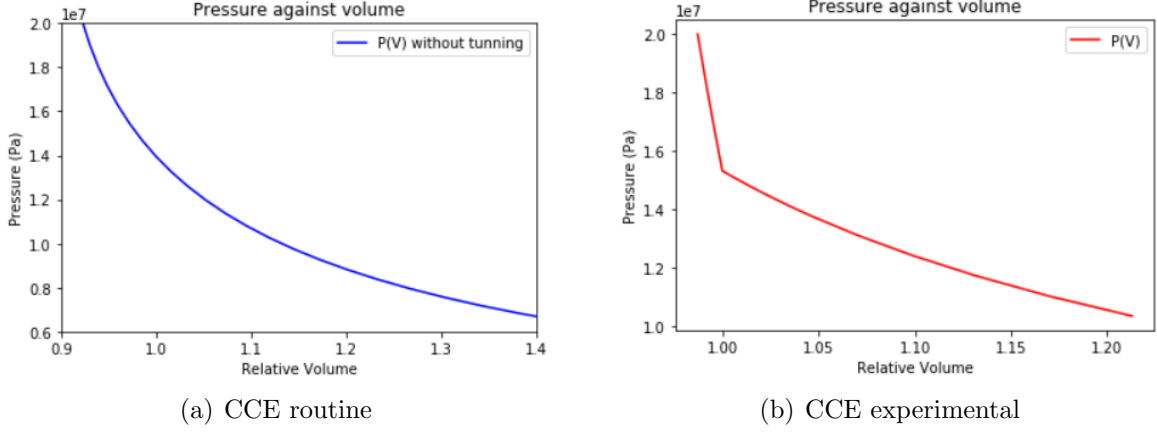(a) CCE routine

(b) CCE experimental

Figure 2: CCE routine (SRK) comparison with experimental results

- Tuning effects on the CCE prediction (PR):

  - Changing the plus fraction density from 245 to 300 g/mol.
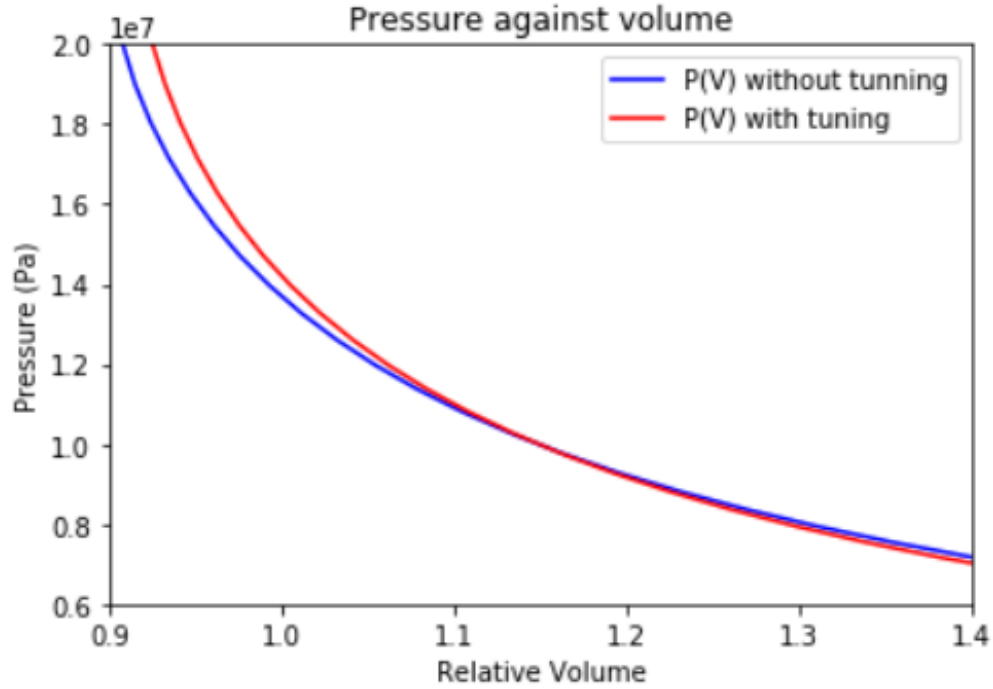

Figure 3: Pressure against Relative Volume - Changing molecular weight of the plus fraction
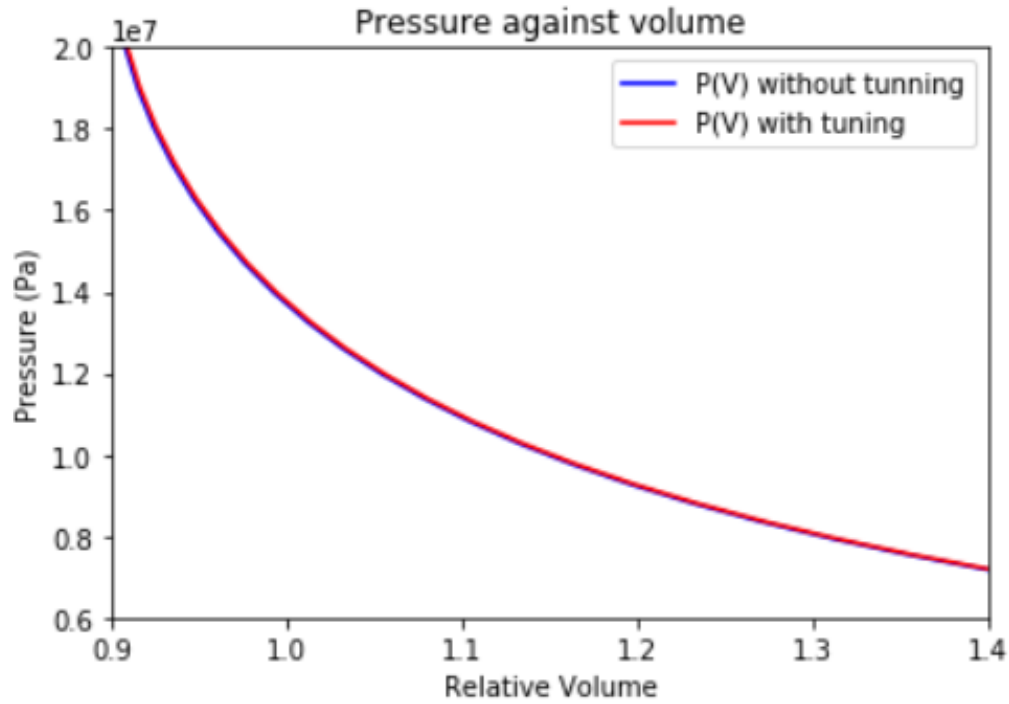
  - Using a non-zero interaction coefficients:

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Figure 4: Pressure against Relative Volume resulting - Changing the binary coefficients

– Using the information about the Heptane plus fraction density as it was used to compute the A, B, C and D for the expansion operation (input table obtained is represented in table 3):
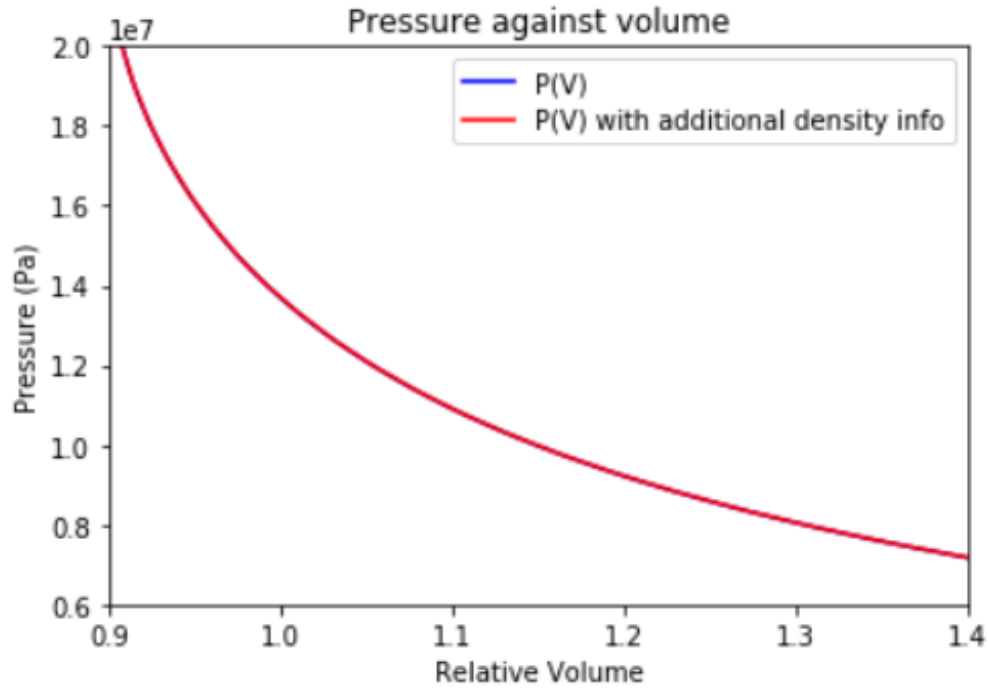
Figure 5: Pressure against Relative Volume resulting - Changing the binary coefficients

- The MMP pressure versus mole fraction of LPG plot, where composition is a percentage in the x axis and Pressure is in Pa at the y axis:
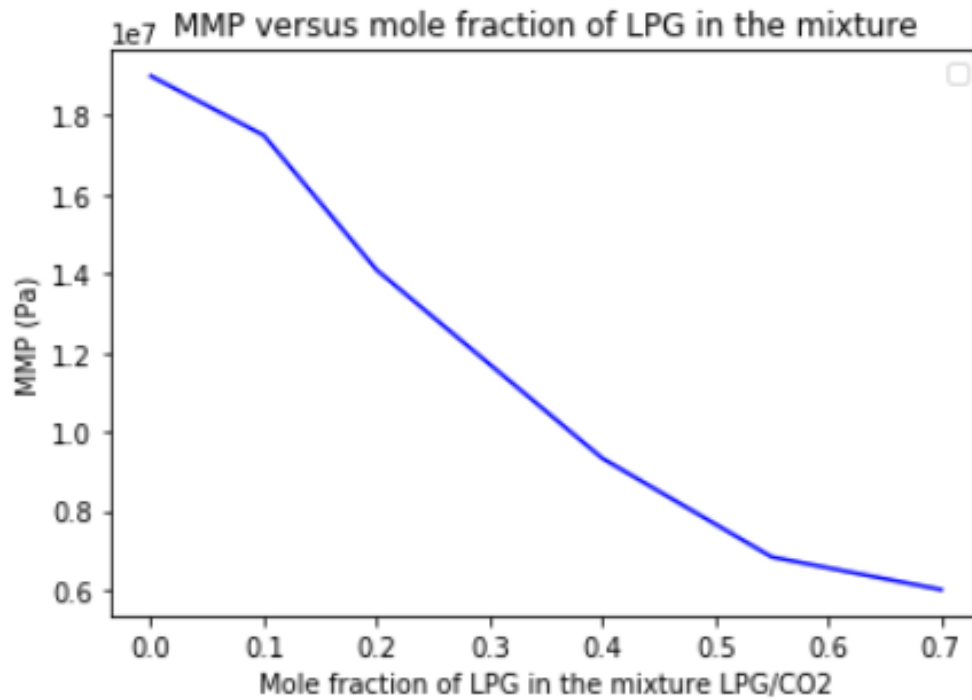

Figure 6: MMP versus the mole fraction of LPG in the CO_2/LPG mixture

- The different viscosity plots are reproduced in the following figures. The first one is using LBC correlation, the second one using corresponding state and the last figure is the viscosity of the different combinations of LPG and CO_2:
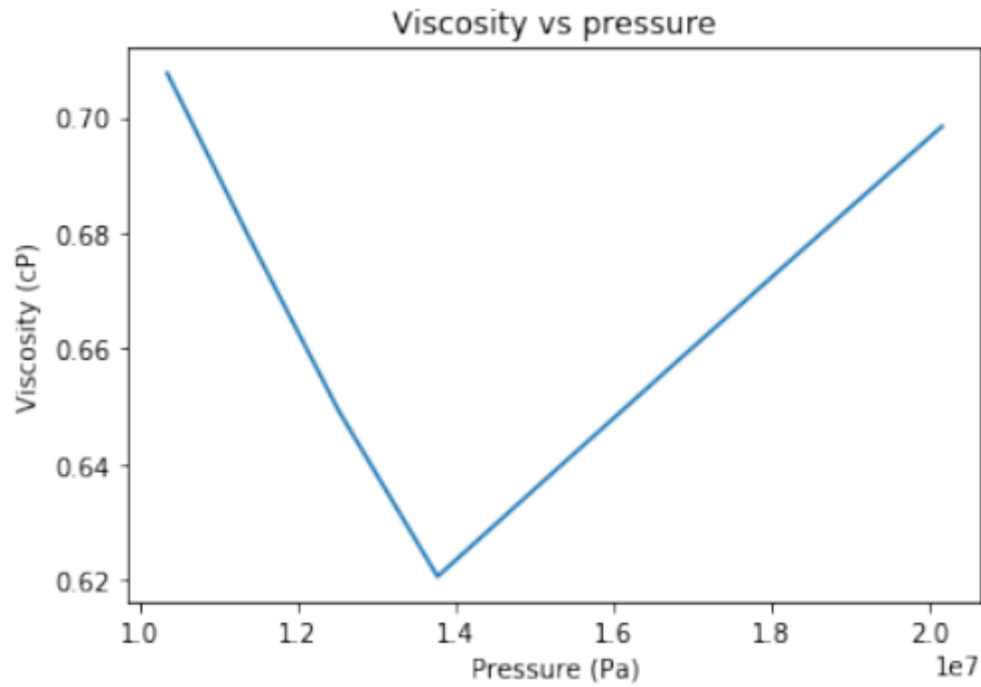

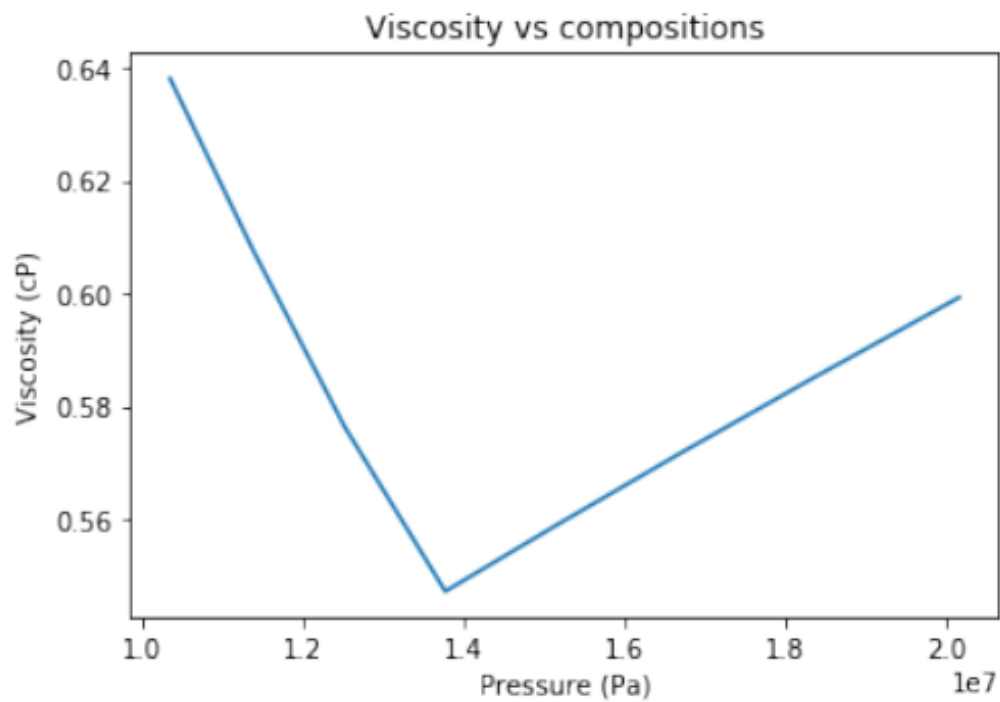Figure 7: Viscosity's evolution with pressure using the LBC correlation

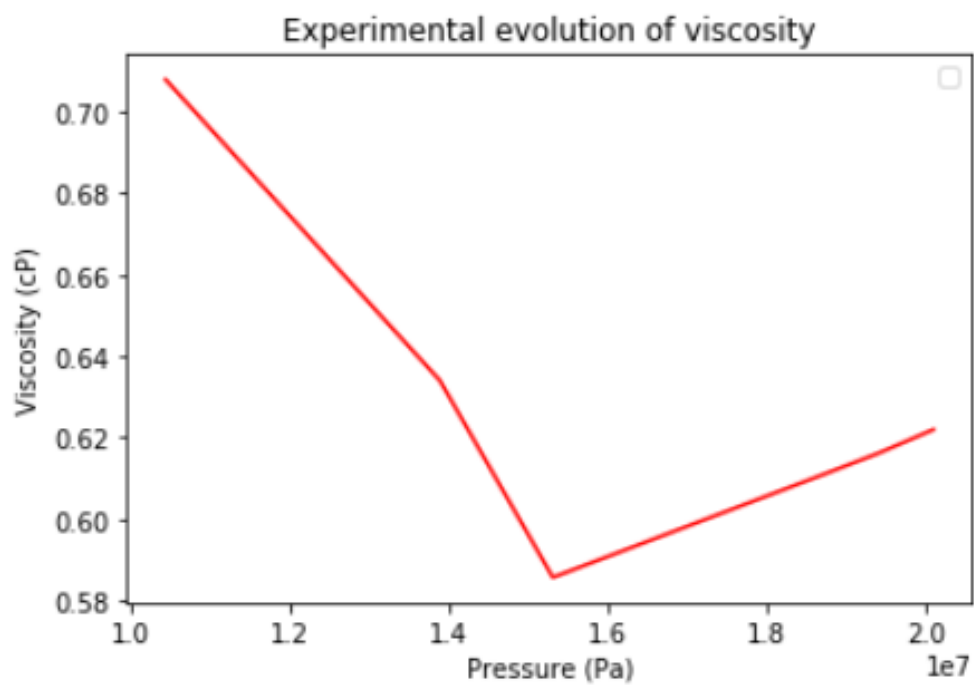Figure 8: Viscosity's evolution with pressure using the corresponding states

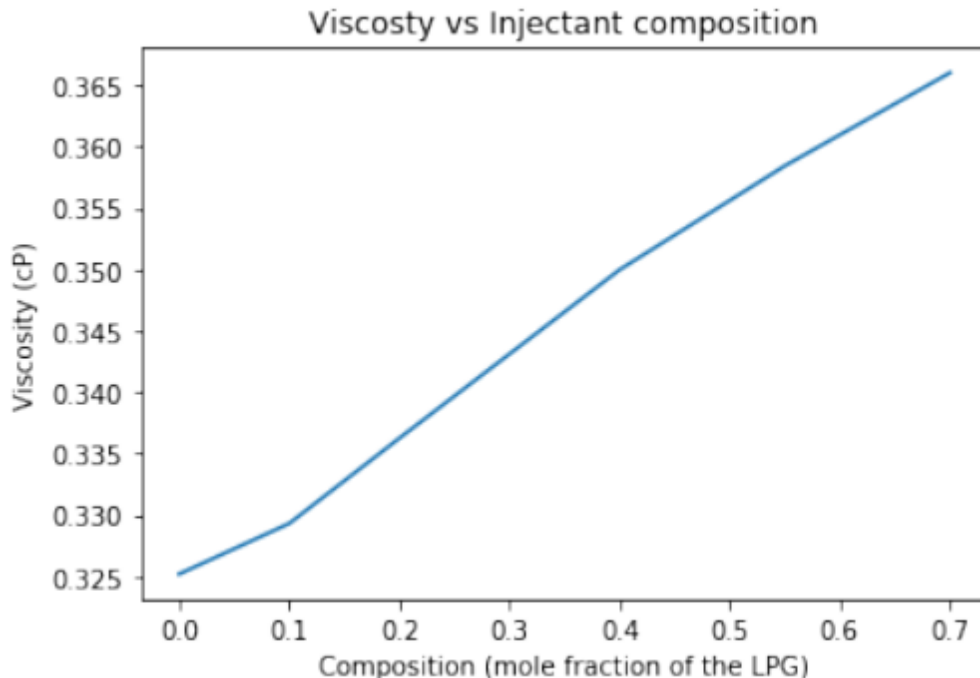Figure 9: Experimental evolution of viscosity

Figure 10: Viscosity for different LPG/CO_2 mixtures at $28\,\text{MPa}$ and $106°$

4   Discussion

There are several aspects of this work that need to be discussed and further investigated. The first point is about tuning, to tune the EOS we can change different parameters: critical parameters (for heavy components), Mw of the plus fraction, binary interaction coefficients, shifting volumes...The idea is to regress on one or more of the mentioned variables in order to match the experimental data and obtain a tuned EOS. I have attempted to do several kinds of tuning as you can see in the results section, we can see that changing the molecular weight has a noticeable impact on the saturation pressure and increasing the plus fraction Mw get us closer to the experimental saturation pressure. However, when I changed the binary coefficients I got only a very small increase in the saturation pressure, I think one of the reasons is that I only changed BIC for non-hydrocarbon components and that if I included methane also it would have given a different result.

For the MMP determination, I tried to increment my pressure using a regression like the one described in the paper where an exponent and two constant are determined, but I haven't found any function capable of doing this, so

to tackle this issue, I looped over the valid range of exponents and I regress each time on the two constant. You can see this part of the code in the MMP determination routine.

Concerning the viscosity determination, I have encountered several problems that needed to be solved to get values close to the experimental ones. For the LBC correlation, the first mistake was taking overall component molar fraction instead of doing the flash each time and taking only the liquid fraction, but if in the flash we get a liquid fraction that is greater than one we should choose the overall molar fractions. One other challenge was the units, the eq 8.8 in the reader did not precise units, so I had to go and read the article to know which units were used and do the conversion in order to get the desired units (the used units in the article were Psia for pressure and Rankine for temperature). Computing the critical molar volume of the mixture was also challenging, at first I wasn't changing the Mw of the C7+ fraction after each flash (compositions changes) and I was keeping constant which was giving me false results, to solve this I did a molar average for the C7+ components after each flash.
For the corresponding states approach, the most challenging part was to compute reference density of methane that is going to be used for the reference viscosity determination. I had once again to find my way through units, especially those related to molar volumes, because in the viscosity function that was provided the density was in g/cm^3, and therefore the reference density that is passed to this function should also be in the same unit. I also added volume correction as it allows to tune the volume to have a better match.
From the different figures of viscosity we can see that we have a match with the experimental data, and we get also the same trend which is a decreasing viscosity until the bubble point pressure and it increases afterwards because the liquid becomes more present.

In fig.6 we can notice that the pressure is increasing with the fraction of CO_2 in the mixture and in the same time the viscosity of the mixture decreases as we can see in fig.10. A good injection mixture should have low viscosity so that it can be more mobile. So, the strategy is the pick the injection mixture with the lowest viscosity but its MMP pressure should not exceed the reservoir's pressure to still have a miscible injection. For our case

we have a reservoir pressure at 18 MPa and the MMP pressure for the mixture with 80% CO_2 is around 14 MPa, so we can use this one as it respects all the conditions and it is the optimal choice.

5 Summary

This project was a great opportunity to apply all what we have learned to a practical case. Facing the different issues that I talked about earlier allowed me to go deeper in understanding the various concept of this course. We can see clearly now that an implementation of what we have studied is not as simple as it sounds. The routines that were developed needed to be rigorously revised and scrutinized because one small mistake can ruin the whole implementation especially that different parts of the code are intertwined.