Thermodynamics of Fluid Phase Equilibria
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Lecture - 28
Thermodynamics Properties from Volumetric Data: Effect of V and T

We have been discussing Thermodynamics Properties from Volumetric Data. And as of now, all the derivations which we have done is considering P and T as independent variable ok. So, now, we are going to move forward and we will be considering how do we calculate thermodynamic properties with volume and temperatures independent variables ok.

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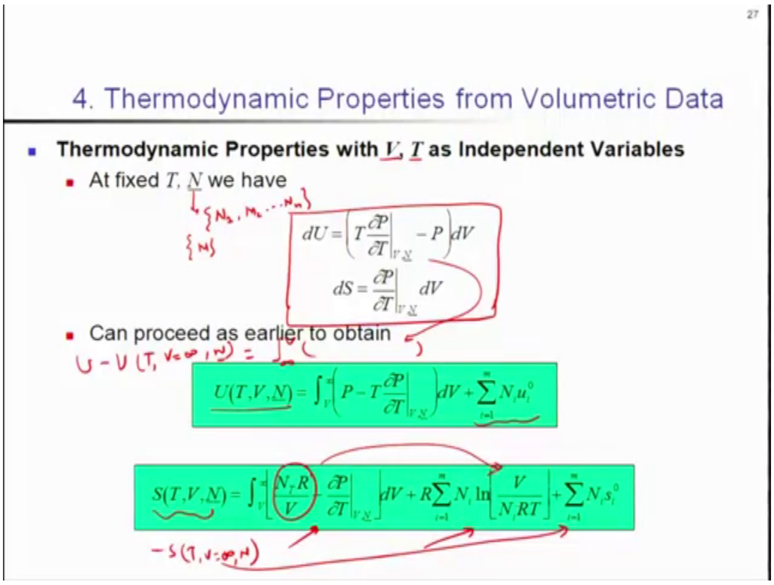

4. Thermodynamic Properties from Volumetric Data

- **Thermodynamic Properties with $\underline{V}$, $\underline{T}$ as Independent Variables**
  - At fixed T, $\underline{N}$ we have

$\{N_1, N_2 \ldots N_m\}$

$\{N\}$

$$\boxed{\begin{aligned} dU &= \left(T \left.\frac{\partial P}{\partial T}\right|_{V,\underline{N}} - P \right) dV \\ dS &= \left.\frac{\partial P}{\partial T}\right|_{V,\underline{N}} dV \end{aligned}}$$

  - Can proceed as earlier to obtain

$U - U(T, V=\infty, N) = \int^{\infty} ($

$$U(T,V,\underline{N}) = \int_V^{\infty} \left(P - T \left.\frac{\partial P}{\partial T}\right|_{V,\underline{N}} \right) dV + \sum_{i=1}^{m} N_i u_i^0$$

$$S(T,V,\underline{N}) = \int_V^{\infty} \left[\frac{N_T R}{V} - \left.\frac{\partial P}{\partial T}\right|_{V,\underline{N}} \right] dV + R \sum_{i=1}^{m} N_i \ln\left[\frac{V}{N_i RT} \right] + \sum_{i=1}^{m} N_i s_i^0$$

$- S(T, V=\infty, N)$

So, as we know and we have done this exercise earlier. So, this is all through a Maxwell relation that for a fixed temperature and mole composition. So, this is nothing, but N 1 N 2 and so forth ok. Earlier we have used this as simply N ok. So, at fixed end mole compositions we can write considering this is a V and T ah; that means, volume is fixed right, now given a volume. So, usually when you consider a volume we automatically consider internal energy when you consider pressure, we consider enthalpy right.

Now, we can look at this differential internal energy which can be written in this is something which we have seen earlier and the derivation is straightforward from the first law and as well as Maxwell's relations right. Now, given these two relation you can integrate this from a volume infinity to V very large volume which corresponds to basically nothing, but ideal gas or pressure. So, if you consider this we can use the same approach as we have done for the case for P and T as an independent variable here V and T are independent variables and you can evaluate U as a function or U as a function of T V N as V to infinity ok. So, you are integrating from infinity to V going from infinity to V, but you can also considering that you can rearrange. So, corresponding to the infinite volume you have a term this ok.

So, this is nothing, but U minus U at T V is equal to V infinity and an integral of infinity to V and this term right. So, you can realize this to get this expression ok. But by rearranging this infinity if you can swap the limits you will get instead of T partial derivative of P with respect to T minus P s simply P minus theta. Similarly you can do the same thing for ds by del P by del T ok, here also you can get S minus T P is equal to V infinity N and this is going to be this term this plus this term, this plus this term right. So, if you take it this other side you are going to get this part.

So, what is this? So, again the earlier if you recall we have added this term and subtracted this term and we plugged in here in this expression. So, this particularly is nothing, but the bracket. So, this is nothing, but a bracket and this term which is nothing, but minus V minus the integral of V to infinity N T R by T here for the mixture can be shown as to be this term ok. This is something which we have done already. So, without going into the derivation I am just writing this.

Earlier if you recall this was based on P when we consider P as a independent variable. So, similarly similar exercise can be done for the case where we are considering V as independent variable ok. So, you can come up with this expression also. So, to avoid derivations I am just writing out what else we can get from there.

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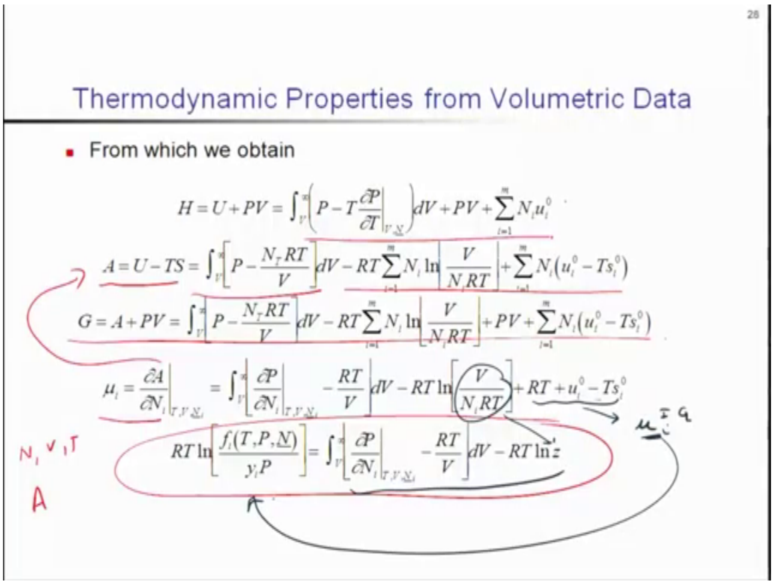

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Thermodynamic Properties from Volumetric Data

- From which we obtain

$$H = U + PV = \int_V^{\infty}\left(P - T\left.\frac{\partial P}{\partial T}\right|_{V,\underline{N}}\right)dV + PV + \sum_{i=1}^{m} N_i u_i^0$$

$$A = U - TS = \int_V^{\infty}\left[P - \frac{N_T RT}{V}\right]dV - RT\sum_{i=1}^{m} N_i \ln\left[\frac{V}{N_i RT}\right] + \sum_{i=1}^{m} N_i\left(u_i^0 - Ts_i^0\right)$$

$$G = A + PV = \int_V^{\infty}\left[P - \frac{N_T RT}{V}\right]dV - RT\sum_{i=1}^{m} N_i \ln\left[\frac{V}{N_i RT}\right] + PV + \sum_{i=1}^{m} N_i\left(u_i^0 - Ts_i^0\right)$$

$$\mu_i = \left.\frac{\partial A}{\partial N_i}\right|_{T,V,\underline{N}_i} = \int_V^{\infty}\left[\left.\frac{\partial P}{\partial N_i}\right|_{T,V,\underline{N}_i} - \frac{RT}{V}\right]dV - RT\ln\left[\frac{V}{N_i RT}\right] + RT + u_i^0 - Ts_i^0$$

$$RT\ln\left[\frac{f_i(T,P,\underline{N})}{y_i P}\right] = \int_V^{\infty}\left[\left.\frac{\partial P}{\partial N_i}\right|_{T,V,\underline{N}_i} - \frac{RT}{V}\right]dV - RT\ln z$$

Now, if you have the information of U and entropy you can get H easily which is nothing, but this term you can get a ok, again this is a is U term U minus you have T s you can get G also. So, once you get G we know that for the case of N V T as an independent variable the corresponding free energy is almost free energy a for the case of N P T the corresponding free energy is G and that is why when we can have an P and T as independent variable to evaluate or to calculate chemical potential we simply take the partial derivative of G with respect to N i.

On the other hand when you have N V T as independent variable we take partial derivatives of a with respect to N i that is what we have done here since a is hey this. Now, we can use this expression to calculate this ok. And from here we can come up with this expression ok.

Now, the question is how do we evaluate this. So, let me just try to explain this or rather derive this part ok. That means, for the case of data where you have V and T are independent variable we can write this fugacity coefficient in this form this is different from the form which we have used earlier where the pressure was independent variables ok. If you recall you know RT lnf by y I P is equal to 0 to P 0 to P V i bar minus RT by P dp right, but here its different why the reason for that is since V is independent variable ok. So, how do we get this? See if you also look at it the left hand side we are saying T P N for a given T P N. Now, this P we cannot control is a wall in which we are controlling, but this P is basically corresponding to the V volume final conditions ok. But the data on the right hand side as a data data is available is based on only volume not on P and that is why we use the right hand side expression to get the integral form, but the left hand side says the fugacity at temperature and pressure given temperature pressure.

So, for example, if the question is for you is that you have a system which you are interested to fare to find out the fugacity and the temperature in pressure and the mole compositions are given to you, but the data from the experiments are available only in terms of the volume volumetric properties have obtained. So, you can you know the data for example, for different different volumes information's are available from extremely small molar you know something like you know 10 to minus 5 molar or litres for example. So, for very very small volume to very large volume; if the things available to you in some form then you may be able to use that so that information you should know.

So that means, for example, if I 100 points corresponding to volume and then other information there that for each volume this is the other properties for each volume in a given temperature I am varying for given temperature and varying the volume from let us say from very V to infinity or rather infinity to V ok, from very very large system infinitely large volume to V and for each volume in the intermediate point I need to find out the partial derivative of pressure as a function of N i.

Now, this is a tricky part. How do you calculate? Because I do not have handle to the pressure right; What I interested is the pressure of the final thing, so P is dependent on the intermediate volume also. But this is the expression which we get and we can make use of it, but before I get to the point and explain how to do that let me first derive this expression. So, we can take a generic expression also. Where does this term come from? So, let me try to simply use this information here itself to derive this part ok. So, if you look at here this is the information of the chemical potential right and you know that mu i minus mu i 0 is nothing, but RT ln f i and by f a 0.

So, this part actually corresponds to mu this is U minus T s plus RT this is nothing, but mu I, i for ideal gas ok. So, this you can show that this is corresponding to ideal gas part and this is nothing, but mu z from mu i minus mu i of ideal gas. So, you can show that this is nothing but this for i, this is something which we have shown earlier also mu i minus mu i ideal gas is nothing, but at here and this. So, this is how it simply can be shown. So, of course, from here, so what is the key thing is basically showing this explained these are the two important things and once you do that the rest of the things are straightforward ok.

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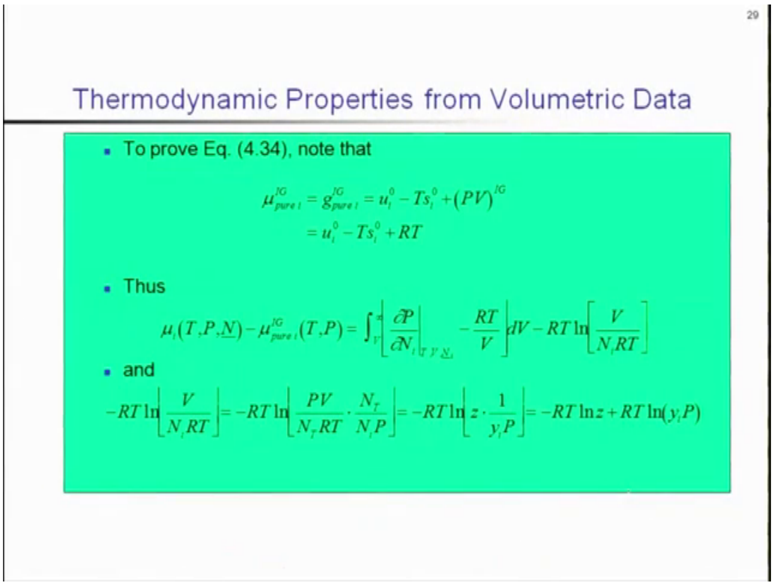

Thermodynamic Properties from Volumetric Data

- To prove Eq. (4.34), note that

$$\mu_{pure\,i}^{IG} = g_{pure\,i}^{IG} = u_i^0 - Ts_i^0 + (PV)^{IG}$$
$$= u_i^0 - Ts_i^0 + RT$$

- Thus

$$\mu_i(T,P,\underline{N}) - \mu_{pure\,i}^{IG}(T,P) = \int_V^\infty \left[\left. \frac{\partial P}{\partial N_i} \right|_{T,V,\underline{N}_j} - \frac{RT}{V} \right] dV - RT\ln\left[\frac{V}{N_i RT}\right]$$

- and

$$-RT\ln\left[\frac{V}{N_i RT}\right] = -RT\ln\left[\frac{PV}{N_T RT}\cdot\frac{N_T}{N_i P}\right] = -RT\ln\left[z\cdot\frac{1}{y_i P}\right] = -RT\ln z + RT\ln(y_i P)$$

Let me consider this expressions and let us say for a pure system, pure fluid ok; for pure fluid if I consider the same expression in terms of the variable. So, again considering V and T these are the independent variables I get the funny expression, f pure i TP by P equal to V by infinity P by N of whatever the component i is ok, minus R T by V T V minus RT and then z plus RT z minus 1 ok.

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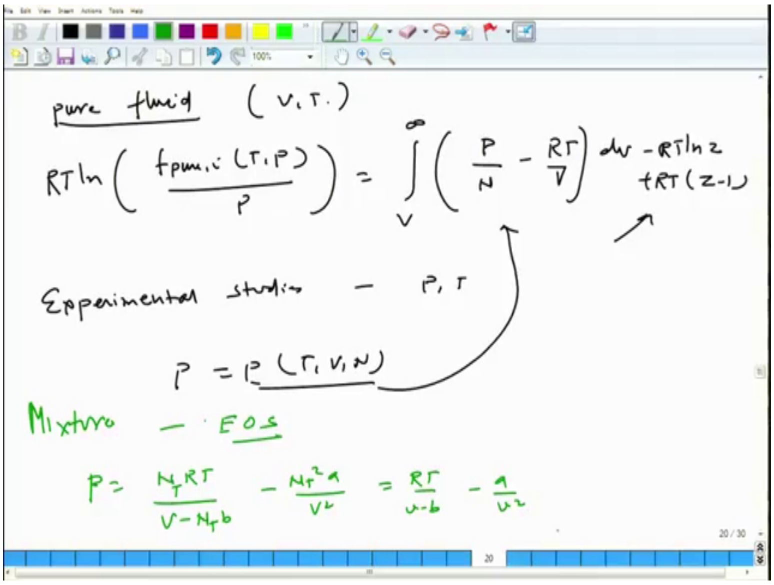

pure fluid (V, T)

$$RT\ln\left(\frac{f_{pure,i}(T,P)}{P}\right) = \int_V^\infty \left(\frac{P}{N} - \frac{RT}{\bar{V}}\right) dv - RT\ln z + RT(z-1)$$

Experimental studies — P, T

$$P = P(T, V, N)$$

Mixture — EOS

$$P = \frac{N_T RT}{V - N_T b} - \frac{N_T^2 a}{V^2} = \frac{RT}{v-b} - \frac{a}{v^2}$$

This is the expression from the earlier expression which you can and this is something which you can derive also ok. Now, this equation becomes very difficult actually ok. The earlier expressions which we have calculated earlier is much more convenient which was nothing, but the integral of V i bar R V minus RT by P right that is more convenient to say that because one of the reason is that mostly experimental study they are done usually considering P and T as independent variable.

So, that is one of the reason that earlier expression is more conveniently to use, but if you have this or particularly for mixtures this expression becomes much more useful and using P as a P T V N, we can easily model such a thing. In other word this is this expression becomes useful when we use equation of states ok.

So, this is more easily you can use equation of state because here you can plug this pressure here in this form and you can do the rest of the things ok. So, similarly you can take for the mixtures the partial derivative of the pressure with respect to N and you can derive all the things ok.

So, for that we can consider an example. So, again some mixtures we can use a equation of state and the wave equation. So, example let us say is let us say this N R T. So, in the case this is a mixture. So, I will put as N T V minus N T b minus N T square a by V square is equal to RT V by may. So, this is something which we can use now, to find out the so this is nothing but molar volume, right this is nothing but V by N T ok.

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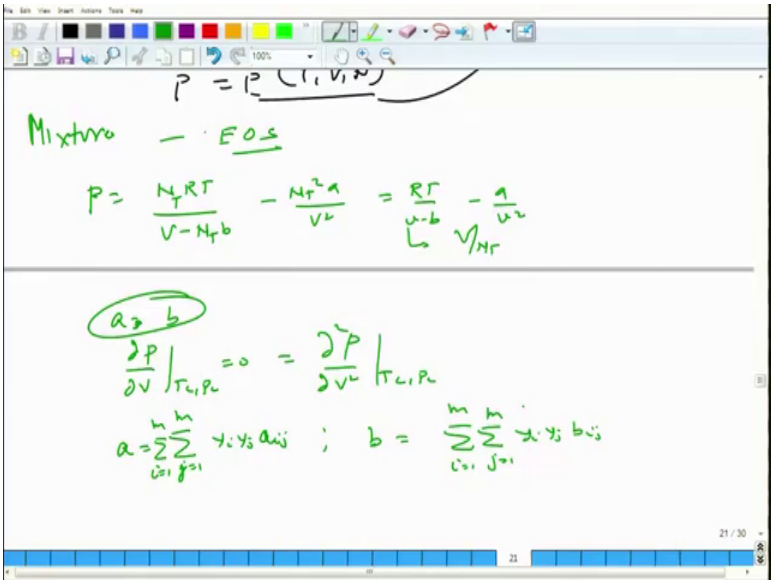

Mixture – EOS

$$P = \frac{N_T RT}{V - N_T b} - \frac{N_T^2 a}{V^2} = \frac{RT}{v-b} - \frac{a}{v^2}$$

V/N_T

a, b

$$\left.\frac{\partial P}{\partial V}\right|_{T_c, P_c} = 0 = \left.\frac{\partial^2 P}{\partial V^2}\right|_{T_c, P_c}$$

$$a = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j a_{ij} \; ; \; b = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j b_{ij}$$

Now, what are the as in this case for the for the van der Waal equation? You can calculate from the critical property. So, if you take their critical property conditions such as. So, to calculate a and b we use the del P by del V, ok. So, for mixtures we have to come up with. So, that is fine, but for mixtures we have to come up with other things also. We have to come up with some kind of a mixing rule because you have many many components. So, usually for b V let me just write for a a we write this expression a ij where this is double summation ok, mi is equal to one to m and i and j is equal to 1 to N ok.

And for b we again use here b ij ok. So, this is one kind of mixing rule to obtain a and b for the mixtures. So, and the question is what is a ij, again many times you cannot evaluate this for example, you can find out a and b for the pure system directly from the critical temperature and you know information's of the phase diagram right, but for for binary mixtures or in general mixtures you do not have just one critical point from any composition you will have any critical point and you can even have a critical line for different composition there will be a specific T C for a constant PC and thus you can draw critical line this it is not directly feasible.

But if you want to model it you have to make understand how to get a ij, but these are difficult part; y's and y js are available because that is how you going to do the experiment. But what about a ij? Again here also we make use of some approximation whether one particular approximation is Berthelot's formula, where we are consider ai j to be a geometric mean of ai and aj and b ij as the arithmetic mean of bi plus bj ok.

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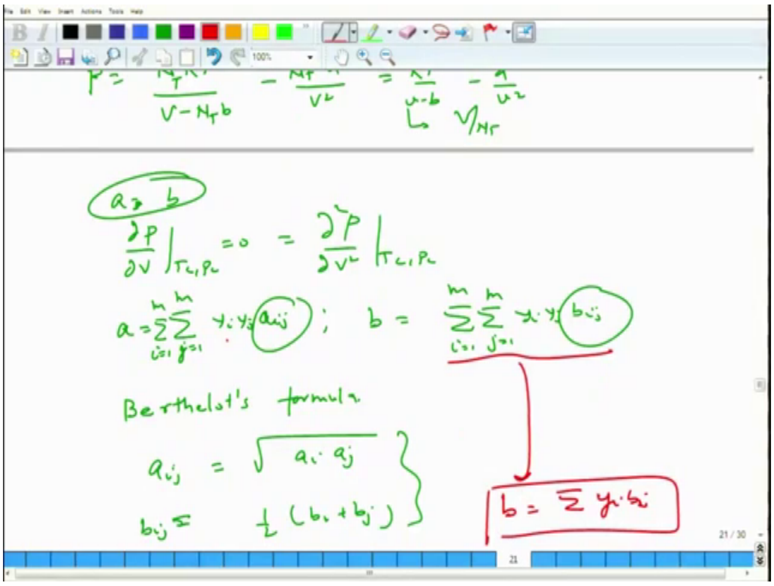

So, this is something once you have these different components pure a and b which you can calculate from their critical properties. For example, if I consider pro propane and butane. So, I can get a of propane and b of propane and as well as for butane and once I mix it I will be using this once I do I have got this a is a ij and bij ok, I can get a of the mixture depending on what is the composition all right. With this approximation this is simplified which it is written as simply y i vi with this approximation.

Now, if you apply this to van der Waals equation of state using this Berthelot's mixing rule the following expression can be written.

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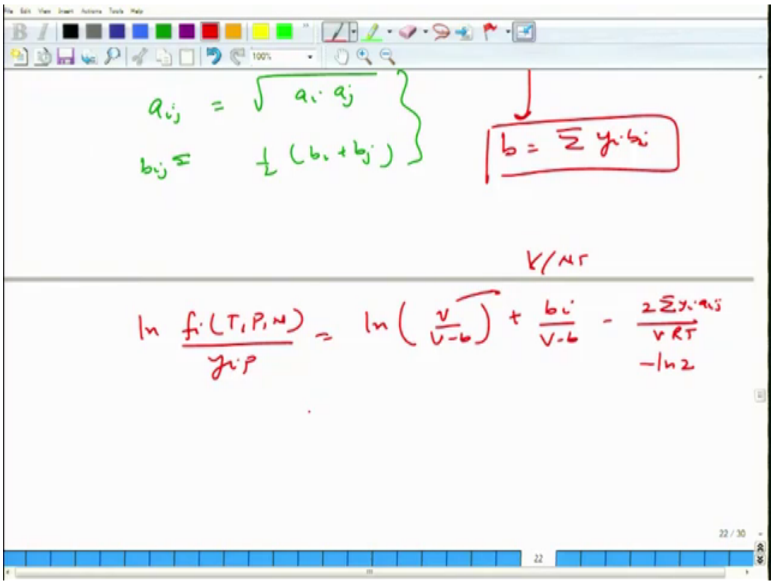

$$\left.\begin{aligned} a_{ij} &= \sqrt{a_i a_j} \\ b_{ij} &= \tfrac{1}{2}(b_i + b_j) \end{aligned}\right\}$$

$$\boxed{b = \sum y_i b_i}$$

V/NT

$$\ln \frac{f_i(T,P,N)}{y_i P} = \ln\left(\frac{V}{V-b}\right) + \frac{b_i}{V-b} - \frac{2\sum y_i a_{ij}}{VRT} - \ln z$$

So, I can get this ln f i again TP N y I P ok. Now, I have the expression of P which is as a function of other terms right, I have to plug in here right and then the fugacity in this following term ln V by V minus b here, V is capital V divided by N T plus b i by V minus P minus 2 summation y i, ai j V R T minus ln z ok.

Now, of course, you cannot remember this equation of state this is very very complicated, but this is how it is derived. Now, if I change this equation of state to other equation of state the expressions are going to be different ok. And there are many popular equations state van der Waal equation is straight for example, is not widely used because it has a limitation as far as what the range of the temperature pressure it can cover; But the popular equation of state such as you Redlich-Kwong. So, I will just going to just make a note of this expression which we are going to get if I had used other equations of state.

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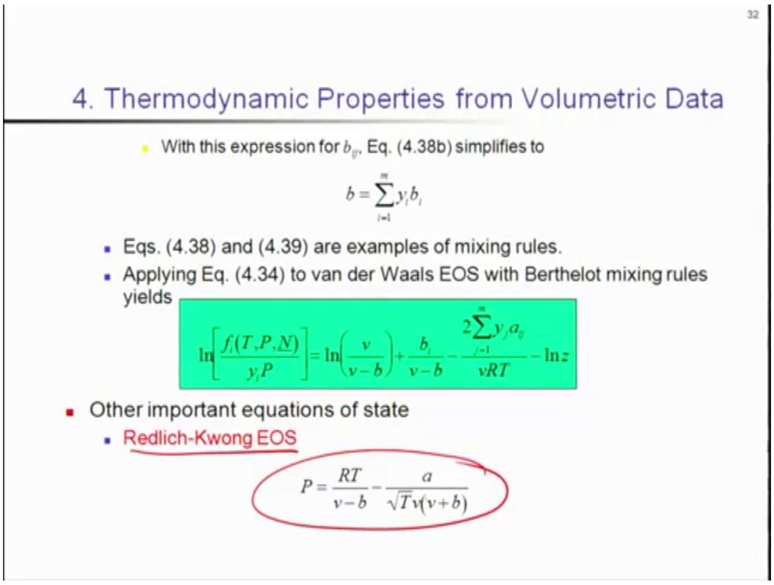

4. Thermodynamic Properties from Volumetric Data

- With this expression for b_{ij}, Eq. (4.38b) simplifies to

$$b = \sum_{i=1}^{m} y_i b_i$$

- Eqs. (4.38) and (4.39) are examples of mixing rules.
- Applying Eq. (4.34) to van der Waals EOS with Berthelot mixing rules yields

$$\ln\left[\frac{f_i(T,P,\underline{N})}{y_i P}\right] = \ln\left(\frac{v}{v-b}\right) + \frac{b_i}{v-b} - \frac{2\sum_{j=1}^{m} y_j a_{ij}}{vRT} - \ln z$$

- Other important equations of state
  - Redlich-Kwong EOS

$$P = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)}$$

So, the other equations of state is Redlich-Kwong equation of state which is this. So, this is the first term is the same term as in the van der Waal equation of state. And, but it has this additional terms which basically is to correct and provide some temperature dependency in this form anyway.

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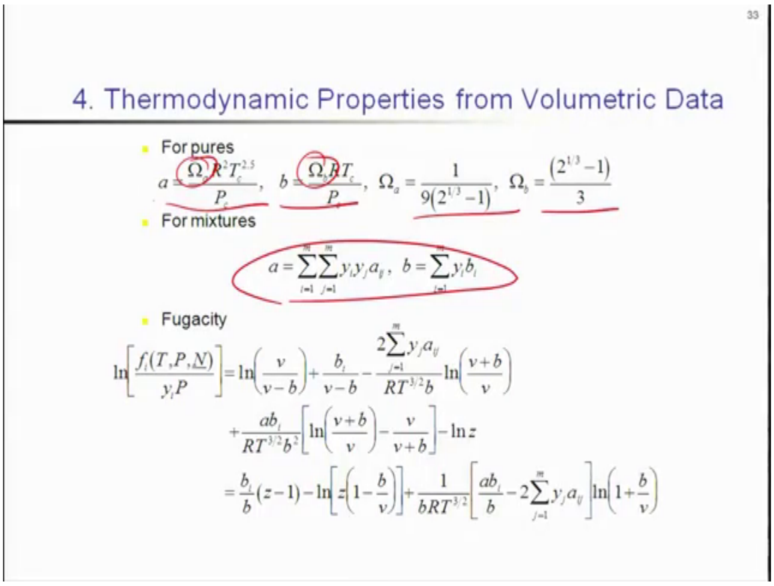

4. Thermodynamic Properties from Volumetric Data

- For pures

$$a = \frac{\Omega_a R^2 T_c^{2.5}}{P_c}, \quad b = \frac{\Omega_b R T_c}{P_c}, \quad \Omega_a = \frac{1}{9(2^{1/3}-1)}, \quad \Omega_b = \frac{(2^{1/3}-1)}{3}$$

- For mixtures

$$a = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j a_{ij}, \quad b = \sum_{i=1}^{m} y_i b_i$$

- Fugacity

$$\ln\left[\frac{f_i(T,P,\underline{N})}{y_i P}\right] = \ln\left(\frac{v}{v-b}\right) + \frac{b_i}{v-b} - \frac{2\sum_{j=1}^{m} y_j a_{ij}}{RT^{3/2} b}\ln\left(\frac{v+b}{v}\right)$$
$$+ \frac{ab_i}{RT^{3/2} b^2}\left[\ln\left(\frac{v+b}{v}\right) - \frac{v}{v+b}\right] - \ln z$$
$$= \frac{b_i}{b}(z-1) - \ln\left[z\left(1-\frac{b}{v}\right)\right] + \frac{1}{bRT^{3/2}}\left[\frac{ab_i}{b} - 2\sum_{j=1}^{m} y_j a_{ij}\right]\ln\left(1+\frac{b}{v}\right)$$

So, if you use this equation state ok, where a is related to this expressions ok, where these are the part of the molecules properties ok and this is something given in this way and this is the mixing rule is same, but a’s and b’s are of the individual molecules is not just dependent on I mean it is not in the same as we have seen in the van der Waals equation.

So, what is the a b for example, a pure system? For a b for pure system is going to be this, for van der Waal equation of state ok.

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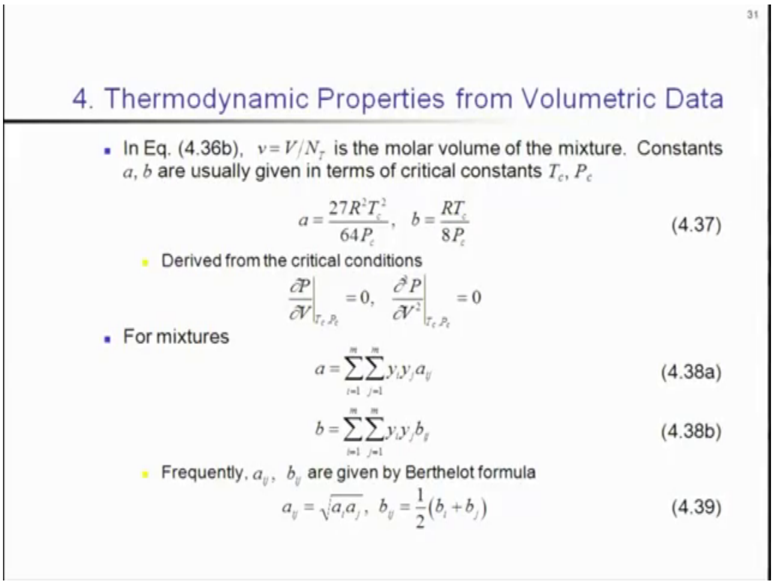

4. Thermodynamic Properties from Volumetric Data

- In Eq. (4.36b), $v = V/N_T$ is the molar volume of the mixture. Constants a, b are usually given in terms of critical constants T_c, P_c

$$a = \frac{27R^2T_c^2}{64P_c}, \quad b = \frac{RT_c}{8P_c} \tag{4.37}$$

  - Derived from the critical conditions

$$\left.\frac{\partial P}{\partial V}\right|_{T_c,P_c} = 0, \quad \left.\frac{\partial^2 P}{\partial V^2}\right|_{T_c,P_c} = 0$$

- For mixtures

$$a = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j a_{ij} \tag{4.38a}$$

$$b = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j b_{ij} \tag{4.38b}$$

  - Frequently, a_{ij}, b_{ij} are given by Berthelot formula

$$a_{ij} = \sqrt{a_i a_j}, \quad b_{ij} = \frac{1}{2}(b_i + b_j) \tag{4.39}$$

For the case of this Redlich-Kwong the expression is different ok, but nevertheless this expression may change because you are changing the equation of state the mixing rule if you use Berthelot’s rule then these are going to be this, but in general we are going to use this as and bs in this form and then you can come up with this expression and look at the complicated expression here you cannot. Remember this, right this expression is finally, the expression ok.

You cannot remember this you can derive this and may and plug it in you in your in the excel sheet or some writing the program there is something which is expected want to do. And now, these are the equations which are already plugged in many software already.

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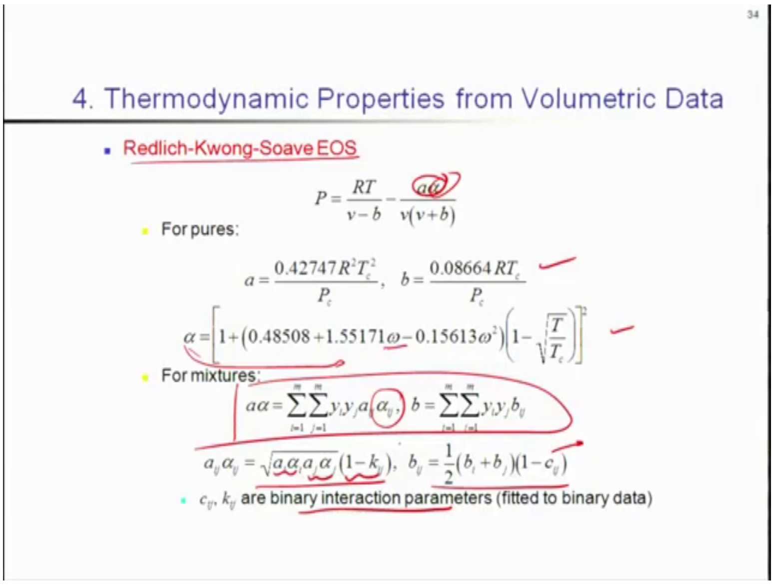

4. Thermodynamic Properties from Volumetric Data

- Redlich-Kwong-Soave EOS

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

- For pures:

$$a = \frac{0.42747 R^2 T_c^2}{P_c}, \quad b = \frac{0.08664 RT_c}{P_c}$$

$$\alpha = \left[1 + \left(0.48508 + 1.55171\omega - 0.15613\omega^2\right)\left(1 - \sqrt{\frac{T}{T_c}}\right)\right]^2$$

- For mixtures:

$$a\alpha = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j a_{ij}\alpha_{ij}, \quad b = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j b_{ij}$$

$$a_{ij}\alpha_{ij} = \sqrt{a_i\alpha_i a_j\alpha_j}\,(1-k_{ij}), \quad b_{ij} = \frac{1}{2}(b_i + b_j)(1-c_{ij})$$

- c_{ij}, k_{ij} are binary interaction parameters (fitted to binary data)

Not a very new equation of state these are already very old. Now, the modification of Redlich-Kwong is rattling Redlich-Kwong or RKs soave equation of state where another term alpha comes into picture which depends on the eccentric factor it talks about the shape of the molecule ok. Now, you have a for the pure system is this with an alpha and again here we are using the similar kind of mixing rules we are basically alpha. Now, for pure is alpha but for the mixtures is going to be alpha ij which is given in the more complicated expressions.

Now, in here the mixing rule is not simply arithmetic average of the b's, but there is another term which is multiplied which adds to corrects the this idle way of kind of averaging the b's by a term which has a interaction parameter ok. So, you it means basically it can get inside a bit also right. Here k ij these are correction to the simple Berthelot's rules ok.

So, this and this is basically geometric mean of a alpha ok. Now, i a alpha is term which is basically. So, a is the typical energetic terms given by the van der Waal right. So, this alpha is basically a bit of corrections to that which depends on the eccentric factors of the molecule which they van der Waal equation is a do not capture because it does not take into account the shape factor. Now, this term together can be written in this way to get an average value or the value for the mixtures a for i and j.

Now, if you do the geometric mean then this would be this, this term multiplied by this and the root of that and then since they would be I mean if they is any specific deviation from this, this is given by this term which has this binary interaction parameter ok. Now, this can be fitted. Now, the question is, now does it has a very significant or does it does this term can be connected to any physical meaning ok. It is difficult to say that. Usually what is done is basically we fit this to the boundary to the data of the experimental and evaluate this tops ok. So, this is the fugacity expression of this.

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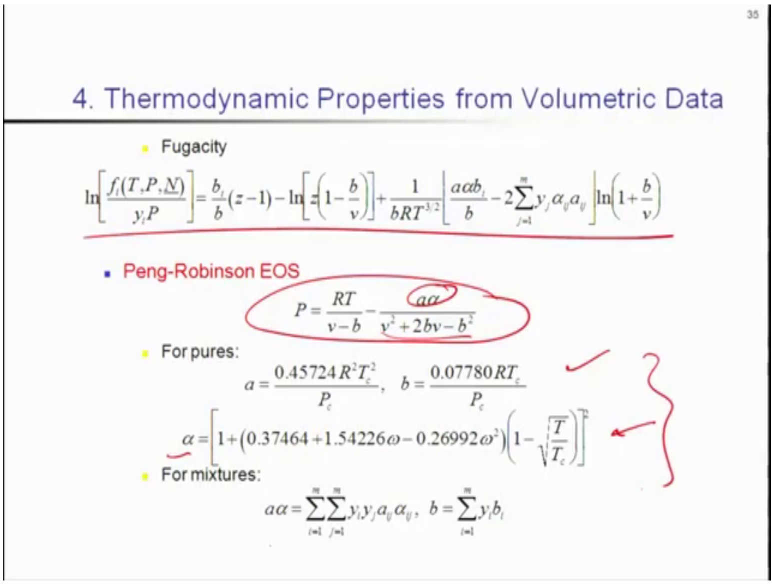

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4. Thermodynamic Properties from Volumetric Data

- Fugacity

$$\ln\left[\frac{f_i(T,P,\underline{N})}{y_i P}\right]=\frac{b_i}{b}(z-1)-\ln\left[z\left(1-\frac{b}{v}\right)\right]+\frac{1}{bRT^{3/2}}\left[\frac{a\alpha b_i}{b}-2\sum_{j=1}^{m}y_j\alpha_{ij}a_{ij}\right]\ln\left(1+\frac{b}{v}\right)$$

- Peng-Robinson EOS

$$P=\frac{RT}{v-b}-\frac{a\alpha}{v^2+2bv-b^2}$$

- For pures:

$$a=\frac{0.45724R^2T_c^2}{P_c},\quad b=\frac{0.07780RT_c}{P_c}$$

$$\alpha=\left[1+\left(0.37464+1.54226\omega-0.26992\omega^2\right)\left(1-\sqrt{\frac{T}{T_c}}\right)\right]^2$$

- For mixtures:

$$a\alpha=\sum_{i=1}^{m}\sum_{j=1}^{m}y_iy_ja_{ij}\alpha_{ij},\quad b=\sum_{i=1}^{m}y_ib_i$$

Now, similarly you have this Peng-Robinson equation again you have this term a alpha this is the denominator is modified a bit alpha has the same expression this is for the pure system is same ok. Here again we are doing the same exercise ok. Here of course, you can see the same term. So, you got an expression like this ok.

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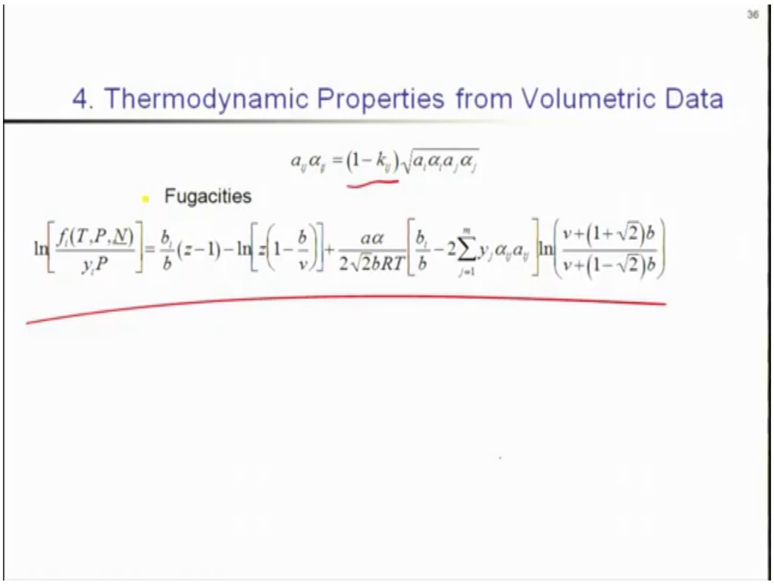

4. Thermodynamic Properties from Volumetric Data

$$a_{ij}\alpha_{ij} = \underline{(1-k_{ij})}\sqrt{a_i\alpha_i a_j\alpha_j}$$

- Fugacities

$$\ln\left[\frac{f_i(T,P,\underline{N})}{y_iP}\right] = \frac{b_i}{b}(z-1) - \ln\left[z\left(1-\frac{b}{v}\right)\right] + \frac{a\alpha}{2\sqrt{2}bRT}\left[\frac{b_i}{b} - 2\sum_{j=1}^{m} y_j\alpha_{ij}a_{ij}\right]\ln\left(\frac{v+(1+\sqrt{2})b}{v+(1-\sqrt{2})b}\right)$$

These are the expressions which you cannot remember, but of course, you have to understand the left hand side expression or the fugacity can be evaluated using different means if you use different equation of state. And not necessarily everything every equation the state will behave equally good. Some may behave better.

So, if you have a given a data you can fit these expressions evaluate it and then you can check whether some equation of state is better or not by comparing with the exact value from the experiment. So, this is something which I expect the later part of the course you would be able to appreciate it. Now, what we can do is we can move to the next part which essentially is the approaches to phase equilibria calculations ok.

So, today's lecture will stop here and will continue in the next lecture different methodology which we can adopt in order to calculate phase equilibria calculation depending on what are the variables available ok. So, you can do a dew point calculation bubble point calculation. So, what are the typical algorithms we should have adopt in order to solve such phase equilibria calculation effectively?

So, see you in the next lecture.