EG3029 Chemical Thermodynamics

Lab Exercise I:

Equations of State using Matlab

Problem 1:

An inexperienced student has conducted an experiment. He pumped a fluid from a gas bottle into a constant volume cell (final specific volume 0.001 m^3 mol^{-1}) which can be heated and is equipped with a thermocouple and a pressure gauge. The aim of his project was to study the *P-T* behaviour at constant volume. For this purpose he increased the temperature in the cell between 400 and 600 K in steps of 20 K and noted the resulting pressure down in his logbook:

T/K	400	420	440	460	480	500	520	540	560	580	600
P/bar	27.0	29.1	31.3	33.3	35.3	37.4	39.3	41.5	43.3	45.4	47.4

After finishing the experiment he put the gas bottle back to the gas storage and went to his desk to start evaluating the data. Unfortunately, he realised that he had forgotten to note down which gas it was. Therefore he went back to the gas storage where he found methane, ethane, propane, and ethylene, but he couldn't identify the bottle he used.

Task 1:

Open Matlab and write a code (m-file) that allows you to calculate the pressure as a function of temperature employing van der Waals EOS, Redlich-Kwong EOS, Soave-Redlich-Kwong EOS, and Peng-Robinson EOS from the generic cubic equation

$$P = \frac{RT}{V-b} - \frac{a(T)}{(V+\varepsilon b)(V+\sigma b)}$$

$$a(T) = \Psi \frac{\alpha(T_r) R^2 T_c^2}{P_c}$$

$$b = \Omega \frac{RT_c}{P_c}$$

EOS	$\alpha(T_r)$	σ	ε	Ω	Ψ
vdW	1	0	0	1/8	27/64
RK	$T_r^{-0.5}$	1	0	0.08664	0.42748
SRK	$\alpha_{SRK}(T_r;\omega)^{\dagger}$	1	0	0.08664	0.42748
PR	$\alpha_{PR}(T_r;\omega)^{\ddagger}$	$1+\sqrt{2}$	$1-\sqrt{2}$	0.07780	0.45724

† $\alpha_{SRK}(T_r;\omega) = \left[1+\left(0.480+1.574\omega-0.176\omega^2\right)\left(1-T_r^{0.5}\right)\right]^2$

‡ $\alpha_{PR}(T_r;\omega) = \left[1+\left(0.37464+1.54226\omega-0.26992\omega^2\right)\left(1-T_r^{0.5}\right)\right]^2$

Task 2:

Use your code to calculate the *P-T* curves of the candidate species (ΔT = 0.5 K) in the range 400-600 K and display the results together with the experimental data. Use the properties from the following table and find out from comparing experimental and calculated data which gas the student used.

	Molar mass	ω	T_c/K	P_c/bar	Z_c	V_c cm^3 mol^{-1}	T_n/K
Methane	16.043	0.012	190.6	45.99	0.286	98.6	111.4
Ethane	30.070	0.100	305.3	48.72	0.279	145.5	184.6
Propane	44.097	0.152	369.8	42.48	0.276	200.0	231.1
n-Butane	58.123	0.200	425.1	37.96	0.274	255.	272.7
n-Pentane	72.150	0.252	469.7	33.70	0.270	313.	309.2
n-Hexane	86.177	0.301	507.6	30.25	0.266	371.	341.9
n-Heptane	100.204	0.350	540.2	27.40	0.261	428.	371.6
n-Octane	114.231	0.400	568.7	24.90	0.256	486.	398.8
n-Nonane	128.258	0.444	594.6	22.90	0.252	544.	424.0
n-Decane	142.285	0.492	617.7	21.10	0.247	600.	447.3
Isobutane	58.123	0.181	408.1	36.48	0.282	262.7	261.4
Isooctane	114.231	0.302	544.0	25.68	0.266	468.	372.4
Cyclopentane	70.134	0.196	511.8	45.02	0.273	258.	322.4
Cyclohexane	84.161	0.210	553.6	40.73	0.273	308.	353.9
Methylcyclopentane	84.161	0.230	532.8	37.85	0.272	319.	345.0
Methylcyclohexane	98.188	0.235	572.2	34.71	0.269	368.	374.1
Ethylene	28.054	0.087	282.3	50.40	0.281	131.	169.4
Propylene	42.081	0.140	365.6	46.65	0.289	188.4	225.5

Problem 2:

Write a Matlab code that simulates the three processes described in Problem 3 of Tutorial 2 and produce a plot of the *PV* diagram.

Deliverables:

Submission of worked example:

Write a report containing a brief introduction and a summary of your results (incl. figures displaying the data) and findings along with concluding remarks. Prepare the report as Word or PDF file and submit it through Turnitin. The filename of the report should be EG3029_Matlab_Lab1_XXX.docx/pdf (XXX to be replaced by your initials). Submit your work by Sunday, October 27th 2013, 23:59 at the latest. Penalties for late or non-submission are as follows: for late submission, 1 CAS mark will be deducted for each day late (including weekends); submission later than 7 days after the deadline will be considered as non-submission and a CAS mark of 0 will be awarded.

In addition, submit a paper copy of your report including a completed plagiarism cover sheet.

Note that the submitted work is part of the continuous assessment which will contribute 20% to your EG3029 mark.