Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 4
Constitutive relations - mass transfer and thermodynamics

Hello, everyone. So, we are going to talk about today in this class from where we left in the previous lecture regarding the derivation of the Maxwell Stephan's theory for multi-component diffusion. Now, if you recall, this is applicable for the scenario when you have more than 2 species, or it is not a binary system. And essentially, we are talking about when it is not a dilute case and concentration of each of the species is important.

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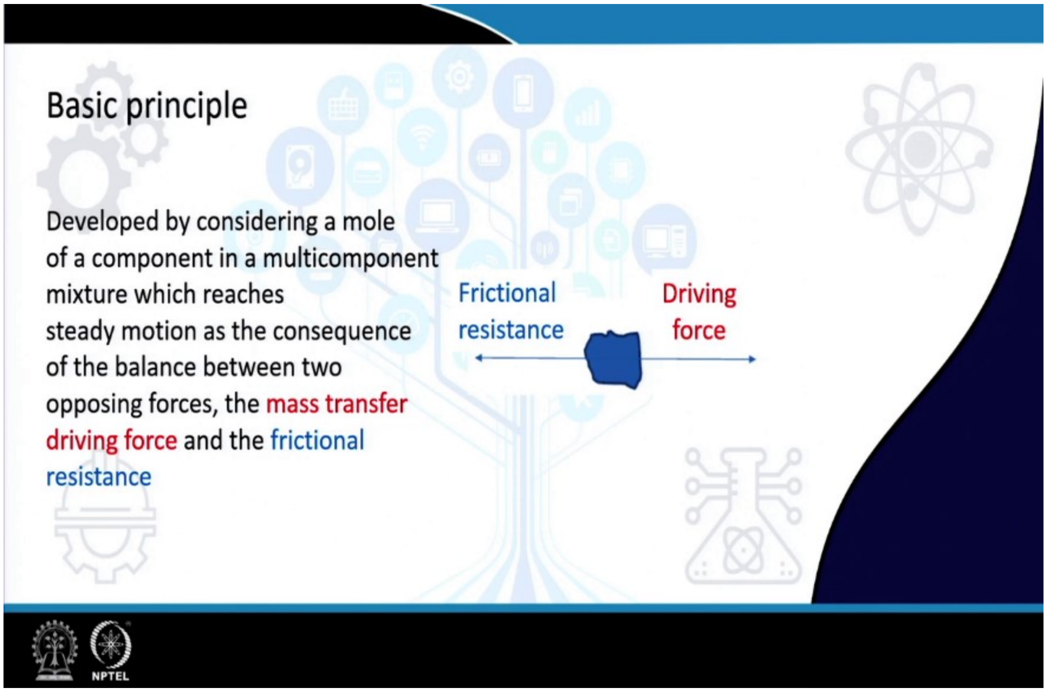

Basic principle

Developed by considering a mole of a component in a multicomponent mixture which reaches steady motion as the consequence of the balance between two opposing forces, the mass transfer driving force and the frictional resistance

Now, in this case let us just quickly get started, and if you recall that this is, there is a balance at the molecular level, there is a balance between the frictional resistance and the driving force So, from this balance, I mean, this is the Genesis of the derivation of this Maxwell Stephan's theory where we try to balance 2 opposing forces, one due to the mass transfer driving force, another due to the frictional resistance.

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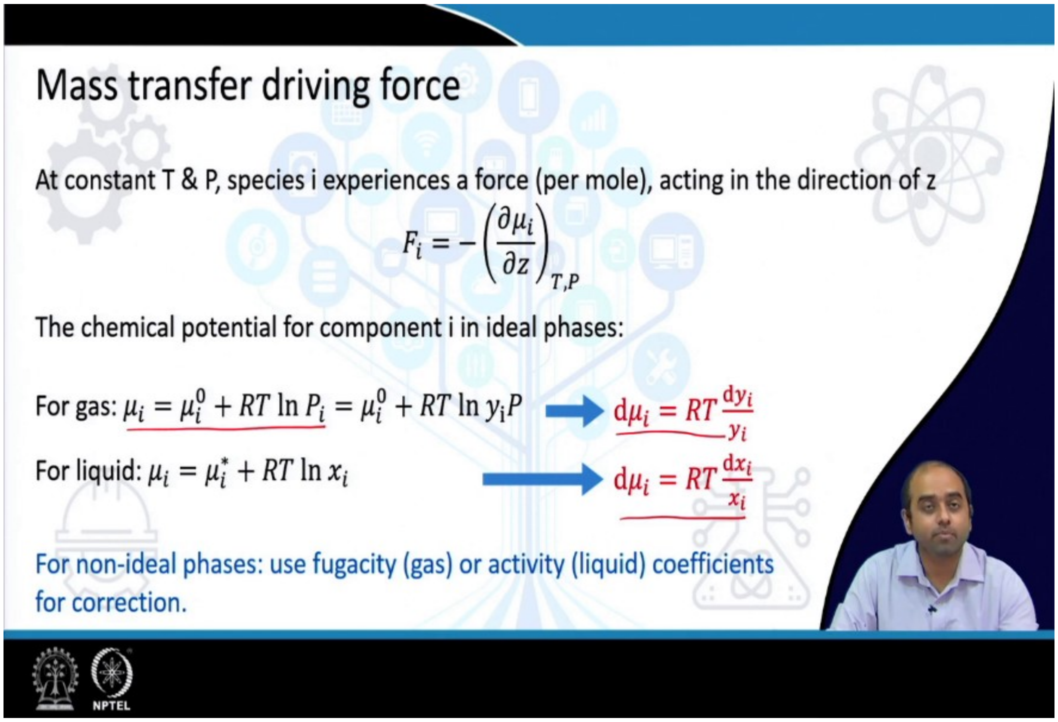

Mass transfer driving force

At constant T & P, species i experiences a force (per mole), acting in the direction of z

$$F_i = -\left(\frac{\partial \mu_i}{\partial z}\right)_{T,P}$$

The chemical potential for component i in ideal phases:

For gas: $\underline{\mu_i = \mu_i^0 + RT \ln P_i} = \mu_i^0 + RT \ln y_i P \rightarrow \underline{d\mu_i = RT \frac{dy_i}{y_i}}$

For liquid: $\mu_i = \mu_i^* + RT \ln x_i \rightarrow \underline{d\mu_i = RT \frac{dx_i}{x_i}}$

For non-ideal phases: use fugacity (gas) or activity (liquid) coefficients for correction.

Now, coming to the mass transfer driving force all of us are aware of the fact that the force acting on this molecule in terms of per mol unit is nothing but the gradient of the chemical potential at constant temperature and pressure. Now, from thermodynamics, we know that the chemical potential for gas or for liquid system is generally represented in terms of RT ln P whereas where you write P for in the case of gas, T and for the case of liquid, with essentially the activity coefficients or for ideal solutions is just a mass fraction, or essentially mole fractions.

Now, from there, we can calculate out the differential d mu i, and you can get an estimation on this force exerted on the molecules due to this mass transport, fundamentally from the thermodynamics.

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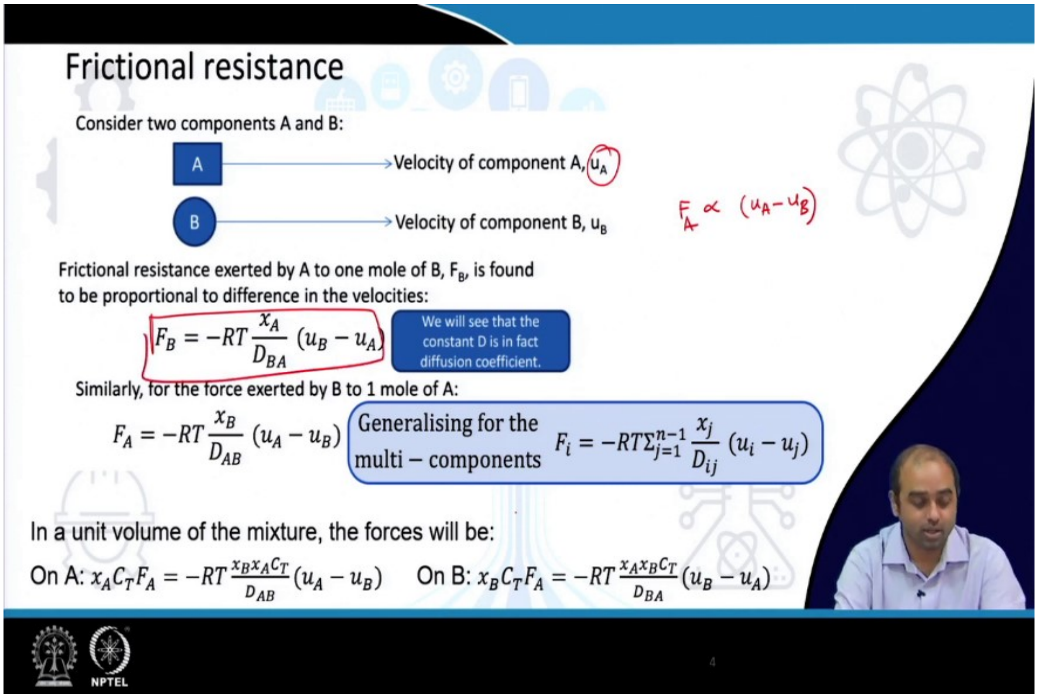

Frictional resistance

Consider two components A and B:

A → Velocity of component A, u_A

B → Velocity of component B, u_B

$F_A \propto (u_A - u_B)$

Frictional resistance exerted by A to one mole of B, F_B, is found to be proportional to difference in the velocities:

$$\boxed{F_B = -RT\frac{x_A}{D_{BA}}(u_B - u_A)}$$

We will see that the constant D is in fact diffusion coefficient.

Similarly, for the force exerted by B to 1 mole of A:

$$F_A = -RT\frac{x_B}{D_{AB}}(u_A - u_B)$$

Generalising for the multi – components $F_i = -RT\Sigma_{j=1}^{n-1}\frac{x_j}{D_{ij}}(u_i - u_j)$

In a unit volume of the mixture, the forces will be:

On A: $x_A C_T F_A = -RT\frac{x_B x_A C_T}{D_{AB}}(u_A - u_B)$ On B: $x_B C_T F_A = -RT\frac{x_A x_B C_T}{D_{BA}}(u_B - u_A)$

The critical part comes when we try to evaluate or understand the frictional resistance. Now, let us consider there are 2 components, and then we will try to extend this idea for multi components. There are, let us say that we have 2 species in the system and we represent their individual molecular velocity as or the molecular level velocity as UA and UB.

Now, it is said, I mean, fundamentally explained by Maxwell in his book on dynamical theory of gases, that the fictional resistance exerted by A onto B is proportional to the relative difference in their velocities, or it is proportional to the relative velocity. So, this F or the force is proportional to the relative velocity of a particular molecule that is acting on the other molecule.

So, this is the case of F, this A. So, similarly it can be written down for this, trying to estimate the relative velocity between any 2 species in the case of multi component systems. Now, you can ask, or you can ask or question, that there is a point that how come this remaining derivation, this, this force, this RT, Xa D_{BA}, how diffusing, etc., is coming into the picture.

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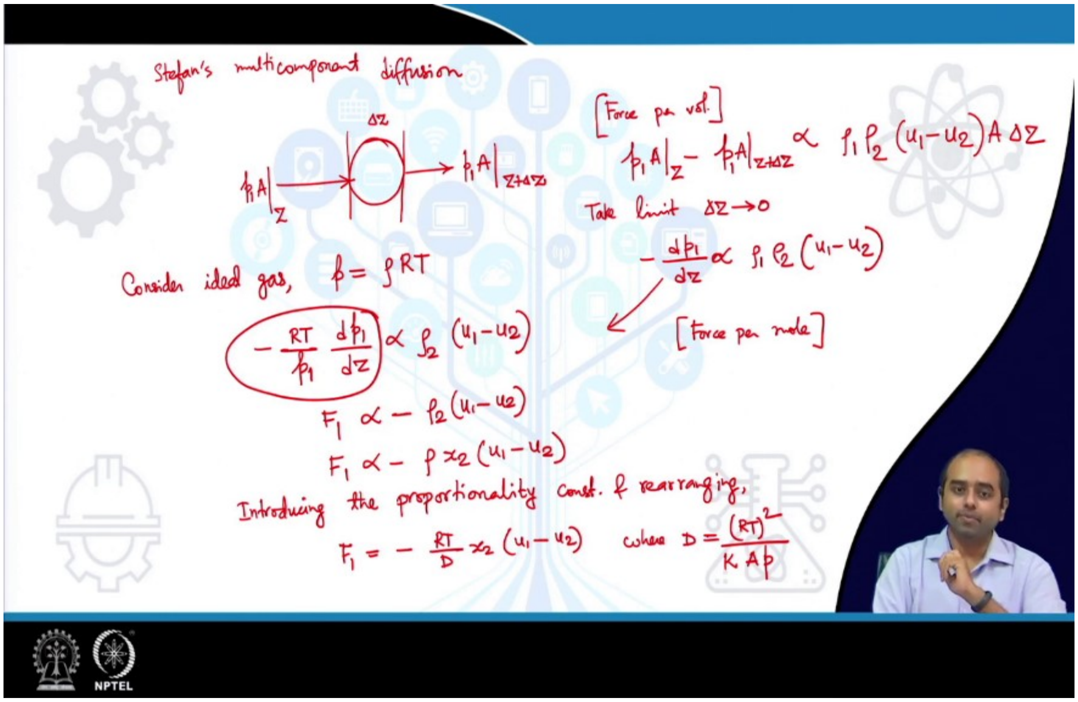


Stefan's multicomponent diffusion

[Force per vol.]

$$p_1 A|_z - p_1 A|_{z+\Delta z} \propto \rho_1 \rho_2 (u_1 - u_2) A \Delta z$$

Take limit $\Delta z \to 0$

$$-\frac{dp_1}{dz} \propto \rho_1 \rho_2 (u_1 - u_2)$$

[Force per mole]

Consider ideal gas, $p = \rho RT$

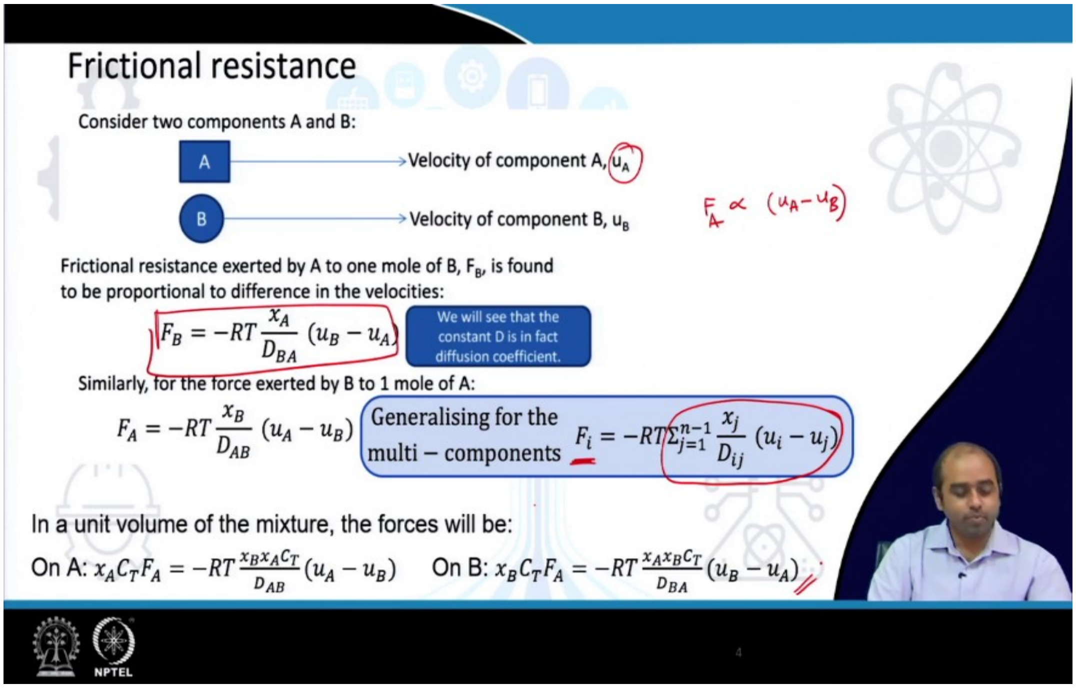
$$-\frac{RT}{p_1}\frac{dp_1}{dz} \propto \rho_2 (u_1 - u_2)$$

$$F_1 \propto -\rho_2 (u_1 - u_2)$$

$$F_1 \propto -\rho x_2 (u_1 - u_2)$$

Introducing the proportionality const. & rearranging,

$$F_1 = -\frac{RT}{D} x_2 (u_1 - u_2) \quad \text{where } D = \frac{(RT)^2}{KAp}$$



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For that, we have to go a little bit into the background of the derivation of this Stephan's multi component diffusion. And it tells you that, let us assume we are having this particle or a molecule and across its boundary it is experiencing a force. So, we write the force in terms of pressure versus the projected area at Z, let us say, this is a small elemental section, please, excuse my drawing, and this is the pressure acting at Z plus Delta Z. So, the force per volume, if I try to write in this terminology is p into A at Z. So, the difference in the force acting at the 2 surfaces is equated, or is proportional to the density of the individual species, the relative velocity and the volume of this small elemental zone or the region.

So, we all know that the rate of change of momentum is actually contributed to the force and that is what is the basis behind this statement. And then if you take the limit of delta Z tending to 0, what we will get is dPi dZ is proportional to rho 1, rho 2, u1 minus u2. Now, if you consider a situation of ideal gases where we know that this pressure is equal to density times the gas constant times temperature in that case, from this expression here, what we can write, I mean, we can write in terms of force per mole as minus RT by p1. So, I am just converting one of the densities in terms of the pressures, dp1 by dz, rho 2, u1 minus u2. So, this entire quantity, (RT by p1) dp, dz. We already know that this is nothing but our what is called this force acting on the particle. It is minus rho 2 u1 minus u2. And this rho 2 can be written down from a Dalton's law as minus rho into X 2, isn't it E 1 minus U.

And then if you invoke this proportionality constant, you can have a proportionality constant, something like a K or something like that. And if you rearrange, so in introducing the proportionality constant and rearranging, you can get F1 is equal to minus RT by D x2 u1 minus u2, where I can write this D is nothing but RT squared by this proportionally constant, this area, A and this rho, sorry not rho this is P.

So, you can just work out the intermediate step and you will, this is what you will be getting in this scenario. So, this is how we get this, what we just have explained you, that F is equal to RT and this constant, I mean, this constant, that balances, the force with respect to the relative velocity actually gives the origin of the diffusivity or the diffusion coefficient.

Similarly, we can write this force acting on the other particle I mean, this is F_B and then we can write for F_A and can easily understand that this can be generalized for multiple components where you need to sum up or take into consideration of all the other species that are in the system considering their relative velocity.

So, if you want to calculate the force exerted on particle A, so what is the relative velocity of a, with all the N minus 1 species, that needs to be taken into account here. So, this is per mole. So, we convert it into per unit volume of the mixture, and this is how the forces or these terms looks like. Now, it is time to balance these 2.

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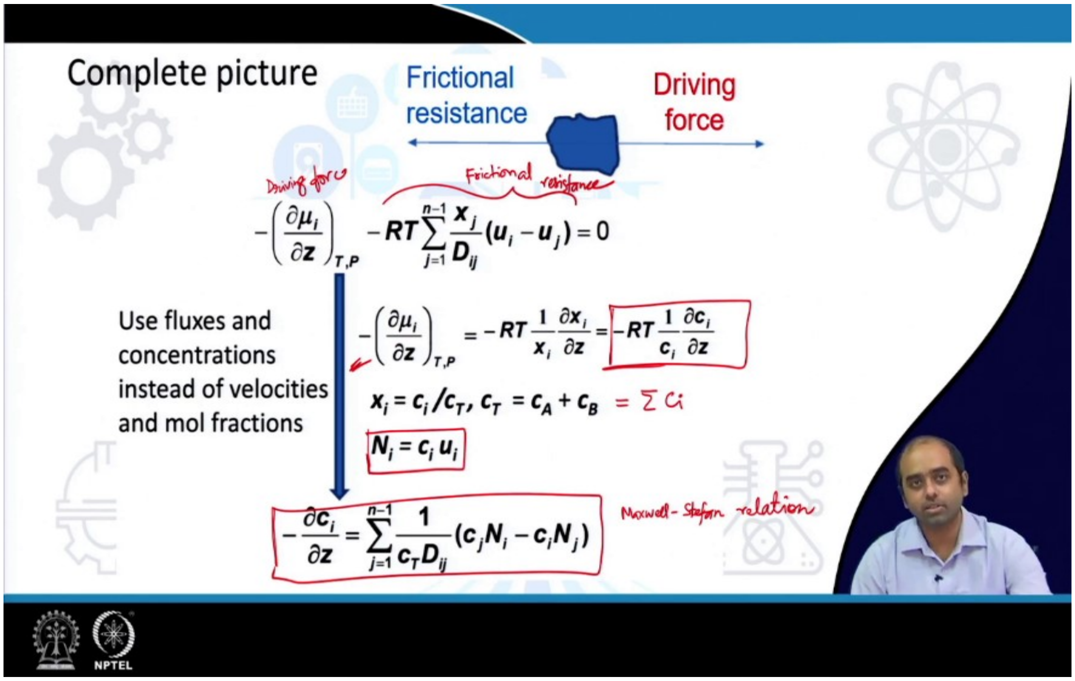

Complete picture

Driving force

$$-\left(\frac{\partial \mu_i}{\partial z}\right)_{T,P} \underbrace{- RT\sum_{j=1}^{n-1}\frac{x_j}{D_{ij}}(u_i - u_j)}_{\text{Frictional resistance}} = 0$$

Use fluxes and concentrations instead of velocities and mol fractions

$$-\left(\frac{\partial \mu_i}{\partial z}\right)_{T,P} = -RT\frac{1}{x_i}\frac{\partial x_i}{\partial z} = \boxed{-RT\frac{1}{c_i}\frac{\partial c_i}{\partial z}}$$

$$x_i = c_i/c_T,\ c_T = c_A + c_B = \sum c_i$$

$$\boxed{N_i = c_i u_i}$$

$$\boxed{-\frac{\partial c_i}{\partial z} = \sum_{j=1}^{n-1}\frac{1}{c_T D_{ij}}(c_j N_i - c_i N_j)}$$

Maxwell-Stefan relation

Now it is time to get the complete picture. So, what we do, we try to balance the, so there is this, this part is the driving force and then you have this part as the frictional, from the frictional resistance, derivation that is what you get. So, then we do some algebraic steps. I mean, you can clearly follow that we try to take in both sides and write this d mu/dz as in this form.

And we write the, instead of writing the individual mole, mass fractions, or the, sorry, the mole fractions, we can write it in terms of the total concentration. So, this CT, whatever we write the CA plus CB, or essentially this is nothing but CI. Now, this flux are the molar flux. So, please note that the molar flux here is written as the concentration into the velocity.

And please note that this velocity is not the bulk velocity, but individual molecular movement, or the molecular scale speed, or the molecular scale velocity of the particles. So please do not get it confused with the bulk scale velocity. So, since we are considering, so there is the confection due to the molecular movements and that in the macroscopic world gets transferred into diffusion.

So, this is that, molecular level conviction or the molecular level, mass transport due to the Brownian motion mostly. So, if you rearrange these equations or these terms, you are likely to get this expression. So, this is the Maxwell Stephan's relation for multi, which is valued for multiple components. And for, I mean, it, the, the condition of this dilute and all those things need not to be invoked. So, now let us look into some of the simplified scenarios based on this equation.

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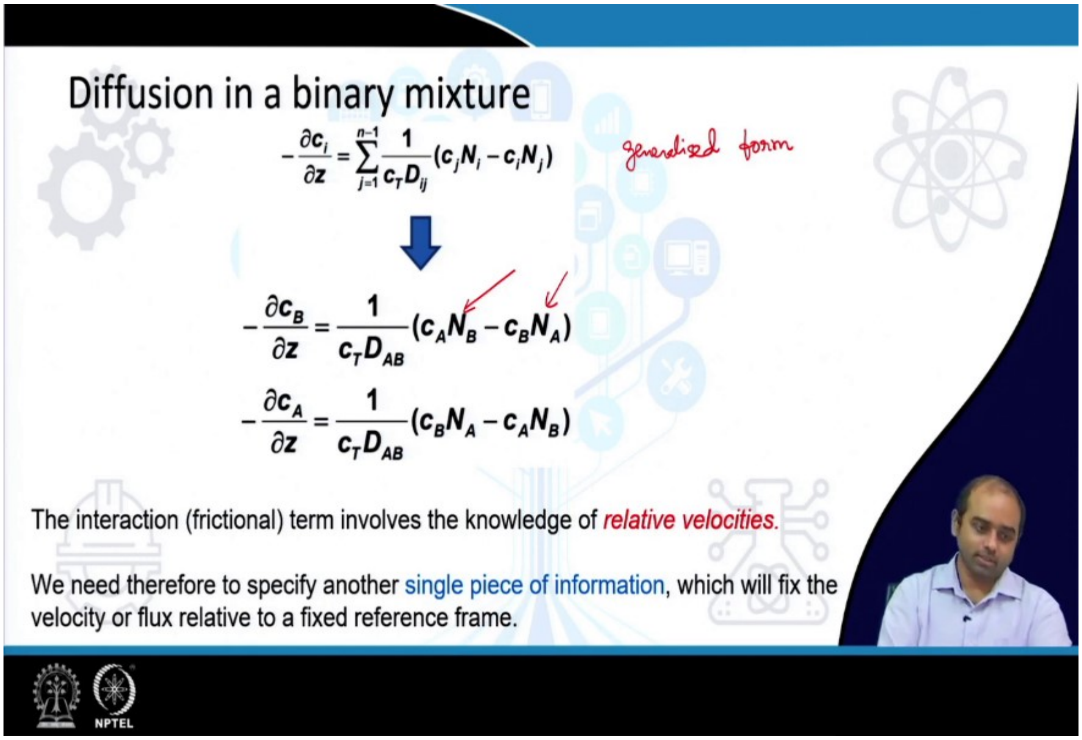

Diffusion in a binary mixture

$$-\frac{\partial c_i}{\partial z} = \sum_{j=1}^{n-1} \frac{1}{c_T D_{ij}}(c_j N_i - c_i N_j)$$

generalized form

$$\Downarrow$$

$$-\frac{\partial c_B}{\partial z} = \frac{1}{c_T D_{AB}}(c_A N_B - c_B N_A)$$

$$-\frac{\partial c_A}{\partial z} = \frac{1}{c_T D_{AB}}(c_B N_A - c_A N_B)$$

The interaction (frictional) term involves the knowledge of *relative velocities.*

We need therefore to specify another single piece of information, which will fix the velocity or flux relative to a fixed reference frame.

For example, what happens when you have a binary system instead of a multi component system? So, this is like the generalized form. So, instead of a generalized form, what happens if we try to write it down in the case of binary system. So, just simply instead of you remove the summation terms and you write the components in terms of CA and CB.

And instead of writing these individual velocities, it is better to write them in terms of the diffusive fluxes. So, this NA and the NB are essentially the diffusive flux. So instead of writing the individual molecular velocities, which is difficult to find out, we write there, diffusive fluxes.

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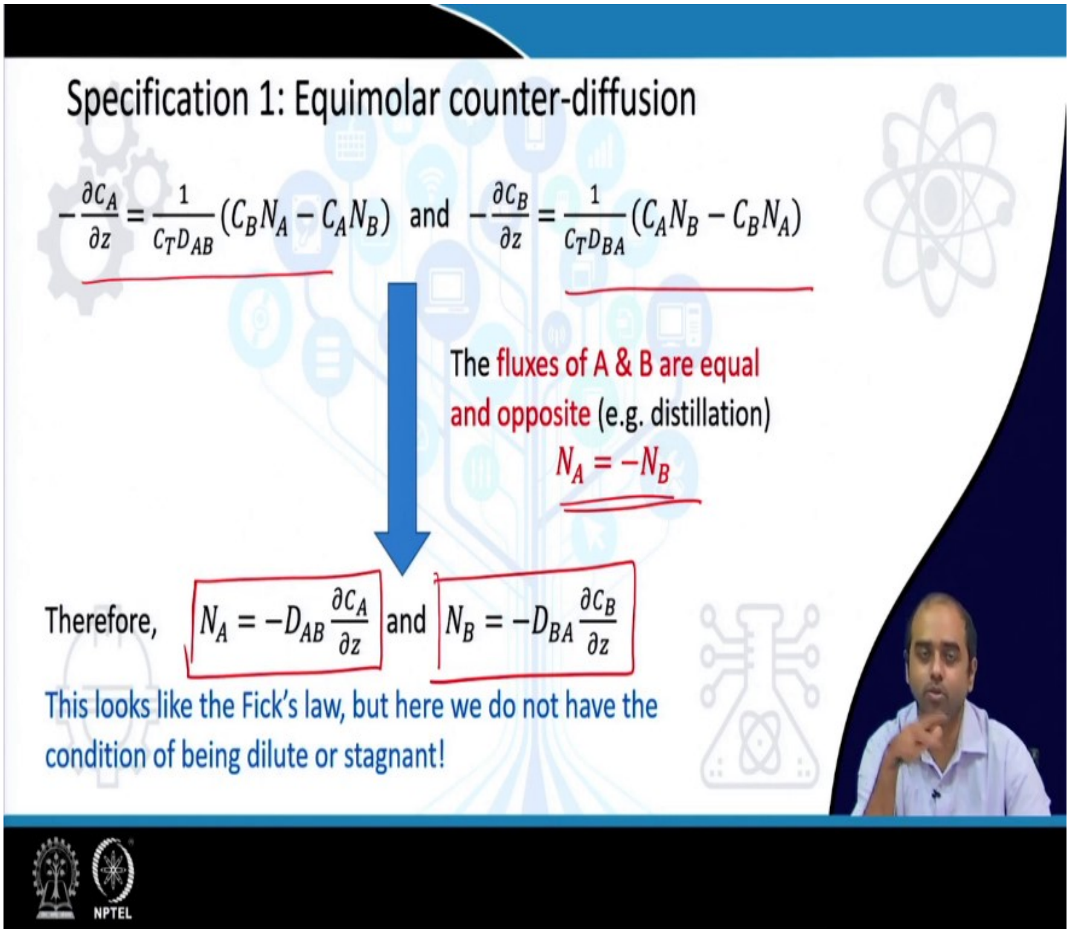

Specification 1: Equimolar counter-diffusion

$$-\frac{\partial C_A}{\partial z} = \frac{1}{C_T D_{AB}}(C_B N_A - C_A N_B) \quad \text{and} \quad -\frac{\partial C_B}{\partial z} = \frac{1}{C_T D_{BA}}(C_A N_B - C_B N_A)$$

The fluxes of A & B are equal and opposite (e.g. distillation)

$$N_A = -N_B$$

Therefore, $\boxed{N_A = -D_{AB}\frac{\partial C_A}{\partial z}}$ and $\boxed{N_B = -D_{BA}\frac{\partial C_B}{\partial z}}$

This looks like the Fick's law, but here we do not have the condition of being dilute or stagnant!

Now, the situation one, when you have equimolar counter diffusion, so what does it means that the flux of A and B are equal and in opposed direction. So, NA is equal to NB isn't it? one of the common situations is that when you have distillations, so the flux of the vapor to the liquid phase and the flux of the liquid transferred to the vapor side are almost equal. So, this is one scenario.

So, from these 2 equations for the binary system, we can write down that if NA is equal to minus B, you just do the simple algebra, and you arrive at these expressions of the diffusive fluxes. And please note that these are very similar, these expressions are very similar to the Fick's law. But here, the condition of being diluted or stagnant medium is not required or is not needed. But it is a specific case where you see that in the condition of equimolar counter diffusion the expression of the flux for binary system converts or simplifies to the Fick's law. I mean, both of these 2 analogous.

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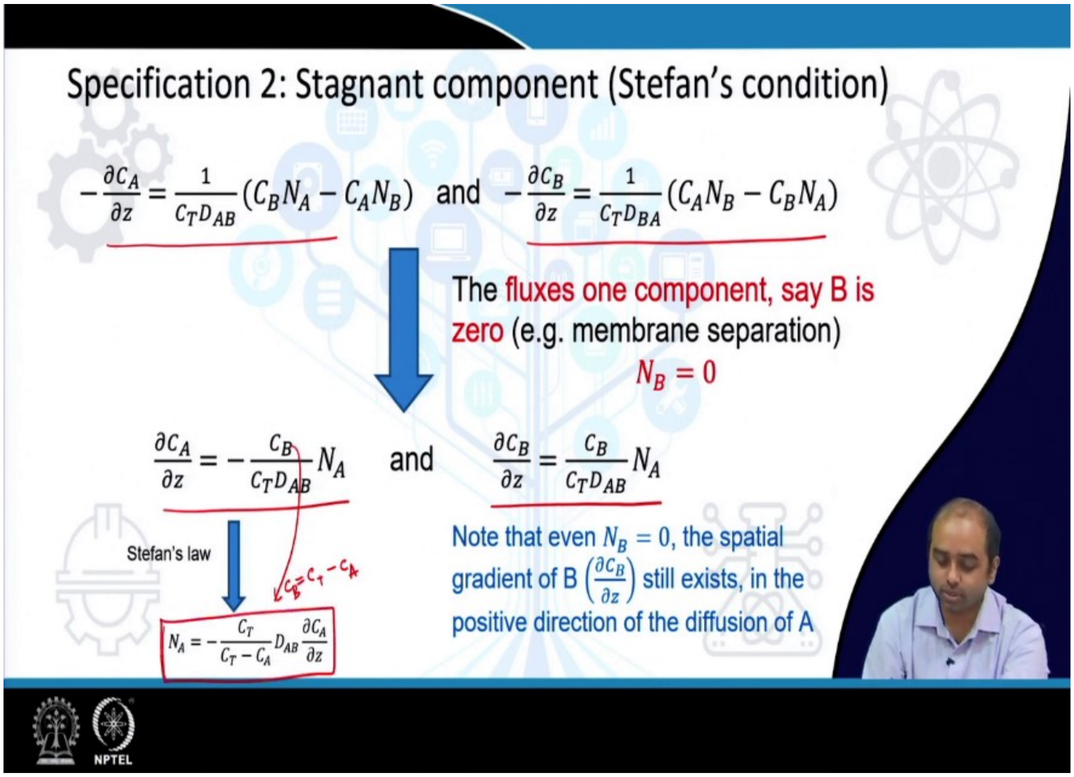

Specification 2: Stagnant component (Stefan's condition)

$$-\frac{\partial C_A}{\partial z} = \frac{1}{C_T D_{AB}}(C_B N_A - C_A N_B) \quad \text{and} \quad -\frac{\partial C_B}{\partial z} = \frac{1}{C_T D_{BA}}(C_A N_B - C_B N_A)$$

The fluxes one component, say B is zero (e.g. membrane separation)

$N_B = 0$

$$\frac{\partial C_A}{\partial z} = -\frac{C_B}{C_T D_{AB}} N_A \quad \text{and} \quad \frac{\partial C_B}{\partial z} = \frac{C_B}{C_T D_{AB}} N_A$$

$C_B = C_T - C_A$

Stefan's law

$$\boxed{N_A = -\frac{C_T}{C_T - C_A} D_{AB} \frac{\partial C_A}{\partial z}}$$

Note that even $N_B = 0$, the spatial gradient of B $\left(\frac{\partial C_B}{\partial z}\right)$ still exists, in the positive direction of the diffusion of A

What happens when you have one of them to be a stagnant component. Let us say the flux of one of the component say B is 0. And this is a scenario that you generally get in a membrane separation. So again, we start from the 2 generalized expression for a binary system, and then we put one of the fluxes to be 0.

So, if you do that, these are the simplified equations. I mean, these are the equations that you are getting. And please note that even though that we set the flux of one of the component to be 0, this NB to be 0 still, there is a existence of the gradient or the spatial gradient of the other component. And that is in the direction or in the positive direction of the diffusion of the other component.

So, this is an important point to note. And of course, this is this you can express the comp, I mean, the concentration CB. So, this CB can be written returned down as CT minus CA. So, everything we are getting in terms of A.

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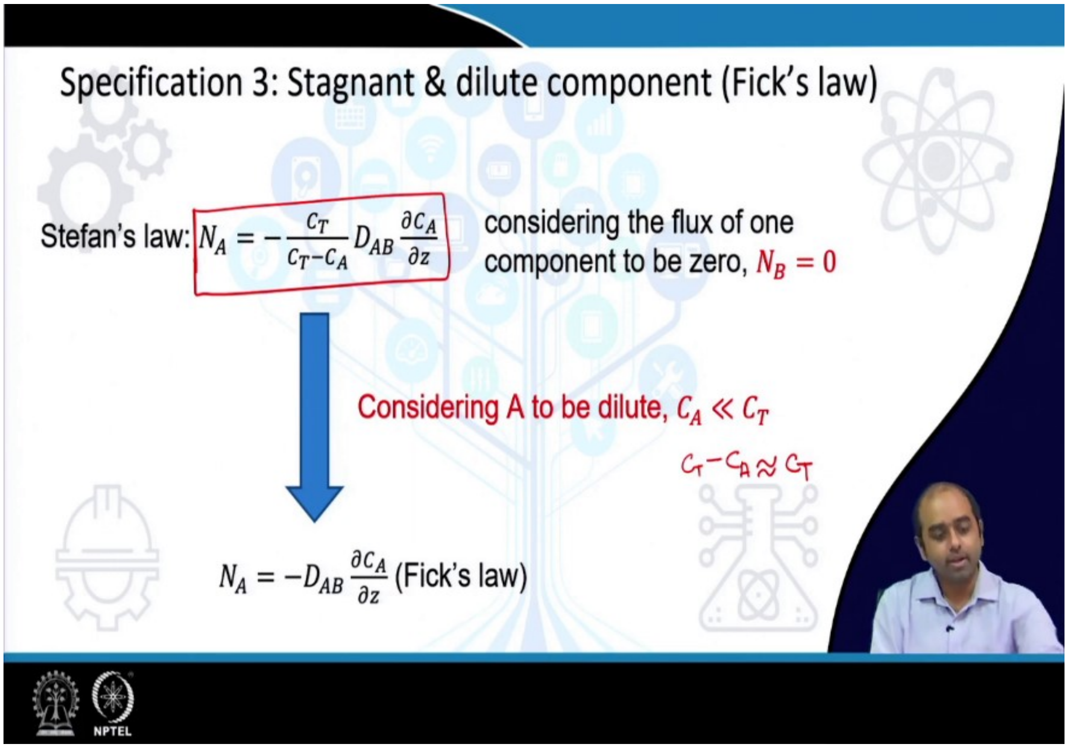

Specification 3: Stagnant & dilute component (Fick's law)

Stefan's law: $\boxed{N_A = -\frac{C_T}{C_T - C_A} D_{AB} \frac{\partial C_A}{\partial z}}$ considering the flux of one component to be zero, $N_B = 0$

Considering A to be dilute, $C_A \ll C_T$

$C_T - C_A \approx C_T$

$N_A = -D_{AB} \frac{\partial C_A}{\partial z}$ (Fick's law)

Now, please note that to this equation, to this equation, if we add the additional, I mean, if we add this extra condition of being dilute is invoked, where CA is much, much smaller than CT provided, one of the component is 0. So, the condition of stagnation is there, and now we are working the dilute condition. So, if this condition is satisfied, CA is much, much less than CT, then what we get that CT minus CA will be close to equal to CT.

So, this equation gets transformed into NA is equal to the infusibility into the gradient of the concentration of A, and which is nothing but the Fick's law. So, now you can see that this, this Stephan's equation can be simplified if you invoke these additional constraints like binary system, stagnant medium, and dilute, you get back your Fick's law. So, this Fick's law is a simplified version of the Stephen-Maxwell law provided certain assumptions are met here.

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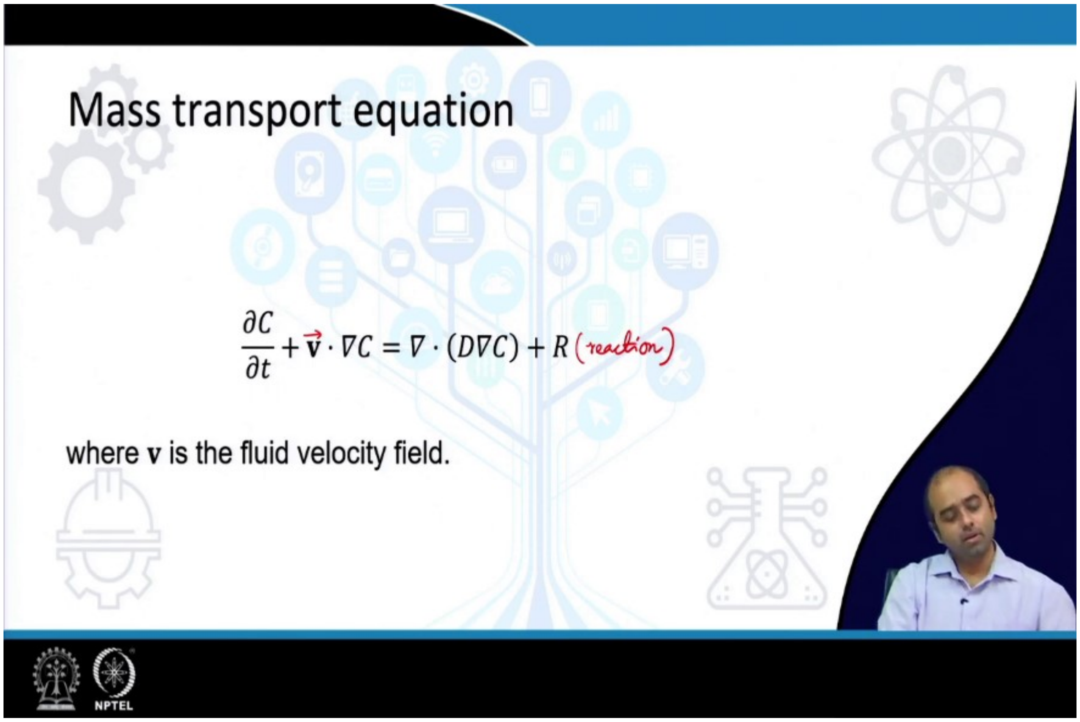

Mass transport equation

$$\frac{\partial C}{\partial t} + \vec{v} \cdot \nabla C = \nabla \cdot (D \nabla C) + R \text{ (reaction)}$$

where **v** is the fluid velocity field.

Moving ahead. This is the mass transport, generalized mass transport equation of the scalar of transport equation, whether you have temperature or whether you have a concentration, this is the generalized equation. R is the additional reaction. So, this R is the reaction term to the bulk of the fluid.

So, depending on whether you are having a homogeneous or heterogeneous reaction, this additional reaction term either could be in the main equation, or it could be present as a boundary condition to this problem. I intentionally written down this diffusivity inside the derivatives because it is seen, or it could be possible that there is anisotropic diffusion in the medium that diffusion in different directions are different, or diffusion is also function of the concentration.

Generally, for most problems, this velocity field is obtained from the momentum conservation equation questions. And that is how this problem is one way coupled when you try to solve a mass transport problem associated with the fluid flow. The fluid flow equations are solved independently and then that is coupled through the mass transport equations. There is one way coupling through this velocity term or the velocity field.

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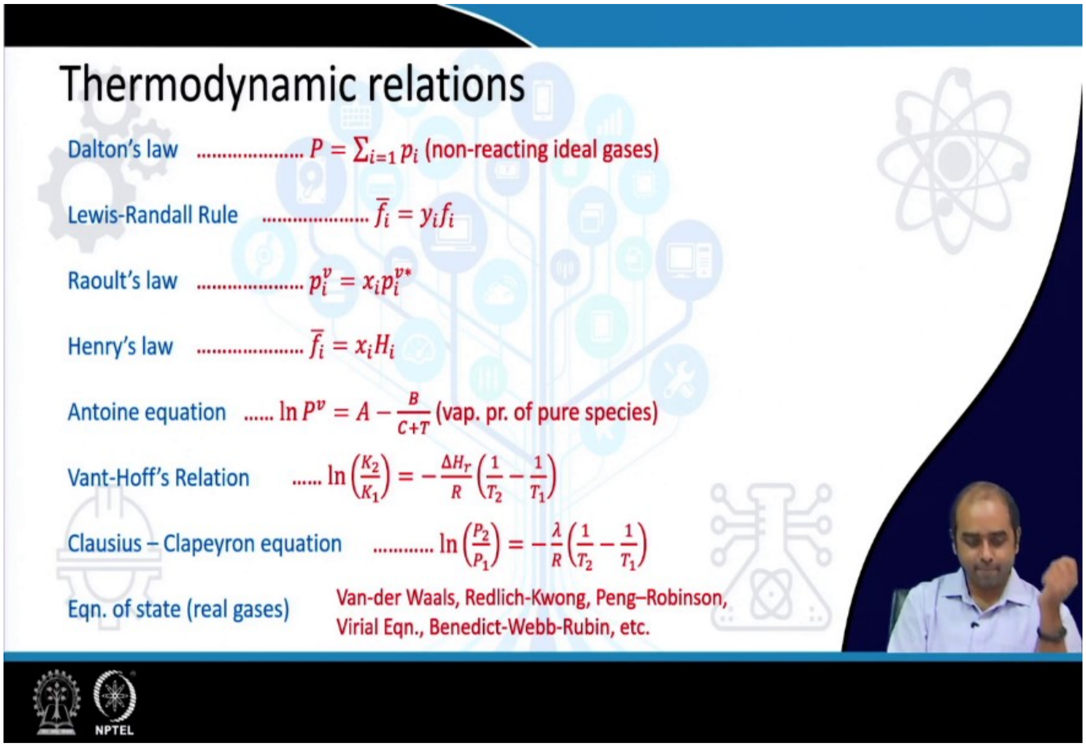

Thermodynamic relations

Dalton's law .... $P = \sum_{i=1} p_i$ (non-reacting ideal gases)

Lewis-Randall Rule .... $\bar{f}_i = y_i f_i$

Raoult's law .... $p_i^v = x_i p_i^{v*}$

Henry's law .... $\bar{f}_i = x_i H_i$

Antoine equation ...... $\ln P^v = A - \frac{B}{C+T}$ (vap. pr. of pure species)

Vant-Hoff's Relation ...... $\ln\left(\frac{K_2}{K_1}\right) = -\frac{\Delta H_r}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$

Clausius – Clapeyron equation .... $\ln\left(\frac{P_2}{P_1}\right) = -\frac{\lambda}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$

Eqn. of state (real gases) Van-der Waals, Redlich-Kwong, Peng–Robinson, Virial Eqn., Benedict-Webb-Rubin, etc.

So next, let us move to the thermodynamic (this) review. So just let us try to recap the different thermodynamic relations that we are all have studied already before by now and it's a time to recap them. So, the Dalton's law is for the case when you have non-reacting ideal gases. The Lewis-Randall rule is generally used to specify the fugacities. The Raoult's law is trying to relate the equilibrium vapor pressures.

Henry's law is balance of the, or is a relation or the connection between the liquid phase concentration to its vapor pressure. Then we have the Antoine's equation that how you can estimate the vapor pressure of pure component from the temperature. Generally, ABC, these are the constants. Then we have the Vant-Hoff's relation. It is to find out the heat of the reactions, as well as the equilibrium rate constants.

And then we have the Clausius-Clapeyron statement where again at different temperatures what is the vapor pressure of the system, and finally the equations of the state which for real gases, because all the systems are not in ideally, so you have the Van-der Waals equation, then you have the more complex, this Redlich-Kwong, Peng-Robinson, Virial type equations.

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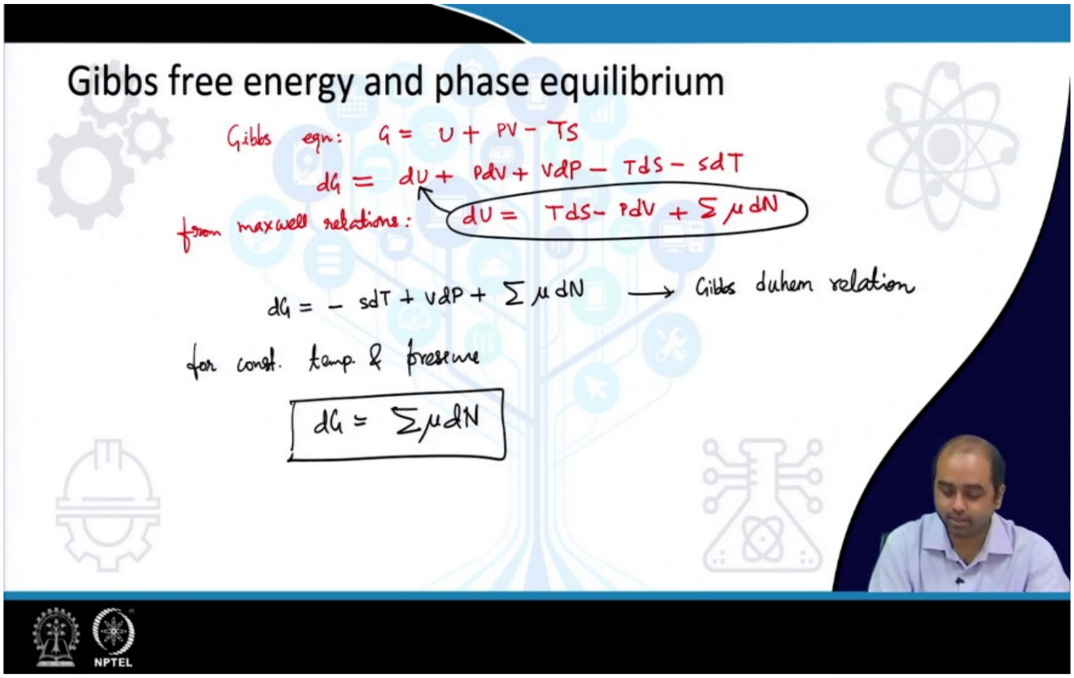

Gibbs free energy and phase equilibrium

Gibbs eqn: $G = U + PV - TS$

$dG = dU + PdV + VdP - TdS - SdT$

from maxwell relations: $dU = TdS - PdV + \sum \mu dN$

$dG = -SdT + VdP + \sum \mu dN$ → Gibbs duhem relation

for const. temp. & pressure

$$\boxed{dG = \sum \mu dN}$$

So, now let us talk about the free energy and the phase equilibrium criteria. So, this Gibb's equation that we know is, free energy is equal to the internal energy PV minus T, and here the symbols represent the usual meaning. So, this pressure, V is volume, this temperature and S is entropy.

So, if we take, try to take the partial derivatives, then this is what we get. So, from Maxwell's relations, we already know that dU can be represented as T dS minus P dV plus the summation of all the components per chemical potential into dN. So, if I try to substitute, if I try to substitute this expression into here, I get dG is equal to minus S dT plus V dP plus this summation term, and this is nothing but the Gibb's Duhem relation. So, for constant temperature and pressure, we get dG is equal to summation of mu dN. Because dT and dP will be equal to 0.

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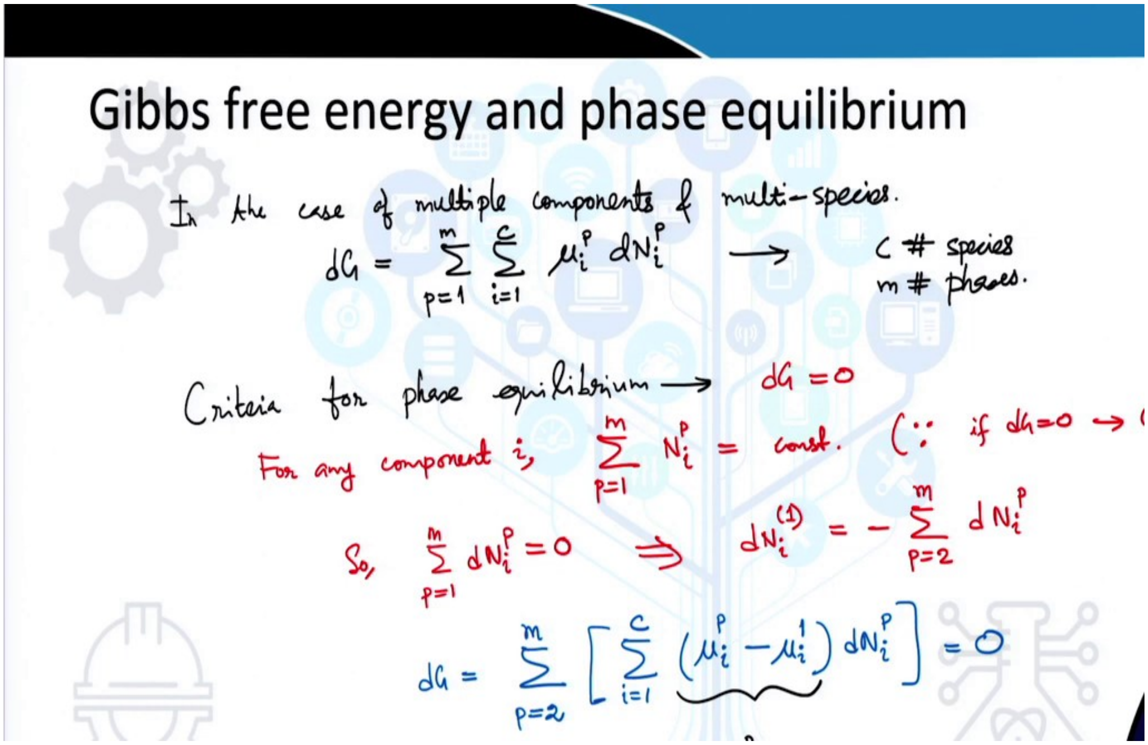

Gibbs free energy and phase equilibrium

In the case of multiple components & multi-species.

$$dG = \sum_{p=1}^{m}\sum_{i=1}^{c} \mu_i^p \, dN_i^p \longrightarrow \begin{array}{l} c \# \text{ species} \\ m \# \text{ phases.} \end{array}$$

Criteria for phase equilibrium ⟶ $dG = 0$

For any component i, $\sum_{p=1}^{m} N_i^p = \text{const.}$ (∵ if $dG=0 \rightarrow$ (

So, $\sum_{p=1}^{m} dN_i^p = 0 \Rightarrow dN_i^{(1)} = -\sum_{p=2}^{m} dN_i^p$

$$dG = \sum_{p=2}^{m}\left[\sum_{i=1}^{c} \underbrace{(\mu_i^p - \mu_i^1)} dN_i^p\right] = 0$$

Now, in the case of multiple components and multiple species. In the case of multiple components and multi-species, this dG is generally written summation of both the species and the component. So here i represents the species and p represents the phases. So here C is the species, the number of species, and m represents the number of phases. So, for any component, so for the criteria, I mean, the criteria for phase equilibrium, all of us know this, the change in the free energy should be equal to 0.

So, the criteria for free energy is del G should be equal to 0. This is fundamentally from the thermodynamics. We know this that it has to be equal to 0. So, for any component, i this summation Ni p will be equal to constant because if del G is equal to 0, it means G is equal to constant, or the summation is equal to constant. And which essentially means that for each individual component, so, for each individual component, and this summation of all the phases of the particular species i has to be equal to constant, isn't it? That is from that idea only we wrote this thing that the summation of all the individual components would be equal to the constant. So, we can rewrite something like this instead. So, this is valid for each of the species, dNi p is equal to 0, isn't it?

If I just take the derivative on both sides, so it will be called to 0. And this implies that I can write dNi for one phase is equal to the minus of the summation of the rest of the phases.

Now, what does this simply imply that from this, what we get is that dG is equal to, this p is equal to 2 to m, I am writing in a slightly different way, instead of writing 1 to m, I take one inside, instead of writing 1 to m, I take one inside, and I try to write this together. So, I can write this to be mu i, so it is mu into N, is not it? It is mu into d into this mu dN. So, I can write dNi to be of phase 1 is equal to the summation of the remaining phases. And from there I can rewrite dG as this is i is equal to 1 to c. I can write this. I hope this is clear to everyone.

Now, what is the immediate implication of this? The immediate implication tells you that this condition, that this equation will be equal to 0 only in the case when we have this to be equal to 0 and if this is equal to 0, it means that mu i of phase 1 is equal to mu i of phase 2 is equal to mu i of phase 3 of all the phases. So, that means the chemical potential of the ith species in each of the phases has to be equal for the condition of equilibrium. So, the del G of the system, the Gibb's free energy is equal to 0, implies that the chemical potential of the ith species of the individual species in each of the phases has to be equal.

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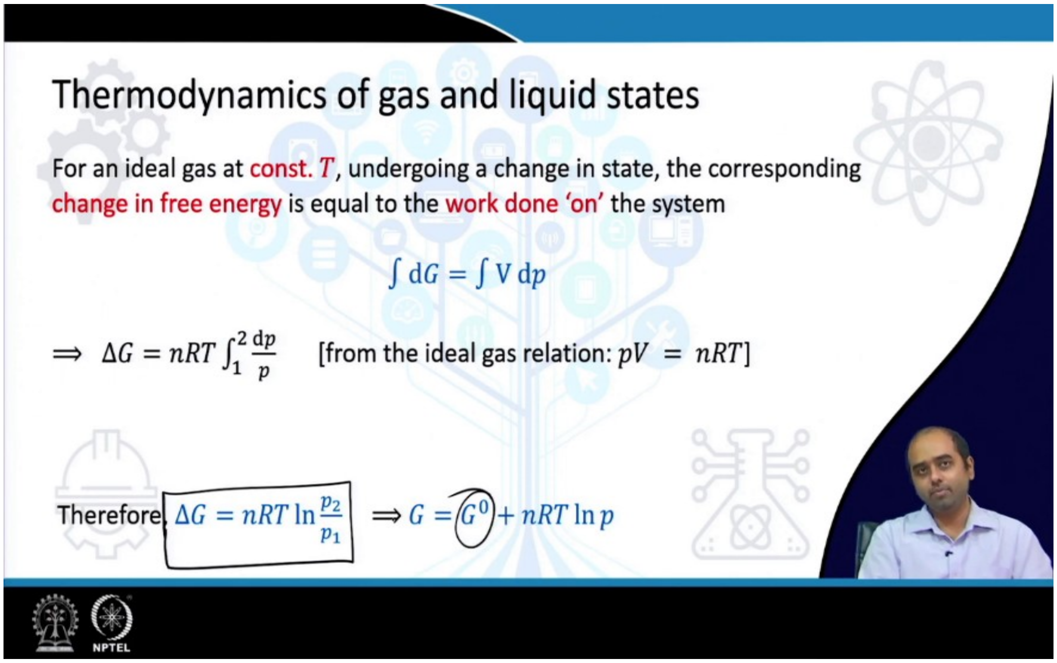

Thermodynamics of gas and liquid states

For an ideal gas at const. T, undergoing a change in state, the corresponding change in free energy is equal to the work done 'on' the system

$$\int dG = \int V\,dp$$

$$\Rightarrow \Delta G = nRT \int_1^2 \frac{dp}{p} \quad \text{[from the ideal gas relation: } pV = nRT\text{]}$$

Therefore, $\boxed{\Delta G = nRT \ln \frac{p_2}{p_1}} \Rightarrow G = G^0 + nRT \ln p$

Now, moving next trying to talk about thermodynamics of gas and the liquid state, we know that, when the ideal gas is at a constant temperature and it undergoes change in the state, the change in the free energy is equal to the work done on the system, not by the system. There is a big difference in the preposition here. So, it is the work done on the system.

And from the relation of the Gibb's driven relation that we have, we can easily write that del G is equal to V dP and if you try to integrate this out, considering the ideal gas relation PV is nRT you can easily get this expression. And we write delta G is the change in the Gibb's free energy. So, our reference state G naught is considered here. And that gives you nRT ln P.

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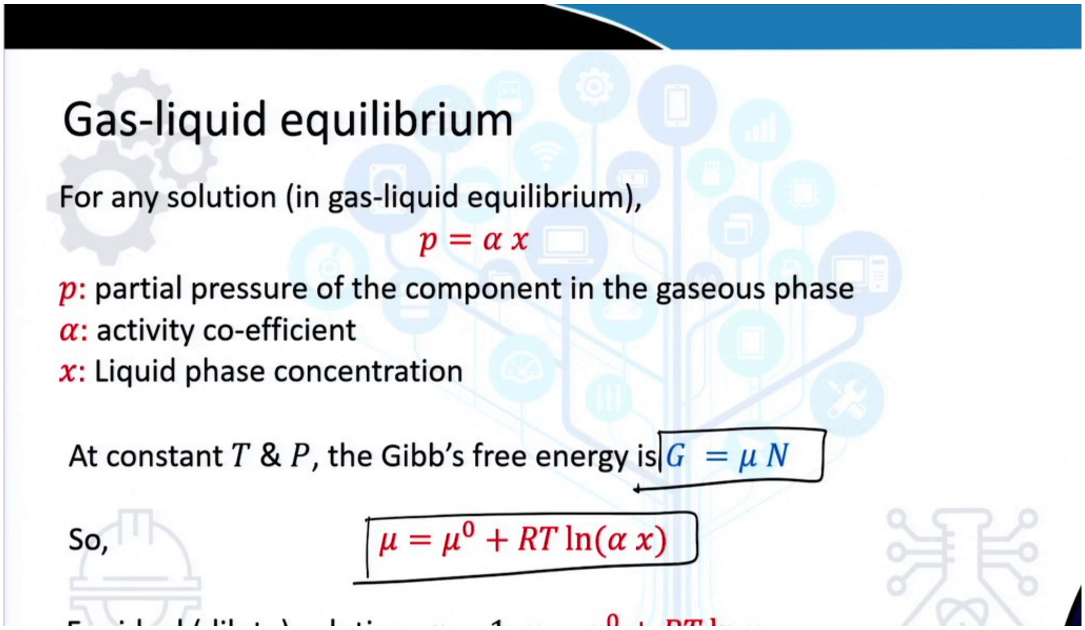

Gas-liquid equilibrium

For any solution (in gas-liquid equilibrium),

$$p = \alpha x$$

p: partial pressure of the component in the gaseous phase

α: activity co-efficient

x: Liquid phase concentration

At constant T & P, the Gibb's free energy is $\boxed{G = \mu N}$

So, $\boxed{\mu = \mu^0 + RT \ln(\alpha x)}$

So, this is generally the case for the gas phase system. And this idea can also be extended for the gas, liquid equilibrium case and this expression that you see is nothing but the this sort of the Henry's law and the partial pressure is equated, or is related to the liquid phase concentration. And then extending this idea, we can tell that at constant temperature and pressure this Gibb's free energy G is equal to mu into N.

We just have seen this and from there, we can write that the chemical potential of the system for the, this liquid state is equal to RT ln this alpha into x. Now, in the case of the dilute or the ideal situation, this alpha is generally close to 1 that is the activity coefficient, and you can write this chemical potential to be RT ln x is the mole fraction of the liquid phase concentration.

So, with this, I would like to close the lecture for this session. And let me just quickly summarize what we have and what we have studied. So, we have studied all the, these details on the mass transport phenomena based on the generalized Maxwell Stephan's theory for liquid for multi-component diffusion. Then we have also reviewed the Gibb's relation and all the little thermodynamic expressions and formulae. Hope you liked it. See you in the next lecture.