Aspen Plus Simulation Software- A Basic Course for Beginners

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Lecture - 17
Practice Problems on Pure Components

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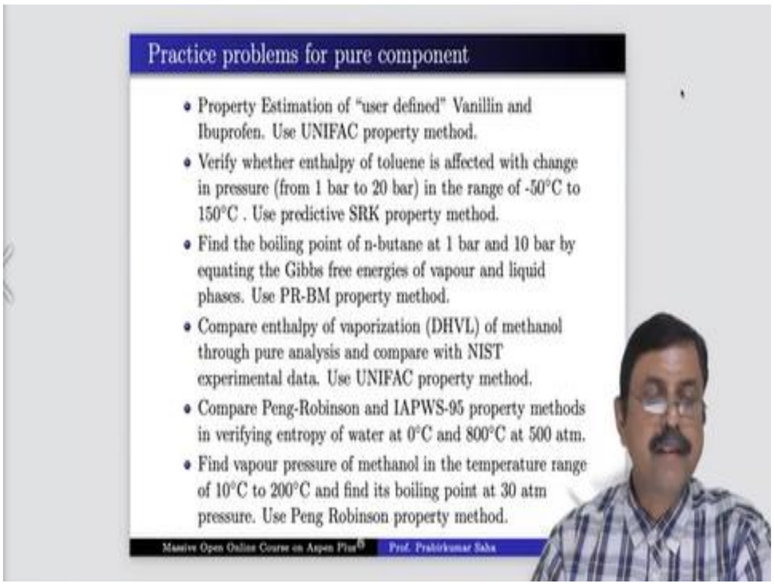

Practice problems for pure component

- Property Estimation of "user defined" Vanillin and Ibuprofen. Use UNIFAC property method.
- Verify whether enthalpy of toluene is affected with change in pressure (from 1 bar to 20 bar) in the range of -50°C to 150°C . Use predictive SRK property method.
- Find the boiling point of n-butane at 1 bar and 10 bar by equating the Gibbs free energies of vapour and liquid phases. Use PR-BM property method.
- Compare enthalpy of vaporization (DHVL) of methanol through pure analysis and compare with NIST experimental data. Use UNIFAC property method.
- Compare Peng-Robinson and IAPWS-95 property methods in verifying entropy of water at 0°C and 800°C at 500 atm.
- Find vapour pressure of methanol in the temperature range of 10°C to 200°C and find its boiling point at 30 atm pressure. Use Peng Robinson property method.

Massive Open Online Course on Aspen Plus® Prof. Prabirkumar Saha

Welcome to the massive open online course on Aspen plus. In today's lecture we shall perform some practice problems for pure component analysis. It is about property methods and property estimations. So, we have a total of six problems that we will solve today. The first problem is about property estimation of user defined Vanillin and Ibuprofen. Now both vanillin and ibuprofen are common components. So, they are available as conventional components in the aspen database.

But in today's problem we will use them as user defined, so for that we will use the UNIFAC property method as it has been asked in the problem.

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So, for that let us go to the aspen plus simulation window. Here we have to set the component as user defined. So, let us say my component is Vani we place them alias save alias is also Vani press next. Here we have to draw or import or edit structure, now for that we do not know the structure of Vanillin. So, we can go to the internet and search for the structure so we write Vanillin over here and we find the structure.

So, here we have all the necessary information for Vanillin. We have molecular weight, boiling point density etc. so this is the structure that we have which we want to draw, so we have one benzene ring; one oxygen over here H the O H O and CH_3. So, we will reproduce it so we have a benzene ring then we have C, we have an O here, and then H and then again, another O and here also we have an O and there is a CH_3 over here.

So, all of them are single bonds, except this one which is a double bond. So, let us connect them so this one connects, these two are connected, these two are connected, these two are connected, these two are connected and these two will be connected with a double bond. So, that will make our structure the same as the vanillin structure. So, we can close it. The structure is now available because we have drawn it.

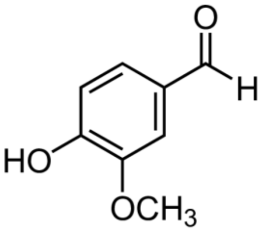

Fig.1 shows Vanillin structure

And molecular weight it is 152.15 so 152.15, the normal boiling point is 285 °C and the specific gravity what is the density it is 1.06 so this is the specific gravity, press, Next. We do not have any additional data or parameters, so we can just ask the aspen to estimate the property and finish. Similarly, we look for ibuprofen let us name it as IBUPR the alias also we give the same name press next.

Now here also we have to draw the structure or import. Now we do not want to do the same exercise again and again of drawing structure, rather we can search for a molecular structure on the internet and download it. So, for that we will go to the internet once again and look for there is a website called chemical book you can even directly go to that website chemical book so it is chemicalbook.com here you can search for the structure ibuprofen.

And here you have the structure in the .Mol file which you can download. And you can see this file has been downloaded. It is a .Mol file so it is a Mol, it contains the molecular structure of ibuprofen so it is available. Now go back and just open that particular structure and bring it over here and this is available with you. Close it you have to give the molecular weight, so again you search for ibuprofen. I think it will be available in Wikipedia, yes, it is available 206.29 g/mol.

So, just write 206.29 g/mol, boiling point it is 157 ℃ and specific gravity is not given but just you can enter Wikipedia I believe it will be available, over here. Yes, the density is available, it is 1.03 g/cm^3 so just write 1.03 press next. Here again we do not have any more data so we just estimate the property finish. Now both the components are defined. Now press next and we have been asked to use the UNIFAC property method.

So, we just write the UNIFAC run so it is available now, the data is available over here just go to the results. So, the critical temperature of vanillin is estimated to be 812.848 K. So, let us check what the critical temperature of vanillin is. So, again we go to the internet and write about the critical temperature. So, critical temperature of vanillin is so here it is available vanillin thermodynamic and transport properties.

We have a critical temperature 777 Kelvin, whereas in the aspen property estimation process it has calculated the critical temperature of varying as 812 K. So, obviously the estimation is always a rough calculation so it will not give the exact experimentally found value. But it has estimated some value of critical temperature which we can always use if the component in question is not available in the conventional list of components in aspen plus database.

Here we have certain temperature dependent properties of vanillin, heat of vaporization, liquid thermal conductivity etc. has been found and for ibuprofen the same thing heat of vaporization is this liquid thermal conductivity they are all available, and for pure component case ibuprofen the critical temperature has been calculated to be 623.705 K. And you can just go and check in the internet what is the actual critical temperature of ibuprofen. That can be taken as a task, and you can just check how close they are.

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The next problem that we have is about verifying whether enthalpy of toluene is affected with the change in pressure from 1 bar to 20 bar and the temperature range is - 50 ℃ to 150 ℃ and we have been asked to use a predictive SRK property method. So, it is a new simulation.

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So, open a new simulation here you have to add toluene and then press next and you have to choose the property method which is predictive SRK, so it is PSRK, run, so the estimation has been done. Now we have to bring in the pure and it is about the enthalpy of toluene. So, just bring in enthalpy which is H enthalpy of a pure component, in J/kmol, right vapour and liquid both, it is from - 50 to 150 °C and the pressure is 1 bar.

So, everything has been given - 50 to 150, 1 bar. So, now we have to run analysis, so it is available the vapour H toluene and liquid H toluene, so we just write it as one bar and this one also we write one bar because both the graphs are for one bar pressure. Now the same exercise we have to do for 20 bars also, so we bring another pure component exercise.

There also we have to choose the enthalpy which is here press toluene - 50 to 150 °C and then here we have to write 20 bars. Everything has been given now run analysis. The second case we convert it into J/kmol and we change it to 20 bar and 20 bar again. Now we merge these two plots so that we can understand them better. Yes, we have merged but we have to use it with a single y axis,

Yes, now you can compare them. You can see that the vapour curves, that is the blue one and red one, are quite apart but the liquid curve they are superimposing on each other for 1 bar and 20 bar. That necessarily means that in the liquid phase the enthalpy does not change with pressure but in the vapour phase definitely the enthalpy changes the pressure. So, our next example is about finding the boiling point of n butane at 1 bar and 10 bar.

By equating the Gibbs free energies of vapour and liquid phases, so as we know that if the Gibbs free energy changes like this in vapour phase and it changes like this in liquid phase. Then the point of intersection where the Gibbs free energy in liquid phase and Gibbs free energy in vapour phase will be equal is actually that is the boiling point of the pure liquid. So, that is about theoretical understanding.

So, in this manner we shall find out the boiling point of pure n butane at 1 bar pressure and at 10 bar pressure. So, we open a new simulation window. So, we have to enter n butane and the property method we will take is the PR-BM, which is the Peng Robinson equation of state with Boston Mathias modifications. And we will run it. So, it is run now we have to find the Gibbs free energies for vapour and liquid phases.

So, we call the pure analysis tool the Gibbs energy for pure component in joules per kilo mole, take both vapour and liquid, select butane, make it 1 bar pressure and begin from - 50 to say 150 and run the analysis. Yes, so this is the temperature at which the Gibbs free energy for vapour and Gibbs free energy for liquid they match. So, let us zoom it a bit so zoom it once again.

So, we can see it is - 0.8 °C, this is - 0.8 °C or between - 1 and - 0.8 we can say - 0.9 or - 0.85 so we conclude that at 1 bar pressure the boiling point of n butane is - 0.85 °C. Now we have to cross check with the actual value so, let us again go to the internet and write here boiling point of n -butane, it is - 1 °C okay, so the normal boiling point is -1 °C.

And we have found it - 0.85 °C but you also have to remember that we have taken it 1 bar not 1 atmosphere pressure and one bar is less than one atmospheric pressure, because one atmosphere pressure means 1.02 bar so this much of error is expected. Now the same thing we can do it for 20 bars as well and run the analysis once again and here we find it over here. So, it is somewhere 114 °C.

So, at that temperature the Gibbs free energy of vapour and liquid they intersect the lines intersect with each other at 20 pressure. So, we can conclude that at 20 pressure the boiling point of n butane is 114 °C.

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So, our next problem is comparing the enthalpy of vaporization of methanol through pure analysis and comparing it with the NIST experimental data set and we can use the UNIFAC property method.

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So, for that let us go to the aspen simulation indoor once again to open a new simulation so it is methanol and enthalpy of vaporization. So, methanol we use the UNIFAC property method to run it. Now you have to bring in the pure analysis so it is enthalpy of vaporization. So, you will find it as DHVL. This is enthalpy of vaporization of pure component joules per kilo mole methanol, this analysis will be done later.

First let us bring in the NIST data. So, NIST data for methanol let us bring it first so it downloads through the internet so it might take some time. It all depends upon the speed of the internet . Somehow today it is quite slow. Now it is available so just close it and here you will find enthalpy of vaporization or sublimation liquid versus gas. Here you find the experimental data and there are actually 59 sets of data and most of them are accepted and a few are rejected as well.

So, we save the data and we save only the accepted data. So, press ok and you will find a data set over here. So, go to the data set and you will find the property and methanol. This is the data and you can compare this data with the property estimation run of aspen plus. But first let us plot their properties versus temperature. So, these are the experimental data that we have found. So, DHVL in J/kmol with temperature K, fair enough so it begins from around 245 K to 480 K.

So, let us run our simulation in this window, 245 K to 480 K and run analysis, yes so it is J/kmol, temperature in kelvin so it is also the same, so now let us compare the graph and merge the plot. Yes, so you just make it a single axis graph, so that is it. So, here we find the result: we have the experimental result all green dots and we have the simulation result the blue line and both of them match.

That means the aspen property estimation method, namely the UNIFAC property method, can properly estimate the enthalpy of vaporization of methanol and it can match the data found through the NIST database.

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So, our next problem is comparison of the Peng Robinson method and the steam table method. These two property methods in verifying the entropy of water at 0 °C and 800 °C at 500 atm.

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So, for that let us open a new simulation window where we find water and we have two estimation methods one is Peng Robinson method which is equation of state method and we also have the IAPWS 95 which is steam table method which is actually ideal for water and steam. So, we use IAPWS. We have to run it twice because we have two property methods.

Yes, now it is done. Now we have to verify the entropy of water at 0 °C and 800 °C. So, just bring in the pure analysis for water and entropy is represented by S entropy of a pure component units J/kmol-K, right both vapour and liquid and there are two values one is 0 °C another is 800 °C and the pressure is 500 atm, now run analysis.

First, we will use the steam table method, we have two property methods over here. So, we are not interested to know about the plot. We will see the result only, so this is the result we have two temperatures and the pressure is 500 atm and we have the vapour entropy and liquid entropy. We have to bring in the pure component once again because we have to do the same thing with the Peng Robinson method.

So, bring in the entropy, sorry it is entropy for vapour and liquid select water a list of values 0 ℃ and 800 ℃, pressure is again it is 500 atm, now you have to run analysis. So, here again you see this one 500 atmosphere for pure input and this one you check, so this is pure 1 this is pure 2 this is for steam table method and this is for Peng Robinson method check the results for both.

So, here you can check the in steam table method we have let us use it as let us take kJ/kmol-K the figures will look better here also take kJ/kmol-K. So, in the Peng Robinson method we have 53.3176 kJ/kmol-K and in the steam table method we have 52.494 kJ/kmol-K, now as it is steam table method at 800 ℃ it is gas. So, I believe this figure is correct. It is 52.4944 kJ/kmol-K and at 0 ℃ it is liquid mostly if it is not solid.

So, it is – 169.87 kJ/kmol-K, in the Peng Robinson method it is calculating - 175.72 kJ/kmol-K obviously it cannot because it is an equation of state method in gas phase. So, it will not predict the liquid phase behaviour properly but the vapour phase it has predicted well because it is – 53 kJ/kmol-K and here it is - 52.5 kJ/kmol-K. So, which are very close enough so we can conclude that Peng Robinson method can very well predict the entropy of water in the vapour phase.

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So, in the last problem we have to find the vapour pressure of methanol in the temperature range of 10 ℃ to 200 ℃ and find its boiling point at 30 atm vapour pressure. That means when the vapour pressure is 30 atm, what is the boiling point that we have to find out. And we have to use the Peng Robinson property method.

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So again, go to the aspen plus simulation window and open a new window, add methanol and Peng Robinson property method run. So, this is the last example of a pure component where we have to find the vapour pressure. So, vapour pressure is represented by PL, pure liquid. So, liquid vapour pressure for pure components is calculated by the specified property method and as in this example Peng Robinson method.

Let us use the atmosphere over here because we have 30 atm we have to calculate and these 10 °C to 200 °C. So, write 10 °C to 200 °C. Choose methanol and we are set. Now run the analysis yes so this is the vapour pressure curve for pure methanol with respect to temperature. So, now you can check at 30 atm the temperature is 185 °C.

So, basically if you hover around it, you can check the value is 30.2 atm and 185 °C. So, actually at 30 °C it should be a little less, maybe instead of 185 °C, it can be 184 or 183.5 not less than that. So, we can conclude that when the vapour pressure is 30 atm then the boiling point of methanol will be 185 °C.

(Video Ends: 35:06)

So, in today's lecture we have done various practice problems on pure component analysis. It is an extension of the property estimation methods that we have learned. So, in the very beginning we have learnt each and every component individually and today we have done some practice problems. So, we end our lecture with these six problems only. We will continue in the next lecture. Thank you.