Aspen Plus Simulation Software: A Basic Course for Beginners

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Lecture – 11
Setup: Components

Welcome to the massive open online course on Aspen Plus.

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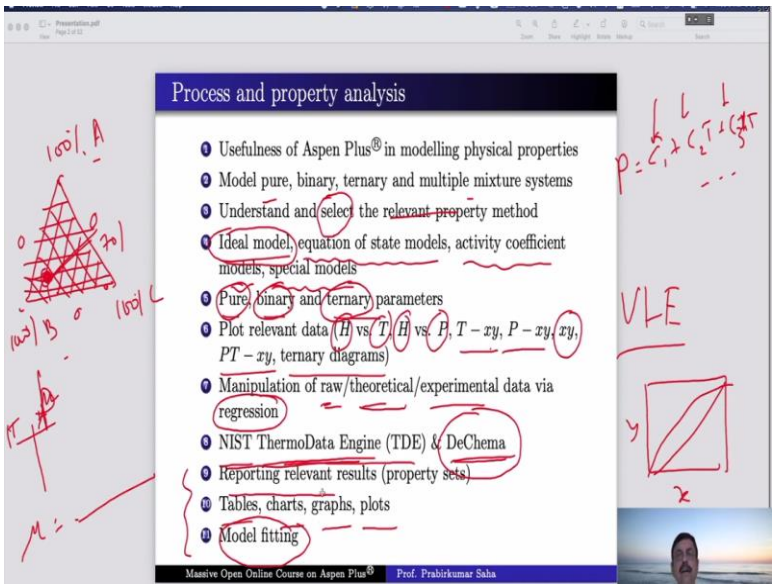

This is the beginning of the third week of this lecture series and in the coming three weeks we shall learn the process and property analysis. Now, we have already learned the property analysis and property data, property methods and other things in the first three weeks of this lecture series, but they were not in detail. We shall learn these things in detail in this three weeks' time mainly we will cover this 11 items.

First, we will learn what is the usefulness of Aspen Plus in modelling physical properties. We will model pure binary and ternary and multiple mixture systems pure means pure components, binary means there will be two components in a system, ternary means three and if we have four or more components we will study it as multiple mixture systems and then we will understand the relevant property methods.

And how to select those property methods in the system basically these property methods will depend upon whether the system is ideal or non-ideal and if it is non-ideal then what kind of property method will fit to the experimental results that we got by studying those systems. So,

we will learn all these things. Basically we know that there are three types of models. One is ideal model if the system is ideal system that means for gases it will follow ideal gas law.

PV = nRT or if it is ideal solution that means if the solution follows Raoult's law and Henry's law then it is called ideal solutions. In such system we will use ideal model, but if that is not if it is real system or real gas or real solution in that case we will use either equation of state model for real gas and activity coefficient model for real solution and we will also have some special models like amines, steam because those are the things which are specific to certain systems where amine components are there or where we have steam.

So, we have special models for that we will also learn them. Basically, we will get the pure binary and ternary parameters because all those models whether it is for pure or binary or ternary or multi component mixtures we will have some kind of model equations. Model means we have a set of equations which will define the whole model. So, if there were models we will have model parameters also.

So, we will find the pure model parameters, binary parameters and ternary parameters as well depending upon what kind of models we are using and then we will learn how to plot the relevant data. We will learn how to find the enthalpy versus temperature (T) or enthalpy versus pressure (P) or we can get T - xy or P - xy diagram that is temperature versus the mole fraction in liquid as well as vapour phases.

Pressure versus xy or simple xy it is VLE that is vapour liquid equilibrium. So, mostly it will have this kind of diagram where this is x, this is y. X means the mole fraction of a component in liquid phase Y means the mole fraction of the same component in vapour phase. We will have P T - xy diagram also and we will have ternary diagrams. Ternary diagram is for tertiary system where we have three components and we will have this kind of diagram.

You might remember that for extraction we use this kind of diagram where this peaks of this triangle they represent 100% of components say this is 100% A, this is 100% B and this is 100% C so where A, B, C are the components and obviously this portion is 0% C, this is 0% B, this is 0% A. Now, if we have a component somewhere here that means it is a 15% of A and 15% of C and it will have 70% of B something like that.

So, that is how it will constitute total 100% of a mixture. Next, we will learn the manipulation of raw, theoretical and experimental data via regression. What is regression? Regression means if we have certain set of data suppose we have temperature versus enthalpy data or temperature versus viscosity data. We know viscosity depends upon temperature or say vapour pressure of a liquid at particular temperature.

We can get that particular relationship so it is

$$P = C_1 + C_2 \times T + C_3 \times lnT + \cdots$$

So, regression means if we have this T versus P experimental data you have to find C_1, C_2, C_3 these are the unknown model parameters that we can find out through regression then we will learn about NIST thermo data engine and DeChema. This is basically a databank or databank of experimental data because everywhere throughout the world research is going on.

And every now and then the researchers are producing loads of data and they are publishing those data in open literature. So, the concern team in this NIST they collect all that data and then they store it. And fortunately, the Aspen users get it free of cost. So, we have a link where if you click it you will go to the NIST thermo data engine. Through that engine you can get loads of information and from that you can choose the correct set of data through which you want to do the modelling.

Similarly, DeChema is also another source of data, but unfortunately this is not free of cost we have to pay this is pay per data basis you can get and finally when you get all those things you have to generate report because working with modelling and getting the parameters is not enough you have to generate certain report which you can show it to your team member for further discussion.

And in that report you have to produce tables, charts, graphs and relevant plots, you have to produce the model fitting parameters also for further calculation or further use for whatever simulation you do. So, this reporting of relevant results also we will learn.

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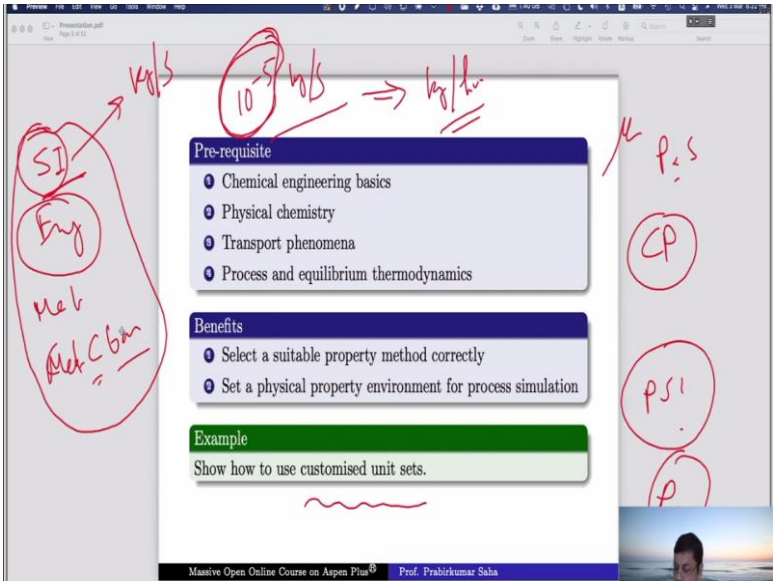

Now to learn this section of property analysis we have certain prerequisites without which we cannot go forward. The first thing is chemical engineering basics. You have to have some basic knowledge in chemical engineering and then also you have to have some knowledge in physical chemistry, transport phenomena and process and thermodynamics. You have to have basic knowledge in order to learn the subject.

What is the benefit you will learn how to select a suitable property method correctly? Because choice of suitable property method is very crucial for correctness of a simulation. If your system is non-ideal and if you use an ideal property method, you will not get an accurate result. Your real life process and your simulated process will be far apart. So, which kind of property method has to be chosen for which kind of system you will learn in this course.

And not only that you have to learn how to set a physical property environment for process simulation. It is not that a process has only one property method. For instance, suppose your reactor is a large system and a large system plant-wide process. It has several unit operations that are connected together, it may have a reactor, it may have a flash tank, it may have a column exchanger.

So, suppose your reactor contains certain components which will produce a non-ideal system. On the other hand, your flash tank may contain certain components which will follow ideal gas law. In such cases you can fix the ideal property method for the flash tank and certain non-ideal property method for the reactor it is possible. So, not that entire plant will follow a single property method.

So, that is called property environment in that you will fix your customized units, you can fix your property method for different units etcetera while I was talking about the customized unit set I define them in this manner basically we have very few numbers of defined system like we can go with an SI unit system or we can use an English unit system or we can use the metric or metric system with centigrade and bar.

We can use centigrade for temperature and bar for pressure. So, these four types of units are available, but your requirements may be different. If you go by SI unit by default your flow rate will be kg/s, but the data may be 10^{-5} kg/s if you use SI units. So, you may not like this particular figure. So, instead of that you may like to have a flow rate of kg/hr.

By doing so, this particular figure will have a higher number. So, depending on your flow rate you may choose kg/hr viscosity. In the SI unit it is Pa.s, but the most common unit for viscosity is cP. Most of the books or literature they report in centipoise. So, you may like to use centipoise not Pascal- second. Similarly, psi for pressure is the most common unit for pressure, but the SI unit is not psi; it will have Pascal.

So, it is possible for you to customize a unit set where you can look for the units which you want to use. So, it may be a mix and match kind of unit set in which we will use some units from SI units, some from the English unit FPS system or some from Metric system (Video Starts: 14:08). For that let us go to the Aspen domain. Now here you see the unit set and you find "define your preferred units for measure of values of all physical types".

So, just click on here, here you have English, Metric, MetricCbar and SI. Here you can say new that means you are looking for a new kind of customized unit. So, you can name it like my unit so create this new ID and it says copy from SI. If you say that most of your units will be SI unit, but some of the units you want to customize to make your life easier. In that case copy everything from SI unit so everything is copied.

Now the mass flow rate instead of kg per second you can take kg per hour. This flow choose kg/hr. You may not like cubic meters for volume, you may like to have litres instead. So, you can say l/hr volumetric flow rate. Temperature you may like to have °C and pressure N/m2 is not your preferred unit, you may like to use psi just use psi.

Similarly, delta P also allows you to use psi. Now these are more general standard units, heat related units instead of joules you can use kilojoules. Similarly, transport units instead of volume you can use litres. This you can use as density g/cm^3. Concentration or size or currency everything you can choose. Viscosity is N.s/m^2, but you may look for centipoise so you just use centipoises. So, you go to the unit set again.

So my unit set is a user defined unit set and this set will have all units as per your choice. That is how you can create and customize a unit set. **(Video Ends: 18:18)**

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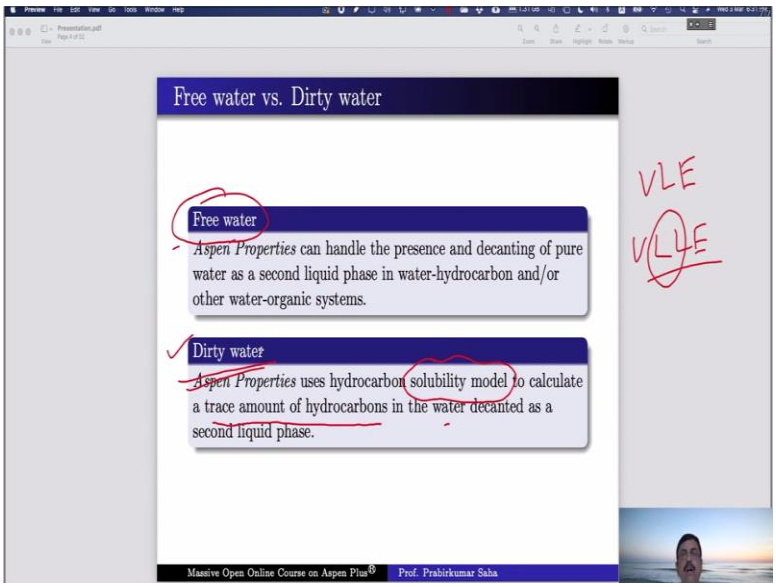

Next, we will discuss about the free water versus dirty water. This free water and dirty water you might have come across in the first three weeks lecture many times we have used free water as a decanted stream. So what is free water and what is dirty water? Free water Aspen properties can handle the presence and decanting of pure water as a second liquid phase in water hydrocarbons and or water organic systems.

So, generally water hydrocarbons are invisible. So, when their mixed stream then many times it might happen that water gets detached from other hydrocarbons and makes a free stream. So, it is no longer vapour liquid equilibrium rather it is vapour liquid-liquid equilibrium where two liquid streams are present in the system and one of them may be a free water which is absolutely pure water which is coming out of the stream as a decanted stream.

On the other hand we have dirty water also where trace amount of hydrocarbon is there in the water because although they are not soluble, but there will be slight solubility of hydrocarbon

in water and we have certain solubility models also available in Aspen property base where the solubility of hydrocarbon in water is calculated and when that kind of system is simulated we can safely call it dirty water.

So, that is the difference between free water and dirty water, free water is absolutely pure and dirty water has a trace amount of hydrocarbon units.

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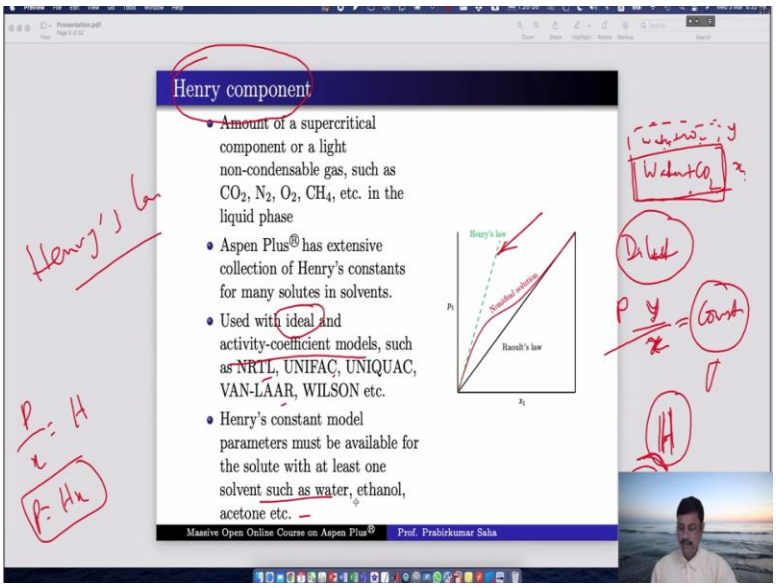


Then many times we have come across Henry's component in simulation. Now what is the Henry component? It is the amount of supercritical component or a light non-condensable gas such as Carbon dioxide, nitrogen, oxygen, methane etcetera in the liquid phase. Liquid phase may be anything it may be organic, it can be inorganic, it can be aqueous solution basically suppose if you have liquid say water if you have water in the liquid phase some amount of carbon dioxide is soluble in water.

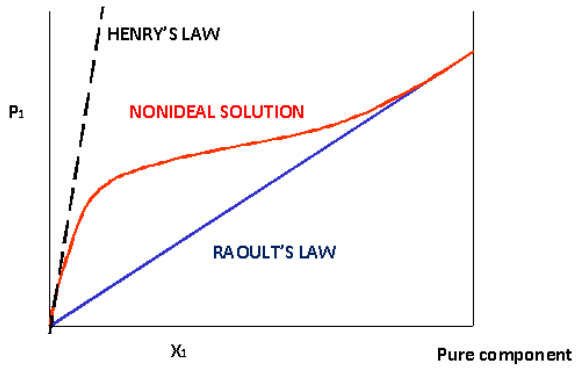
Now this is true only for dilute systems, very dilute systems. Now very little trace amount of carbon dioxide is dissolved in water. So, suppose its mole fraction of carbon dioxide in water solution is x. Now, if you take this kind of system obviously there will be a vapour phase above this and if it is a binary solution then obviously there will be water plus CO_2 in the vapour phase as well and the carbon dioxide in this vapour phase.

Suppose, its component its mole fraction is y. So, x is mole fraction of carbon dioxide in liquid phase, y is mole fraction of carbon dioxide in vapour phase. In both the cases water is the solvent then for a dilute solution y versus x is equal to constant this is Henry's law and this

constant is called the Henry's constant and this is fixed for a particular temperature. So, Henry's constant does not have a unique unit.

If this mole fraction both of them are mole fraction then Henry's component is dimensionless, but sometimes we replace y with partial pressure. So, if it is partial pressure versus x then Henry's component will have a certain unit it will not be a dimensionless thing. So, this is called Henry's law and this Henry's law is true only for dilute systems and this Henry's constant is temperature specific.

So, if temperature changes Henry's constant will also change. Now Aspen Plus has an extensive collection of Henry's constant for many solutes and solvent.



We can graphically show Henry's law over here it is a straight line because if P / x = Henry's constant then P = H into x this is a straight line so this is the straight line we have. Now Henry's law can be used with ideal as well as activity coefficient models.

Such as NRTL, UNIFAC, UNIQUAC, Van-Laar, Wilson etcetera and Henry's constant model parameters must be available for the solute with at least one solvent such as water, ethanol, acetone etcetera.

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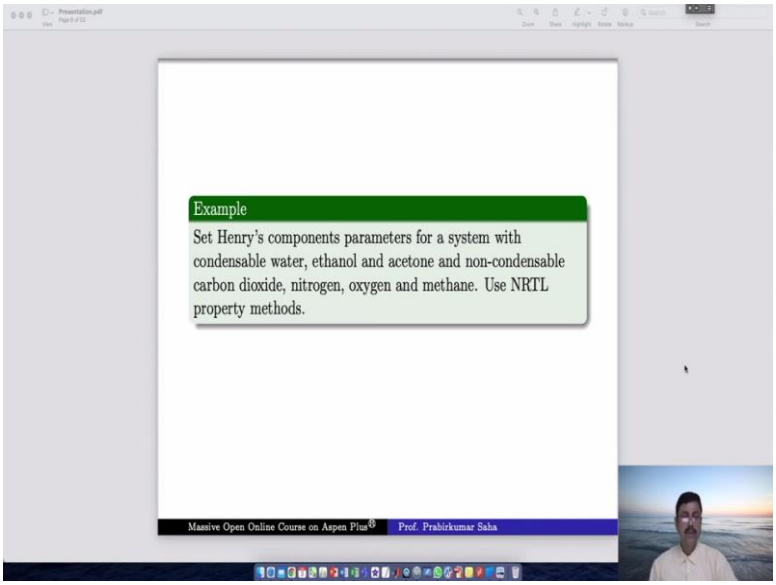


Now we will take a small example where it is asked to say the Henry's components parameters for a system with condensable water, ethanol and acetone and non-condensable, carbon dioxide, nitrogen, oxygen and methane and it has been asked to use NRTL property method. So, let us go to the Aspen simulation window. (Video Starts: 25:00) So, let us go to the components. So, we have water, ethanol and acetone.

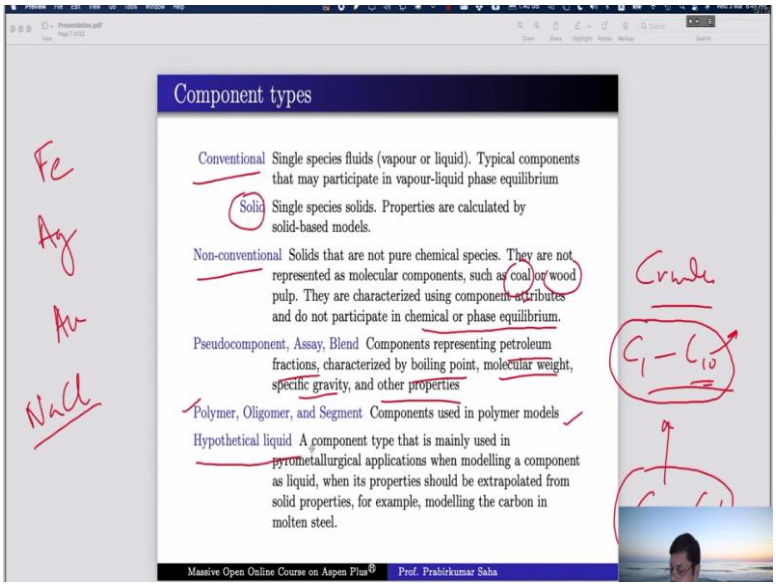
And we have non-condensable gases carbon dioxide, nitrogen, oxygen and methane. So, carbon dioxide, nitrogen, oxygen and methane. Now, we press next and here we can fix Henry's component. We can directly go there and ask for Henry's component or we can choose a method like NRTL. It has been asked to do NRTL and Henry's component we can choose.

Now we do not have any Henry's component defined so we can say new. So, select a new, say HC 1 this is the name of this Henry's component press okay then you can see a new Henry's component has been produced over here. So, this is Henry's component press next. Now say CO_2, N_2, O_2 and methane all of them are Henry's components. So, immediately you can find a Henry's component, binary interaction has been produced over here.

So, these binary interaction parameters are temperature dependent so this is T dependent now we can run it and see we have all Henry's components, temperature dependent, Henry's parameters are available. So, there are four gases CO_2, N_2, O_2 and methane and there are three solvents. So, carbon dioxide with three solvents, nitrogen with three solvents, oxygen with three solvents and methane with three solvents.

So, 3 into 4 so total 12 combinations of components I and J their Henry's parameters AIJ, BIJ, CIJ, DIJ and their temperature limit. So, this is the limit of temperature within which Henry's parameters are valid and all these temperatures are in degree centigrade. So, this is how you generate the Henry's component you said the Henry's components and Henry's parameters are available. Now you can run it and all the property methods are set with NRTL.

Now, if you wish you can add other methods also like you can add the ideal method, you can add UNIQUAC method, there is a new UNIQUAC that has come up, you can use Van-Laar method, the new Van-Laar has come. Now, if the UNIQUAC method is there then you have to get the parameters for UNIQUAC also. So, this is the UNIQUAC parameters. **(Video Ends: 29:42) (Refer Slide Time: 29:43)**



Next, we will learn about the component types. What are the component types? There are basically six types of components; the most common is conventional type components. It is single species fluid either vapour or liquid and typical components that may participate in the vapour-liquid phase equilibrium almost 90% components fall under this category they are conventional.

Also we have solid component type this is also species solid property are calculated by solid based model and most of the metals they come under this say iron or silver or gold sometimes the common salt NACL that also we can use as a single species solid then non-conventional solids that are not pure chemicals because they are not represented as molecular component such as coal or wood pulp.

Now you see what coal is? Coal is not a single species, coal is composed of carbon, other volatile components and ashes among others. So, it is not a single species, it is a combination of various chemicals, the same as for wood pulp. So, they are characterized using component attributes and they do not participate in chemical or phase equilibrium so they are all non-conventional.

Then the fourth category that we have is pseudo component assay or blend. Mostly they represent the petroleum fractions. So, they are characterized by boiling point, molecular weight, specific gravity and some other properties also. The fifth one is polymer, oligomer and segment and these components are used in polymer models for those who work with polymer chemistry or polymer engineering. These kinds of component types are very useful for them and lastly we have hypothetical liquid.

It is a component type that is mainly used in pyrometallurgical application when modeling a component has a liquid and its property should be extrapolated from solid properties for example modeling of carbon in molten steel.

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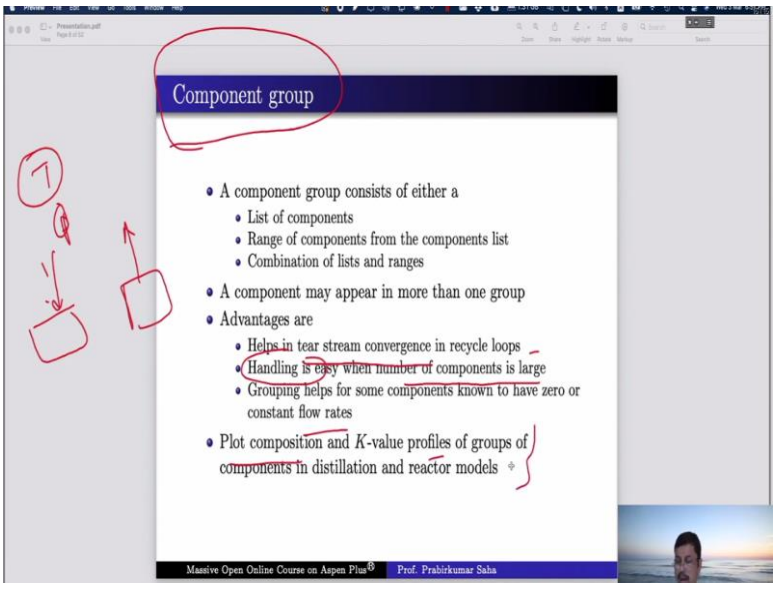

Then comes the component group. What is a component group? Component group consists of either a list of components or a range of components from the component list or combination of list and ranges. So, as we have seen in our list of components that we have used in the example of Henry's component we have water, we have ethanol, we have acetone, we have CO_2, nitrogen, oxygen and methane.

So, among this component list we can make certain groups and the groups maybe something like condensable or non-condensable or groups maybe gas or liquid or the groups maybe organic or inorganic something like that and sometimes the groups may not be mutually exclusive. In certain cases, a component may appear in more than one group when the groups are not mutually expensive.

I will give an example for that. Now what are the advantages of making the component group? It helps in tear stream convergence in the recycle loop. Now to understand this tear stream concept we have to understand what is a recycle loop? Suppose, we have a reactor whose output is passed through a flash tank. The lower portion of the flash tank it is a product and the higher portion of the flash tank it is unreacted substance which can be recycled back to the reactor.

So, that it does not go waste and in this kind of system it is very difficult to converge in the very first go because converging a recycle loop is not very easy for what we need to do? We need to tear that stream in the very first place. So, as if we have two distinct streams like this is the reactor and this is the flash tank where this independent stream is the input and this independent stream is output.

And we have to do some trial and error method where this particular stream the input condition of this particular stream is somewhat close to the output condition of this particular stream. When these two streams are almost close with all its components and their properties such as temperature, pressure and all, then we can join these streams as a recycle stream. So, this is the concept of tear stream convergence in the recycle loop.

And component groups come very handy in this kind of situation because when we do the inlet and outlet analysis of two different streams then setting the component group and assigning a single temperature or single pressure in all of them becomes very easy and also this kind of grouping becomes very effective when large number of components are present in the system.

Then handling of the components becomes very easy and also the grouping helps for some components known to have zero or constant flow rates. Finally, the plotting of composition and K-value profiles of groups of components in distillation reactor models is very easy when we group the component.

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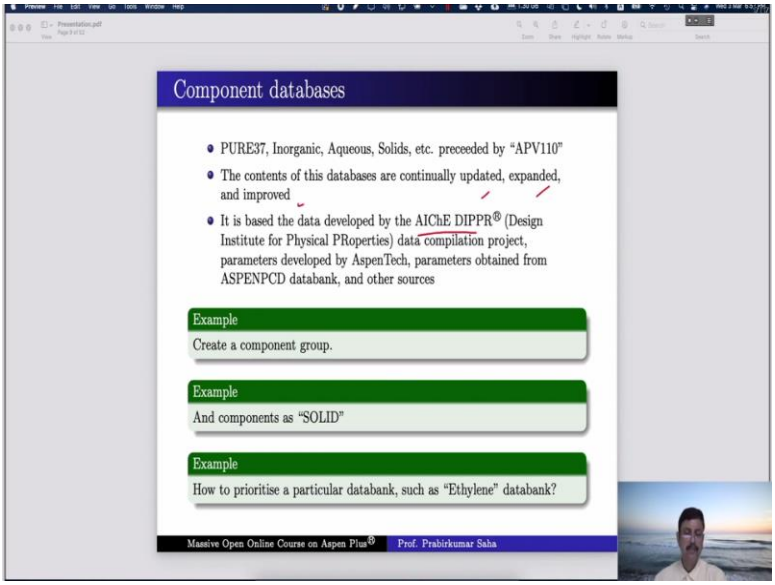

Now where these components are available. As we know they are available in component data basis and some of the data basis already we are aware that is PURE 37, inorganic, aqueous, solids etcetera and we will find all of them are preceded by APV 110. Now what APV 110?

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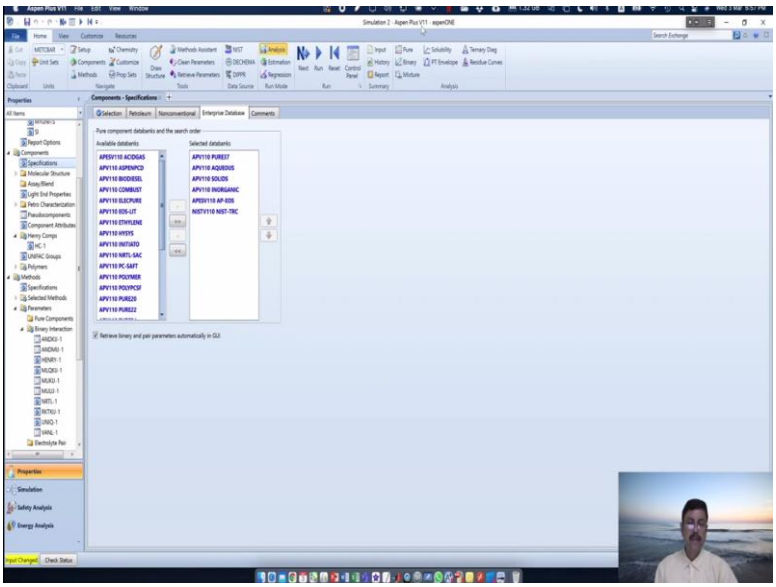

Just go to the component setup see enterprise database all these data banks are APV 110 most of them APV 110. APV 110 is Aspen Plus V 11 version 11 11.0 APV means Aspen Plus version 11.0 and under this category we have PURE 37, aqueous, solids, inorganic and so on and the contents of this database they are not fixed, they continually update, expand and improve the database because all over the world the researchers continuously work on these components.

They publish literature and whenever a new dataset appears the Aspen Plus team takes those data and improves the database periodically. Now all this data are developed by AIChE DIPPR

AIChE means American Institute of Chemical Engineers and DIPPR is the short form of Design Institute for Physical Properties and they are developed by AIChE DIPPR data compilation project.

The parameters are developed by Aspen Tech. Now, we will take three small examples where we will create a component group and we will set certain components as solid and we will find how to prioritize a particular databank. In order to do that let us first go to the Aspen Plus domain. Now the first example creates a component group. **(Video Starts: 40:21)**. So, let us go to the components so we have seven components from our previous example.

We go to the component group and click on new. Given a name, suppose we want to create a group of condensable and non-condensable components. So, we give a name CON so this is a condensable component. We chose this one, this one and this one (water, ethanol and acetone). So, this is the component list having a condensable group. Go to component groups once again, create another new NCON that is a non condensable group.

Now here you can choose anything between CO_2, N_2, O_2 and methane. Now, instead of choosing one by one we can go to the component range. As we see over here it can be chosen by either list of components or range of components from the component list or combination of them. So, we can say component CO_2 to component methane. So, anything between them will be included in the component list so all of them are NCON.

Now as I said, a component may appear in more than one group. For instance, you create a component group where you want to take up all the organic components. So, you just enter an ID ORG and there you take ethanol, you take acetone and you take methane because they are organic. So, they are available over here so that you can open various component groups. Now, the next example is how to set components as solid.

I will go back to your specifications and add a component for instance let us add sliver. Now here if you just write silver it will add as a conventional item, but you can set it here as solid. That means you want to use silver as a solid item only, not liquid, not vapour. So, the temperature range in which it will work is also set by a solid then how to prioritize a particular data bank such as ethylene databank.

Now ethylene is available as conventional material or as in ethylene databank. So, just find ethylene now see it has been asked in pure component databank. So, APV 110 dot PURE 37 so it is asking the compound name ethylene is looking in APV 110 PURE 37 databank, but suppose you do not want to take it from here so what you can do there is a databank of ethylene APV 110 ethylene databank.

You just take it over here and this databank you prioritize at the top. So, it is coming ahead of PURE 37. Now you find this ethylene once again. So, you will expect the ethylene to be found in ethylene databank first not in PURE 37. Let us see find now. So, it is asking in the ethylene databank. So, that is how you prioritize your databank where you want to search a particular component. **(Video Ends: 45:49)**.

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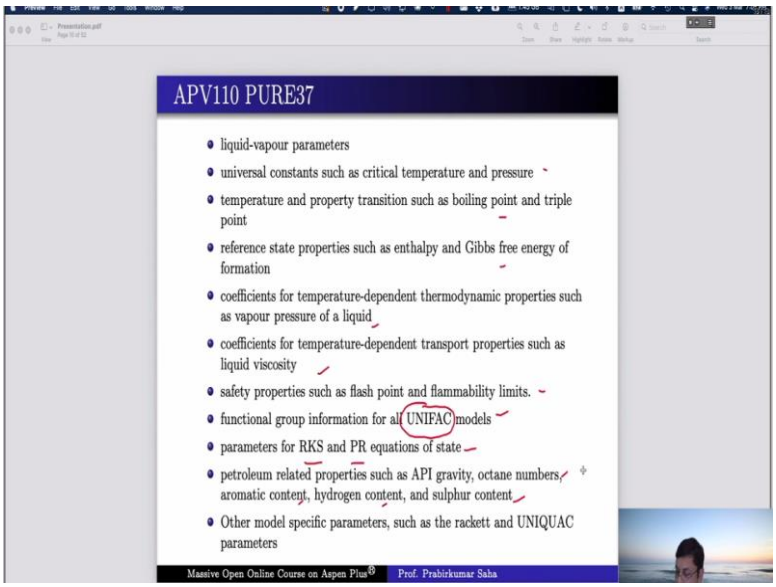

So, these are the few databanks that we can further discuss. APV 110 PURE 37 it consists of liquid vapour parameters and universal constant such as critical temperature, critical pressure. Temperature and property transition such as boiling point, triple point etcetera. It contains reference properties such as enthalpy, Gibbs free energy of formation, coefficient for temperature dependent, thermodynamic properties such as vapour pressure of a liquid.

Coefficient for temperature dependent, transport property such as liquid viscosity, safety property such as flash point, flammability limit, functional group information for all UNIFAC models. Now I will explain UNIFAC models in a future slide, parameters for Redlich-Kwong-Soave and Peng-Robinson Equation of State, petroleum related properties such as API gravity,

octane number, aromatic content, hydrogen content and Sulphur content and other model specific parameters such as rackett and UNIQUAC parameters.

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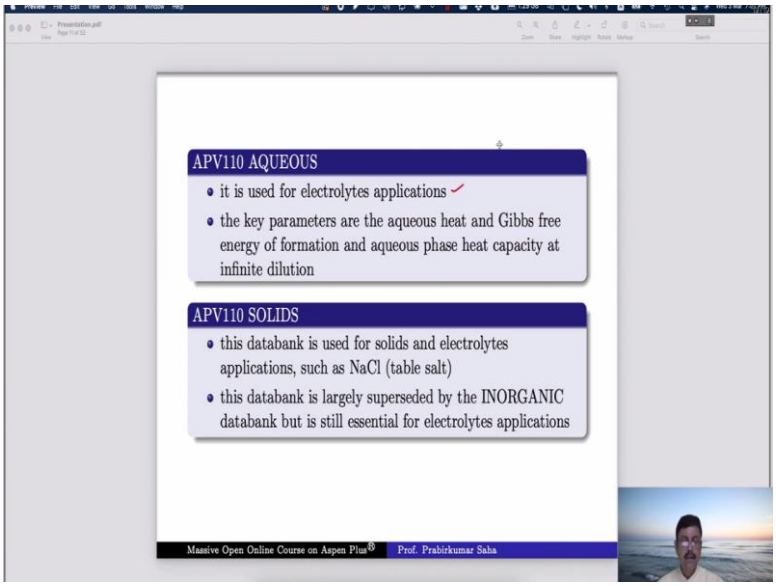

Similarly, we have APV 110 aqueous and APV 110 solids databank. In the first databank it is used for electrolyte application the key parameters are aqueous, heat and Gibbs free energy formation and aqueous phase heat capacity at infinite dilution whereas in solid databank it is used for solids and electrolytes applications such as table salts etcetera and this databank is largely superseded by inorganic databank.

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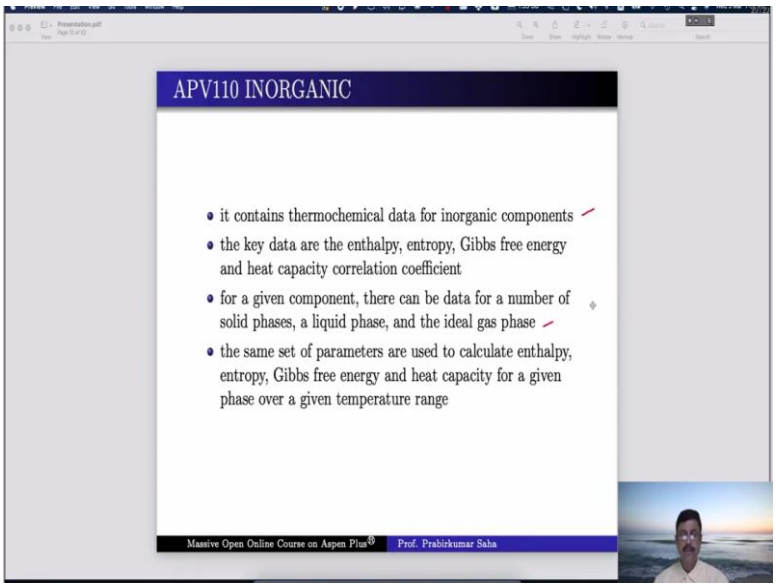

So, this is the APV 110 inorganic database; it contains thermochemical data for inorganic components. The key data are enthalpy, entropy, Gibbs free energy and heat capacity correlation coefficient. For the given component there can be data for a number of solid phases,

a liquid phase and the ideal gas phase. The same set of parameters are used to calculate enthalpy, entropy, Gibbs free energy and heat capacity for a given phase over a given temperature range. So, we end our lecture at this point. We will continue in the next lecture. Thank you.