Aspen Plus Simulation Software - A Basic Course for Beginners
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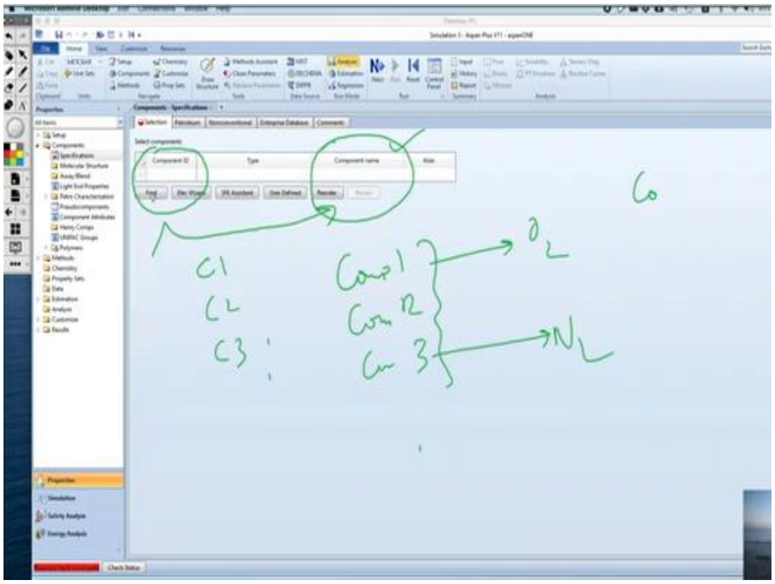
Lecture - 03
Overview of setting up of property environment

Welcome to the massive open online course on Aspen Plus. In today's lecture, we will discuss about the setting up of property environment. Now, this portion will be discussed in detail in the fourth week of this lecture series, when we will discuss about the process and property analysis. But today, we will have an introductory session. So, the first thing that we have to do in setting up of property environment is to select the components or the selection of chemical compounds with which we will do the simulation in Aspen plus. For that, let us go to the Aspen Plus software. **(Refer Slide Time: 01:15)**



So, this is the window where we need to select the components or the chemical compounds. Now, each chemical compound or each component that we select have a unique component name and a component id, which the user has to assign. Now, this component id can be anything. One can use C1, C2, C3, etcetera or Comp 1, Comp 2, Comp 3, etcetera. But it is wise to assign a component id whose name matches with the actual component name.

Because in this fraction if you write then in future, you may not remember whether component 1 is oxygen or component 3 is nitrogen, it is very difficult to remember in that manner. So, the component id has to be given which matches with the component name to some extent or its abbreviation sort of. So, one thing that we have to remember a component Id should be not more than eight letters long.

So, there is a limitation in the number of alphabet for naming the component id. But if the component name itself is very short that is within eight letters, then you can directly write the component name in place of component id, and Aspen is smart enough to identify the desired component itself. For instance, if you want to write or if you want to choose water, then you can directly write water in place of component id.

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And the moment you enter it, component name water or H_2O that will be taken as it is conventional. Similarly, if you place ACETONE which is again within eight-letter, then it will take up as ACETONE. But suppose you want to work with Methyl Isobutyl Ketone. This is a long name. So, you cannot write it in component id. So, the question is, how can we set this Methyl Isobutyl Ketone?

For that, we have to use this find button, and it will find the desired component name from its database. So, for that, you have to press find and here there are several search criteria available. For instance, if you say name or alias equals Methyl Isobutyl Ketone and say find now, it will actually look for the methyl isobutyl ketone, and it will dig out the actual component that you are looking for and suggest you. What do you need to do? You need to choose it and add selected component then the component Id will be automatically fixed.

So, here you can change the component id also. But it might so happen that methyl isobutyl ketone is not your desired component. A derivative of that or some other ketone is the one which you are looking for. So, you want to search for a component that has ketone in its name. So, name or allies that contains the word ketone, if you say find now, then you will get all the components that have ketone in its name, the first one is cyclohexyl methyl ketone, then isobutyl heptyl ketone, ethyl methyl ketone oxime, Amyl methyl ketone, etcetera.

So, you have to choose your component from this list. It is a long list of components from which you have to choose. Now, the search criteria give you the option to choose from molecular weight or boiling point. For instance, if you want to find out the components whose boiling point is between 99 and 101 degrees centigrade so, what you can do? You can simply write a boiling point from 99 to 101.

So, it will give you the list of components that is boiling point is between 99 and 100. And you can very well see one of them is water whose boiling point is 100 and not only water there are so many other items whose boiling point is between 99 and 101. All of them are listed over. So, you can use the molecular weight also as search criteria. Anyway, you have inserted methyl isobutyl ketone over here, and this component id has been automatically chosen by Aspen.

But you can rename it as per your choice. For instance, you may say that you want to call it methyl isobutyl ketone, and then methyl isobutyl ketone will be renamed. So, this component id is given by you. Now you may be curious to know these components have been taken from some database, but what are those databases? For that, you have to go over here enterprise database. So, just go there, and you will find these are the selected data banks from where these components have been searched.

And these data banks are searched in this order PURE37 first and then AQUEOUS, SOLIDS, INORGANIC, AP-EOS, and NIST-TRC. These are the most common database, and for all practical purposes mostly you will get your desired component from them. But in case this is not sufficient, you may look for your desired component from here. For instance, if you want to search your component from polymer, then you just choose polymer and then use this particular button polymer will come from here to here.

That means, this database also is being included within your search criteria. Now, let us see what these data banks are PURE37 AQUEOUS, SOLIDS, INORGANIC, AP-EOS and NIST-TRC.

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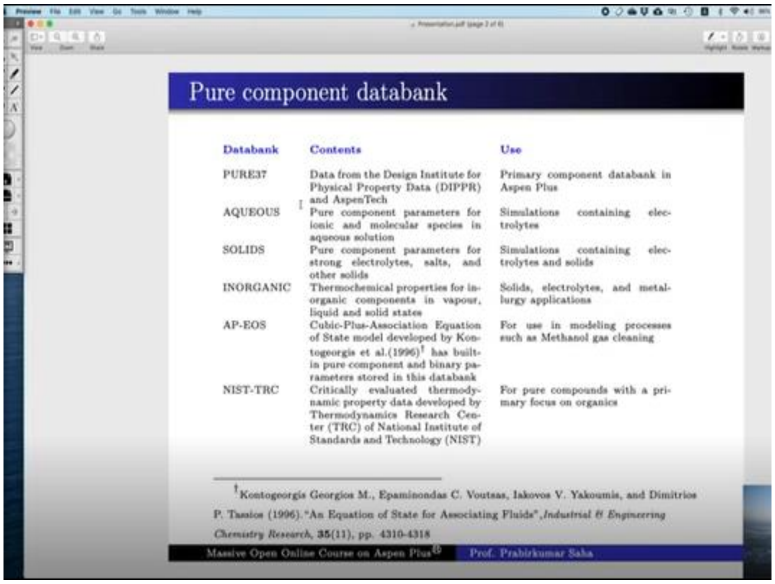

Pure component databank

Databank	Contents	Use
PURE37	Data from the Design Institute for Physical Property Data (DIPPR) and AspenTech	Primary component databank in Aspen Plus
AQUEOUS	Pure component parameters for ionic and molecular species in aqueous solution	Simulations containing electrolytes
SOLIDS	Pure component parameters for strong electrolytes, salts, and other solids	Simulations containing electrolytes and solids
INORGANIC	Thermochemical properties for inorganic components in vapour, liquid and solid states	Solids, electrolytes, and metallurgy applications
AP-EOS	Cubic-Plus-Association Equation of State model developed by Kontogeorgis et al.(1996)† has built-in pure component and binary parameters stored in this databank	For use in modeling processes such as Methanol gas cleaning
NIST-TRC	Critically evaluated thermodynamic property data developed by Thermodynamics Research Center (TRC) of National Institute of Standards and Technology (NIST)	For pure compounds with a primary focus on organics

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† Kontogeorgis Georgios M., Epaminondas C. Voutsas, Iakovos V. Yakoumis, and Dimitrios P. Tassios (1996). "An Equation of State for Associating Fluids", *Industrial & Engineering Chemistry Research*, **35**(11), pp. 4310-4318

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So, these are the data banks you just saw in the Aspen plus software. First one is PURE37. It contains the Data from Design Institute for Physical Property Data or DIPPR in abbreviation and aspen tech. So, actually, it is a primary component databank in Aspen Plus. The next one is AQUEOUS it contains pure component parameters for ionic and molecular species in an aqueous solution.

They are used in simulations containing electrolytes. The solids databank, they contain your component parameters for strong electrolytes, salts and other solids. They are also used for simulations containing electrolytes and solids too. Fourth one is INORGANIC databank; it contains thermochemical properties for inorganic components in vapour, liquid, and solid states. They are used for solids, electrolytes, and metallurgy applications.

Next one is AP-EOS, they contain Cubic Plus Association Equation of State model developed by Kontogeorgis et al. This is the paper industrial engineering chemistry research. It has been published in 1996, and this databank has built-in pure component and binary parameters, and they are used for modelling processes such as methanol gas cleaning. And finally, NIST-TRC databank, the full form of NIST is National Institute of Standards and Technology TRC is Thermodynamics Research Centre.

They have critically evaluated thermodynamic property data and it is used for pure compounds. We primarily focus on organics. Now, once the selection is done, you have to press next, and it will come at setting up of property method. So, it is property methods and options. Now when building a simulation, it is important to ensure that the properties of pure components and mixtures are being estimated appropriately.

In fact, selecting the proper method for estimating properties is one of the most important steps that will affect the rest of the simulation. Therefore, it is important to carefully consider the choice of methods to estimate the different properties. In Aspen plus, the estimation methods are stored in what is called a property method. And the property method is a collection of estimation methods to calculate several thermodynamic and transport properties.

The transport properties are like viscosity, density, thermal conductivity, diffusion coefficient, surface tension etcetera. And thermodynamic properties are like fugacity, enthalpy, entropy, Gibbs free energy etcetera. And in addition, the Aspen Plus stores a large database of introduction parameters that are used with mixing rules to estimate mixer properties. Now, one of the key calculations performed in process simulation is phase equilibrium calculation.

The basic principles of several unit operations such as flash tanks, distillation column, extraction, etcetera. They are all based on multi-phase equilibrium and phase equilibrium is calculated using fugacity.

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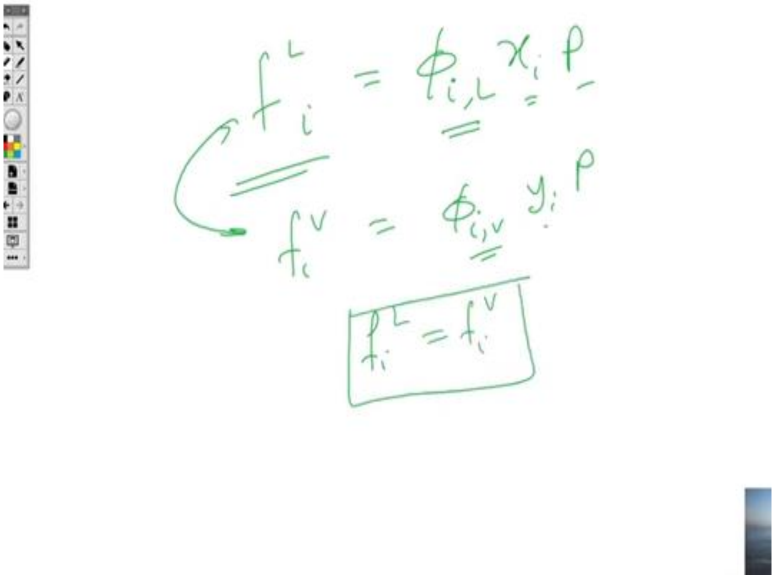

Now, the phase equilibrium is calculated using fugacity which is a measure of NNC of a component ‘i’ to live its phase. And the equilibrium is achieved when the fugacity of the component is equal in all phases. Now, say the fugacity of a component ‘i’ in liquid phase is given by

$$f_i{}^L = \Phi_{i,L} x_i P$$

where this is the fugacity coefficient x_i is definitely the mole fraction of ‘i’ in liquid phase, and P is the pressure.

Similarly, fugacity of component ‘i’ in vapour phase is

$$f_i^V = \Phi_{i,V} y_i P$$

y_i that is the coefficient of component i in vapour phase. Now, at equilibrium these two are same that means

$$f_i{}^L = f_i^V$$

If the fugacity is in two phases are same that means, the equilibrium has been achieved.

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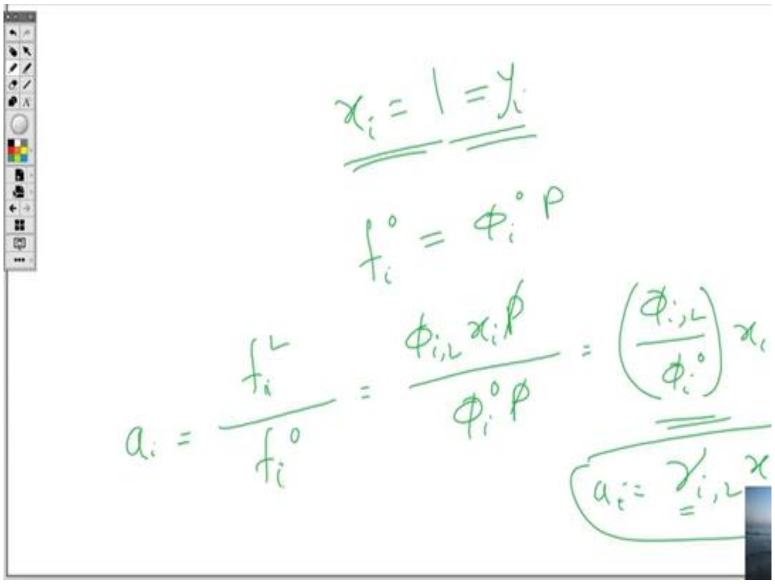

Now, at pure state when there is no other component in the mixture only component ‘i’ then obviously x_i will be 1, so, is y_i. So, both in liquid phase and vapour phase the mole fraction of component will be 1, because the pure component. In such cases the fugacity will be represented by,

$$f_i{}^0 = \Phi_i^0 P$$

because x_i is equal to 1 and y_i also equal to 1 and for non-ideal liquid solutions the fugacity of the components in solution deviates from that of pure component.

So, if you find the ratio of $f_i{}^L$ and f_i^0, so, this is the ratio you will find f_i^L is not equal to f_i^0 it deviates a lot. So, the ratio of them is called the activity which is

$$a_i = \frac{f_i{}^L}{f_i{}^0} = \frac{\Phi_{i,L} x_i P}{\Phi_i^0 P} = \left(\frac{\Phi_{i,L}}{\Phi_i^0}\right) x_i$$

Where,

$$\gamma_{i,L} = \left(\frac{\Phi_{i,L}}{\Phi_i^0}\right)$$

This is called the activity coefficient ($\gamma_{i,L}$).

$$a_i = \gamma_{i,L} x_i$$

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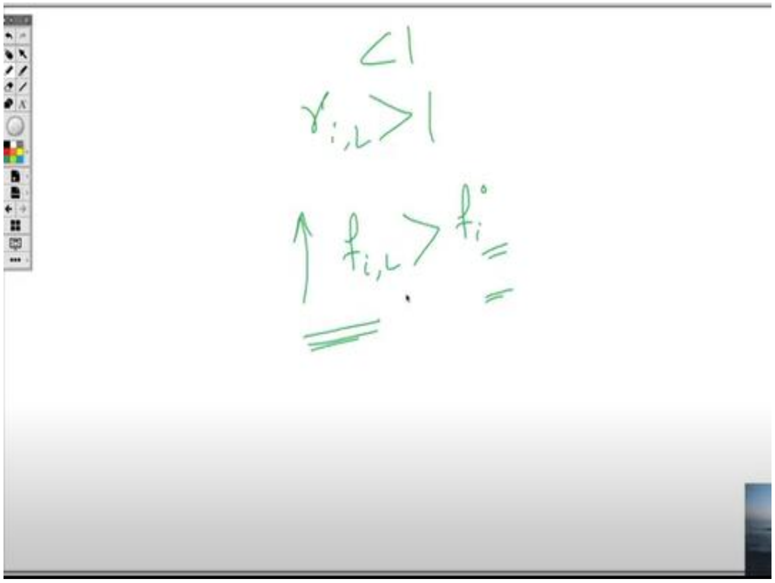

So, all the non-ideal cases are dealt with activity coefficient. Now, in general this activity coefficient is higher than 1. That means, the fugacity of component in solution is greater than fugacity of the pure component. That means, the same liquid will have a higher tendency to vapourise when in the mixture than in the pure state, and this can be attributed to the increased repulsion between the molecules in the mixture then in pure state.

Obviously, in a few cases, the activity coefficient will be lower than one indicating that there will be increased attraction between molecules in the solution state and it will yield less, tendency to vapourise.

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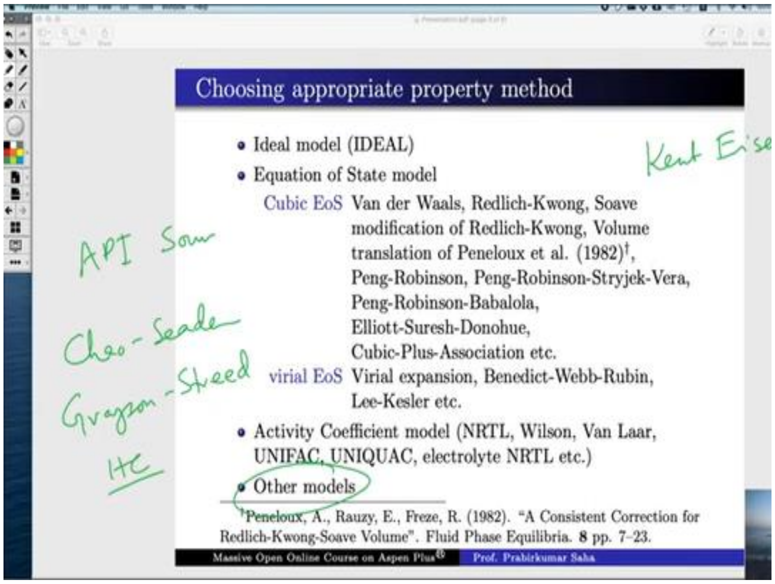

Choosing appropriate property method

- Ideal model (IDEAL)
- Equation of State model

Cubic EoS Van der Waals, Redlich-Kwong, Soave modification of Redlich-Kwong, Volume translation of Peneloux et al. (1982)†, Peng-Robinson, Peng-Robinson-Stryjek-Vera, Peng-Robinson-Babalola, Elliott-Suresh-Donohue, Cubic-Plus-Association etc.

virial EoS Virial expansion, Benedict-Webb-Rubin, Lee-Kesler etc.

- Activity Coefficient model (NRTL, Wilson, Van Laar, UNIFAC, UNIQUAC, electrolyte NRTL etc.)
- Other models

Kent Eise

API Sour

Chao-Seader

Grayson-Streed

HC

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†Peneloux, A., Rauzy, E., Freze, R. (1982). "A Consistent Correction for Redlich-Kwong-Soave Volume". Fluid Phase Equilibria. **8** pp. 7–23.

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In general, there are four choices for choosing appropriate property method, Ideal model, Equation of State Model, Activity Coefficient model and other models. The Ideal model is applicable for a system composed of ideal gases and liquids. As you might know, the ideal gas it follows the ideal gas law PV = n RT. And here, the fugacity is equal to one, and an ideal liquid it has the activity coefficient 1.

Now, when will you assume ideal behaviour of a system? When you have a vacuum or low pressure or when you have a system with very high temperature and when there is very small interaction or negligible interaction in liquid. Now interactions are negligible when molecules of similar size and character mixed together in the liquid phase. In that case Ideal model will be applicable.

And the non-ideality as a general rule of thumb will appear when you have systems that involve materials such as water, organic acids, amines, alcohols, esters, ketones, aldehydes, ethers, etcetera. I mean, when you have them, you are necessarily handling polar molecules, and there is a good chance that your system will deviate from ideality. In such a situation, you will use either equation of state model or the activity coefficient model.

Now, in case of gases you will generally use equation of state model. Equation of state models are PVT models. You might remember from the knowledge in thermodynamics you have mainly cubic equation of state model and variable equation of state model. A few popular cubic EoS models are Van der Waals, Redlich-K Wong, Peng-Robinson, and their extensions. You have Cubic Plus Association also among Virial equation of states you have Virial expansion, Benedict-Webb Rubin, Lee-Kesler etcetera.

And usually when you have pressure less than 10 bar where you can use equation of state model. On the other hand, the activity coefficient models can be used for liquids there are many NRTL, Wilson, Van Laar, UNIFAC, UNIQUAC, electrolyte NRTL etcetera. You might be knowing NRTL means non-random to liquid model and this NRTL model is used for polar mixtures. And in these models;

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And in these models, the activity coefficient approach is used to calculate the liquid properties while the vapour phase properties are calculated using an equation of state model, and if you have supercritical component in the mixture, then you can use Henry's law in activity coefficient model. Finally, the other models, there are still many other property models available and they are classified as vapour pressure liquid fugacity models.

And the found applications in many specific processes among these models are API sour model, and it is developed for sour water treatment applications, and two popular models are Chao Seader model or a Grayson Streed model they are applicable for heavy hydrocarbons. They are also Kent Eisenberg model they are used for amine sweetening units.

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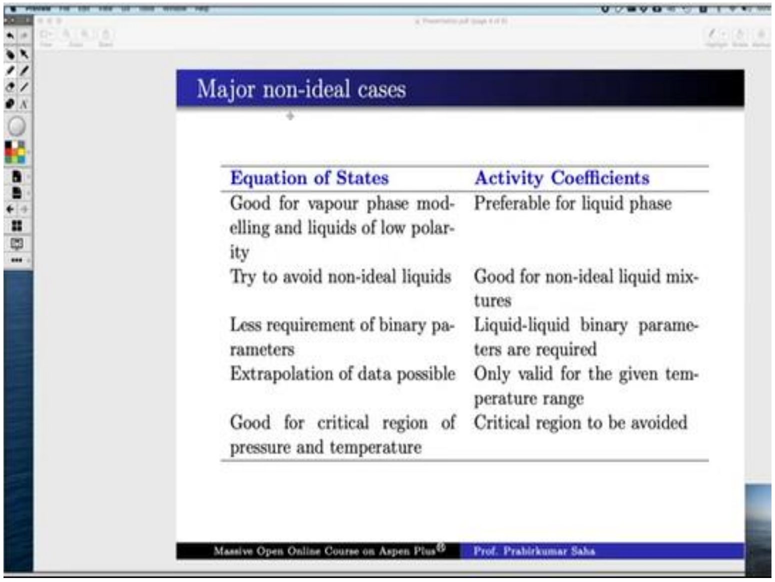

Major non-ideal cases

Equation of States	Activity Coefficients
Good for vapour phase modelling and liquids of low polarity	Preferable for liquid phase
Try to avoid non-ideal liquids	Good for non-ideal liquid mixtures
Less requirement of binary parameters	Liquid-liquid binary parameters are required
Extrapolation of data possible	Only valid for the given temperature range
Good for critical region of pressure and temperature	Critical region to be avoided

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Here we have a comparative assessment of two major non-ideal cases. That is an equation of state model and activity coefficient model. The first one is equation of state model, they are good for vapour phase modelling and liquids of low polarity and activity coefficient models they are preferable for liquid phases. Equation of state models, are not used generally for non-ideal liquids, but activity coefficient models are good for non-ideal liquid mixtures.

They use less number of binary parameters and for activity coefficient model binary parameters are required. Here extrapolation of data is possible, but for activity coefficient model, they are only valid for the given temperature range. Equation of state models they are good for critical region of pressure and temperature whereas, activity coefficient model the critical regions are to be avoided.

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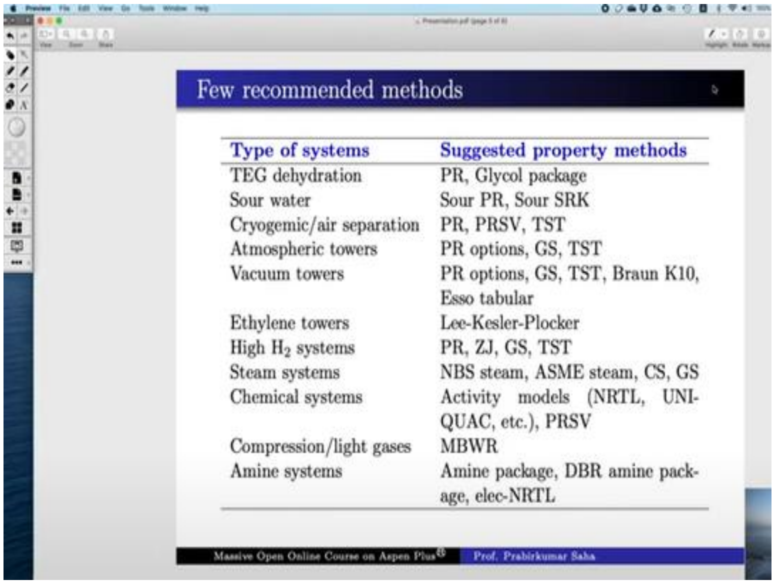

Few recommended methods

Type of systems	Suggested property methods
TEG dehydration	PR, Glycol package
Sour water	Sour PR, Sour SRK
Cryogemic/air separation	PR, PRSV, TST
Atmospheric towers	PR options, GS, TST
Vacuum towers	PR options, GS, TST, Braun K10, Esso tabular
Ethylene towers	Lee-Kesler-Plocker
High H_2 systems	PR, ZJ, GS, TST
Steam systems	NBS steam, ASME steam, CS, GS
Chemical systems	Activity models (NRTL, UNIQUAC, etc.), PRSV
Compression/light gases	MBWR
Amine systems	Amine package, DBR amine package, elec-NRTL

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Here we have few recommended methods for a few types of systems. For instance, TEG dehydration, the suggested property methods are Peng Robinson and glycol package. For sour water system we have sour Peng Robinson or Sour Suave modification of Redlich-K Wong and so on.

(Video Starts: 21:03)

Now, even after knowing all of them, you may still need some kind of assistance to choose the appropriate property method and Aspen has a ready assistant for you that is called method assistant. So, here it is called property methods selection assistant. If you click on it, it will open up so, this is a property method selection assistant and you can start by selecting one of these two following options.

You can specify the component type or specify the process type. If you go by process type, you can choose either chemical process whether your process or application has an electrolyte, whether it is for environmental application, gas processing, oil and gas, mineral and metallurgical, etcetera. If you go by component type, it will ask whether it is for a chemical system, whether for hydrocarbon, whether it has a special system or refrigerant.

So, for instance, if we have hydrocarbons in the system, then we have hydrocarbon mixtures. Does the mixture contain petroleum as a pseudo component? You can say yes or no, suppose we say no we do not have. Then these are the options that we have Peng Robinson, SRK, LKPLOKE etcetera. For instance, if you choose Peng Robinson Equation of State for it then by default, the method name will come as Peng Robinson Equation of State.

Now, you may be curious to know what are the equation that govern that particular method that is operating. So, this Peng Robinson method you can see the equation of state it is showing as ESPRSTD. So, just go for help and type here ESPRSTD. So, here you see ESPRSTD is standard Peng Robinson method. So, this is the standard Peng Robinson equation for this model. So, basically, FM plus is using this model to do the property calculation.

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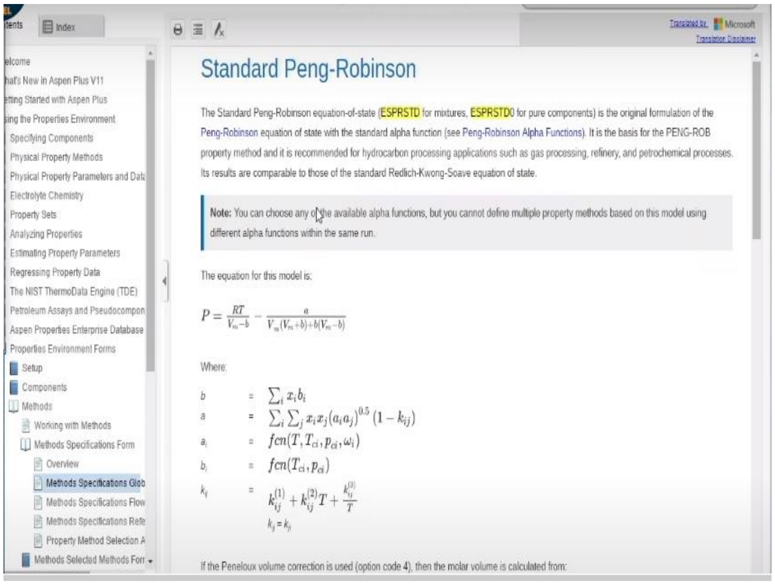

Standard Peng-Robinson

The Standard Peng-Robinson equation-of-state (ESPRSTD for mixtures, ESPRSTD0 for pure components) is the original formulation of the Peng-Robinson equation of state with the standard alpha function (see Peng-Robinson Alpha Functions). It is the basis for the PENG-ROB property method and it is recommended for hydrocarbon processing applications such as gas processing, refinery, and petrochemical processes. Its results are comparable to those of the standard Redlich-Kwong-Soave equation of state.

Note: You can choose any of the available alpha functions, but you cannot define multiple property methods based on this model using different alpha functions within the same run.

The equation for this model is:

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m(V_m+b)+b(V_m-b)}$$

Where:

$b = \sum_i x_i b_i$

$a = \sum_i \sum_j x_i x_j (a_i a_j)^{0.5} (1 - k_{ij})$

$a_i = fcn(T, T_{ci}, p_{ci}, \omega_i)$

$b_i = fcn(T_{ci}, p_{ci})$

$k_{ij} = k_{ij}^{(1)} + k_{ij}^{(2)} T + \frac{k_{ij}^{(3)}}{T}$

$k_{ij} = k_{ji}$

If the Peneloux volume correction is used (option code 4), then the molar volume is calculated from:

And this model has been taken from this journal paper, Peng Robinson a new to constant equation of state which has been published in industrial engine chemistry fundamentals in 1976. This means, the source of information or source of modelling is authentic, Aspen plus is using some authentic source of modelling technique to do all the calculations. So, it is quite reliable. Now, in case you are not happy with this standard Peng Robinson equation of state.

(Video starts: 24:45)

Rather you want to modify this. So, what you need to do is? You need to say modify, and you have to enter a new property method name. For instance, you can give a name like my Peng Robinson or you say my Peng Robinson. So, that is the name you want to give to that property method. And immediately, it will open up some options for you. So, you can change the equation of state from Peng Robinson to something else you can use Peng Robinson equation of state with PSRK mixing rule or Peng Robinson equation with state with image MHV2 mixing rule.

Now, if you want to know what is MHV2 mixing rule? Again, you can go there and look for MHV2. Then, Aspen will tell you what MHV2 mixing rule is, so, just click on that it is Dalh and Mikkel shun 1990. This is the relationship equivalent to one used by Huron and vital. So, this is the MHV2 mixing rule that is used in that type of Peng Robinson extension. And this has been taken from this paper Dalh and Mickelson paper from AICH journal published in 1990.

Again, an authentic source. So, that is how you can change the Peng Robinson equation of state as per your wish; if you do not want to use the default one, it will give you the options. And here also, there are several equations for the calculation of liquid molar enthalpy. All these equations you can search in the help file and get relevant information. Anyway, let us not modify it; let us delete this modification and let us go by the standard Peng Robinson and see what happens.

Now here usually Aspen plus does not give the parameters of its own. If you want to know the pure component parameters, you have to choose retrieve parameter. So, it will retrieve all the pure component parameters used in the calculation and display them on the parameters and results form. So, if you say retrieve parameter and press OK. Then you will find them in this form. Let us first see what the parameters are?

These are selected method Peng Robinson and these are the property calculation. What is PHIVMX? Let us see, PHIVMX, so, if you click on this it is vapour fugacity coefficient of a component in a mixture. Similarly, PHIV it is vapour pure component fugacity coefficient SV and SL they are vapour and liquid pure component entropy. Similarly, you have notations for Gibbs free energy, molar volume enthalpy, etcetera. All of them you can get from the help file.

Then you have pure components it is CPIGDP 1. It is methods parameters pure component. What is CPIGDP 1? Again, you go to the hell file and you write CPIGDP and check what it is. It is actually general pure component ideal gas heat capacity. Just click on that we will get CPIGDP ideal gas heat capacity polynomial the DIPPR 107 or 127. Let us see what is 107 127? Here it is DIPPR equation 107 DIPPR ideal gas heat capacity equation 107 by Ellie and Leigh 1981.

So, Ellie and Lee in 1981, they have published a paper in fluid phase equilibrium on self-consistent equations for calculating the ideal gas heat capacity enthalpy entropy. So, on that basis, this equation has been taken. Here in this equation, you may find that ideal gas heat capacity is expressed as a polynomial where coefficients C_1, C_2, C_3, C_4, C_5 are there. And this equation is valid only within this temperature region, which is within C_6 and C_7.

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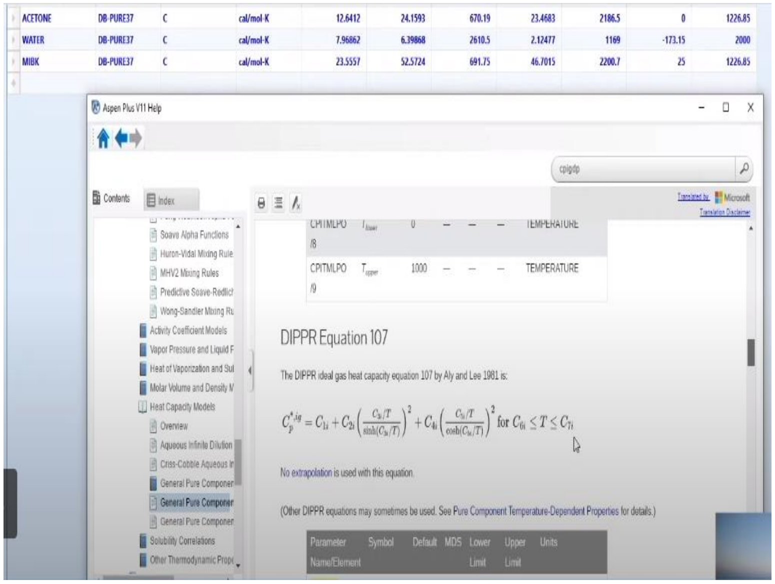

ACETONE	DB-PURE37	C	cal/mol-K	12.6412	24.1593	670.19	23.4683	2186.5	0	1226.85
WATER	DB-PURE37	C	cal/mol-K	7.96862	6.39868	2610.5	2.12477	1169	-173.15	2000
MIBK	DB-PURE37	C	cal/mol-K	23.5557	52.5724	691.75	46.7015	2200.7	25	1226.85

Aspen Plus V11 Help

cpigdp

CPITMLPO /8	T_{lower}	0	—	—	—	TEMPERATURE
CPITMLPO /9	T_{upper}	1000	—	—	—	TEMPERATURE

DIPPR Equation 107

The DIPPR ideal gas heat capacity equation 107 by Aly and Lee 1981 is:

$$C_p^{*,ig} = C_{1i} + C_{2i}\left(\frac{C_{3i}/T}{\sinh(C_{3i}/T)}\right)^2 + C_{4i}\left(\frac{C_{5i}/T}{\cosh(C_{5i}/T)}\right)^2 \text{ for } C_{6i} \le T \le C_{7i}$$

No extrapolation is used with this equation.

(Other DIPPR equations may sometimes be used. See Pure Component Temperature-Dependent Properties for details.)

Parameter Name/Element	Symbol	Default	MDS	Lower Limit	Upper Limit	Units

So, you go back to the Aspen domain temperature dependent correlation parameters. Actually, these are the correlation parameters from C_1 to C_7. So, what are C_1, C_2, C_3, C_4, C_5? The first five components are C_1, C_2, C_3, C_4 and C_5. What about the C_6 and C_7? They are also there; they are actually temperature. If you put the values of C_1 to C_5 in this equation that means, when you are talking about acetone, you put C_1 is equal to 12.6412, C_2 you put 24.1593, C_3 you put 670.19, C 4 you put 23.4683 and C_5 you put 218 6.5.

Then only thing that you need to do is to put the temperature value. So, whatever is the temperature value you put over here the temperature unit is C. So, the moment you put in the value of temperature T the entire equation is defined, you will get the value of CP. That means, the ideal gas heat capacity of acetone at that particular temperature and this particular equation is valid from C_6 to C_7 0 to 1226.85.

That means, this is temperature unit. So, this particular equation is valid between 0 degrees centigrade to 1226.85 degree centigrade. So, the range of temperature within which this equation is valid that is also given. Same is there for water and methyl isobutyl ketone. Similarly, you will get other things like thermal conductivity, viscosity etcetera. Then go to binary interaction. Now, you might remember that equation of state requires very less number of binary parameters whereas, activity coefficient models they use a lot of binary parameters.

You can see this from this result Peng Robinson equation it is an equation of state model. It does not have any binary introduction parameter. Instead, if you use say NRTL method, suppose you use NRTL method. Then the binary interaction parameters are available. For that you have to again run this equation and all the binary interaction parameters are now available. So, acetone water component i component j.

So, the binary interaction parameters are there. For acetone water acetone, methyl isobutyl ketone and water methyl isobutyl ketone. For each pair you will have the binary interaction parameters. And if you want to see the results, this here you will find your component results. So, the freezing point of water you know this is the freezing point, it is zero degrees centigrade unit is C, so, e to the power minus 14.

So, this is actually the calculated or computed based on the correlations they have found the freezing point of water is nearly zero and that is right actually. Freezing point of acetone is minus 94.7. Similarly, we will have other parameters also when they are pure. Here you will have DCPLS again you can look for the value, what is DCPLS? It is difference between liquid and solid heat capacity and the triple point DG form DGFORM it is ideal gas; Gibbs free energy of formation add to 98.15 kelvin.

(Video Ends: 35:48)

So, wherever you have some doubt, you can just click on this help button and get the appropriate help information. So, that is how we use the property method. And we will learn about this property method in detail in our fourth-week lectures of this lecture series. Thank you.