Aspen Plus Simulation Software: A Basic Course for Beginners

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Lecture – 13
Property Methods and Property Sets with Example

Welcome to the massive open online course on Aspen Plus.

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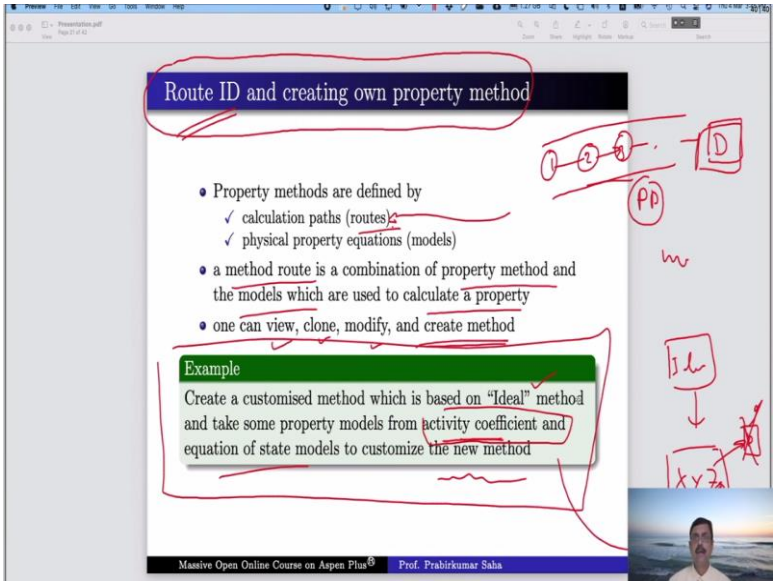

In this lecture, we shall study about the route ID and creating one's own property method. In the last lecture, we discussed the property methods in detail, but they were already available property methods in Aspen plus domain. But in today's lecture we shall discuss how to create one's own property based on the available models we have or customized models that we can edit.

Now, before that we have to find out what is the route? The route is as we know that the property method is nothing, but a combination of different models and the models are nothing, but a set of equations. Now, while calculating a physical property we have to use these model equations judiciously one by one. There should be a protocol that the dataset goes from the first set of equations to the next set, from the next set the result will go to the third set and so on.

Until we get the desired properties that we have. So, the calculation path is called the route and each and every route has a separate ID. By choosing the route ID we can set that we want to

go through this route to arrive at this desired physical property. So, this method route is a combination of property methods and the models which are used to calculate the property.

Now, one can view, clone, modify and create one's own route that means you can clone already present routes and then you can edit them to create your own. So, we shall see an example which says create a customized method which is based on an ideal method and take some property models from activity coefficient and equation of state models to customize the new method.

What does it mean? We will clone the ideal method first, we will name it some xyz model and then we will know that the ideal model has some route ID where some property methods are described. We shall choke them out and take up some activity coefficient model method and add into this so that will be your new property method obviously it is for advanced users who can make this thing work.

So, we will learn how to do this so that we have to go to the Aspen domain. **(Video Starts: 04:00)**. Let us take a system, say benzene and toluene press next let us say ideal model, run yes. Now just go to the selected model and you will find the ideal. Now what I need to do is create a new thing. So, my new model is to say I use it as MYPROP so it is my property method and my property method the best property. That is the property from which I want to clone it. We will use the ideal property method.

The moment I do it all the ideal property routes, route ID and properties they come over here. Now what is this? This is the vapour fugacity coefficient of a component in mixture and what is this? This is the vapour fugacity coefficient calculated using the ideal gas model. Now let us change it. So, instead of this I will use the vapour fugacity coefficient calculated using the Redlich-Kwong-Soave model.

So, instead of 0, 0 if I choose this one it is no longer an ideal method. The base is ideal, but I have changed the route ID. We can create a route ID in the very first place so for that we just take my route and what is my route. What is the property name let us say property is vapour fugacity coefficient of a component in a mixture. Clone route from this is from ideal gas, vapour fugacity coefficient calculated is in ideal gas model.

So, we have clone the route this is the model name, ideal gas equation state model this model is used for ideal property method let us change it. Let us change it to let us look for the Redlich-Kwong-Soave. Polymer Soave Redlich-Kwong equation of state model this model is used for POLYSRK property method. So, let us use it. So, MYRO route is fixed. Now go back to our property method.

Select the route ID, choose MYRO. This is my route ID. That way I have changed it from the ideal method to the Redlich-Kwong-Soave method, but only for vapour fugacity not for others. Now let us say I want to change this liquid mixture surface tension. Liquid mixture surface tension I do not like this one. So, I go to route, create a new, liquid surface tension with this ID.

Let me check liquid surface tension, clone it from say this one and change the model to this one. So, this is our LST route. Now go back to my prop and instead of SL00. So it is for pure components I believe so pure component liquid pure component and here I find my model user defined LST. So, like that I can change a lot of them and we can create my prop.

Now in the specification method instead of ideal I can use MYPROP method which is user defined and I can use it to run the property method. So, it gives some result now this result maybe very stupid because while changing them I did not give enough thought process. So, this particular example may not mean anything, but for an advanced user this changing the property method is a very good and very effective method to target more and more accuracy for simulation. **(Video Ends: 11:03)**.

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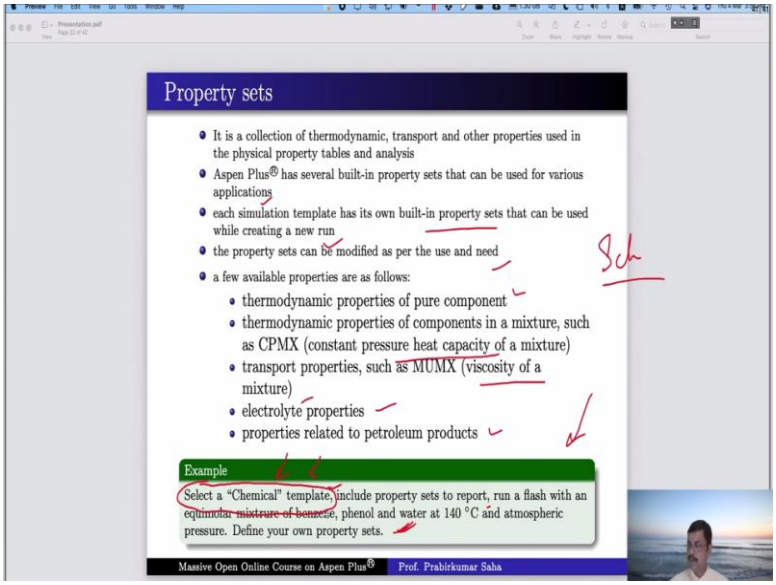

So, next is the property set. Now what is the property set? It is a collection of thermodynamic, transport and other properties used in the physical property tables and analysis. So, Aspen Plus has several built in property sets that can be used for various applications. Each simulation template has its own built in property set that can be used while creating a new run or you may not use any one of them you can start from scratch.

I will give an example like that and we can try one. This property set can be modified as per use and need. Few available properties are as follows like thermodynamic properties for pure components, thermodynamic properties in the mixture such as constant pressure heat capacity of a mixture or viscosity of a mixture, electrolyte properties, properties related to petroleum products.

Now this example has been given: select a chemical template including property sets to report, run a flash with an equimolar mixture of benzene, phenol, water and at 140 °C and atmospheric pressure define your own property set. Now we may not use this, we may start from scratch because if you learn how to start from scratch then you can definitely do how to begin from chemical template because in chemical template already some basic work will be done.

Let us learn how to do it from scratch. **(Video Starts: 13:04)** For that let us go back to our flowsheet. What do we have here? We have benzene and toluene, but here it is written equimolar mixture of benzene, phenol and water. So, we have to add phenol and water then we have to run a flash 140 °C atmospheric pressure. So, go to simulation we do not have anything so let us add flash, bring in material, streams let us name this as feed vapour and liquid.

Press next this is 140 ℃ one atmosphere pressure. So, 140 ℃ and one atmosphere pressure and it is an equimolar mixture so write benzene, phenol and water all of them one then go to next it will ask for flash options. So, let us say duty is 0 and pressure remains in one atmosphere with the flash tank. Go back to properties again. First, we can delete this toluene because toluene does not add to our system.

So, delete it. Select the ideal property method and then run. Now the results are available, just go to the result. Sorry we have not run the simulation so run the simulation first now the results are available so go to stream result and here you will find this information. So, what is the stream result information we have? We have temperature, pressure, molar vapour fraction, molar liquid fraction, solid vapour fraction, enthalpy, entropy, density and so on.

Molar flow rate we have mole fractions, we have mass flows, we have mass fractions we have. In the vapour phase we have this information and in the liquid phase we have this information, but we do not have any more information which you might want to know for that we have to generate a property set. Here create a new property set. So, we can name it as MYPSET.

Now it is said what are the property sets that you want physical property you may want to know the set the free energy of a pure component or say free energy of a mixture. You can set the unit in kJ/kmol. You may ask for CPMX and MUMX that is constant pressure heat capacity and viscosity of a mixture. So just write CPMX and MUMX so CP you can check the unit as kJ/kmol K and MU you can choose centipoise not a problem.

And a qualifier you have to choose liquid phase or gaseous phase. So, let us say we wanted a vapour phase. Now let us go and run the simulation. Now go check the simulation results here you have to add the properties here you do not have anything you can add properties. While adding the properties you will have the combination at the bottom MYPSET Gibbs energy, MYPSET heat capacity, MYPSET viscosity.

So, you can click all of them and click okay then you have these things added along with all of them press okay the moment you press you have these things in vapour phase. So, what is the Gibbs energy, what is the heat capacity and what is the viscosity of the mixture? But I have got

in vapour phase. We do not have the same thing in the liquid phase. Do we have a liquid phase? No we do not have it in the liquid phase because we have not asked for it.

If you go back to MYPSET you can check we have a qualifier and this qualifier is only in vapour phase, but if you want the same information into liquid phase as well we have to choose liquid. So, both vapour and liquid are available. So, just go and run it once again, go to stream results, add properties, come at the bottom, click them once again, press 'Okay' and then press 'Okay' again.

And then you get all of them in the vapour phase as well as in the liquid phase. So, that is how you can create your own property set and for each simulation you can drag those property sets from the definition to its result section so that every time you do not have to repeat it. Once the property set is met that is fixed over there only during the simulation you have to add it. **(Video Ends: 22:35)**.

So, we end our lecture at this point. So, in tomorrow's lecture we shall start with analysis tools. Thank you.