

Microscale Transport Processes
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Lecture No. # 35
Transport Processes and Their Descriptions

In today's lecture, we are going to talk about the different transport processes and their descriptions. Now, when we talk about transport processes we not only mean heat transfer momentum transfer or mass transfer, we also going to talk about the mechanism of these transport processes. For example, in some situations, the convective transport processes may become important; in some other cases, conductive and in some cases both would be important. So, when we talk about conductive transport process or molecular transport process, in which the transport is going to be proportional to the gradient of a quantity that can be measured. For example, it could be velocity for momentum transfer temperature or concentration.

And the corresponding phenomenological equations such as Newton's law of viscosity or Fourier's law of conduction or Fick's law of diffusion, they essentially define a transport coefficient, which could be the viscosity or the thermal conductivity or the diffusion coefficient. So, these are a cluster of transport processes, in which the transport is due to the presence of a gradient in a direction perpendicular to the flow. So, if we have a difference in temperature and we for example, in a solid, then the heat transport is going to be proportional to the temperature gradient. And the proportionality constant is a thermal conductivity of the fluid.

So, there will be some situations in which the transport is primarily going to be governed by the **molecule by the** molecules, without those molecules actually displaced from their average positions. In some other cases, it is the bulk convection, bulk transport of material between point one and two, and they will carry with them the corresponding momentum energy or material transport from one point to the other. So, whenever we have transfer of material from one point to another and thereby causing some transport of

mass momentum or energy, that kind of processes are known as convective transport process.

The convective transport processes are predominantly they are the mode of transport in liquids though in liquids the conduction is also present. And these type of coupled convection and conduction problems are quite important and we are also going to look at the effects of transport effects of convective and conductive transport in micro systems. So, we would see in this is the transport processes their classifications and the properties, the coefficients which are important in some such processes the governing equations for momentum transfer, heat transfer and mass transfer. And the relative importance of convections and conduction as specified by some engineering parameters and similarity parameters.

And their relative importance which would tell us that which process is going to take longer to establish a fully developed condition. And when mass let us for example, mass and heat transfer are taking place simultaneously then we would like to know which process is faster. For example, in the case of condensation from a vapour on to the surface of a on to a cold surface, we would like to know what are what whether it is governed by the thermal process. Or it is going to it is governed by the diffusion of the vapour molecules from the bulk to the cooler surface and thereby creating an ideal condition for condensation. So, these differences we would also like to look at in today's class.

Furthermore we would also like to see what would be the and just one applicative example is for example, if we have flow, simultaneously flow and heat transfer in a slender micro channel. A micro channel which is thin yet long and we would like to see, what would be the governing equations for such cases and how additional forces could be incorporated into the governing equation. For example, how the surface forces can big play a prominent role in such cases and finally, we would also like to see the application. Engineering application of these equations for example, in terms of finding out what would be the pressure difference between points one and two and not in a straight pipe as we have already known from all undergraduate fluid mechanics.

But in a system in which we have a there would be large number of mains, there would be internals and we are going to concentrate on smaller dimension pipes. In which the

length is going to be large compared to the cross section and the cross section itself has many is following a tortuous path. So, the pressure drop is going to be more.

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Elementary transport processes and their description


The entire change of a state variable is described by the transport processes of conduction in the immobile phase (solids or resting fluids), convection in the fluid phase (gases and liquids), and by the generation or depletion in the control volume.

$$\left[\begin{array}{c} \text{Total Flow} \\ \text{Density} \end{array} \right] = \left[\begin{array}{c} \text{Conduction over} \\ \text{the boundary} \end{array} \right] + \left[\begin{array}{c} \text{Convection over} \\ \text{the boundary} \end{array} \right] + \left[\begin{array}{c} \text{Source} \\ \text{or} \\ \text{Sink} \end{array} \right]$$

Conductive transport

convective transport

Transfer coefficients: $D, \nu = \mu/\rho, \alpha = k/\rho c_p$ (m^2/s)



So, you are going to study first start with the transport processes and we would see how it changes (No audio from: 05:58 to 06:13) since it is taking some time for to load. Then let us talk about the relevant equations when in transport process and their descriptions. See for example, all of us know that the governing process in fluid mechanics is if we go by elementary transport process and their descriptions, what we see here is the change of a any variable is described by the transport process of conduction in the immobile phase. But essentially the governing equation can be written as total flow of any parameter it could be energy, it could be mass or it could be the momentum.

Is if we define a control volume consisting of six phases in through, all these six phases there can be transport of momentum. For example, into the control volume and there could also be conviction due to flow of fluid into the control volume and there could be some source or sink. So, let us think of what happens in an in a system in which momentum transport is taking place. So, as a result of all the momentum which are coming to the control volume the density, the flow density the momentum total momentum contained in the control volume will change. And how would it change there can be six phases through, the six phases we can have conduction molecular transport of momentum into the control volume.

And they exist because of the gradient in velocity in a direction perpendicular to the flow. So, I have a x phase and x plus and another phase at x plus Δx . So, the area of the x phase could be Δy times Δz . So, x phase is the area which is perpendicular to the x direction. So, I have another phase which is at x plus Δx . So, if I have flow in this maybe it is easy to find out what is the total amount of momentum being added by conduction into the control volume. So, it would simply be the component velocity v_x in this direction multiplied by the area which is Δy times Δz . So, v_x times Δy Δz would give me the amount of fluid which is coming into this control volume per unit time.

So, multiply that with ρ and what I get is the amount of mass which is coming into this control volume per unit time. So, this mass flow rate when again multiplied by v_x one more time would give me the x momentum the x component of momentum which is entering the control volume. So, the expression for momentum coming into the control volume would simply be equal to ρ times v_x times Δy Δz and a v_x again everything evaluated at x . Similarly, the momentum which is leaving through the x plus Δx phase would be all these quantities, but they are evaluated at x plus Δx .

Similarly, for the y phase and for the z phase one would be able to obtain what is the y component of momentum being added to the system and the z component of momentum being added to the system. Similarly, through all these phases due to a difference in velocity the momentum can enter the x momentum can enter because of the presence of a gradient those are the conductive transport of momentum. So, through all these six phases due the presence of velocity gradient and applying Newton's law, I should be able to find out what are the expressions of τ_{xy} τ_{xz} and τ_{xx} similarly, for three y components and for three z components. So, together we then would be able to find out all the components of this stress tensor.

So, sum this over the boundary for the conduction and for the convection plus there would be source or sink. In these source or sink it is simply going to be the forces, which are present in the system now for a momentum transport situation the sources or sink. That are relevant are due to surface forces and the surface forces for macroscopic systems would simply be equal to the pressure forces and the shear forces. And when we talk about the body forces it could be the gravity or the electrostatic forces or some other

such forces, which are applied on the entire volume, entire mass of the control volume. So, based on that, I can write the source or sink components of this equation.

So, we know what are the conductive transport and as a sum of all these the total flow density or the total energy contained or the total amount of species inside the control volume may be different. And this would give us the a complete description of the flow physics in terms of either mass, heat or momentum. And the transfer coefficients are defined as the diffusivity D the kinematic viscosity which is μ/ρ . And a thermal diffusivity which is $k/\rho c_p$ where k is the thermal conductivity ρ is the density and c_p is the heat capacity. All three transport coefficients namely the diffusivity the kinematic viscosity and the thermal conductivity and the thermal diffusion coefficient has have units of meter square per second.

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The dynamic behavior of viscous fluids is governed by $Re = wd\rho/\mu$


Species transfer in convective flow, both Re and $Sc (= \mu/\rho D)$

Sc - ratio between momentum and species transfer.

If $Sc = O(1)$, as with gases, momentum transfer and species transfer are in the same order-of-magnitude.

Concentration gradients behave similar to velocity gradients.

If Sc is large, such as for liquids, concentration gradients are slower to develop than velocity gradient.



Now, if we look into the dynamic behaviour of viscous fluids we will see I mean this I think we have covered before a dimensionless number or a similarity parameter namely Reynolds number would appear in all the equations. And the dimensionless number Reynolds number is defined as a length scale the velocity, the density divided by the viscosity. Now, the importance of similarity parameters are simply that if the similarity parameter of two different fluids under two different conditions are equal. Then the process be it heat transfer, mass transfer or momentum transfer, then the process can be described by governing equations which are identical.

The if so, if we express the dimension the if we express the equations governing equations in a non dimensional form then these similarity parameters. For example, Reynolds number would appear automatically and the moment, the process conditions if the process conditions are such that for two different fluids. The values of the Reynolds number are the same then the governing equations describing the process would be equal. So, Reynolds number typically tells us about the is important for viscous fluids and it tells us it is basically gives us some ratio of inertial forces and viscous forces.

Similar to Reynolds number in fluid mechanics we have a convective flow. For example, defined by Schmidt number in mass transfer denoted by S_c here, which is defined as $\frac{\mu}{\rho D}$ where μ being the viscosity and D being the diffusion coefficient. So, if you look carefully the Schmidt number is nothing but a ratio between momentum transfer and mass transfer or specifically it is a species transfer. So, the values of these numbers would tell us something about, which process is important, is it the momentum transfer process? That is more important compared to the mass transfer or otherwise. So, if we can also see that if Schmidt number is of the order of one, which is happens for the case of gases.

Then the momentum transfer and the species transfer are in the same order of magnitude. So, let say we have a flow of a gas through a pipe through a let say small slit and that slit is made of a material, which can sublimit. For example, it is a naphthalene slit two plates of naphthalene which are kept close to each other and we have flow. So, there is going to be the formation of a hydrodynamic boundary layer and the formation of a mass transfer boundary layer. Now, we do not know priority which one is going to linger for longer; that means, we are not sure whether it is the mass transfer, which is going to be the faster or the momentum transfer, which is going to be which is going to take place at a higher rate.

So, if we see the value of Schmidt number which is $\frac{\mu}{\rho D}$. So, if the value of Schmidt number is let say about one, then the viscous transport of momentum and the species transport are of the same order of magnitude. And both these boundary layers will grow together and the fully developed condition. In terms of momentum transfer and in terms of mass transfer are going to attain at the same point or at very close to each other. That means, both these processes momentum transfer and specie transfer will take

place at the same rate. So, concentration profile and the velocity profile as they grow will be similar in nature.

So, similarly one can also see that if Schmidt number is large now the value of Schmidt number being large; that means, the value of the diffusion coefficient which is in the denominator would be small. And if the value of the diffusion coefficient is small, then it will take longer path for the concentration gradient or the concentration profile to become fully developed. That means, for large Schmidt number cases such as for liquids the concentration gradients will develop slowly compared to the velocity gradient. So, the velocity will be hydro dynamically fully developed, but not fully developed as far as the mass transfer mass transport is concerned.

So, these similarity parameters the values of these similarity parameters tells us important information about the not only the nature of the process, but how fast the different components of the processes are. So, the same contribute same conclusion that we can made about mass transfer and momentum transfer can also be made for momentum transfer and heat transfer. The corresponding similarity parameter of interest in that case would be Prandtl number which is $c_p \mu / k$ or in other words it is the it can be expressed as the momentum diffusivity by thermal diffusivity. So, if the value of Prandtl number is large then the momentum diffusivity is going to be quite large compared to the thermal diffusivity.

And same as in Schmidt number the flow is going to be fully developed hydro dynamically, but the thermally it is yet it will still be developing.

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Convective heat transfer – both Re and Pr


Low Pr numbers indicate low k , as in oils or organic liquids.

The Pr numbers of air or water have the order of $O(1)$, permitting a heat transfer as fast as momentum transfer.

Liquid metals behave differently

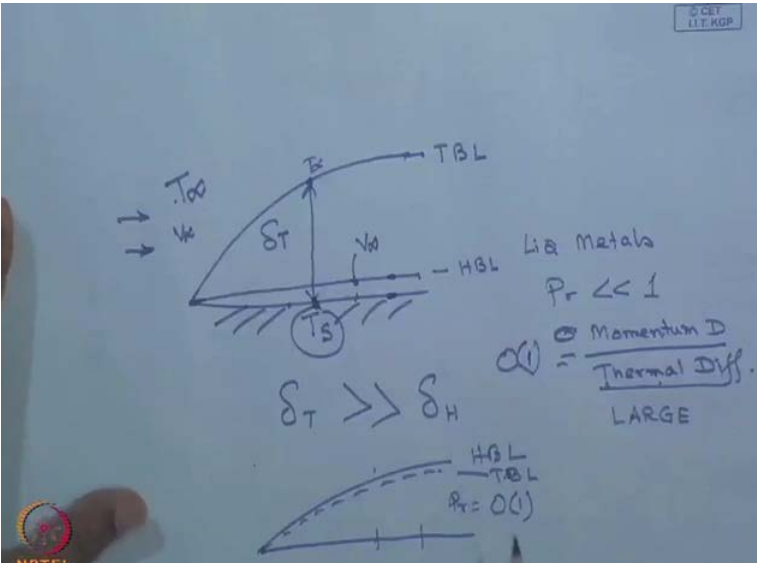
Coupled heat and mass or species transfer, are combined to Lewis number $Le (=Sc/Pr) = \alpha/D$, ($\alpha=k/\rho c_p$)

A high Le number allows droplet generation from vapor cooling, while for low Le numbers, vapor will directly condense at the wall.



So, similar such similar such cases similar such analogies can be drawn between heat transfer and fluid flow as well as between convective heat transfer cases where both Reynolds and Prandtl number are going to be important. And where the Prandtl number is going to be of the order of one which would tell us that the process is as fast as in momentum transfer. But different situation would arise when we are dealing with liquid metals, the liquid metals are behave will behave completely differently in the case when we talk about the growth of these layers.

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Li_q Metals
 $Pr \ll 1$
 $\Pr = \frac{\text{Momentum Diff.}}{\text{Thermal Diff.}}$
LARGE

$\delta_T \gg \delta_H$

HBL
TBL
 $Pr = O(1)$



For the case of liquid metals let us say if we see the for the liquid metals the value of Prandtl number is going to be very, very small compared to one. So, this would tell us that the thickness of the hydrodynamic boundary layer is going to be quite small compared to the thermal boundary layer. Now, if you see that Prandtl number is momentum diffusivity divided by thermal diffusivity. So, if the value of Prandtl number is quite small then it only tells us the value of thermal diffusivity is quite large. Now, if the value of thermal diffusivity is large then it simply tells us that the effect of the temperature of the plate, solid plate which is in contact with a liquid since T_s is different from the T_w .

Then the effect of the plate hot plate will be felt at a much greater depth compared to the effect of the plate when we talk about velocity. So, it will take this much of distance for the temperature to become equal to T_∞ . Whereas, only this much of distance, this much of boundary layer thickness is necessary for the velocity over here to become equal to V_∞ . So, we have a liquid which is approaching a solid plate whose temperature is different from that of T_∞ and due to no slip condition the velocity at this point would be equal to 0. So, there is going to be simultaneous development of hydrodynamic boundary layer and thermal boundary layer.

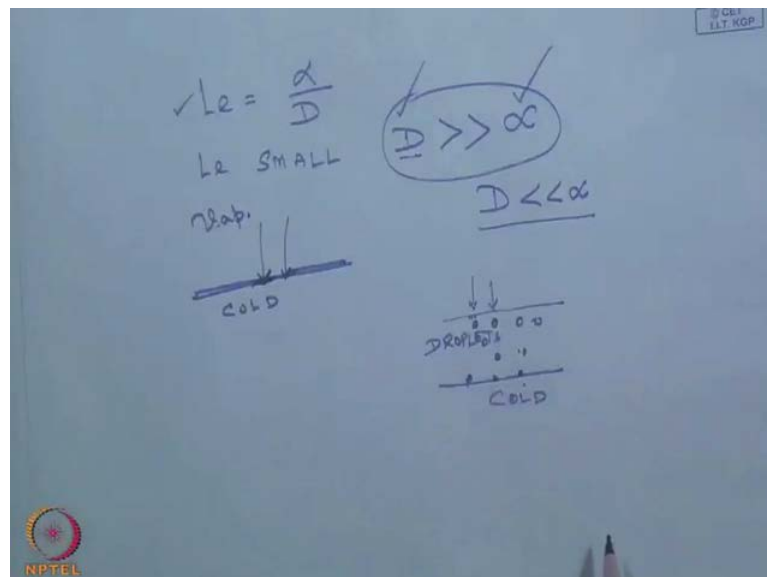
For the case liquid metal we can say that the δ_T that is the thickness of the thermal boundary layer is going to be much much greater than the thickness of the hydrodynamic boundary layer. So, this liquid metals therefore, behave in a different way, but if these two are of the order of one momentum diffusivity by thermal diffusivity, then what you would see is that both the hydrodynamic boundary layer and the thermal boundary layer will probably be of the same thickness. That means, the boundary layer thickness is at any thick at any axial position for these two cases would be of the would be almost equal, if the value of Prandtl number is of the order of one. So, the Prandtl number Schmidt number or similar such numbers they carry information about the basic physics of the process.

And not really they allow us to compare between seemingly different transport process, their values will also give us such important information. So, this is a case of coupled momentum transfer and heat transfer, the processes are there are also processes which are coupled heat and the species transfer. Now, they are expressed in terms of Lewis number which is nothing, but the ratio of Schmidt number and Prandtl number or alpha

the thermal diffusivity divided by D the species diffusivity. So, obviously we can say that if the value of Lewis number is large, then the diffusion the species diffusion is going to be slower compared to heat transfer.

On the other hand if Lewis number is small then the diffusion species transport is going to predominate over heat transport, which would give rise to some interesting phenomena, which can be explained by high or low values of Lewis number. A high Lewis number allows droplet generation from vapour cooling where whereas, for low Lewis number the vapour will directly condense on the wall.

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So, the vapour will diffuse very fast because if the value of Lewis number is small, Lewis number is nothing but α by D . So, if the value of Lewis number is small then it simply tells us that D is going to be quite large compared to the thermal diffusivity. So, if I have a surface which is cold and if I have a vapour which is in contact with the cold surface. Then due to it is high diffusion coefficient the vapour molecules will reach the cold surface before it feels the change in temperature. So, the vapour molecules will directly come in contact with cold surface and condense and form a film. On the wall on the other hand if D is quite small compared to the thermal diffusivity, then the effect of the cold wall temperature wise will be felt at a greater distance.

So, the vapour which was coming towards this it will sense the lowering temperature there will thereby will start condensing. And droplets will be generated from the vapour

and these droplets will then come and condense on the cold surface. So, simply by looking at the values of Lewis number from by tuning the value of Lewis number one can make the vapour come and condense on the cold surface; or one can one if the value of Lewis number is large then the droplets are going to form. So, all are connecting with the relative values of the two diffusion coefficients, the species diffusion coefficient and the thermal diffusion and the thermal diffusion parameter.

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Two-film model for the fluid/fluid exchange of mass, species, energy

Species transport equations

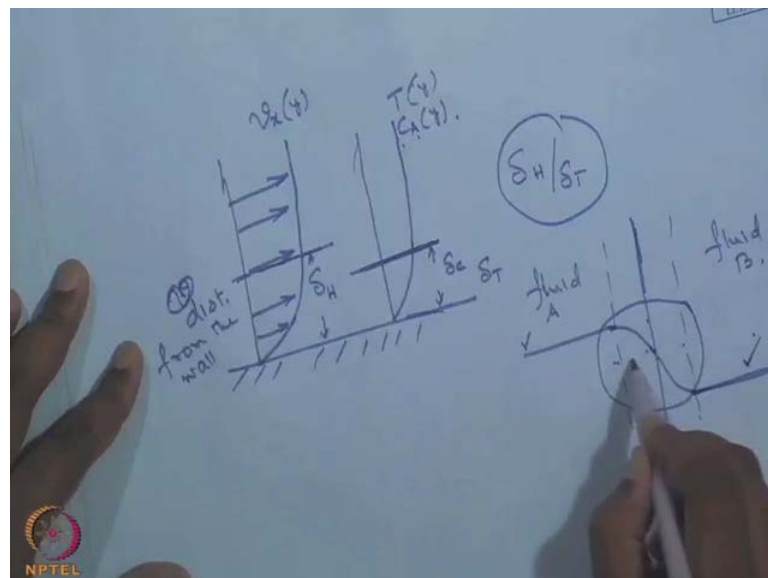
$$J_i^A = \beta_i^A A (c_{i,bulk}^A - c_{i,int\,erface}^A); \quad J_i^B = \beta_i^B A (c_{i,int\,erface}^B - c_{i,bulk}^B); \quad \beta_i = D_{Ai} / \delta_i$$

For the absorption of a gas into a liquid Henry's law $p_{i,g} = H_i c_{ij}$

For the evaporation or condensation of a binary mixture (distillation, rectification), Raoult's law $p_i = p_t y_i = \pi_i x_i$



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Now, there are several models by which one can predict what would be the species transport and (()) this is just a case of a two film model. And the two film model can be expressed as like a as I mentioned before then if I let say I am plotting the velocity profile and as so, this. So, what you would see is that the velocity will sharply change and it is going to become more or less parallel. So, this is the distance from the wall and these are the velocities. So, you can see that there would be some arbitrary distance beyond which the velocity almost becomes invariant.

Similarly, for the case of thermal temperature profile or species profile so, this could be either the T as a function of y or it could be concentration of one species as a function of y. Whereas, this is velocity in the x direction main flow direction as a condition of y. So, there would be some portion, some point, some plane beyond which the temperature or the concentration does not vary. So, this is known as the hydrodynamic boundary layer thickness and this could be the concentration boundary layer thickness or the thermal boundary layer thickness. And the relative magnitudes of ΔH or ΔT can be expressed in terms of the similarity parameters that we know.

So, when we if simply think of when we talk about the species transport equations and two film models let us say this is the interface which separates between which separates these two liquids. So, for fluid A and over here I have fluid B and let us say I am talking about the temperature profile which is uniform in fluid A, but in a layer very close to the surface the temperature falls and over here the temperature again decreases to ultimately it is going to become a constant. So, these are this will be the bulk temperature or bulk concentration of B and that of A. But over in this region near these two interfaces there would be two films on other side on either side of the interface where the change in temperature or change in concentration takes place.

So, one can therefore, express as we see over here that the flux or the amount of transport of species. One is going to be can be expressed as proportional to the distance of concentration of a in the A th fluid at the bulk minus at the interface and similarly, from the interface to the B th fluid. So, this way one can find out using a two film model the distribution of the transport of a across these two the across these interfaces.


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Molecular velocities and macroscopic fluid properties

Macroscopic gas properties from kinetic theory and molecular behavior

Bird, Stewart, Lightfoot

Viscosity from the kinetic theory of gases : Chapman and Cowling

$$\mu = 0.499 \rho \lambda \bar{c}_m \quad \lambda = \text{mean free path}; \bar{c}_m = \text{mean molecular velocity}$$
$$\mu = \frac{M_m}{\sqrt{6} \pi \sigma^2} \sqrt{RT} \quad \mu \neq f(p), \mu \uparrow \sqrt{T}, \text{ unlike liquids where } \mu \downarrow \text{ with } \uparrow T$$
$$k = \frac{k}{\pi^{3/2} \sigma^2} \sqrt{RT} \quad D_{AB} = \frac{1}{3} \lambda \bar{c}_m$$


Now, when we have there are simple there are many equations there are relations which have been postulated derived from this two film model. For absorption of gas into a liquid we all know that Henry's law can be used and for evaporation or condensation of a binary mixture. For example, in distillation the Raoult's law, that is also quite common and these molecular velocities and macroscopic fluid properties can be obtained theoretically. For example, the properties can be obtained from kinetic theory and I would request you to look at the textbook the famous textbook of transport phenomena by Bird Stewart and Lightfoot, which would give us, which will tell us about the values possible values of the viscosity, thermal conductivity, based on molecular contributions based on kinetic theory of gases.

And there are certain relations, which are available for viscosity of gases, the variation of viscosity of gases with temperature. From the corresponding equation can see that μ increases with increases in temperature and the dependencies root over T . Whereas, in liquids you can see that the we know that viscosity decreases with increase in temperature and similarly, one can find relations based on kinetic theory from many of these textbooks for thermal conductivity and so on.

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Limits of linear transport properties

Linear relationship between force and the corresponding flux

In small structures, these linear coefficients may be limited due to the influence of the surface, which plays a major role for gases.

The viscosity of a liquid is higher in the vicinity of a surface - visco-elastic effects

The solid surface of a dielectric material induces, due to its electrical charge, an adsorbed layer of molecules from the liquid, the Kelvin-Helmholtz electro-kinetic double layer - EDL.



But one important thing that we must keep in mind is that. So, far we are talking about when we talk about Newton's law of viscosity or let us say Fourier's law conduction or similar such laws that we expect a linear relationship between the force and the corresponding flux. So, when you are talking about the heat transfer it is the amount of heat transfer is proportional to the gradient or the amount of shear stress is going to be proportional to the velocity gradient. And this linear relation this is the values of viscosity, the values of thermal conductivity or of diffusivity. So, till now we have assumed that there is a linear relationship between the cause and the effect, the temperature gradient and the amount of heat transfer.

And the proportionality of this linear relation is a thermal conductivity, but these linear relationships will not be valid as the system dimensions is becoming smaller or if the temperature gradients for example, are too large. So, when you have a large value of gradient or the system dimensions becoming smaller, then the linear relationship will not be valid. And additional terms are to be added to those relations to make the equation more equations, more realistic and to increase the applicability region of applicability of these equations. So, in as I as we were saying the you when you talk about small structures the linear coefficients are going to be limited as the surfaces are going to play an increasingly important part for example, in gases.

In liquid it is an increasing phenomena which is known as the viscoelastic effects. So, the viscosity or the truly speaking the liquid molecules behaves differently in a vicinity of a surface, which is termed as the viscoelastic effects.


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This layer extends approximately three molecular layers from the wall into the bulk fluid and induces a charge orientation in the adjacent fluid.

This layer of mobile, charged molecules is called the Stern layer.

In very small channels ($d_h \approx 100$ nm) and for relatively large molecules, this layer may influence the flow and the transport processes at the wall increasing the wall friction.

The EDL also influences the local Nusselt number Nu. In micropolar flow, for example, the Nu number is approx. 7 % smaller than in laminar flow.



Now, when we talk about flow of a let us say a liquid in contact with dielectric material then the dielectric material due to it is electrical charge will create an adsorbed layer of molecules from the liquid. So, that adsorbed layer of molecule will not move and it is known as the Kelvin Helmholtz electro kinetic double layer or E D L in short. So, the presence of E D L presence of an immobile layer of liquid very close to a dielectric material creates a situation which is different from the bulk flow that we have been discussed so, far. So, obviously this very thin layer of thickness few molecules become relevant in describing the process, if the system dimensions are smaller.

So, few molecules adsorb to the a dielectric surface will not be will not have any significant effect. If you are talking about a conduit which is few centimetres in size, but when we reduce the size to hundred nanometre or even smaller of the conduit of the tube or the capillary. Then a few molecular thick layer at adsorbed on the surface due to the electric due to and the formation of the electric double layer is can cause significant changes to the flow properties. Not only the EDL there would be additional changes because this layer this EDL extends approximately three molecular layers from the wall

into the bulk fluid and induces a charge orientation in the adjacent fluid. So, this layer of liquid which is mobile, but charged is called the stern layer.

So, since they are they are charged yet mobile the movement or the velocity of these molecules would be different when compared to the situation in which the walls do not have any charge. So, this relatively if we talk about very small channels and large molecules then a few molecule thick layer of adsorbed layer on the surface and the presence of a stern layer. So, that is why it is called double layer the presence of an immobile layer and the presence of the stern layer their combined thickness could be significant compared to a hundred nano meter diameter channel.

Now, what would this give rise to this is going to create a situation in which as if a more viscous liquid, but uncharged more viscous uncharged liquid is flowing through that hundred nanometre tube. So, these two situations are comparable a dielectric with surface charges inducing an apparent increase in viscosity that is known as the viscoelastic effect. So, as if the viscosity of the liquid certainly near the wall has increased and this has given rise to less flow for the same value of Δp . So, there is a difference between the flow based on depending on whether the tube is charged or it is neutral. So, the presence of charge induces some induces an ordering or in or slows down the fluid close to the surface. Additional slowing down of the fluid close to the surface thereby it would appear as if the viscosity of the liquid has increased.


The wall friction has increased you require more Δp than that predicted by the ordinary equations which are to be used for bulk flow. So, this is another effect which one has to keep in mind and effect of the transport property how the transport there can be additional changes in the transport property for systems which are very small in size. So, if we it not only changes the wall friction since the velocity near the wall for such cases would be smaller and therefore, the convection is going to be smaller. And if the convection is smaller than the value of Nusselt number will turn out to be smaller as well. So, for micro polar flow the Nusselt number could be as about ten percent smaller in laminar flow when there is no EDL.

So, the EDL influences the flow EDL and heat transfer for flow through micro flow through very small systems. So, these properties of the transport parameters need to be looked into while thinking about flow through small systems.

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Modeling, Calculation Methods, and Simulation

1. Physical variables and dimensional analysis
2. Similarity laws and scaling laws
3. Order-of-magnitude analysis
4. Lumped element modeling
5. Numerical simulation and analytical modeling



Now, when we talk about modelling we are going to talk about now in about modelling the calculation methods and simulation. So, one can find out first what are the physical variables and try to do some dimensional analysis is there any similarity law. That can be used whether or not if there are any scaling laws one can start with an order of magnitude analysis would we would also like to see if a lumped element modelling. That means, assuming that let say for example, the temperature is space wise isothermal inside a solid which is in contact with liquid. So, if we could say that the temperature is not a function of x y z inside a solid then that simplifies our calculation to a great extent. And that is what is the lumped element or lumped capacitance modelling.

There will be some situations in which these kind of approximations would be could not be made. And then we will probably have to go for full scale numerical simulation and or analytical modelling.


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Momentum Transfer

In single-phase flow, the fluid motion in microchannels is determined by wall friction, viscous forces and inertial forces.

Continuity Equation
$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \text{div}(\rho \bar{w})$$

Equation of motion
$$\frac{\partial(mw)}{\partial t} = \left(\dot{mw} \right)_in - \left(\dot{mw} \right)_out + (pA)_in - (pA)_out + mg + F_z$$



So, we are if we if we think about once a single phase flow in the relevant equations are; obviously, continuity equation and equation of motion and so on. So, the continuity equation; obviously, we know that the substantial derivative that is capital D D t. Substantial derivative of density is going to be function of the del t of rho and the divergence of the mass flow vector. Similarly, for the case of equation of and if it is a steady state then you will simply know that the dot product of velocity times area would be the same which would give rise to rho 1 rho 1 v 1 A 1 should be equal to rho 2 v 2 A 2 and so on.


For a case of equation of motion what we have on the left hand side is a transient effect which is del t of m w and on the right hand side it is basically a sum of several factors. The first two are the amount of momentum the net addition of momentum to the control volume as a result of convection as well as conduction. So, the first two terms represent the addition of momentum to the control volume, the next two that which that contain the pressure.

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Using the correlations between pressure p and shear stress τ as well as between tension σ and strain, the momentum equation or Newton's law is written as:

$$\rho \frac{D\vec{w}}{Dt} = -\text{grad } p + \text{Div} \left[\mu \left(2 \text{grad } \vec{w} - \frac{2}{3} \vec{\delta} \text{div } \vec{w} \right) \right] + \rho \vec{g}$$

$\vec{\delta}$ is the Kronecker unit tensor



They are the effect of surface forces in this case identified as the pressure. The next term is the body force $m g$ and the last term is the additional forces which are acting or which are present in such in systems. So, using the correlations between the pressure and the shear stress these are fundamental fluid mechanics then and using Newton's law, one can write the equation of motion in this in the following compact vector form.

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For one-dimensional differential channel elements with viscous flow, the momentum balance can be written as


$$\frac{\partial(\rho A w)}{\partial t} = -\frac{\partial(\rho w A w)}{\partial z} - \frac{\partial(p A)}{\partial z} + p \frac{\partial A}{\partial z} - \tau L_c - \rho A g$$

L_c is the perimeter of the differential channel element

With continuity equation, the above equation can be simplified for all space co-ordinates as (\vec{k} is the sum for external forces)

$$\rho \frac{D\vec{w}}{Dt} = \rho \left(\frac{\partial}{\partial t} + \vec{w} \cdot \text{div} \right) \vec{w} = -\text{grad } p + \mu \nabla^2 \vec{w} + \vec{k}$$

The 2nd term on LHS is also called the inertial term and describes convection. It is the only nonlinear term in the Navier-Stokes eqn.



So, for one dimensional if we take just an one-dimensional differential channel element with viscous flow the momentum balance is simply a balance between momentum in the

change in pressure in the flow direction. The change in area in the flow direction and the effect of pressure so, the pressure between two points can be different and not only that the area at the two points could be different. So, if you have a curved area and then we would also have to consider the component of pressure which is acting on the additional area additional curved area. And then the next term corresponds to the shear stress so, the shear stress opposing the flow and the last term would be the gravity forces.

So, for flow through a channel element this kind of approach can be used to find out what is **the what is** going to be the total amount of what is going to be the velocity distribution and so, on. So, with in incorporating the continuity equation this equation can be simplified and the compact expression for momentum transfer as we all know can be obtained. The second term on the left hand side is called the inertial term and it describes convection and the second term on the right hand side it denotes the viscous forces the first term on the right hand side is a pressure forces. And the second term on the left hand side or the inertial term is the only non linear term in Navier stokes equation.

And under certain special conditions this inertial term can be neglected and we get simpler solution of the Navier stokes equation. So, there would be some situations for example, when the flow is very slow so, the convection will not have any bearing any effect on momentum transfer. So, one can make a creeping flow assumption and get rid of all the convective terms on the left hand side and therefore, it would then probably be possible to obtain an analytic solution for such situations. So, a creeping that will be several such approximations which can be made to simplify Navier stokes equation.

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The energy equation for fluid dynamics

The total energy conservation can be expressed as the sum of Mechanical and thermal parts.

Mechanical Energy


$$\frac{\rho}{2} \frac{D\bar{w}}{Dt} = \rho \bar{w} \cdot \bar{g} + \frac{\partial \rho}{\partial t} \frac{Dp}{Dt} - \Phi$$

Thermal Energy

$$\rho \frac{Dh}{Dt} = -\text{div} \bar{q} + \frac{Dp}{Dt} + \Phi$$

The dissipation Φ of mechanical energy is accompanied by entropy production - inner product of the viscous stress tensor and the velocity gradient tensor.

$\Phi = \tau : \text{grad} \bar{w}$



On the other hand when we talked about the energy equation for fluid dynamics then we have to think about the mechanical energy equation and the thermal energy equation. So, combining these two one get the total energy conservation which is nothing but the sum of mechanical and thermal energy equations. And the last term phi on the right hand side is nothing but the dissipation, which is similar to fluid friction similar to friction in solids. So, it can also be termed as the amount of dissipation that would result because of fluid friction and this fluid friction increases entropy. So, in some cases phi in some books textbooks phi is also referred to as the entropy generation.

So, the larger the value of phi it is the larger would be the pressure drop, the larger would be the temperature rise, the larger would be the frictional force opposing the flow in such systems. So, this entropy generation has to be kept to a minimum and in order to build an efficient system.


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Relevant boundary conditions

- no wall slip, i.e. zero normal and parallel velocity at the wall (for gases with $Kn < 0.01$),
- no temperature jump at the wall

For constant density, non-viscous flow in all three directions, the momentum balance can be written as

$$\frac{\partial \bar{\mathbf{w}}}{\partial t} = -(\bar{\mathbf{w}} \text{div}) \bar{\mathbf{w}} - \frac{\text{grad } p}{\rho} + \bar{\mathbf{g}} \quad \text{Euler equation}$$

 Additional forces in microchannel flow may occur with surface effects in multiphase flow, such as bubbles and droplets.

Now, as you can see when we have a micro channel and we have several bends in the micro channel there will be more dissipation and the more and more entropy will be generated. So, the design of a micro channel will also requires a knowledge about how we can reduce this entropy generation, how you can keep this entropy generation to a minimum. And the boundary conditions that one use these are for no slip condition no temperature jump at the wall and so on. And if we are dealing with this is already must be well known to you that if we have a situation in which there is no viscosity it is a non viscous flow.

Then Navier stokes equation can be simplified as the simplified by dropping the terms containing viscosity and it is known as the Euler equation. But in micro channel flow we may have additional forces and this will have to be taken to account.


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Momentum Transport of Single-Phase Flow

Basic equations for long, small channels

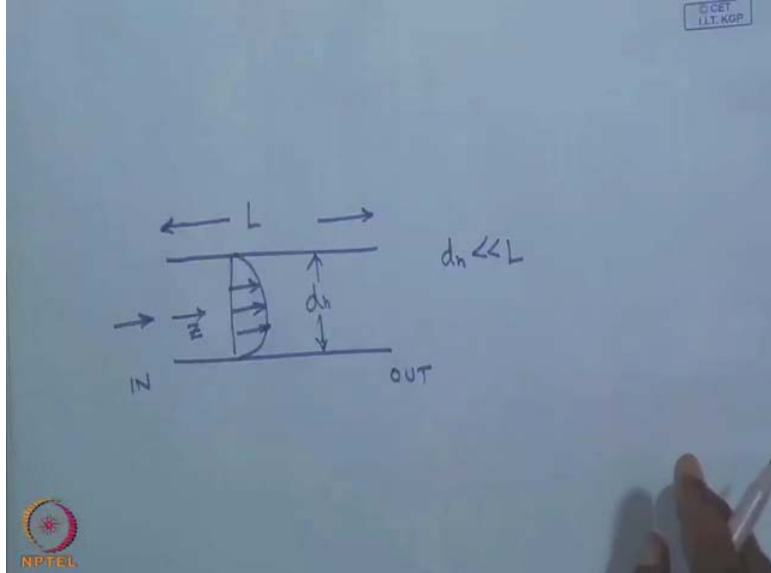
Slender microchannel with rectangular cross section.

Length in flow directions is much larger than cross-sectional dimensions



So, we are going to give I am going to give you a very quick example of modelling for flow in long and small micro channels long and small micro channels. So, we have a slender micro channel with a rectangular cross section and length in flow direction is much larger than the cross sectional dimensions.

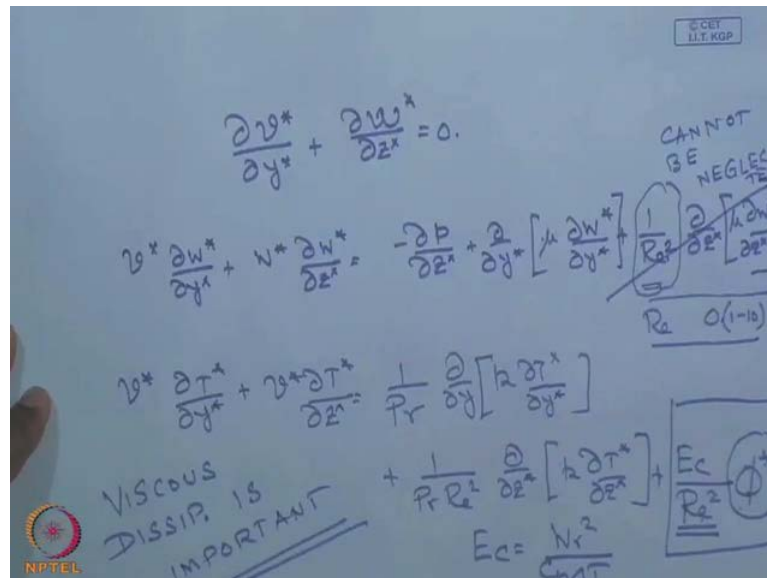
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So, roughly the this system would look like this that I have a micro channel which is this will be the velocity profile and this is flow in and I have flow out from here. And this is the flow direction and this is the diameter hydraulic diameter of the channel and this is

the length of the micro channel. Now, when we say slender micro channel we are going to assume that d is much much smaller than l . So, this is the system that we are going to model in using the equations that we already know.

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So, obviously, the continuity equation would be $\frac{\partial v^*}{\partial y^*} + \frac{\partial w^*}{\partial z^*} = 0$. So, that is the continuity equation in dimensionless form and the Navier-Stokes equation would be (No audio from: 50:49 to 50:59) the pressure gradient plus the viscosity (No audio from: 50:07 to 50:14) this is Reynolds number (No audio from: 50:17 to 50:24) and the z momentum equation. So, one can write the thermal energy equation for this case as well if the temperatures are different the T refers to the T^* refers to the dimensionless temperature. This is the Prandtl number, thermal conductivity, Prandtl number and Reynolds number square this Ec refers to Eckert number and this is the dissipation function.

So, these are the three equations which you are one has to find one has to use and this Eckert number is simply the flow rate square divided by $Cp \Delta T$.


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The y – momentum equation

Thermal energy equation

Reynold's number = $\rho w_r l / \eta_r$; Prandtl number = ν / α

Eckert number = $w_r^2 / c_p \Delta T$



Now, in flow regimes when you have large Reynolds number this term can then be neglected. Now, so in most of the macro flow problems the values of Reynolds number are quite large and therefore, this entire term can be neglected, but in micro flows the Reynolds number is generally of the order of one to ten. So, since in micro flows the Reynolds number are small then this term cannot be neglected. And that creates additional problems for solution of this thing so, the full Navier Stokes equation must be taken into consideration and the effects of the velocities the u both u and v are is not going to be negligible. Similarly, the while dealing with the viscous dissipation the Reynolds since the Reynolds number is small the effect of this term cannot be neglected.

So, one would expect that since the velocity is small since the so, the viscous dissipation which is similar to liquid friction would also be small. So, we should be able to neglect viscous dissipation for most of the cases of flow in micro channels, but that is not going to be the case because of the presence of Reynolds number square in the denominator. So, a small value of Reynolds number would lead to a large value of viscous dissipation even though the velocity is small. So, therefore the important message is that viscous dissipation is important in micro channel flows is extremely important in micro channel flows even though the velocity is going to be very small and.


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The describing PDEs of the velocity w through a certain cross section area is comparable to the displacement of a thin membrane or the stress function in a bar under torsion. That means for the velocity

$$w(x, y) = \frac{\Delta P}{\eta L} \phi$$

with $\Delta p/L$ as pressure loss per length and ϕ as the torsion function.

A solution for the torsion function on a rectangular cross section can be found with a Fourier series:


$$\phi = \sum_{m,n=1}^{\infty} \frac{16(2r_x)^2(2r_y)^2}{mn\pi^4(n^2 4r_x^2 + m^2 4r_y^2)} \sin\left(\frac{m\pi x}{2r_x}\right) \sin\left(\frac{n\pi y}{2r_y}\right),$$

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with $2r_x$ and $2r_y$ as the width and depth of the channel. The sum of the first 4 elements is sufficient for rectangular channels with an aspect ratio of approx. $a = 1$.

Higher order elements are negligible, but must be considered for flat channels.

The basic equations are valid for laminar flow with a typical Re number below the critical Re number at the transition from laminar to turbulent flow.

The critical Re numbers for internal flows are in the range of $Re_c = O(10^3)$.




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circular pipe flow: $Re_c = 2300$ (diameter)

rectangular channel flow: $Re_c \approx 2300$ (hydraulic diameter $d_h = 4A/l_p = 2bh/(b+h)$)

plane channel flow: $Re_c \approx 2000$ (distance of the walls)

plane Couette flow: $Re_c \approx 1800$ (distance of the walls)



This equation these three equations have been solved for a different situation and the solution which is there in some of the text the solution is given over here the last solution as a Fourier series. And when one can look at a this solution which is for stress function of a bar under torsion and this would give the solution, this would give the velocity for laminar flow with typical Reynolds with a small value of Reynolds number. Now, we all know that as Reynolds number increase so, this is just an example of how complex the situation could be in the case of micro scale processes. Since we have to solve the full form of the energy equation and the full form of full form of Navier stokes equation.

Now, there are critical Reynolds number for internal flows which are available in most of the text is that for a circular pipe flow when the Reynolds number is of the order of 2300 we get a change in flow regime. So, for plane Couette flow the Reynolds number could be as small as 1800 when we get this change in phase and in all cases the length scales are defined. For example, for the case of pipe flow the length scale is a diameter for the case of rectangular it could be the hydraulic diameter for plane channel flow, the length scale of relevance is the distance from the wall and so on.

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The governing equations can be simplified for long channel geometries with established mean values for the velocity and for constant fluid properties.

For different locations 1 (at the inlet) and 2 (at the outlet) of the channel, the basic equations can be written as:

continuity equation: $\rho w_2 A_2 = \rho w_1 A_1$

momentum equation or mechanical energy equation, also called the Bernoulli equation

$$\frac{w_2^2}{2} + \frac{p_2}{\rho} + g y_2 = \frac{w_1^2}{2} + \frac{p_1}{\rho} + g y_1 + w_{t12} - \phi_{12}$$



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Thermal energy $e_2 = e_1 + q_{12} + \phi_{12}$

The Bernoulli equation, is complemented by the technical energy and the dissipation. It represents the momentum balance and the mechanical energy balance.

Technical work, positive for added work (pump, actuator, etc.) and negative for produced work (turbine, opened valve, etc.)



So, the governing equations can be simplified for long channel geometries and using continuity equation Bernoulli's equation and so, on. And one would be able to obtain the total energy balance the technical incorporating the technical work that we all know that technical work is going to be positive for the case of if work is done on the system. For example, in pumps and all and if it is negative, if it is produced work if the if it done by the system for example, in turbines and so on.

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q_{12} : specific heat, positive for added heat and negative for cooled fluid between locations 1 and 2

φ_{12} : specific viscous dissipation, linked to the pressure loss Δp .

The pressure loss Δp_{12} in a slender channel is determined from the Bernoulli equation (neglecting technical work).

$$\Delta p_{12} = \rho \varphi_{12} = p_1 - p_2 + \frac{\rho}{2} (w_1^2 - w_2^2) + g (y_1 - y_2)$$



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For a constant cross section and negligible gravitation forces, the viscous dissipation in a channel element correlates with the pressure loss:

$$\varphi_{12} = \frac{p_1 - p_2}{\rho}$$

The pressure loss is approximated by the sum of individual losses consisting of fittings, bends, valves and straight pipes of length l_i

$$\Delta p = \sum_i \left(\lambda_i \frac{l_i}{d_{h,i}} + \zeta_i \right) \cdot \frac{\rho}{2} w_{ref,i}^2$$

Reference: Transport Phenomena in Micro Process Engineering. N. Kockmann, SPRINGER 2008

The reference velocity $w_{ref,i}$ must be determined for each channel element i .




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The channel friction factor λ of the straight pipe is determined by the flow regime and the cross section.

The pressure loss coefficient ζ_i is affected by flow internals, such as curves, bends, fittings, and other channel joints.


Flow friction factors for straight channels with a rough surface according to Moody (Reynold's number based on constricted flow)



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Channel friction factor coefficients in fully developed flow through straight microchannels with different cross-sections.

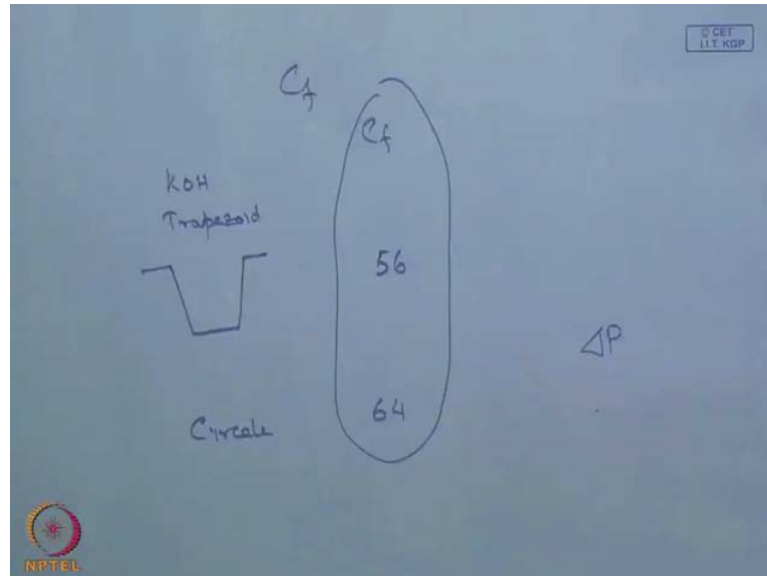
Values of C_f can be obtained for different geometries from standard books such as Transport Phenomena in Micro Process Engineering, N. Kockmann, SPRINGER 2008



So, the viscous dissipation is incorporated in Bernoulli's equation as an additional term as an head loss and for the system of our interest. This equation has been provided in a book by of title transport phenomena in micro process engineering by Kockmann and he has given that the pressure drop for a micro channel with a large number of fittings, bends, valves and straight pipes. It is going to be a factor two factors, one is due to the straight pipe and the other is due to the curved nature of the pipe. And the channel straight friction factor can be easily evaluated using moody diagram whereas; the pressure loss coefficient has to be evaluated experimentally.

And we all know that how to obtain the channel friction factor and the other factors are values of these friction factors are given in that textbook values of C_f for the systems; for example, the value of C_f as given for K O H trapezoid silicon.

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So, if we make a micro channel like this then what would be the value of C_f this value of C_f is given to be about 56 whereas, we know that for a circle the value of C_f is about 64. So, with the knowledge of C_f as given in the textbook one would be able to obtain what is the total pressure drop as per the equation for flow in a micro channel. So, that is all I wanted to cover today and so, this gives us a concise approach, concise description of the complexities associated with flow heat transfer and mass transfer in micro channels and we are going to continue with that in our subsequent classes, thank you.