Fundamentals of Combustion

Prof. V. Raghavan

Department of Mechanical Engineering

Indian Institute of Technology, Madras

Lecture - 18

Mass Transfer Basics – Part 03

Steady Evaporation (The Stefan Problem)

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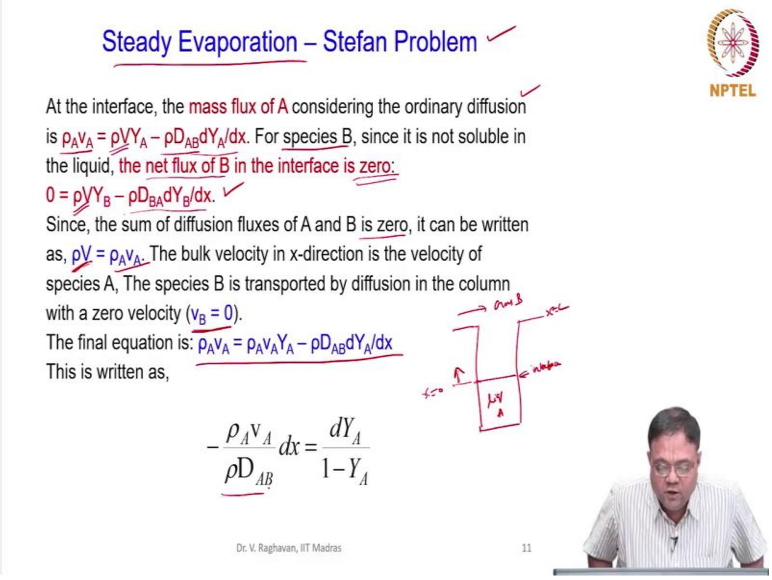

Steady Evaporation – Stefan Problem

At the interface, the mass flux of A considering the ordinary diffusion is $\rho_A v_A = \rho V Y_A - \rho D_{AB} dY_A/dx$. For species B, since it is not soluble in the liquid, the net flux of B in the interface is zero:

$0 = \rho V Y_B - \rho D_{BA} dY_B/dx$.

Since, the sum of diffusion fluxes of A and B is zero, it can be written as, $\rho V = \rho_A v_A$. The bulk velocity in x-direction is the velocity of species A, The species B is transported by diffusion in the column with a zero velocity ($v_B = 0$).

The final equation is: $\rho_A v_A = \rho_A v_A Y_A - \rho D_{AB} dY_A/dx$

This is written as,

$$-\frac{\rho_A v_A}{\rho D_{AB}} dx = \frac{dY_A}{1-Y_A}$$

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So, let us continue with the steady state evaporation problem which is the Stefan problem here. So, we considered a beaker in which liquid is present and over which a gas is flowing. When this level is maintained a constant, then it will be a steady state problem. So, that is what we saw. Let us focus our attention on the interface now.

At the interface there is evaporation from the liquid. So, this is liquid A and this is say, gas B and you can see that this is interface. So, at the interface a mass flux of A considering ordinary diffusion, so, ordinary diffusion we do not take into account of thermal diffusion etcetera which we will see later.

So, this is given by the Fick's law. That is the flux $\rho_A v_A$, that is the density of the vapor A into v_A, velocity at that interface.

The flux means you are dividing by the area that will be equal to the convective flux. So, this is the bulk convection $\rho V \times Y_A$ plus this diffusion flux.

So, $\rho D_{AB}dY_A/dx$; obviously, at interface Y_A will be higher and when you go upwards that is x, in this direction when you go upwards you can see that it will be decreasing. This gradient is negative. So, negative of negative will be positive. We are trying to add the convective flux and the diffusion flux to get the total flux of A at the interface.

Now let us do it for this species B. Now, species B as I told you this is a gas and it is not going to condense and it is not soluble in the liquid. In this case what happens is there is no bulk flow of B into the interface. This means that at the interface the net flux of B is zero that is $\rho_B v_B = 0$.

But, due to other convection etcetera we can see that the how B is transported; that is the bulk flow $\rho V \times Y_B$ plus this diffusion flux. So, Y_B will have a value at $x = L$ which is at the top of the tube. So, $x = 0$ at the interface.

So, $x = L$ is the top of the tube. We can see that Y_B will be higher and it reduces towards $x = 0$. So, that will trigger the transport of B. This will be the net flux of B.

Now, since the sum of diffusion fluxes of A and B is zero, that we have already proved, it can be shown that $\rho V = \rho_A v_A$. Obviously, we can see that the only convection in the y direction (perpendicular direction) is the flow of gas B at the top of the tube.

But, in the x-direction the only convection is due to the transport of A only. So, the bulk convection $\rho V = \rho_A v_A$. The bulk velocity in the x-direction is the velocity of species A. The species B is transported by diffusion in the column and its velocity will be zero, that is $v_B = 0$.

So, when I say v_B this is the x-direction velocity. As I told you in y-direction, which is perpendicular to x there may be a species velocity for that. So, the final equation we can write the same what we have written above as this then we try to use this for further analysis.

So, $\rho_A v_A$, the net flux of species A will be equal to ρV, now ρV is written as $\rho_A v_A \times Y_A - \rho DAB(dYA/dx)$. Now, separate the variables and try to integrate.

So, - $\rho_A v_A$, please understand we are talking about steady evaporation that means, $\rho_A v_A$ will be steady state flux. So, that will be constant.

Similarly, we have already taken the properties to be constant. So, ρD_{AB} will be constant. So, left hand side $-(\rho_A v_A/\rho D_{AB}) \times dx$ and right hand side, I am connecting the terms involving Y_A. So, $dY_A/(1-Y_A)$, so, this we are going to integrate. So, the separation is done. We are going to integrate this now.

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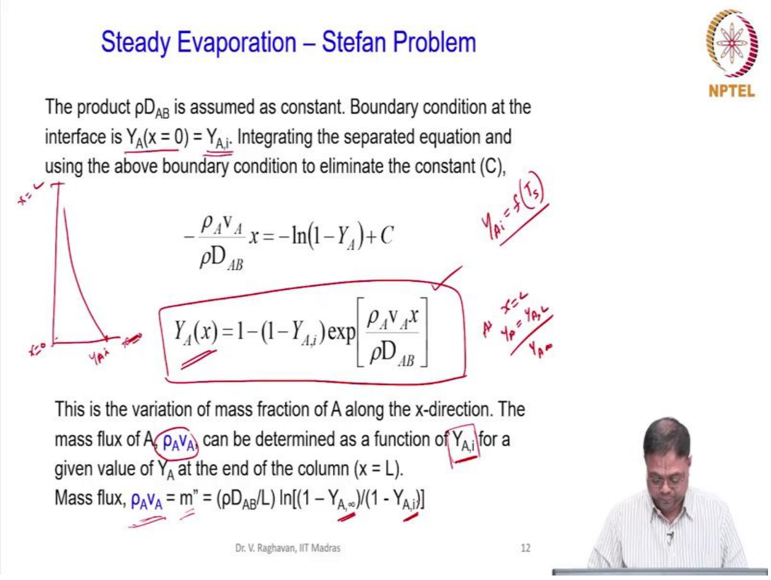

Steady Evaporation – Stefan Problem

The product ρD_{AB} is assumed as constant. Boundary condition at the interface is $Y_A(x = 0) = Y_{A,i}$. Integrating the separated equation and using the above boundary condition to eliminate the constant (C),

$$-\frac{\rho_A v_A}{\rho D_{AB}} x = -\ln(1 - Y_A) + C$$

$$\boxed{Y_A(x) = 1 - (1 - Y_{A,i}) \exp\left[\frac{\rho_A v_A x}{\rho D_{AB}}\right]}$$

This is the variation of mass fraction of A along the x-direction. The mass flux of A, $\rho_A v_A$, can be determined as a function of $Y_{A,i}$ for a given value of Y_A at the end of the column (x = L).

Mass flux, $\rho_A v_A = m'' = (\rho D_{AB}/L) \ln[(1 - Y_{A,\infty})/(1 - Y_{A,i})]$

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So, the product ρD_{AB} is assumed to be constant. Anyway, when you try to integrate we need some boundary conditions. So, at the interface $Y_A(x = 0)$ is Y_{Ai}. In fact, I do not know this value now because this is dependent on temperature of the surface. That is Y_{Ai} is a function of surface temperature T_s.

So, this is one of the boundary conditions I will incorporate. Now, integrating the separated equation and applying the boundary condition at the interface should eliminate the constant. So, $-(\rho_A v_A/\rho D_{AB}) \times x = -\ln(1-Y_A) + C$.

Now, when I apply the boundary condition at x = 0 you see that Y_A will be Y_{Ai}. When I invoke that I get the expression for the mass fraction of species A along x. So, that will be equal to $Y_A(x) = 1-(1-Y_{A,i})\exp(\rho_A v_A x/\rho D_{AB})$. So, this is the variation of the mass fraction.

So, when you say this is surface, x = 0. We can see this is Y_F. We can see the Y_{Fi} I will say Y_{Fi} at this point. So, this is the typical variation. So, non-linear variation of Y_A along this a line.

So, Y_{Ai} will be at the interface and it slowly reduces when you go upwards. This is the variation of mass fraction of A along the x-direction; the mass flux of A, $\rho_A v_A$, can be determined as a function of Y_{Ai}.

We can see that the variation of mass fraction of A along the x direction is a function of the interface quantity Y_A and obviously, the value of $\rho_A v_A$ is going to determine that also. One more variable ρD_{AB} also is going to be involved in this.

So, from this how to get the mass flux? The mass flux of A can be determined as a function of Y_{Ai} for a given value of Y_A at the end of the column. So, at x = L, Y_A will be equal to $Y_{A,L}$. So, based upon this or I can say $Y_{A,\infty}$ if L is very large. So, I can say $Y_{A,\infty}$.

So, if I apply that boundary condition, then the mass flux $\dot{m}''$, $\rho_A v_A$ will be equal to $(\rho D_{AB}/L)\times\ln[(1-Y_{A,\infty})/(1-Y_{Ai})]$. So, this will be the mass flux of the A.

So, by the simple analysis we are able to get the profile of mass fraction of A in the tube. What is Y_B then? Y_B will be $1-Y_A$ because there are only binary species A and B. So, once you calculate the value of Y_A as a function of x, Y_B will be equal to $1-Y_A$ at the particular x.

Flux is calculated for A, $Y_A\rho_A v_A$ in terms of the $Y_{A,\infty}$ which is the value of Y_A at L and the interface quantity. So, anyway interface quantity is yet to be determined.

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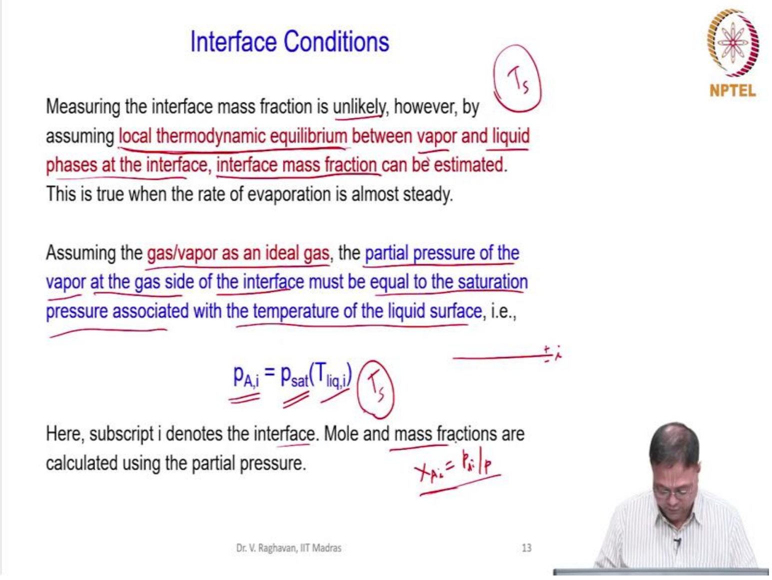

Interface Conditions

T_s

Measuring the interface mass fraction is unlikely, however, by assuming local thermodynamic equilibrium between vapor and liquid phases at the interface, interface mass fraction can be estimated. This is true when the rate of evaporation is almost steady.

Assuming the gas/vapor as an ideal gas, the partial pressure of the vapor at the gas side of the interface must be equal to the saturation pressure associated with the temperature of the liquid surface, i.e.,

$$p_{A,i} = p_{sat}(T_{liq,i}) \quad T_s$$

Here, subscript i denotes the interface. Mole and mass fractions are calculated using the partial pressure.

$x_{A_i} = p_i/p$

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Now, interface conditions; measuring the interface mass fraction is very tough. We can say it is unlikely, it is not going to be accurate also it will involve lot of uncertainties. So, we cannot measure the interface mass fraction but we can measure the temperature at the interface with some accurate techniques.

So, by getting the interface temperature, we can apply local thermodynamic equilibrium because we are already envisaging the steady state evaporation here.

So, local thermodynamic equilibrium we can assume; that means, the evaporation takes place with the thermodynamic equilibrium prevailing between vapor and the liquid phases at the interface.

So, given a fixed temperature of the interface you can see that the number of molecules leaving the liquid phase to the vapor phase will be same as the number of molecules entering the liquid phase from the vapor phase. So, that is the local thermodynamic equilibrium where T_s, the surface temperature is fixed.

Once the surface temperature is known I can get the interface mass fraction. What I try to measure or I try to calculate is the surface temperature based upon that I can calculate the mass fraction of the species A at the interface. Now, for this in several problems involving combustion I can invoke gas or vapor which is prevailing above the interface as an ideal gas.

Then I can say the partial pressure of the vapor at the gas side of the interface that is a vapor side of the interface just above this we can say this interface i, I will say plus or minus, I will put just above the interface and below the interface to represent the gas side and the liquid side.

So, partial pressure of the vapor at the gas side of the interface must be equal to the saturation pressure associated with the temperature of the liquid surface.

When I say saturation pressure, that is the pressure at which phase change occurs at the given temperature of T_s. When there is a phase change there is a definite relationship between the pressure and the temperature. So, applying that, given T_s as the temperature of the interface surface, we can say there is a particular saturation pressure. That will be taken as a partial pressure of the species A at the interface.

So, partial pressure of the species A at the interface will be nothing but the saturation pressure of the liquid at the interface temperature. So, I have given interface temperature as $T_{liq,i}$ this is also same as the T_s, the surface temperature what I am referring to.

Actually, there will be continuity in the surface temperature. At the interface the gas phase temperature and the liquid phase temperature should be the equal. So, that is the criteria here. So, I can just say instead of just saying liquid side of interface having a temperature of $T_{liq,i}$ that will be same as the $T_{gas,i}$. So, we can give a common notation as T_s here that is not a problem.

So, subscripts i here is the interface or I can also use s, subscript s. So, once I know the partial pressure, mole fraction is straight away got. So, X_A at the interface will be equal to $p_{A,i}$ by total pressure at which the evaporation takes place. So, evaporation can take place at any pressure, that is the total pressure or the gas phase mixture I can say.

So, $X_{A,i}$ will be equal to $p_{A,i}$ which I calculate as the saturation pressure at the given temperature divided by the total pressure. So, once I know this, I know what are the species, in this very simple case only the binary species A and B are present.

So, once I know that molecule weight of the mixture can be got, once the mole fraction is known molecular weight of the mixture is known I can calculate the mass fraction at the interface.

So, this is the way we try to calculate this pressure here, that will give you the mass fraction. So, once T_s is known, I can calculate the saturation temperature that is a thermodynamic relationship you can use, any equation like a Clausius-Clapeyron equation to get the partial pressure or the mole fraction of the species at the gas phase of the interface.

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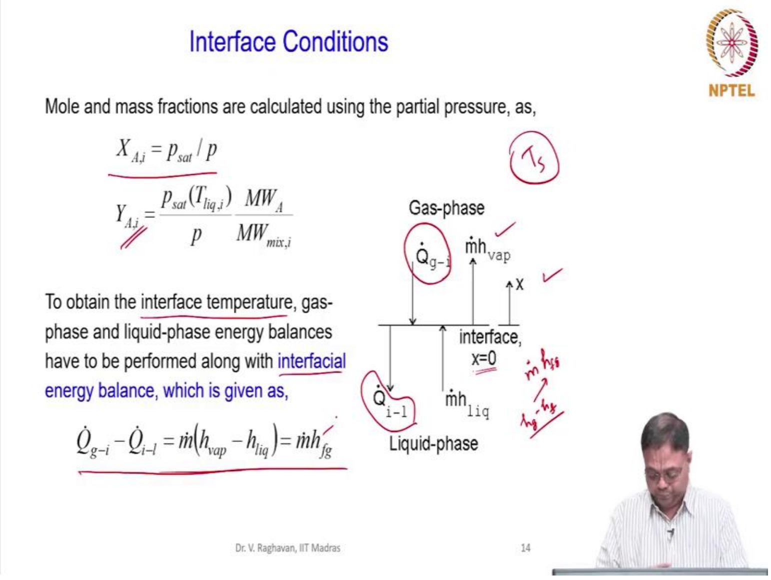

Interface Conditions

Mole and mass fractions are calculated using the partial pressure, as,

$$X_{A,i} = p_{sat} / p$$

$$Y_{A,i} = \frac{p_{sat}(T_{liq,i})}{p} \frac{MW_A}{MW_{mix,i}}$$

To obtain the interface temperature, gas-phase and liquid-phase energy balances have to be performed along with interfacial energy balance, which is given as,

$$\dot{Q}_{g-i} - \dot{Q}_{i-l} = \dot{m}\left(h_{vap} - h_{liq}\right) = \dot{m}h_{fg}$$

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Now, that is what I have just covered here. $X_{A,i}$ is nothing, but the $p_{A,i}$ which is the saturation pressure divided by the total pressure at which the evaporation takes place.

So, $Y_{A,i}$ is nothing, but $X_{A,i} \times MW_A / MW_{mix}$. So, you what is the mixture whatever be the mass fraction of the A, mass fraction B will be one minus that.

So, you know we can calculate the molecular weight of the mixture and use this to calculate $Y_{A,i}$. So, our $X_{A,i}$ is known. From the $X_{A,i}$ you can calculate $X_{B,i}$ and calculate the molecular weight of the mixture and so on. However, what is to be applied to get T_s or the T liquid interface that is the challenge you have.

So, to obtain the interface temperature gas phase and liquid phase energy balances have to be conducted. That is what is illustrated in this figure. If you note it; the interface is designated x = 0 and gas phase is positive x and negative x will be the liquid phase you see the for evaporation to takes place, I need some heat from the gas phase to the interface.

So, that is designated as $\dot{Q}_{g-i}$; g is gas phase, i is interface. $\dot{Q}_{g-i}$ is nothing but the heat which is coming in from the gas phase to the interface. So, this is the heat which is coming in to the liquid phase, taking the control volume around the interface, this is the heat coming into the control volume.

Now, part of this heat is going to go from the interface to the liquid phase which is designated as $\dot{Q}_{i-l}$ interface to the liquid phase, predominantly by conduction. When you comment on $\dot{Q}_{g-i}$ it may be due to conduction as well as radiation also but if you take the liquid phase $\dot{Q}_{i-l}$ is predominantly due to conduction within the liquid.

So, $\dot{Q}_{i-l}$ which is the part of the heat which is coming in is transmitted to heating up of the liquid phase. Now, the remaining part will be used for vaporization. We can see that some mass is going to vaporize at the rate. So, $\dot{m}$ and when it goes out it takes its latent heat of vaporization that is h_{fg}. What is h_{fg}? h_g - h_l or we can say h_{fg}.

So, this is h_{fg}. So, this will be the second portion of the heat which is going to vaporize some substance equal to $\dot{m}$. So, we can see that the total heat which is coming in from the gas phase to the interface is $\dot{Q}_{g-i}$, part of that is going to be used for sensible heating of the liquid $\dot{Q}_{i-l}$, then the remaining part will supply for the latent heat which will evaporate a particular mass $\dot{m}$ to the gas phase.

So, we can see that some mass leaving the to the vapor phase has a enthalpy of h_g or h vapor and that is coming to the interface through the liquid h_l into m dot. So, that is the balance here.

So, the entire balance mathematics is written like this. In the last we can see that $\dot{Q}_{g-i}$ - $\dot{Q}_{i-l} = \dot{m}h_{fg}$. So, that is the interfacial balance.

So, if you can do the interfacial balance you know what are the modes of heat transfer here that we have to understand So, generally in liquid phase conduction will be a predominant heat transfer from the gas phase to the interface. So, we can write this as a conduction flux or conduction flux into the area of the surface.

So, that will be the total heat which is coming from the gas phase to this. So, that will involve the gas phase thermal conductivity into the gradient of the temperature at the interface. Similarly, conduction in the liquid phase also can be demonstrated by using k_l that is the liquid phase thermal conductivity into gradient at the interface.

So, you know h_{fg}; now one more thing is h_{fg}, at what temperature will it be calculated. That will be calculated at its surface temperature because the h_{fg} will vary with the temperature. So, at given temperature you have to calculate h_{fg} and plug in So, this is not a linear problem it is slightly non-linear you have to iterate it to get the correct value of T_s.

So, once T_s the surface temperature is got, then we will be able to have some vaporization. So, due to some vaporization some heat is removed from the interface. So, the temperature will change. This is not a straight forward process, but anyway there are procedures to do this.

But, by conducting a complete energy balance between the gas phase and liquid phase, we can estimate the interface temperature. And once interface temperature is got then we can calculate the saturation pressure and the mole fraction and mass fractions.