Combustion in Air Breathing Aero Engines
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Lecture – 12
Transport Phenomena

Hello, welcome back to this course on combustion in air breathing aero engines. So, as we have seen in last 2 last few classes last; quite a few classes that we have done, we have covered chemical equilibrium we have covered the theory of chemical kinetics the collusion theory, then we have covered by transition state theory law of mass action, and then in the last class; last 2 classes, we have seen that how we have essentially gone over the concepts, how the theories of the chemical kinetics can be used to understand combustion kinetics.

How actual fuels like hydrogen carbon monoxide, methane actually they undergo oxidations then under what state they can basically undergo rapid oxidation to release large amount of energy in a very short amount of time. So, we have gone over that. So, we have covered quite some amount of ground on chemical kinetics; both from a theoretical view point as well as from a practical fuel view point, then we have also seen how pollutants have formed nox soot etcetera, and how we can actually reduce the mechanisms. But it is actually not only just chemistry not only just kinetics or chemistry that is happening inside combustor and combustion is much more than chemical kinetics why? One of the thing is that the flow inside a combustor if you just consider an snapshot of the flow state of the flow inside any combustor say a gas turban engine or a scramjet engine rocket engine any even a car engine, it is hardly homogeneous.

So, far we discussed basically chemistry or combustion from a; in a state where it everything is homogeneous and basically it is a perfect mixture of different kind of species there can be more species, but there is no spatial variation or the spatial non uniformity of the species in the state. So, that is what we have studied so far, but what I want to say is that this is not the reality inside a combustor, the flow inside a combustor is hardly homogeneous it is strongly non homogeneous in terms of temperature that is in terms of enthalpy, in terms of sensible enthalpy in terms of momentum and also in terms of species concentration why? Because you see in a combustor what is there combustor the flow is essentially more or less the flow is axial flow.

So, there is strong shear. So, the momentum of one region of the combustor the momentum overflow one region of the combustor is different from the momentum of the flow in the; another part of the combustor. For the more the energy the combustor contains a flame. So, the region inside the flame the flame where the flame is located the temperature is high or also the temperature is high in the product gases, but outside in the cold reactance there is no high temperature those are cold cold means that not compare to the cold compare to the product gases. So, there is strong temperature gradients there is strong gradients of velocity, and also there is strong variation in species concentration why because in flame region you have consumption of the fuel and the oxidizer. So, those goes to zero, but outside you have got very strong concentrations of fuel and a oxidizer outside the flame, but so similarly inside the flame and inside the product you have strong concentration of CO2 and water, but outside you do not have this species.

So, flow inside a combustor is non homogeneous in all possible ways, it is non homogeneous in temperature non homogeneous in species concentrations, non homogeneous in momentum. So, what happens when there is non homogeneity? If you consider the non homogeneity inside a system it is a system does not allow on homogeneity. So, the system acts in such a manner that this or non homogeneity of this non homo or this non uniformity of this temperature or this species concentration or this momentum is homogenized or it is made uniform in some possible ways.

Now, why this must happen this is because from a microscopic point of view you know that this u that even though we have this field equations so, but in microscopically they all this gases contains a large amount of molecules, and this molecules are always in a state of motion. So, these molecules always collide. So, as the collide this information of this or this high temperature or this high energy, high temperature, high concentration region that this is basically this is this non homogeneity in this type of parameters is basically uniform a is made uniform through this continues collusion of this molecules. If there was no collision then this could have this non uniformity could have persisted, but because there is strong always this molecules are in motion and because there is continuous collusion among them this non uniformity of this properties of in terms of enthalpy, in terms of species concentration, in terms of momentum is not tolerated.

But how does it happen. So, that is what we are going to understand today by this topic called transport phenomena.

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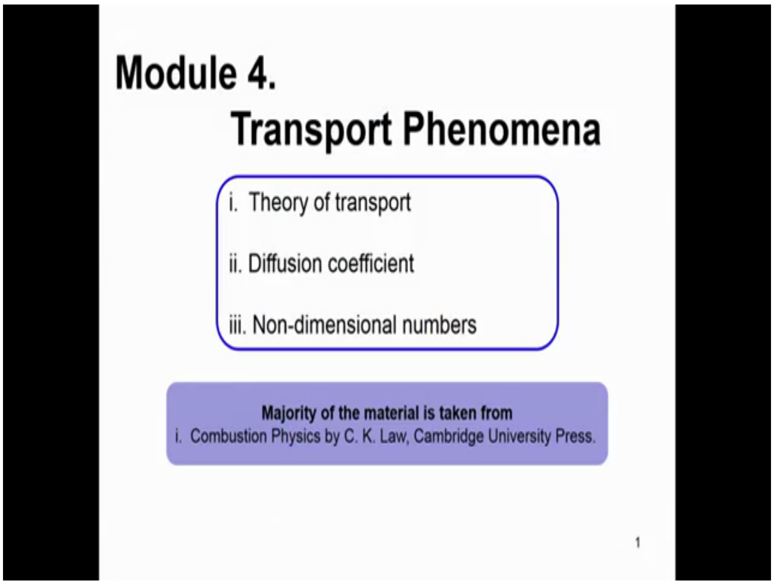

Module 4.

Transport Phenomena

i. Theory of transport

ii. Diffusion coefficient

iii. Non-dimensional numbers

Majority of the material is taken from

i. Combustion Physics by C. K. Law, Cambridge University Press.

So, we will to understand the theory of transport and then we will look in to the coefficients which control this transport, which are parameters of the which are functions of the composition of the gas or the nature of the molecules of the gas present in the gas and then we will find some non dimensional numbers useful non dimensional numbers, that will be used in this that will you utilize this diffusion coefficients or this transport coefficients are to and these non dimensional parameters you will see that will be useful by in terms of understanding the different kinds of governing equations, and the flow systems that we encounter a inside a practical combustor.

So, as we said that that if we go to the introduction we will say that this transport phenomena.

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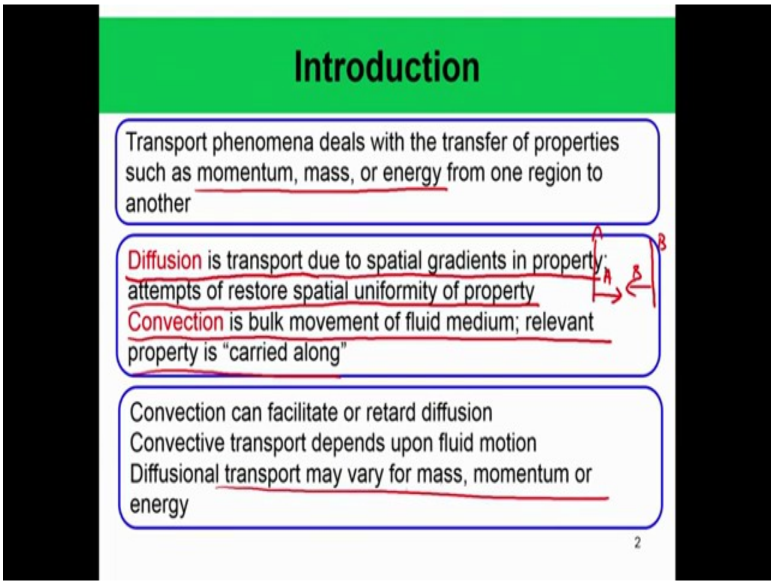

Introduction

Transport phenomena deals with the transfer of properties such as momentum, mass, or energy from one region to another

Diffusion is transport due to spatial gradients in property; attempts of restore spatial uniformity of property

Convection is bulk movement of fluid medium; relevant property is "carried along"

Convection can facilitate or retard diffusion

Convective transport depends upon fluid motion

Diffusional transport may vary for mass, momentum or energy

The transport phenomena what does it deal with? This deals with a transfer of the prosperities such as momentum mass or energy from one region to the other. So, this and this as I said this occurs when there is this transference occurs when there is strong non uniformity in these things in this momentum mass or energy. Now there are can be 2 kinds of essentially transport; diffusion transport which is the topic of this class this diffusion is transport due to spatial gradients in it is property.

So, mathematically how do we say that this some property or some parameter is non uniform over a field? It is it is quantified by the spatial gradients right. So, if the gradients is 0 we can say that this quantity is uniform or this homogeneous where as if there is a non homogeneous they will this will characterized by the spatial gradients of that property; and these process basically attempts to restore spatial uniformity of the property. Now in contrary to in contrast to diffusion convection is essentially bulk movement of the fluid medium. So, it is diffusion is not bulk movement diffusion is essentially one species moves from a region of high concentration to region of low concentration, but one there is low concentration of species; that means, a high concentration of species B.

So, essentially species A is moving in this direction, and species B is moving in this direction wherever we say that this is in this region there is a high the concentration of species A and this high concentration of species B. So, there is no bulk transport as such that is what we want to say. It is only that this particular species move in different directions where as convection is characterized by bulk movement of the fluid medium and relevant property is carried along with it. So, that is a bulk that is a difference between the diffusion and convection, one is movement of certain kind of species where as conviction is a bulk movement of the entire fluid medium.

Now, convection this can facilitate or retard diffusion depending on the sign of that depending on the direction in which the diffusion is happening, I mean in with respect to the reduction of the flow convection can facilitate or retard diffusion and convective transport depends upon fluid motion, where as diffusion does not depend upon fluid motion. So, that is how essentially we will see that it is the entire fluid and kinetics will be connected, it convection is basically contains the fluid information of fluid motion and then will see diffusion essentially connects with that property over small length scales, and then this thing will connect with the reaction. So, will see that when we go in to the governing equations in the next few classes.

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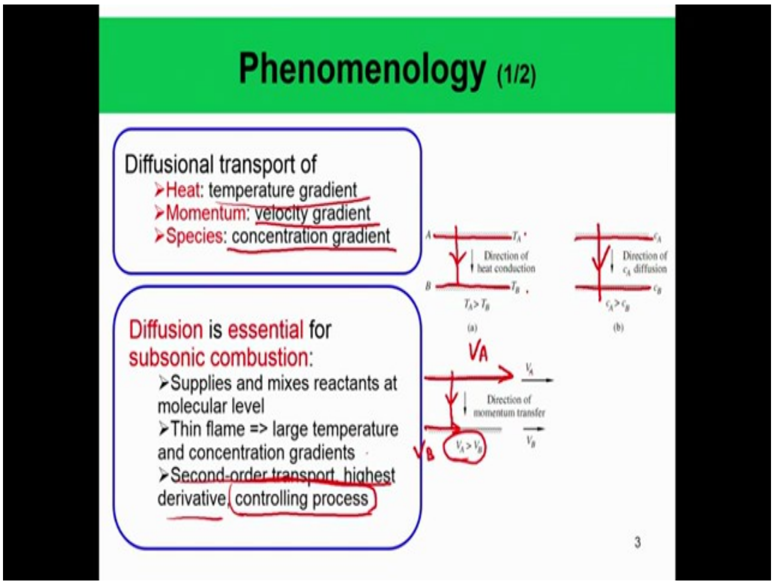

Phenomenology (1/2)

Diffusional transport of
- Heat: temperature gradient
- Momentum: velocity gradient
- Species: concentration gradient

Diffusion is essential for subsonic combustion:
- Supplies and mixes reactants at molecular level
- Thin flame => large temperature and concentration gradients
- Second-order transport, highest derivative, controlling process

Let us diffusion transport may vary from mass momentum or energy alright. So, phenomenology the we basically by diffusion we do not mean only in diffusion of species, we mean a diffusion transport of essentially heat which is happens when there is a temperature gradient, diffusion transport momentum will happens there is a velocity gradient, and diffusion transport of species when there is a concentration gradient. Now to just to give an example I am sure all you are aware of this.

Now, let us consider these 2 parallel plates which are at 2 different temperature; T A and T B and T A is greater than T B and of course, if this the there is a gap between this 2 this 2 plates this 2 different temperature plates is filled up with the fluid medium not a solid medium such a also possible suppose we consider a fluid medium, then we know that there will be transfer of heat from this high temperature region to the low temperature region and this we call diffusion of heat. Now similarly if there is a concentration difference so this is at high concentration suppose these are like porous plates and this inside these there is a this high concentration of C A and this is a concentration of the concentration of certain species C A and then the concentration of the same species on this plate B is essentially C B.

So, and then there they are separated by a fluid medium. So, then because C A is greater than C B which are the concentration of the same fluid and. So, then there will be a net transfer of this species from this plate to this plate and that is a direction of diffusion. And momentum is suppose that this plate is now moving this plate is now moving with a velocity V A whereas, this plate is moving with a velocity V B and if the velocity V A and V B are related by V A greater than v B. So, then we know that momentum will be transferred from this from the fluid from this e to B. So, these are the different modes of transport heat momentum and species.

Now this diffusion is essential for subsonic combustion ok why? Because we will see that one of the reasons is that my diffusion is essentially is that because we know that combustion you see have seen that combustion is characterized by large activation energies, and we have seen that previously when we have large activation energies these reactions become concentrated in very thin regions. So, as a result of this because the reactions are concentrated in a thin region, the change was species and the change of temperature also occurs in a reasonably thin region thin not thin medium, but thin region as such.

So, what I want to say is that this because large activation energy, the reactions the reactions that characterized combustion are concentrated in very thin regions in space or in time, and because this thin region because if they are consider in thin regions space then it automatically means the gradients of this properties of either the temperature or the species are very high, and when there is a sharp gradient or there is a sharp change in concentration or in there is a sharp change in temperature, then it means that as we see that then it means that this diffusion property diffusion becomes very important and this second order transport of this high order second order derivatives which is characterized which characterizes the diffusion transport, will see that diffusion transports appear as second order derivatives in the species equation or in the energy equation and they become the controlling process instead of convection inside a flame.

Outside the flame convection can be important, but inside the flame typically we can see we will see that diffusion processes of heat and species become very very important alright. So, that is why we need to understand diffusion and here we will see that the phenomenology of diffusion and will what we will do is that, we will derive the how we can characterize the flux of a of a property, how the property is transported across the across a plane and how we can arrive at a very fundamental from using just basic principles how we can arrive at a that how will the rate of how the rate of change of that or the flux of the property across a plane, how that quantity can be derived from very basic first order principles. On that we can we will use to basically find out the diffusivity.

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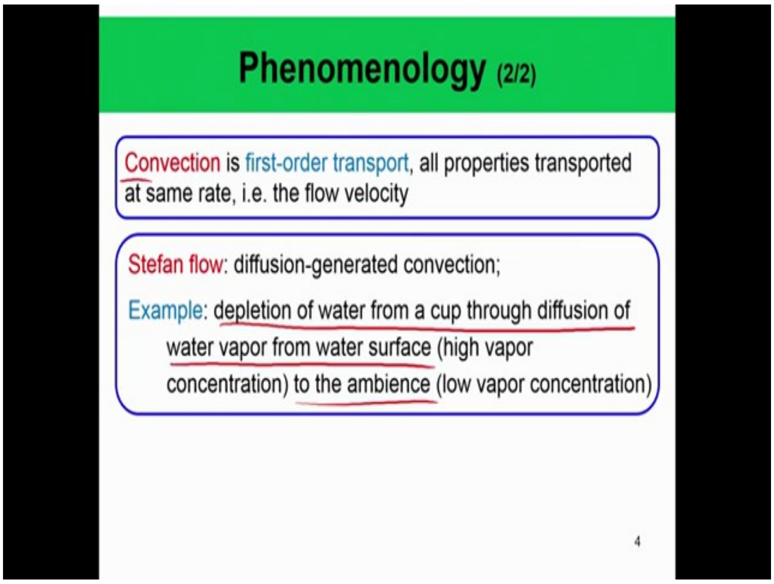

Phenomenology (2/2)

Convection is first-order transport, all properties transported at same rate, i.e. the flow velocity

Stefan flow: diffusion-generated convection;

Example: depletion of water from a cup through diffusion of water vapor from water surface (high vapor concentration) to the ambience (low vapor concentration)

So, as we have said that before that as we see here that convection; convection is first order transports right in all properties are transported at the same rate that is with the flow velocity. So, there is no problem. So, if we have any even if we have different species a different convection different concentrations, convection will transport them with the same fluid velocity which is and, but we will also see that in certain cases especially when it comes to like things like multiphase flow or this 2 place flow when it we have we will study this droplet combustion, then there can the bulk flow velocity can be induced by diffusion. So, diffusion can generate convection in certain cases and as an example we can will say that the depletion of water from a cup through diffusion, water vapor from the surface. So, as we know that the there is continuous evaporation of water vapor from the surface.

Now, for continuous evaporation to take place there must be continuous supply of bulk supply of water from the entire fluid and that basically is the Stefan flow and that will do. So, this depletion of water from a cup to diffusion of water vapor surface to the ambience will be high vapor concentration to low vapor concentration, will see that is that will induce flow and that will be essentially the Stefan flow. So, there can be diffusion generated convection alright.

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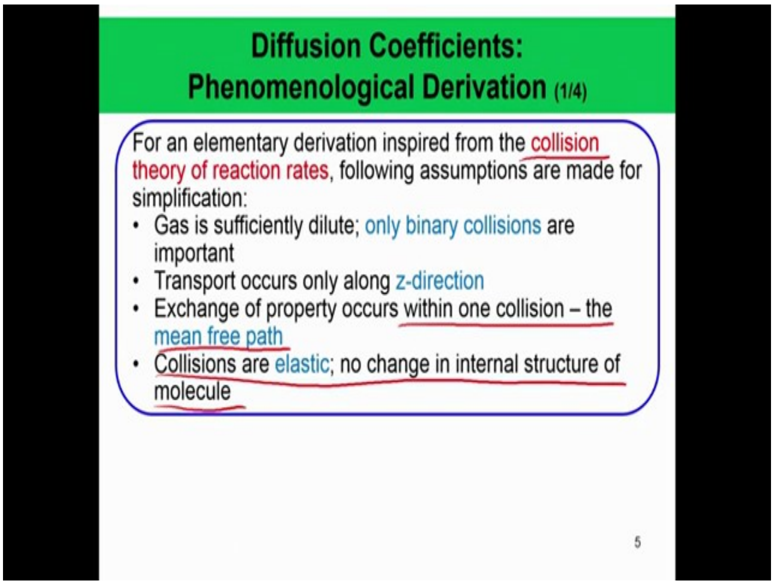

Diffusion Coefficients:
Phenomenological Derivation (1/4)

For an elementary derivation inspired from the collision theory of reaction rates, following assumptions are made for simplification:

- Gas is sufficiently dilute; only binary collisions are important
- Transport occurs only along z-direction
- Exchange of property occurs within one collision – the mean free path
- Collisions are elastic; no change in internal structure of molecule

And then we will study that that the diffusion will were look into diffusion coefficients from an elementary point of view and for an elementary derivation will in will use this collusion theory of reaction rates, and following assumptions are will be made for the simplification.

So, what will do now is that we will derive the formula for diffusivity that is the parameter that controls the rate of diffusion. So, for an elementary derivation we should as we said that this will be inspired from the collusion theory of reaction rates, and the following assumptions would be made for simplification. So, will assume that the gas in which the diffusion is taking place that is sufficiently dilute, and only binary collusions were important. Now if you remember that we have also use the collusion theory in in deriving the reaction rate constant k. So, this is also we can we can ask that what is that is also derived using collusion rate theory or collusion theory diffusivity also is derived using collision theory, I mean yes both are actually happen due to collision between molecules.

But then when you have reaction you basically have change in the electronic structure of the molecule in diffusion there is no such change, and we will accommodate in the theory doing this by saying that only when the collusion energies of beyond the certain kind of energy that is activation energy collusions are trigger reactions. But in this case will just find out that; what is the flux of species concentration that is happening because of these collusions? So, and of course no such concept of activation energy coming, alright so, that is the difference and will assume that gas is sufficiently dilute and only binary collusion are important all right and so, that only there is no three buddy collusions as such because if the gases dilute that all three molecules cannot be at the same place at the same time, and we will see that this transport will only occur in the z direction which will the vertical direction and the exchange of property occurs within one collision and that is the mean free path.

So, will this diffusion is essential in exchange of property that is high concentration goes to the molecules of high concentration basically travel this if we have a 2 region separated by high concentration and low concentration, then after certain time this there will be uniform concentration that is the proper basic essence of diffusion and this. So, we need this to equilibrate this property we need basically collision of molecules, and we will assume that this exchange of property this occurs within one collision that is that is within one mean free path. And will assume that collisions are elastic and no change in the internal structure of the molecule alright so, basic then using this we go back to our previous discussion of the same.

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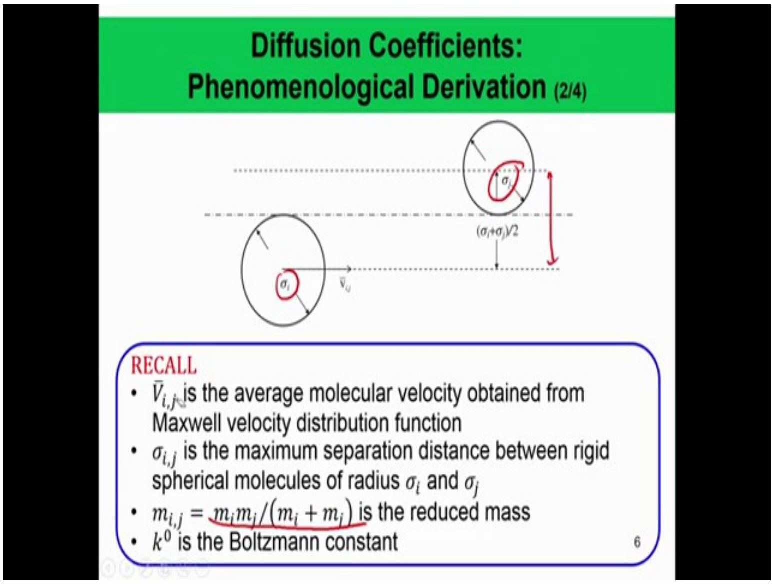

Diffusion Coefficients: Phenomenological Derivation (2/4)

RECALL

- $\bar{V}_{i,j}$ is the average molecular velocity obtained from Maxwell velocity distribution function
- $\sigma_{i,j}$ is the maximum separation distance between rigid spherical molecules of radius σ_i and σ_j
- $m_{i,j} = \underline{m_i m_j/(m_i + m_j)}$ is the reduced mass
- k^0 is the Boltzmann constant

Basically same schematic, these are the 2 molecules which will which are essentially colliding one has a diameter of sigma i one has a diameter of sigma j and there reduced mass is given by this sigma this there reduced mass will be given by m i j is given by this m i times m j divided by m i plus m j where as this collision diameter will this given by this sigma I plus sigma j and also if you remember that we used this thing that is V i j for mean V i j is the average molecular velocity obtain from Maxwell velocity distribution function, and sigma i j as you remember is a diameter of the of the collision volume that this the maximum diameter within which this 2 molecules must be located for collision to happen and as you remember that k 0 is the Boltzmann constant.

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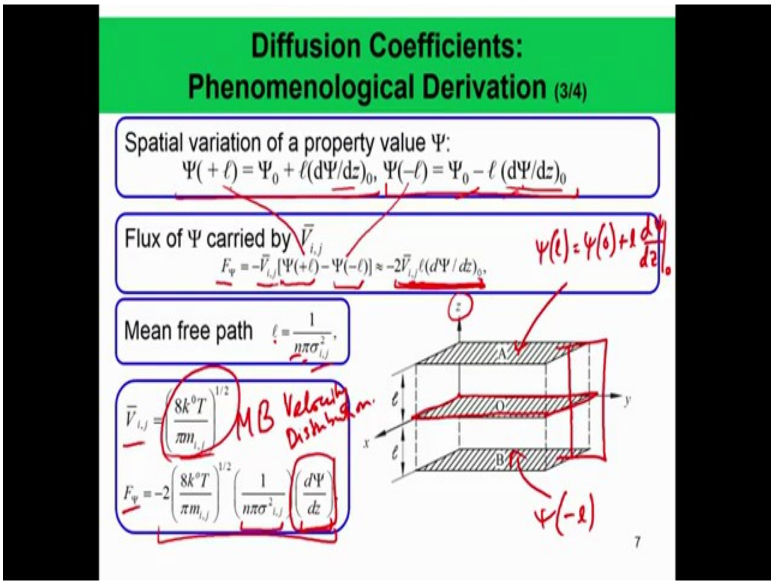

Diffusion Coefficients: Phenomenological Derivation (3/4)

Spatial variation of a property value Ψ:

$$\Psi(+\ell) = \Psi_0 + \ell(d\Psi/dz)_0,\ \Psi(-\ell) = \Psi_0 - \ell(d\Psi/dz)_0$$

Flux of Ψ carried by $\bar{V}_{i,j}$

$$F_\Psi = -\bar{V}_{i,j}[\Psi(+\ell) - \Psi(-\ell)] \approx -2\bar{V}_{i,j}\ell(d\Psi/dz)_0,$$

Mean free path $\ell = \frac{1}{n\pi\sigma_{i,j}^2},$

$$\bar{V}_{i,j} = \left(\frac{8k^0T}{\pi m_{i,j}}\right)^{1/2}$$

$$F_\Psi = -2\left(\frac{8k^0T}{\pi m_{i,j}}\right)^{1/2}\left(\frac{1}{n\pi\sigma^2_{i,j}}\right)\left(\frac{d\Psi}{dz}\right)$$

$\Psi(\ell) = \Psi(0) + \ell \frac{d\Psi}{dz}\Big|_0$

MB Velocity Distribution.

$\Psi(-\ell)$

So, now, let us consider this schematic where we have essentially 3 parallel planes all right. So, our this is the z coordinate, this is x coordinate, this is y coordinate say this our origin and through the origin this plane o passes and now from l distance from the origin we have another plane a and from l distance belong origin we have below o plane we have another plane b all right. So, now, we can write by using kinesis expansion that this property at this psi l is equal to psi 0, plus l times d psi d z at plane 0 right. So, this is what we have written and this can be easily obtain by Taylor series expansion and also we can write up to first order Taylors series expansion and we can also write psi minus l is equal to psi 0 minus l times d psi d z at 0.

So, the at both that we can write this at both of plane l and this is psi at plane of minus l as well as this psi this can be any property as such here we do not specify the property; and we just consider a generalized property and then the flux of this psi carried by this mean velocity, there is a average particle average molecular velocity is given by nothing, but this F psi which is a flux of psi carried by mean V i j is given by minus mean V i j the minus sign comes as you know because this flux is travelling from the from region of high psi to a region of small psi large psi to small psi. So, that is where the minus sign comes in. So, it is given by this F psi is equal to minus V i j times psi plus l minus psi minus l.

So, this is basically the; it is basically the flux of psi is nothing, but the difference between these of this property between these 2 planes and that is carried over by a mean molecular velocity mean V i j. So, then it is given by you can substitute this thing we can substitute this from this and this from this and we can write this one which is minus 2 V i j times l, l is the distance between these 2 planes times d i d z at this plane 0. Now what is l? Now if you remember that we assume that the exchange happens within one collision itself now then what is the distance between one collision happens that distance of one collision of course, mean free path there is average length of course, average distance and that is given by this numbered density times by times sigma i j square.

So, sigma i j once again it is diameter of the collision volume all right. So, and then of course, we know that mean V i j that is given by this 8 k 0 T times divided by pi m i j to the power of half which comes from the Maxwell Boltzmann velocity distribution. We use this formula in the previous kinetics class also when we derive the formula for the k the. So, we can substitute l we can substitute V i j in to this equation and then we get this form that is a F is in f psi is nothing, but minus 2 times 8 k 0 t divided by pi m i j to the power of half times 1 by n pi sigma i j square i j which substitute i j times d psi d z and this derivative d psi d psi d z as you see comes from essentially this from the Taylors series expansion from here and here from here and here.

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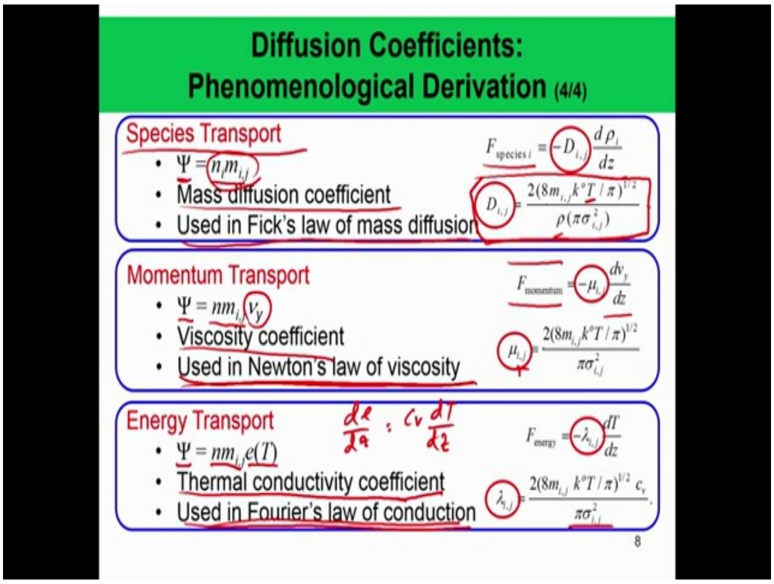

Diffusion Coefficients:
Phenomenological Derivation (4/4)

Species Transport
- $\Psi = n_i m_{i,j}$
- Mass diffusion coefficient
- Used in Fick's law of mass diffusion

$$F_{\text{species}\,i} = -D_{i,j}\frac{d\rho_i}{dz}$$

$$D_{i,j} = \frac{2(8m_{i,j}k^{o}T/\pi)^{1/2}}{\rho(\pi\sigma_{i,j}^{2})}$$

Momentum Transport
- $\Psi = nm_{i,j}v_y$
- Viscosity coefficient
- Used in Newton's law of viscosity

$$F_{\text{momentum}} = -\mu_{i,j}\frac{dv_y}{dz}$$

$$\mu_{i,j} = \frac{2(8m_{i,j}k^{o}T/\pi)^{1/2}}{\pi\sigma_{i,j}^{2}}$$

Energy Transport
- $\Psi = nm_{i,j}e(T)$
- Thermal conductivity coefficient
- Used in Fourier's law of conduction

$\frac{de}{dq} : c_v\frac{dT}{dz}$

$$F_{\text{energy}} = -\lambda_{i,j}\frac{dT}{dz}$$

$$\lambda_{i,j} = \frac{2(8m_{i,j}k^{o}T/\pi)^{1/2}c_v}{\pi\sigma_{i,j}^{2}}.$$

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So, now we can consider now instead of this generalized we this generalized formula that we have derived we can use this for different kind of transport we can use this for species transport we can use this for momentum transport, we can use this for energy transport or thermal transport. So, here as we see that this psi now we write this psi is equal to n i times m i j, n i is nothing, but the number density of this i th species n m i m i j is the reduced mass m i times m j divided by m i plus m j and this is the species transport and then this is psi and we can then supplement.

We can then substitute d psi d z and then the associated derivative of this that is d n i d z and we can write d n i d z into d rho i d z we can convert those things with appropriate constants and then we can try to find out the mass diffusion coefficients, and if you do that you will find that this f species I the flux of the species I is essentially given by minus D, i j times d rho i d z where as d is given by this formula. So, essentially this is the binary diffusion coefficient which is 2 times 8 m i j times k 0 t divided by pi to the power of half, and divided by rho times pi i sigma i j square.

So, the 2 most important thing that you see this gives a t to the power of half power dependence and 1 by rho power dependence. This m i j power dependence is actually we can this is not fully refined this we have made many assumptions and we will see that this can be have a more defined formula if we introduce some more complexes, but this is also itself good it shows very importantly that D i j is temperature to the power of half. So, as we increase the temperature diffusivity increases, the reason is simple the reason is that the essentially that we increase the diffusion your mean molecular speed V i j which is 8 k 0 t divided by pi m i j the; this one this one essentially is increasing. So, there is clearly there is very fast transport happening when there is more d more d i j.

So, that that is where this t to the power of half coming all right now also on momentum transport if you say momentum transport now we write this property psi, psi which was a generalized property as n times m i j which is for the mass and then times then the v i V y and then we will when you take d psi d z is essentially becomes d v y d z and then if we have find out the viscosity coefficient. So, if we write this the flux of momentum transport is given by minus mu i j and d v y d z, which actually comes from the previous formula of F psi is equal to something times d psi d z. So, this something as we as you as who put in different forms of psi whether it is species transport.

Whether it is momentum transport this parameter changes and also this one changes this one essentially changes and the associated change in this actually becomes the change in the coefficient. So, this viscosity mu i j that is also now given by 2 times 8 m i j times k 0 t to the power by to the power of half divided by pi sigma i j square, now you see importantly this rho is missing here. So, it does not depend on rho. Now energy transport here once again we see that now for energy transport we can write this generalized property psi as essentially n m i j times e t, e t where is internal energy and then we can write d e d z we will of course, when we should do d psi d z will arrive at d is d z and we can write d e d z is equal to C v d T d Z.

So, d is equal to C v d T we can use that one and then we will arrive at this thing that that this well if energy is equal to minus lambda i j d T d Z lambda i j is nothing, but 8 m i j k t are divided by pi to the power of half time c v by this thing. You can this lambda is nothing, but this thermal diffusion coefficient or this thermal not thermal diffusion coefficient this is thermal conductivity coefficients. So, this is used in Newton’s law of viscosity the previous one is you know as Newton’s law of this one is actually Newton’s this energy transport is actually this Fourier’s law of conduction, the momentum transport is actually Newton’s law of viscosity and the species transport is actually Fick’s laws of mass diffusion so, but now one thing that you can see the most interesting thing is that.

Because these are similar origin all of them are similar kind of dependence. So, the all of them are temperature t to the power of half dependent and all of them have this kind of similar things. So, that is how we can derive it in a simplified manner, but it is very illuminating in the sense that is gives us why it should dependent temperature, the answer is a as you have as we have discussed that basically it because depends on the mean molecular velocity all right which comes from the Maxwell Boltzmann distribution that is essentially t to the power of half.

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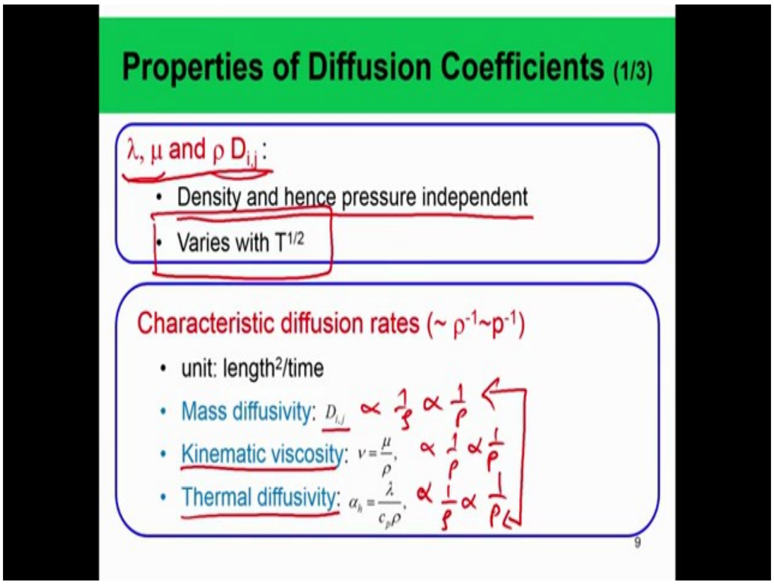

Properties of Diffusion Coefficients (1/3)

λ, μ and $\rho D_{i,j}$:

- Density and hence pressure independent
- Varies with $T^{1/2}$

Characteristic diffusion rates ($\sim \rho^{-1} \sim p^{-1}$)

- unit: length²/time
- Mass diffusivity: $D_{i,j} \propto \frac{1}{\rho} \propto \frac{1}{p}$
- Kinematic viscosity: $\nu = \frac{\mu}{\rho}$, $\propto \frac{1}{\rho} \propto \frac{1}{p}$
- Thermal diffusivity: $\alpha_h = \frac{\lambda}{c_p \rho}$, $\propto \frac{1}{\rho} \propto \frac{1}{p}$

Now, so, what we find is that that density this lambda mu and rho D i j that is if we take this rho to here.

So, all this things and you will see later that instead of D i j this rho D i j is sometimes a better choice for defining diffusion. So, we see that this both this things this lambda and mu and rho D i j these things are density and hence pressure independent. Now why this is density independent suppose you give you in you will increase the density by twice that you put in twice number of molecules species i. So, you think that yes now my transfer of will increase we as that increases, but you see the distance between which them collide that l the mean free path that also decreases now by half right. So, as a result of this now as you know that the mean free path appears proportional here.

So, the flux actually depends is directly proportional to the mean free path. So, as a result of this, this as the mean free path decreases you are this increased stuff increase of that particular species actually is counter acted, and hence there is no change there is no in there is no this parameters lambda mu and rho D i j do not depend on a such on density and pressure, but the most interesting thing is that they vary with t to the power of half actual variation is even stronger, but this t to the power of half gives as a quiet of good quality divider that it should be increasing with temperature at all the time.

And as you see that the characteristics diffusion rates, now the diffusion rates that might be of choice is sometimes D i j. So, D i j is proportional to 1 by rho. So, it is can be written to a proportional to 1 by p, if you use kinematic viscosity of course that is essentially proportional to 1 by rho. So, that also becomes proportional to 1 by p and thermal diffusivity which is lambda thermal conductivity divided by c p times rho divided by rho C p that also is proportional to 1 by rho and proportional to 1 by p. So, then if you consider this kinds of properties that is characteristics diffusion rates mass diffusivity instead of rho d kinematic viscosity instead of dynamic viscosity, and thermal diffusivity in terms of instead of thermal conductivity because of the density dependent because they are all proportional to rho to the power of minus 1 they essentially become pressure dependent, alright.

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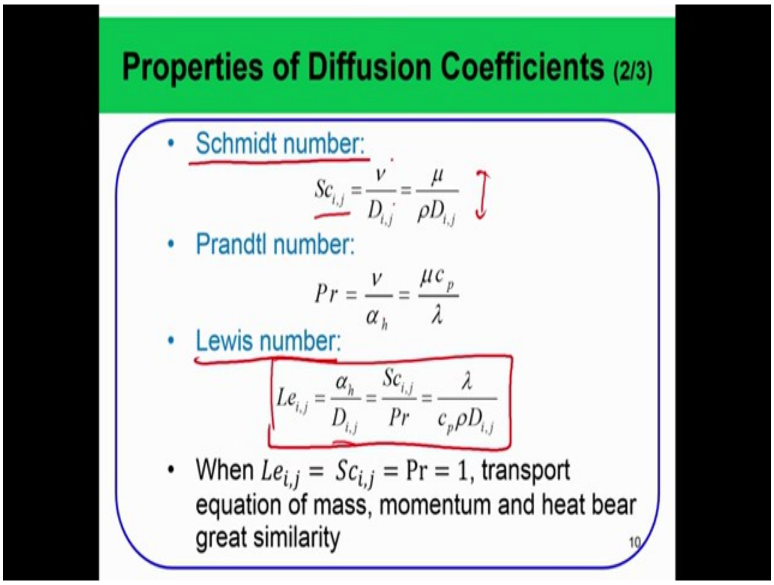

Properties of Diffusion Coefficients (2/3)

- Schmidt number:

$$Sc_{i,j}=\frac{\nu}{D_{i,j}}=\frac{\mu}{\rho D_{i,j}}$$

- Prandtl number:

$$Pr=\frac{\nu}{\alpha_h}=\frac{\mu c_p}{\lambda}$$

- Lewis number:

$$\boxed{Le_{i,j}=\frac{\alpha_h}{D_{i,j}}=\frac{Sc_{i,j}}{Pr}=\frac{\lambda}{c_p\rho D_{i,j}}}$$

- When $Le_{i,j}=Sc_{i,j}=\mathrm{Pr}=1$, transport equation of mass, momentum and heat bear great similarity

So, now the properties we are always look for non dimensional numbers. So, the non dimensional numbers of choice of importance in combustion will also encounter them later the other things other non dimensional numbers, which are essentially non dimensional numbers in terms of chemical kinetics we already have encountered one which is the Arrhenius number for kinetics, but here we are talking about non dimensional numbers in terms of transport and for that we see that the numbers of importance are Schmidt number which is nothing, but S c i j is nothing, but the ratio of the kinematic viscosity to the to the binary diffusivity, nu by D i j and we can also write it is in this form that is dynamic viscosity divided by rho density times D i j.

We can of course, Prandtl number is important Prandtl number does not change too much, but still this nu divided by alpha h this is very very important when it comes to combustion which is essentially Lewis number. Lewis number is a ratio of a thermal diffusivity alpha by molecular diffusivity that is or the binary or the species diffusivity that is D i j. Now this is very very very important because in combustion there is always competition between thermal energy transport heat transport and molecular transport. So, this quantifies that compete which one is actually stronger which one is a expectedly will be stronger because if the Lewis number is greater than one it means that the thermal diffusivity wins over this species diffusivity.

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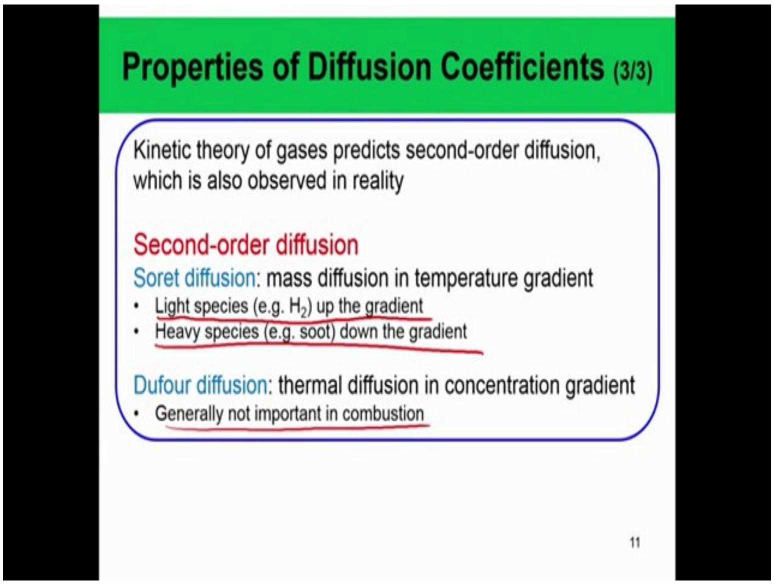

Properties of Diffusion Coefficients (3/3)

Kinetic theory of gases predicts second-order diffusion, which is also observed in reality

Second-order diffusion

Soret diffusion: mass diffusion in temperature gradient

- Light species (e.g. H_2) up the gradient
- Heavy species (e.g. soot) down the gradient

Dufour diffusion: thermal diffusion in concentration gradient

- Generally not important in combustion

If Lewis number i j is less than one then it means that species diffusivity is winning over thermal diffusivity so on and so forth. So, that is very important number; now there are this kinetic theory if we use there also second order diffusion, which is actually observed in reality what is second order diffusion. Second order diffusion is that when you when there is a temperature gradient and you are considering a multi components species. So, not only heat transfers of course, heat is transfer, but that is also mass transfer there is mass diffusion when there is a temperature gradient in a multi component species, and a good example is that there is a light species like hydrogen goes up the gradient and heavy species like soot goes on the gradient. We will come back to this again later when we discuss about the constitute revelation that come into the different diffusive processes inside the governing equations.

And before diffusion is thermal diffusion in concentration gradient and this generally not too much important in combustion, alright.

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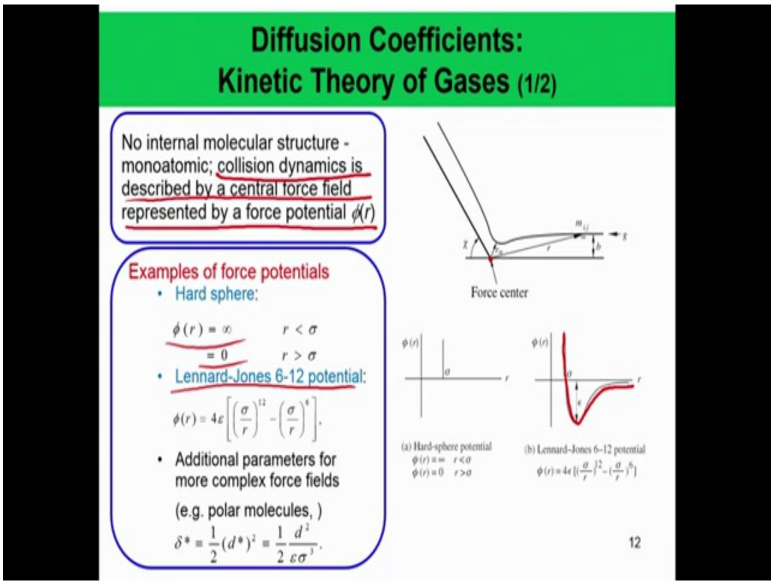

Diffusion Coefficients: Kinetic Theory of Gases (1/2)

No internal molecular structure - monoatomic; collision dynamics is described by a central force field represented by a force potential $\phi(r)$

Examples of force potentials

- Hard sphere:

$$\phi(r) = \infty \qquad r < \sigma$$
$$= 0 \qquad r > \sigma$$

- Lennard-Jones 6-12 potential:

$$\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right].$$

- Additional parameters for more complex force fields

(e.g. polar molecules,)

$$\delta^* = \frac{1}{2}(d^*)^2 = \frac{1}{2}\frac{d^2}{\varepsilon\sigma^3}.$$

So, now as we said that this all this properties of course, stay to the power of half dependence is nice, but this m i j this diffusivity is not really proportional to m i j. Larger the mass of the molecule it your diffusivity should not be large and there are actually 2 two simplified assumptions as we have seen in kinetics also we need transition state theory to properly explain, different things similarly here also the refined theory is can be used using kinetic theory of gases. So, here I will not go into details of this, but what will just do is that we will just give you a brief over brief on what are the parameters how does the calculated properties look like.

So, here the interesting thing is that again we had the; what is the difference; the difference is that when we are talking about collision theory. So, we were actually meaning that this molecule goes and hits this molecules right we are actually considering the counting the number of collisions that was happening. So, but here we say that that there is the, but actually this molecules are not billiard balls right they have a 4 field surrounding them they have an electron cloud, and those electron clouds when has force associated with them. So, we consider that that yes we do not consider molecular structures in these ones, but then the collision dynamics in this case instead of this hard collision is described by a central force field which is represented by a force potential.

So, here this instead of these hard collisions we consider central force field which is which we consider a force potential, which describes actually the force field. So, we actually consider this molecular molecule to be point mass, we do not have an need to consider the molecular structure and then the force potential will describe how much collision can happen. And this as you can understand that if we consider a hard sphere basically it means that the inside the sphere this potential goes to infinity, but outside this sphere there no effect as such. So, only after the collision then there is the molecules response, before that it does this molecule does not sense the another molecule is coming, but in reality that does not happen of course, the molecules have one electron cloud as is said and as a result.

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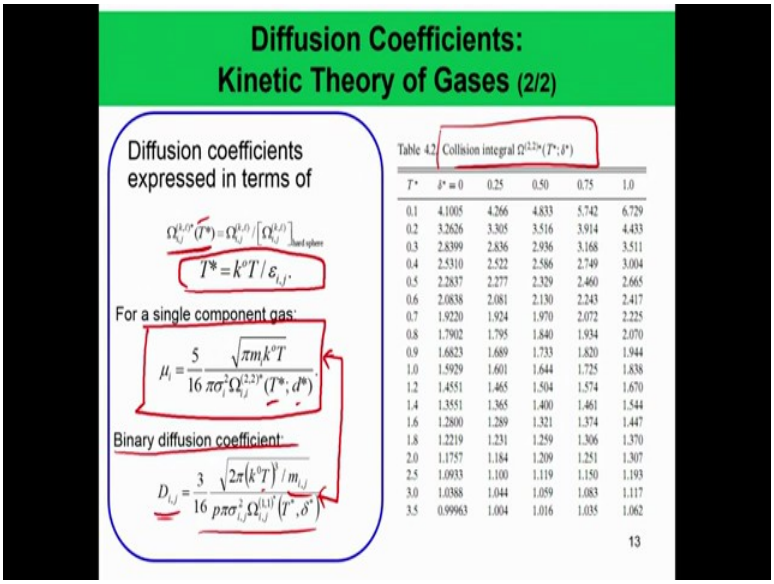

Diffusion Coefficients: Kinetic Theory of Gases (2/2)

Diffusion coefficients expressed in terms of

$$\Omega_{i,j}^{(k,l)*}(T^*) = \Omega_{i,j}^{(k,l)} / \left[\Omega_{i,j}^{(k,l)}\right]_{\text{hard sphere}}$$

$$\boxed{T^* = k^o T / \varepsilon_{i,j}.}$$

For a single component gas:

$$\boxed{\mu_i = \frac{5}{16} \frac{\sqrt{\pi m_i k^o T}}{\pi \sigma_i^2 \Omega_{i,j}^{(2,2)*}(T^*; d^*)}.}$$

Binary diffusion coefficient:

$$D_{i,j} = \frac{3}{16} \frac{\sqrt{2\pi \left(k^0 T\right)^3 / m_{i,j}}}{p \pi \sigma_{i,j}^2 \Omega_{i,j}^{(1,1)*}\left(T^*, \delta^*\right)}$$

Table 4.2 Collision integral $\Omega^{(2,2)*}(T^*;\delta^*)$

T^*	$\delta^* = 0$	0.25	0.50	0.75	1.0
0.1	4.1005	4.266	4.833	5.742	6.729
0.2	3.2626	3.305	3.516	3.914	4.433
0.3	2.8399	2.836	2.936	3.168	3.511
0.4	2.5310	2.522	2.586	2.749	3.004
0.5	2.2837	2.277	2.329	2.460	2.665
0.6	2.0838	2.081	2.130	2.243	2.417
0.7	1.9220	1.924	1.970	2.072	2.225
0.8	1.7902	1.795	1.840	1.934	2.070
0.9	1.6823	1.689	1.733	1.820	1.944
1.0	1.5929	1.601	1.644	1.725	1.838
1.2	1.4551	1.465	1.504	1.574	1.670
1.4	1.3551	1.365	1.400	1.461	1.544
1.6	1.2800	1.289	1.321	1.374	1.447
1.8	1.2219	1.231	1.259	1.306	1.370
2.0	1.1757	1.184	1.209	1.251	1.307
2.5	1.0933	1.100	1.119	1.150	1.193
3.0	1.0388	1.044	1.059	1.083	1.117
3.5	0.99963	1.004	1.016	1.035	1.062

We consider this Lennard Jones potential which is given by this kind of a potential curve, and then we have we do some calculations and this is the final results that you obtain. So, these are nothing, but do not get worried about this these are nothing, but the collision integrals and this is some non dimensional temperatures as you see here, and this collision integrals are essentially one can find tabulated as a function of this t star and d star which is another length and what we find here is that the for a single component gas the dynamic viscosity mu i s now given by pi m i k 0 T of course, this T you see then you compare this with the collision theory this t is essence this t dependence means half to the power of half.

But when you go the binary diffusion coefficient there is 2 interesting deviations from the collision theory, we see that now this diffusion we did D i j essentially has a T to the power of 3 pi 2 dependents, and also this m i j has come down stairs. So, larger the larger the m smaller is the diffusivity which makes sense now right so, but there are other similarities also. So, with this an as I said that one can find this collision integrals tabulated; now and from that we can find a good estimate of this different properties.

So, with that we will end this transport will end this transport theory topic and next we will go on to discuss the governing equations where we will see that how this transports as well as this kinetics basically comes and along with the convection. So, the basically we will see that the governing equations we can describe essentially any flow field of choice and that is a purpose of a governing equations, which is a very central theme of any combustion course and of course, it is a very central thing of our course also. So, we will come back to that in a short amount of time.

Thank you.