Tutorial 1

Excel Applications

1. Calculate the change of the vapour pressure with volume for methane at 250 K.
   a) Using the ideal gas model to calculate $p = f(v)$.
   b) Using the Soave EoS for real gases that is given below.

$$p = \frac{RT}{v-b} - \frac{a \times \alpha}{v(v+b)}$$

where

$$a = \frac{0.42748 R^2 T_c^2}{p_c};\ b = \frac{0.08664 R T_c}{p_c};\ \alpha = \left(1 + (0.48508 + 1.55171\omega - 0.15613\omega^2)\left(1 - \left(\frac{T}{T_c}\right)^{0.5}\right)\right)^2.$$

   c) Plot the results as $p = f(v)$ and $error = \frac{(p_{cal} - p_{exp})}{p_{exp}} \times 100$
   d) Briefly discuss implications of you results.

Base your calculation on the experimental data at 250 K from the following table.

v (m³/mol)	*p* (bar)	*v* (m³/mol)	*p* (bar)	*v* (m³/mol)	*p* (bar)	*v* (m³/mol)	*p* (bar)
5.39E-05	400	4.39E-05	900	4.01E-05	1400	3.77E-05	1900
5.21E-05	450	4.34E-05	950	3.98E-05	1450	3.75E-05	1950
5.06E-05	500	4.30E-05	1000	3.95E-05	1500	3.73E-05	2000
4.93E-05	550	4.25E-05	1050	3.93E-05	1550	3.72E-05	2050
4.83E-05	600	4.21E-05	1100	3.90E-05	1600	3.70E-05	2100
4.73E-05	650	4.17E-05	1150	3.88E-05	1650	3.68E-05	2150
4.65E-05	700	4.13E-05	1200	3.86E-05	1700	3.67E-05	2200
4.58E-05	750	4.10E-05	1250	3.83E-05	1750	3.65E-05	2250
4.51E-05	800	4.07E-05	1300	3.81E-05	1800	3.64E-05	2300
4.45E-05	850	4.04E-05	1350	3.79E-05	1850	3.62E-05	2350

Experimental data for methane are obtained from NIST:

T_c = 190.564 K, p_c = 45.992 bar and ω = 0.01142.

2. Calculate the pressure of CO_2 at the conditions indicated in the table by using the van der Waals equation:

$$p = \frac{RT}{v-b} - \frac{a}{v^2}$$

where the constants a and b for CO_2 are: a = 3.59 bar·l²/mol² and b = 0.0427 l/mol.

v \ *T*	250 K	260 K	270 K	280 K	290 K	300 K	310 K

0.05 l/mol							
0.10 l/mol							
0.15 l/mol							
0.20 l/mol							
0.25 l/mol							
0.30 l/mol							
0.35 l/mol							
0.40 l/mol							
0.45 l/mol							
0.50 l/mol							

Note: use F4 to keep a reference cell, row or column in your equation.

3. A mixture of 80% of methane and 20% of propane reacts with oxygen in an incomplete reaction to produce CO, CO_2 and water. Plot methane and propane contributions to the heat of combustion for temperatures from 298 to 900 K.

4. Create Excel functions to search for the critical properties of a given compound. Use these properties to calculate the pressure for a given specific volume and temperature using Peng-Robinson EoS.

Formula	**Name**	**Mol Wt (g/mol)**	**T_c (K)**	**p_c (bar)**	**v_c (cm^3/mol)**	ω
CH_4	methane	16.043	190.56	45.99	98.6	0.011
CH_4O	methanol	32.042	512.64	80.97	118	0.565
CO	carbon monoxide	28.01	132.85	34.94	93.1	0.045
CO_2	carbon dioxide	44.01	304.12	73.74	94.07	0.225
C_2H_6	ethane	30.07	305.32	48.72	145.5	0.099
C_2H_6O	ethanol	46.069	513.92	61.48	167	0.649
C_3H_8	propane	44.097	369.83	42.48	200	0.152
C_3H_8O	1-propanol	60.096	536.78	51.75	219	0.629
C_6H_6	benzene	78.114	562.05	48.95	256	0.21

5. The amount of instant coffee per can is usually expressed as mass. The standard deviation of the packing operation is 20 g. Use the information in the table below to develop a quality control chart of the operation and indicate if the process is under control or not. The table represents a collection of data for 30 samples. 5 cans are collected for each of the samples.

Sample #	Observations (g)				
1	199.42	185.99	190.08	183.33	180.87
2	212.91	185.53	194.66	188.84	181.71
3	202.07	208.70	201.15	189.57	203.26
4	186.35	218.41	191.58	212.57	191.28
5	202.61	218.63	206.64	211.22	188.08

6	203.13	188.78	196.68	194.03	201.06
7	216.27	202.27	210.12	215.10	192.37
8	205.94	186.06	190.71	189.78	192.49
9	182.91	182.30	204.82	204.12	200.50
10	210.26	206.77	216.55	193.21	215.18
11	198.38	212.89	197.60	185.60	181.04
12	217.74	217.96	198.74	190.48	187.34
13	205.63	207.09	209.32	184.86	190.65
14	191.73	189.47	212.46	188.99	209.30
15	218.58	190.46	185.11	216.78	195.40
16	180.93	196.41	187.46	219.42	202.37
17	208.72	196.14	184.62	204.28	216.22
18	208.87	216.30	195.80	215.95	201.21
19	190.28	204.21	180.86	209.33	214.70
20	200.81	183.03	203.51	185.62	203.34
21	184.06	181.24	215.34	188.60	195.32
22	182.89	184.56	211.30	210.84	191.36
23	191.36	214.61	196.58	191.16	214.72
24	213.83	206.73	195.95	213.26	195.97
25	190.43	198.05	202.54	207.21	206.64
26	195.86	209.45	218.35	185.18	211.27
27	214.40	195.83	213.47	200.56	198.10
28	186.90	197.15	204.89	219.92	181.95
29	188.82	182.64	215.70	211.38	210.82
30	196.41	184.58	191.18	190.63	191.34