Fundamentals Of Combustion (Part 1)
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Lecture – 33
Lennard-Jones potential model (Contd.)

Let us start this lecture with thought process given by Elon Musk.

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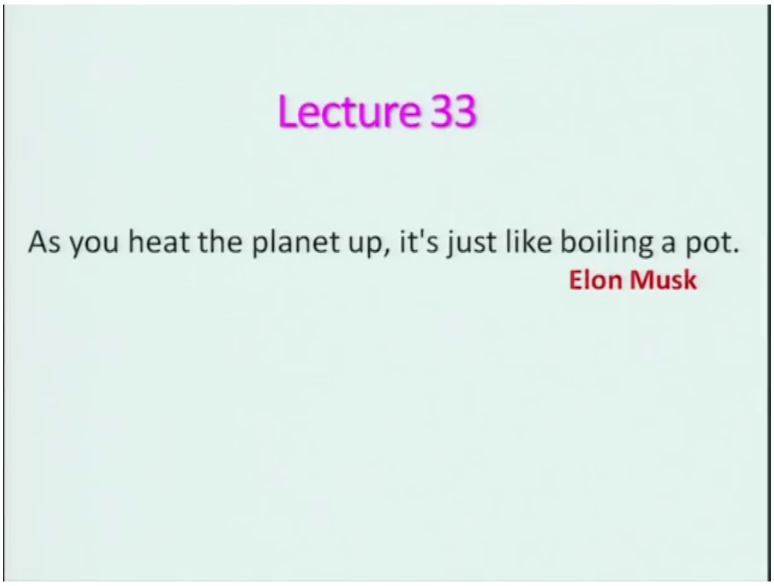

Lecture 33

As you heat the planet up, it's just like boiling a pot.
Elon Musk

As we heat of the planet, it is just like boiling pot. That we could you know experience now days. And if you recall that in the last lecture, we look that how to take care of the effect of real gases in calculating the properties right, and using a model known as the Lennard Jones you know 6 12 potential model, and we also look that how we can calculate you know diffusivity of a i-th species, in particular species, in a mixture of gases, and we will also look at now how we will you know take care that in the thermal conductivity.

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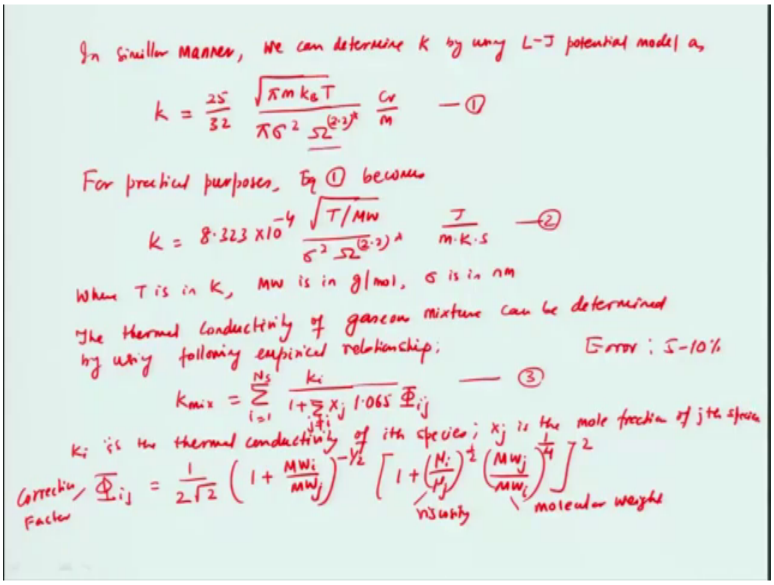

In simillar manner, we can determine k by using L-J potential model as,

$$k = \frac{25}{32}\frac{\sqrt{\pi m k_B T}}{\pi \sigma^2 \underline{\Omega^{(2\cdot 2)*}}}\frac{C_v}{M} \quad — ①$$

For practical purposes, Eq ① becomes

$$k = 8\cdot 323 \times 10^{-4}\frac{\sqrt{T/MW}}{\sigma^2 \Omega^{(2\cdot 2)*}} \quad \frac{J}{m\cdot K\cdot s} \quad — ②$$

Where T is in K, MW is in g/mol, σ is in nm

The thermal conductivity of gaseous mixture can be determined by using following empirical relationship; Error : 5-10%

$$k_{mix} = \sum_{i=1}^{N_s}\frac{k_i}{1+\sum_{j\neq i} x_j\, 1\cdot 065\, \Phi_{ij}} \quad — ③$$

k_i is the thermal conductivity of ith species; x_j is the mole fraction of jth species

Correction Factor, $\Phi_{ij} = \frac{1}{2\sqrt{2}}\left(1+\frac{MW_i}{MW_j}\right)^{-1/2}\left[1+\left(\frac{\mu_i}{\mu_j}\right)^{\frac{1}{2}}\left(\frac{MW_j}{MW_i}\right)^{\frac{1}{4}}\right]^2$

viscosity

molecular weight

So, in the similar manner we can determine the thermal conductivity K by using L J model, potential model right what is that L J means Lennard Jones potential model, as k is 25 by 32 pi M k B T divided by pi sigma sigma A B square into 2.2 star C B by M A B.

I think O need not to use because as it A B (Refer Time: 02:27). So, if you look at like we can look at this, and what is the difference if you look at only this is the what you call integral constant right function, this difference is that collision integral correction factor right. And for practical purposes, if I say equation 1 equation 1 becomes K is 8.323 10 power to minus 4 root over T molecular weight, 2 by 2 star, and this will be joules metre Kelvin second right, and where T is in Kelvin M W is in gram per mole and sigma is in nanometre right.

So, this is of course, if you look at it is corresponding to 1 species, but there might be several of them right. So, you need to calculate the mixtures right. So, thermal conductivity of you know the mixtures, gaseous mixture, consists of different species right can be determined, by using empirical by using following empirical relationship.

Keep in mind that in the text there are several you know the literature, there several empirical relationships are there. So, I am just using one of them right k mixture i is equal to 1 number of species, right N S is the number of species k i divided by 1 plus sigma x j 1.065 phi i j, and k i i is basically k i is the conduct thermal conductivity of i-th species.

And x j is the mole fraction of j-th species right, and keep in mind that j is not equal to i ok, let us say you are considering methane you should not consider methane in these terms, in the denominator right, when you are summing it up you should not take, and this phi i j is again another semi empirical formula you are using divide by 2 root over 2 1 plus M W i by M W j minus half into 1 plus mu i mu j half M W j M W i power to the 1 by 4 square, and if you look at this is a basically correction factor which depends on the coefficient of viscosity; that means, this mu is viscosity right, and also it depends on the molecular weight of the and the this M W is molecular weight. So, keep in mind that this is the formula which you can use for finding out mixture.

But the error if you know it will be involved in this relationship let us say if I say this is 2, and this is your three what will be error here, error in this will be around something 5 to 10 percent are you getting, in each step we are incurring some error even, if you are doing a very nice competition or the you know kind of thing.

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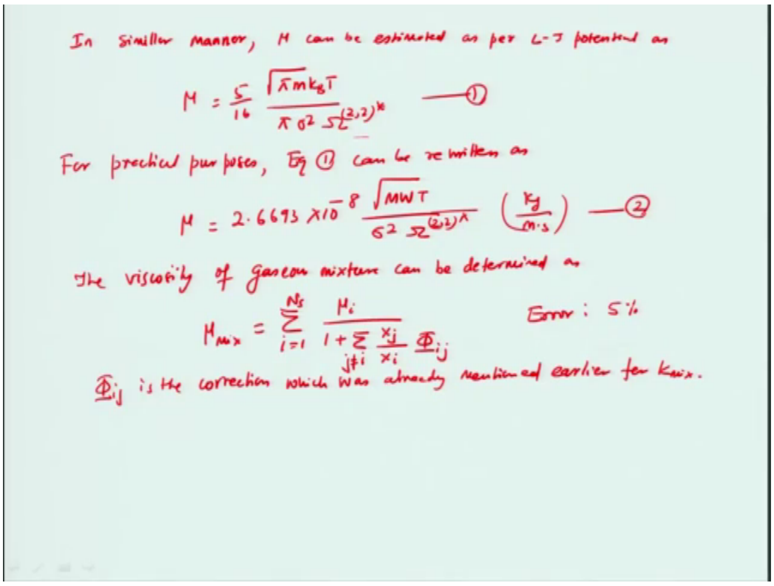

In similler manner, μ can be estimated as per L-J potentel as

$$\mu = \frac{5}{16}\frac{\sqrt{\pi m k_B T}}{\pi \sigma^2 \Omega^{(2,2)*}} \quad \text{—①}$$

For practical purposes, Eq ① can be rewritten as

$$\mu = 2.6693 \times 10^{-8}\frac{\sqrt{MWT}}{\sigma^2 \Omega^{(2,2)*}}\left(\frac{kg}{m\cdot s}\right) \quad \text{—②}$$

The viscosity of gaseous mixture can be determined as

$$\mu_{mix} = \sum_{i=1}^{N_s}\frac{\mu_i}{1+\sum_{j\neq i}\frac{x_j}{x_i}\Phi_{ij}}$$

Error : 5%

Φ_{ij} is the correction which was already mentioned earlier for k_{mix}.

So, in the similar manner we can also look at the viscosity, mu of you know can be estimated as per Jones potential, as mu 5 by 16 pi M k B T pi sigma square, 2 by 2 star right.

And only difference is this one that is your integral factor right, and for practical purposes equation 1 can be rewritten as 2.6993 10 power 8 M W T, this is molecular weight into temperature sigma square 2 coma 2 star, and this will be kg metre second right this unit.

So, I am in we can also find out in the similar like using semi empirical relationship, for finding out a viscosity of the mixture right of gaseous mixture can be determined as mu of mixture 1 i is equal to 1 to N S, N S is the number of species, this is mu I divided by 1 plus sigma x j x i phi i j, and j is not equal to i ok. And already I have had you know this given relationship for the phi i j which is same for both the thermal conductivity, and viscosity this phi i j right.

Is the correction factor, which is correction factor, which was already mentioned earlier for conductivity right conductivity of mixture, that already same relationship can be used, and keep in mind that when you do this thing this error what you will get is something around 5 percent right, that is the error you can get less than in the range of 5 percent not exactly 5 percent ok. The range of 5 percent you should expect. So, by this you can find out basically mixture you know like sorry viscosity of the gaseous mixture right.

Now, if you consider that one thing I want to summarise now, and look at that you know diffusivity what we have considered right. So, if you look at the mass diffusivity, we have considered because there will be something concentration gradient right is not it, because of that there will be diffusion process taking place, but there will be some diffusion process which is due to the temperature gradient right yes or no, and there will be also some kind of energy transfer due to the concentration gradient that we have not looked at like consider, but in some of the combustion problem particularly the thermal diffusion that diffusion of mass due to temperature will be consider right. So, let us look at that.

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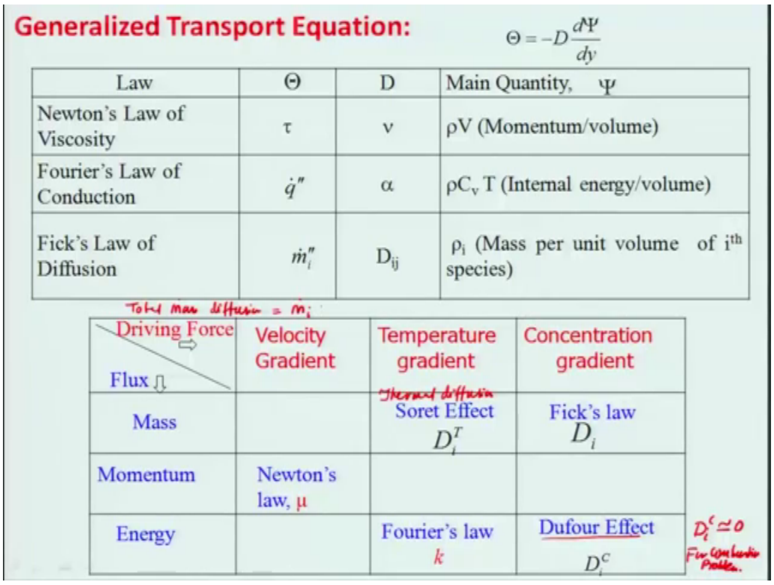

Generalized Transport Equation: $\Theta = -D\frac{d\Psi}{dy}$

Law	Θ	D	Main Quantity, Ψ
Newton's Law of Viscosity	τ	ν	ρV (Momentum/volume)
Fourier's Law of Conduction	$\dot{q}''$	α	$\rho C_v T$ (Internal energy/volume)
Fick's Law of Diffusion	$\dot{m}_i''$	D_{ij}	ρ_i (Mass per unit volume of ith species)

Total mass diffusion = $\dot{m}_i$

Driving Force ⇨ / Flux ⇩	Velocity Gradient	Temperature gradient	Concentration gradient
Mass		Thermal diffusion Soret Effect D_i^T	Fick's law D_i
Momentum	Newton's law, μ		
Energy		Fourier's law k	Dufour Effect D_i^C

$D_i^c \simeq 0$ For Combustion Problem.

That is basically what i had told you that that effect is known as the Soret Effect, and this is due to the temperature gradient, and this Soret Effect is also known as the thermal diffusion, and there will be also the what you call, because of the concentration gradient right, there will be some energy transfer will be taking place or the transport of energy that is known as Dufour Effect, and Dufour Effect generally is negligible is small in combustion problem. So, D i C is approximately 0 for combustion problem.

However this D i T that is Soret effect has to be considered particularly when you are using the hydrogen oxygen system, where the hydrogen right H and some other molecules right will be having some effect right, because those are lighten molecules lighten molecules you know will be travel due to the temperature gradient. So, therefore, the Soret effect has to be taken care so.

Student: Natural convection.

Which one?

Student: Soret effect.

No it is not natural convection as such right, but; however because of you know one molecule you keep in mind that let us say propane, propane is heavier molecule. So, it will be travelling at lower velocity as compared to.

Student: Hydrogen.

Hydrogen or the helium, or you know H radical. So, therefore what will happen in combustion problem, because the temperature will be there, then be temperature gradient, and that will be order of something 2000 200 to 300 you know that kind of so therefore, those molecule will be moving towards you know some place, where you know like kind of things whether, as a result there will be some super adiabatic temperature will be coming; that means, you will get local temperature more than the adiabatic, you know kind of things.

Which we are done some computation in our as a part of research work, we found it is quite interesting so, but those things will be go you know will be more predominant particularly hydrogen oxygen system, or air system we consider. So, therefore when will consider that this effect, then will have to consider the total mass diffusion, right total mass diffusion, diffusion kind of thing right of lets molecules A or i-th species right due to 2 effects what are those things one is or maybe I will write down in the next show.

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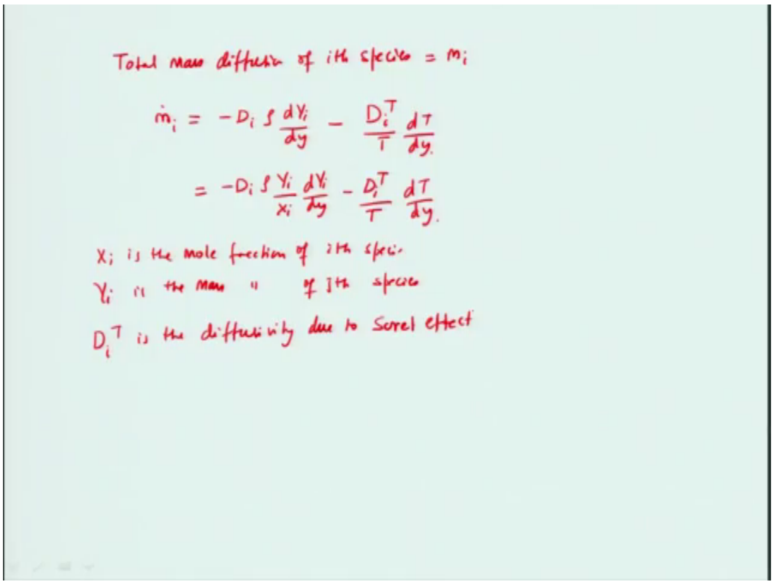

Total mass diffusion of ith species = m_i

$$\dot{m}_i = -D_i \rho \frac{dY_i}{dy} - \frac{D_i^T}{T}\frac{dT}{dy}$$

$$= -D_i \rho \frac{Y_i}{X_i}\frac{dY_i}{dy} - \frac{D_i^T}{T}\frac{dT}{dy}$$

X_i is the mole fraction of ith species

Y_i is the mass " of ith species

D_i^T is the diffusivity due to Sorel effect

So, if you look at that total diffusion right total mass diffusion of i-th species right is equal let us say m dot i right m dot i. So, what it would be then, we know that is D i rho d Y i by y plus, there will be also a Soret diffusion divide T into d T by d y ok. Now I can of course, write this as D i rho Y i, x i, d Y i by d y minus D i T by T, and d T by d y.

If you look at what is this x i is the mole fraction of i-th species Y i is the mass fraction of j-th species, and rho is your density and D i T is the diffusivity due to what due to Soret effect right, Soret effect means it is due to temperature or thermal diffusion whatever you call temperature gradient, and D i is your mass diffusivity whatever you call due to concentration right this is a mass diffusion right. And if you look at this is generally being considered that is the Soret effect and the Dufour effect which is energy transfer due to the concentration gradient you know is not being considered, and there will be also some mass D diffusion due to the pressure that also is not considered in combustion ok.

So, now you know like the mass diffusivity and is due to the Soret effect, and also the pressure effect, but we are not considering pressure effect Soret effect will be considered, and the Dofour effect is not being considered. So, it this we will now moving to basically the governing equations right, and keep in mind that I will be also revisiting this mass diffusion or the mass transfer particularly when will be driving equation for species conservation right, or species transport equation. So, now will get back into basically fluid mechanics part, and will be looking at the mass conservation equation right.

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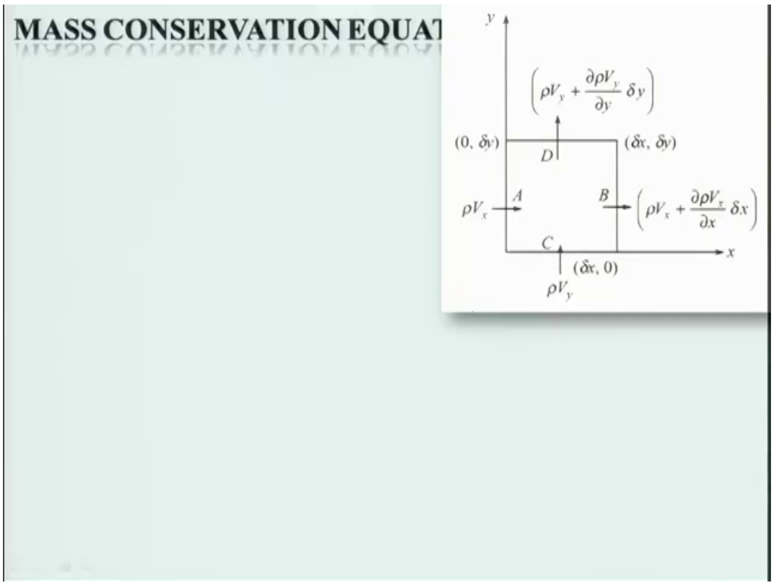

MASS CONSERVATION EQUAT

So, with this we will stop over here, and then will continue in the next lecture ok.

Thank you.