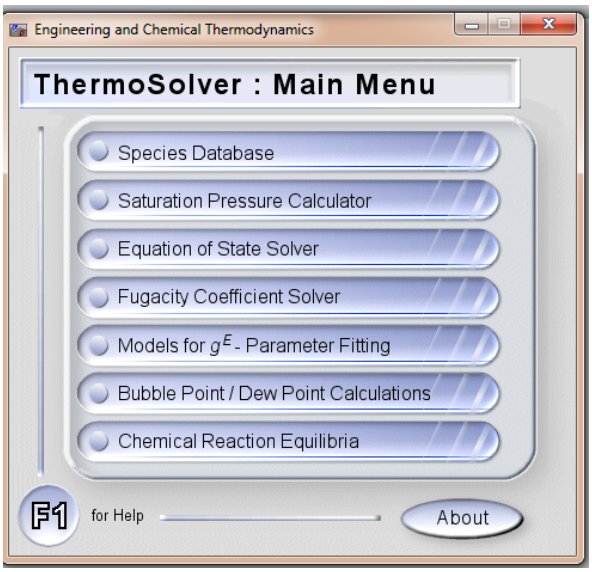
Fugacity and fugacity coefficient excersise

Problem statement

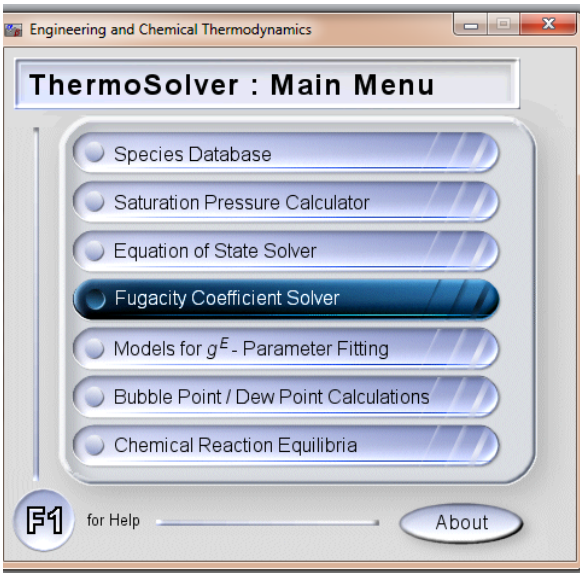
Prepare a graph that shows the change in the fugacity and fugacity coefficient (both in the same graph) when the composition changes for natural gas. Determine the change of the fugacity and fugacity coefficient of natural gas (considering it's a mixture of ethane and propane) at 50 bar and a temperature of 20ºC.

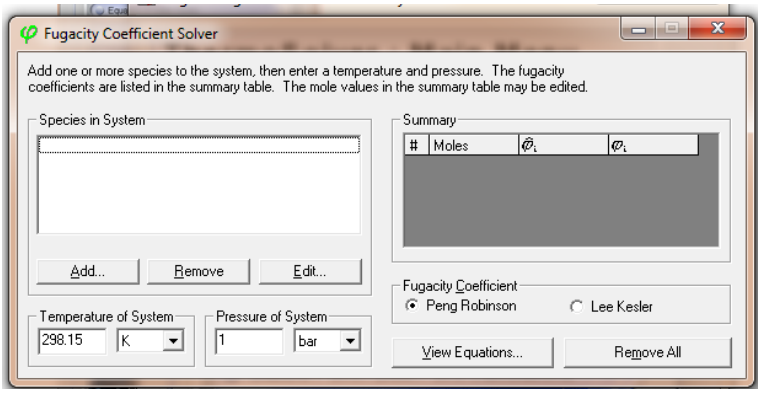
Development

1. We open the *Thermosolver Software*.

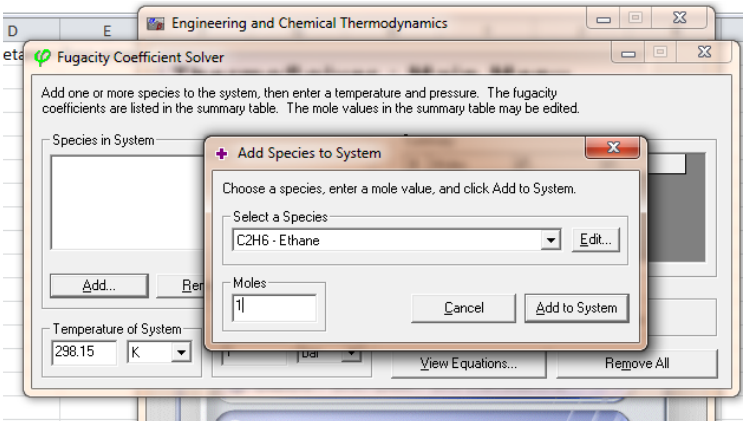


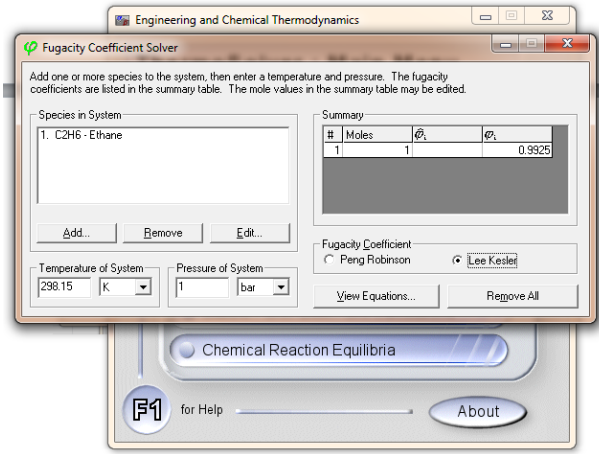
2. We picked the Fugacity Coefficient Solver option.

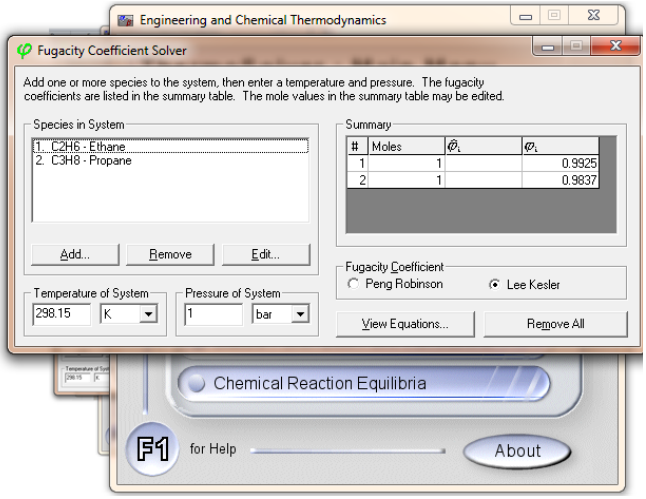


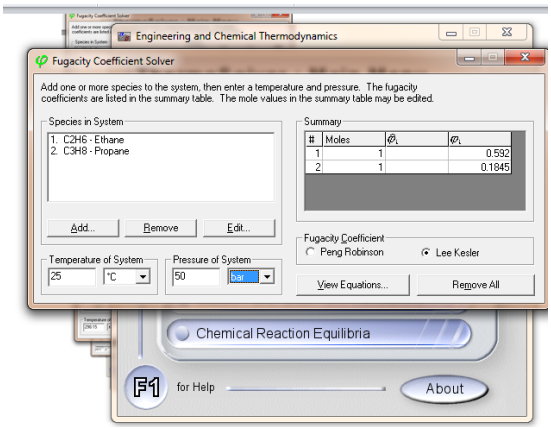


3. We add the two components that we are going to use: ethane and propane for 1 mol and we choose Lee Kesler equiaton.

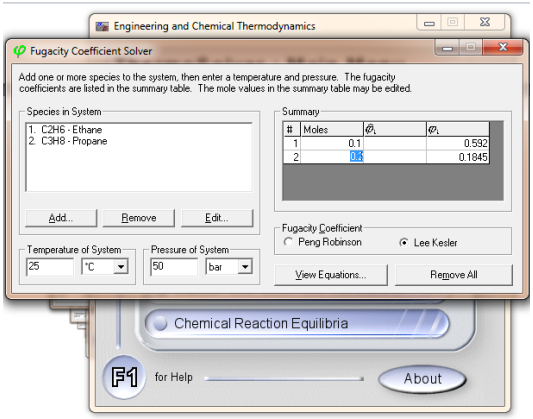








4. We observed that if we change the number of moles the fugacity coefficient does not change at all, and this makes sense because these two component are not interacting. This is becasuse we take the statement that the activity coefficient behavies equal in the mixture as is does in the pure state.



5. With this two constants:

Fugacity coefficient Ethane (∅): 0.592

Fugacity coefficient Propane: (∅) 0.1845

We could create the graph.

$$f = y * \emptyset * P$$

So fist we calculate $y * \emptyset$, from 0 to 1 moles.

$$\emptyset = (x_{ethane} * \emptyset_{ethane}) + (x_{propane} * \emptyset_{propane})$$

For example:

∅ =(0.1*0.592)+(0.9*0.1845) , then (0.2*0.592)+(0.8*0.1845) …

Always with the fugacity coefficients constant.

Then we multiply all the expression by P (50 bar) and so we obtain the fugacity.

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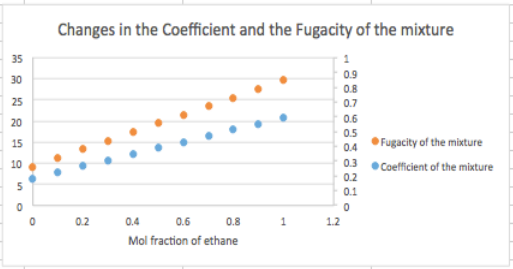
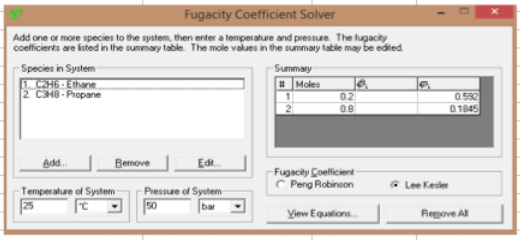
	A	B	C	D	E	F	G	H
1	Mol fraction of ethane	Coefficient of ethane	Mol fraction of propane	Coefficient of propane	Coefficient of the mixture	Fugacity of the mixture	Presión (bar)	Temperatura (°C)
2	0	0.592	1	0.1845	0.1845	9.225	50	25
3	0.1	0.592	0.9	0.1845	0.22525	11.2625		
4	0.2	0.592	0.8	0.1845	0.266	13.3		
5	0.3	0.592	0.7	0.1845	0.30675	15.3375		
6	0.4	0.592	0.6	0.1845	0.3475	17.375		
7	0.5	0.592	0.5	0.1845	0.38825	19.4125		
8	0.6	0.592	0.4	0.1845	0.429	21.45		
9	0.7	0.592	0.3	0.1845	0.46975	23.4875		
10	0.8	0.592	0.2	0.1845	0.5105	25.525		
11	0.9	0.592	0.1	0.1845	0.55125	27.5625		
12	1	0.592	0	0.1845	0.592	29.6		
13								





		Pure Ethane	Ethane in the mixture
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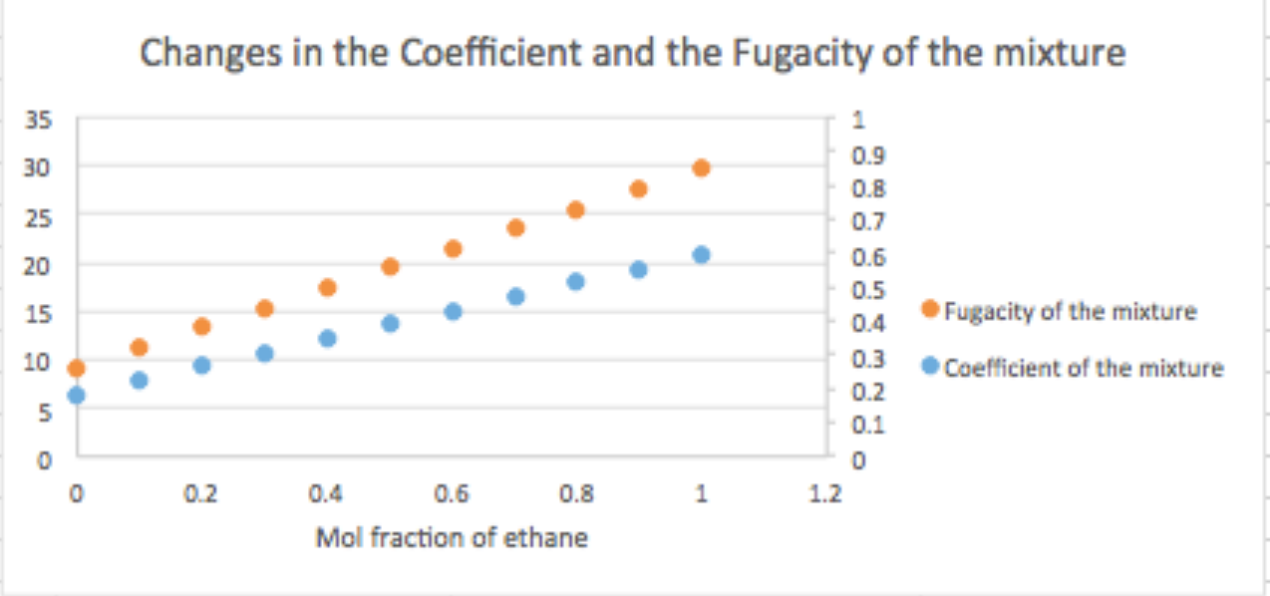
30	Fugacity Coefficient	0.5998	0.592
31	Fugacity (bar)	29.99	29.6
32			



6. Conclusions

Activity coefficient for mixture	Fugacity for mixture	Deviation from ideality
0.1845	9.225	0.8155

0.22525	11.2625	0.77475
0.266	13.3	0.734
0.30675	15.3375	0.69325
0.3475	17.375	0.6525
0.38825	19.4125	0.61175
0.429	21.45	0.571
0.46975	23.4875	0.53025
0.5105	25.525	0.4895
0.55125	27.5625	0.44875
0.592	29.6	0.408

As we know, the fugacity for an ideal mixture is 1. Taking this into account, we can notice that the deviation from the ideality, obtaining the difference between the fugacity of the mixture and the ideal mixture. The greater is the concentration of ethane, the greater the deviation of the mixture. This is due to the molecular interactions, because we have greater molecular interactions between our components. In addition, the ethane is a compound that presents the greatest deviation to the ideality instead of the propane at 50 bars.