Aspen Plus Simulation Software- a Basic Course for Beginners
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Lecture - 16
Data and Regression (Part 2), Property Estimation

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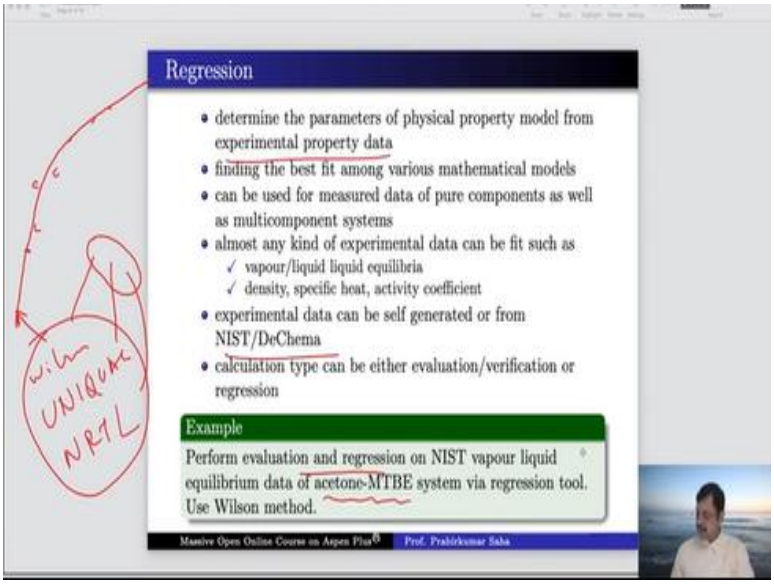

Then we come to regression. It is about determining the parameters of physical property model from experimental property data and we have to find the best fit among various mathematical models. So, say if you have a data set of this nature, so this is the data set now you may think that this is the best fit curve that you can get. So, this curve may be Wilson model or it may be unique or NRTL I am talking about only the activity coefficient models. Now it can be anything.

So, each and every model they have different types of equations and those equations have their own parameters, so these parameters can be obtained through regression of this data. So, where from we can get the data? We can get the data either from your own experiment or you can get it from NIST, DeChema or any other model. So, here we have got an example where we have to perform evaluation and regression on NIST vapour-liquid equilibrium data of acetone MTBE system via regression tool and they have asked us to use Wilson method. Now for that let us go to a new simulation.

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So, we have acetone and MTBE there are two components acetone MTBE. It is methyl tert butyl ether. And the process is done by Wilson method. So, Wilson method press next find the binary parameters. So, it has found the binary parameters of Wilson model. This is temperature dependent binary parameters. Now you may be willing to know what is the Wilson model? So, for that let us go and check the exchange what is Wilson model.

So, this is Wilson activity coefficient model. So, click on this so, this is the Wilson activity coefficient model, so you can see the activity coefficient is a function of Aij and Aji with x j and x k where x j is the mole fraction of a component j in the liquid phase. So, this is binary parameter aij, bij, cij ,dij and eij there are 5 parameters. And they are unsymmetrical parameters that means you have aij and you also have aji and they are not same.

So, that is why it is called it is unsymmetrical. So, any pair they should have 5 into 2 10 parameters. So, 5 a b c d e into 2 so there should be 10 parameters. Now for that we have got the data and here we find the model given by aspen A does not have any value b ij has some values C and D do not have any value and E also does not have any value. So, Wilson model that is proposed by aspen does not have or any other parameters other than bij and bji.

So, basically out of 10 parameters this model has given weightage on only 2 parameters rest of the parameters they do not exist at all. So, they have considered them to be 0. Now if you consider this Wilson model to be right then let us see whether this Wilson model actually defines our acetone MTBE data. For that let us go to NIST binary mixture acetone MTBE retrieve data. We have only one source of binary really isobaric.

So, let us choose this we have binary data liquid mole fraction of acetone and vapour mole fraction of acetone at this temperature range and pressure is 94 kPa. It is not one atmosphere less than one atmosphere. So, you will just save the data. So, this is the data set we have. This is the data set we have. Now let us choose the T x y diagram. So, the experimental value of y and x at 94000 Pascal 94 kPa we have this two data set.

Now we want to evaluate our Wilson model given by aspen and check whether the Wilson model fits the experimental data. For that we have to go to binary T x y diagram mole fraction and here we have to place 94 kPa. So, property method Wilson let us do the analysis. So, run analysis. So here we have T x y diagram for acetone and MTBE and this is the model output this is not the experimental output.

Experimental output is here, this is the experimental plot and this data has been recovered from NIST. And this is the binary plot it is actually from the Wilson model suggested by aspen. Now let us change it to kelvin and let us merge these two plots. Now first let us merge this in a single axis. Now you can check the experimental data are here. Now you can see the difference between the experimental data and the simulation data.

Here this is the actual experimental data and this is the regression or this is the evaluation data. This is the evaluation data that we are getting. Now these two are not matching. Now we want to do the regression once again so that our Wilson model matches with the experimental data set. For that we will do the regression first. So, press new Wilson model data set you have to choose. So, this is the data set we have chosen.

Now first you have to do some evaluation whether the data are consistent you can give a tolerance value of say 3%. And check whether the evaluation can be done. So, evaluation is done go to results and see the consistency test. So, it has passed the consistency test so thermodynamic consistency test for binary failing data has been passed because the value is within 3% tolerance limit. Now we will do the regression first, so for that we will call the recreation once again.

It is a new DR1 the data set is BVLE001. And this time we will do regression because we want to find out the aij aji bij bji etc. Go to parameters. Now here the type of parameter obviously will check binary parameters. Now you might remember that Wilson model that we had checked it had only bij and bji only these 2 parameters were there in the Wilson model that we had. It did not have aij aji or c or d or e those things are not there.

But in our regression, we will add all of them. So, total we will have 10 parameters and those 10 parameters will be aij, aji, bij, bji, cij, cji, dij dji and eij eji. So, for that let us choose Wilson element one component acetone and MTBE that is, it. And set aji aij equal to 0, no it there is it is not. So, we have to press, so just copy them for 10 parameters. So, this will be MTBE. First, we have to check it to be 2. So, this should be 2 this should be 3 this should be 4 and this should be 5.

So, 5 parameters a b c d e all of them are here. So, acetone MTBE, acetone MTBE, acetone MTBE, acetone MTBE. Now the same thing you have to do for the MTBE acetone. So, here we have done for aij, bij, cij, dij and eij. Now here you have to do MTBE and acetone. So, it is aji. So, copy paste and so this is 2 this is 3 this is 4 and this is 5. Here it should be acetone, acetone, acetone, acetone. So, 1 2 3 4 5 1 2 3 4 5. Now we have to do the regression.

So, basically, we have set the parameters all the parameters now we have to do the regression. For that run the regression, so it will take some time we have to patiently wait. So, it has done very fast. It says value of parameter Wilson already exists in the component acetone MTBE on the parameters form. You can choose to replace it with request results from DRS. So, we will say yes, yes to all. That means all the parameters will be changed including bij, bji.

So, go to Wilson once again and here it is no longer the previous thing that we were using it is no longer APV 110 LGE. We have got R DR1. It is value retrieved from R DR1 so this is DR1 result. So, in the previous case we had only bij and bji no other parameter was there. But when you do the regression and you will find all of them aij aji, bij bji, cij, cji and up to eij and e ji they are not regressed.

Anyway, so without them only the regression is complete and this source is DR1 that is the result of regression. Earlier you might remember that we were using this one. Now we will not use this we will use only this. Now we do the binary study once again. So, we have T x y data, calculation option Wilson and run analysis. So, this is the binary analysis but we have done a mistake we have done it at 1 atmosphere pressure.

But we should not do it at one atmosphere pressure we have to do it at 94 kPa. So, it should be 94 kPa and do the analysis once again. So, we have the data set over here, and with this data set let us calculate T x y plot it and the binary plot we have to make it in kelvin and then match with the previous one. So, merge plot with this one, so make it y axis it is not needed because they are the same but still. So, we have got single axis.

So, you can find the experimental data of y is given by the red dots and the Wilson model has been given by the green dot and green line. So, they go through almost through the data set, the same thing can be said about the experimental data of x it is square and this versus this, this is the model with revised parameter after the regression. And we have plotted both of them together and the Wilson model after our regression, it is following the data in a proper manner.

So that is how we can do the regression for model fitting. If we are not happy with the model given by aspen plus.

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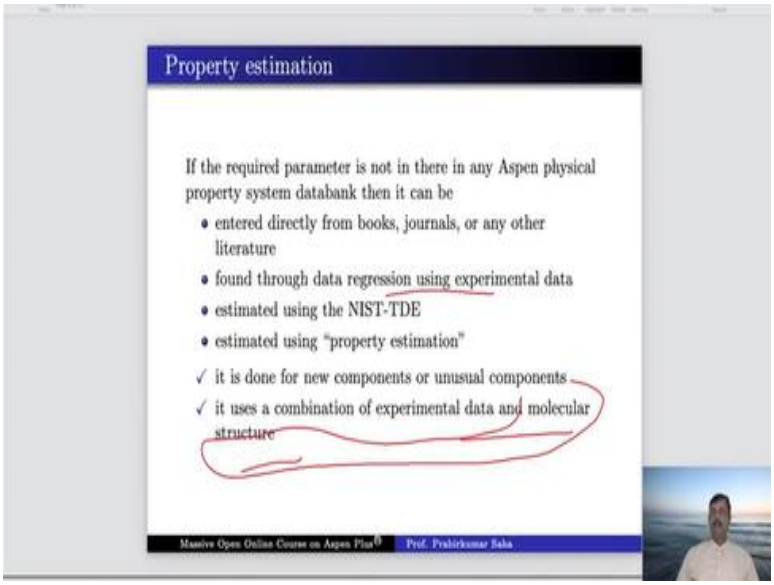

Now we will learn about the property estimation, now if the required parameter is not there in any of the aspen physical property system data bank, then it can be done by entering directly from books and journals or any other literature or it can be found through regression analysis the way I

have done just a couple of minutes back. And then it can be a combination of experimental data and molecular structure. Now we will learn about this molecular structure in the coming slide.

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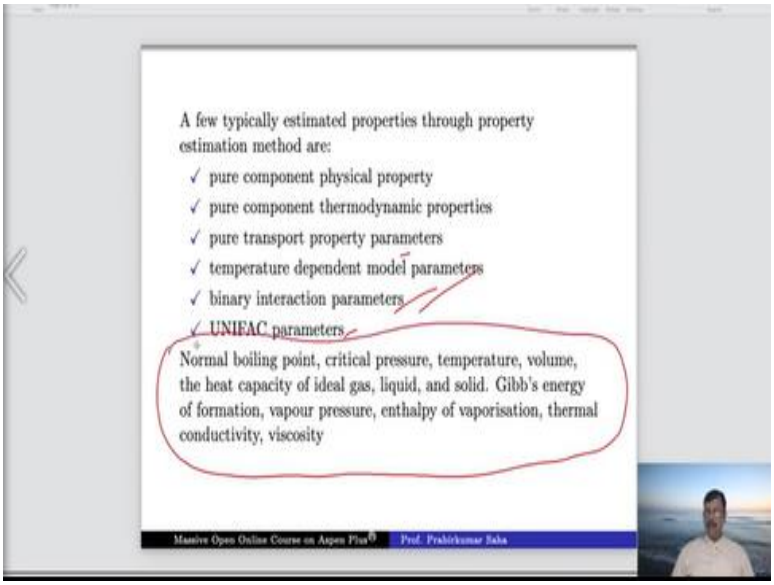

Now a few typically estimated properties are pure component physical property, thermodynamic property, transport property, temperature dependent and binary interaction parameter, UNIFAC parameters and lots of parameters that you can think of.

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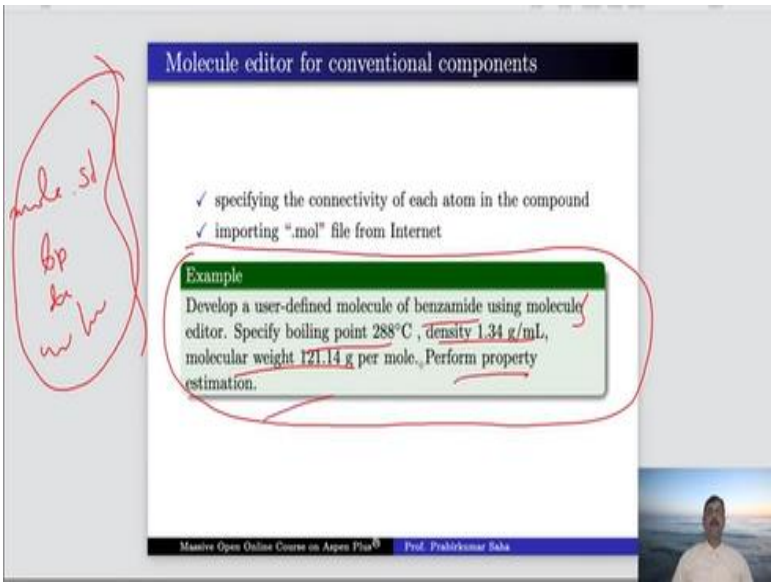

Now this is molecule editor for conventional component. So, conventional components suppose that particular component that you are talking about that component is not there in aspen database. But you have certain information minimum information such as you know the molecular structure

you know the boiling point of the substance, density, molecular weight and so on. So, as many information that you give about that particular component it will be better for aspen to get an idea about how to do.

The concept is something similar to tab poly. Now we will best learn it through this example, here we have a user defined molecule benzamide using molecule editor. So, we have the information boiling point of benzamide, density, molecular weight. Now we have to perform property estimation. Now let us do it for that let us go to the aspen window.

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Let us find original benzamide. So benzamide, this is the benzamide molecule. So, aspen plus has all the information about this benzamide. Because it has the it is a conventional component and aspen plus has the information about benzamide. But suppose you want to define a component called Benz and you want to give all the properties of benzamide, whatever the properties that you have you want to give it to it.

So, give benzamide, so this is the user defined component Benz press next. Here it asks for intermolecular structure, so here you draw or import or edit structure. Suppose you can draw a structure. Now how the benzamide looks like, so this is how benzamide looks like. It is a benzene with amide and wedge group. This is the structure of benzamide with the chemical formula of $C_6 H_5CNH_2$. So, its molecular weight is 121.14 solubility is 13 g/L melting point, flash point everything is given.

Now we are interested to know about the structure, so we just want to place this structure over there. So, we just place this structure so, this is the benzene ring this is C this is amide and we have an oxygen and we have the bond. So, there is a single bond between them and there will be another bond with this and there will be a double bond between these two. So, now it is same as this one. So, molecular editing is complete.

Now sometimes you it is very difficult to draw molecular structure like this, it may be cumbersome. In such situation you may try in the internet you will find certain molecular structure in the form

of mol file. So, it will have a name say ben mol file. So, that molecular structure file you can import, so there is a there is an option to import the structure. So, import is possible. Now we have defined the structure is available just now we have given.

Mmolecular weight yes, we know molecular weight is 121.14. So, give this information boiling point we had the information over here it is 288 ^{0}C and specific gravity it is 1.34 g/cc density. So, obviously the specific gravity is 1.34. Now this information you do not have but suppose if you have this information, you can feed in. Then aspen will calculate the missing parameters of Benz quite easily and more accurately.

If you do not have do not worry press next. Here, click buttons 1 to 5 to enter additional data or parameters. So, do you have molar volume data if you have you can give in vapour pressure data the way we have given in tap poly same thing we can give extended Antoine vapour pressure coefficient, ideal gas heat capacity, ideal gas heat capacity polynomial coefficient etc. So, you can evaluate it using NIST data or you can estimate using aspen property estimation system.

So, finish saving the property data you entered in the component. So, now Benz has been defined as conventional comp. Now let us go to the method and in this kind of situation it is best to use UNIFAC because lot of estimation has to be done and if you run it, now we can go to estimation and see the results. Here, we have the results so we have pure component benz, we have not given the data for critical temperature we have given the data for boiling point.

But it has estimated the critical temperature of benzamide which is 822 k it has calculated. Now let us check what is the benzamide critical temperature in the net. So, it is said critical temperature of benzamide is 749.85. So, here we find the critical temperature of benzamide is 749.85 whereas aspen calculates it at 822.039. Although it is quite far apart but still, we can work with and more data that we can give for the particular benzide component we will get more and more accurate result.

And there are some temperature dependent parameters heat of vapourisation it has calculated liquid thermal conductivity has calculated and you can check the net whether they are very close to the real parameters or real data.

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So, with this we come to the end of this lecture. Thank you.