Microscale Transport Processes
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Lecture No. # 32
Scaling Dimensions and Issues (Contd.)

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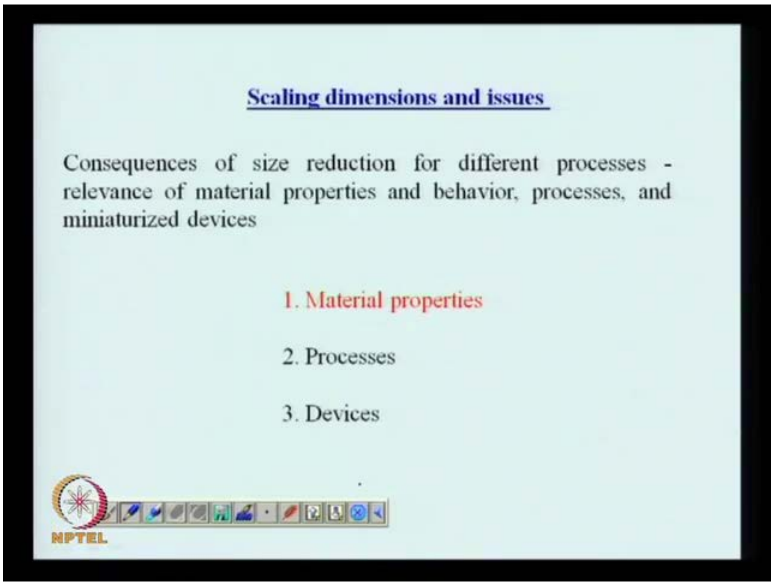

Scaling dimensions and issues

Consequences of size reduction for different processes - relevance of material properties and behavior, processes, and miniaturized devices

1. Material properties
2. Processes
3. Devices

Good morning. We are going to continue with our studies on scaling dimensions and issues, we had an introduction about scaling - the scaling laws and whatever is involved in the initial part of our lecture, we concentrated on material properties. Now, there are three things which needs to be things which need to be looked into one would be the material properties that we have already covered. The second would be the processes how the processes at microscale are going to be different are going to be affected, when we reduce the scales, when you reduce the size of the device from centimetre to millimetre to micron and beyond.

So, we are going to look at different processes and how do they get affected due to the reduction of the device to micrometre lengths. And finally, we will see a few devices and the peculiarities of their operation in terms of different scaling, and how the equations the governing equations, which are valid. For example, navier stokes equation in fluid flow; how the navier stokes equation can be modified the should be modified and which are the terms which would be important I mean the system size is reduced. So, just an example right when we think of navier stokes equation means a body force term. And that body force term will not get affected no matter whatever be the system size, but the viscous and the convective terms will change or the magnitude of them will change as you reduce the system size.

So, one has to look at the contribution of the different terms and their related processes in the overall scheme of things; that means certain process may become important at microscale, which we need not have considered in the macroscale process. So, we will identify certain phenomena, which will be more prominent in microscale systems in today's class.

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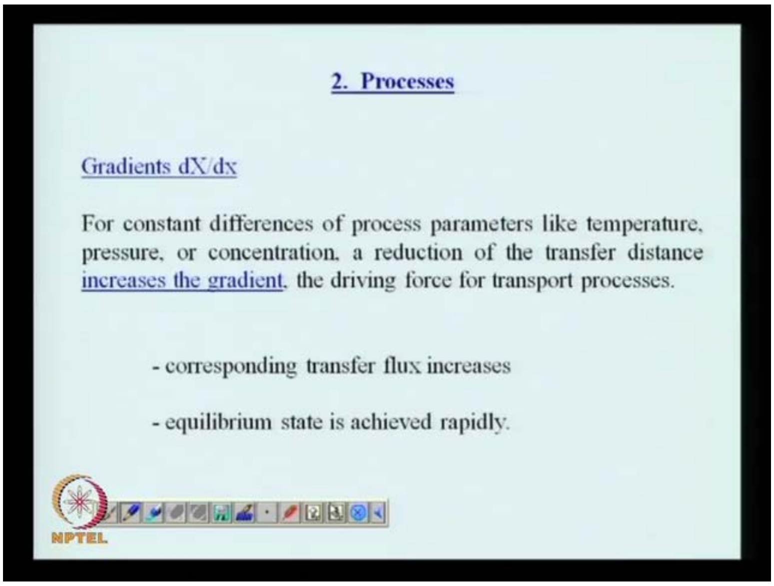

2. Processes

Gradients dX/dx

For constant differences of process parameters like temperature, pressure, or concentration, a reduction of the transfer distance increases the gradient, the driving force for transport processes.

- corresponding transfer flux increases
- equilibrium state is achieved rapidly.

So, first we think about the root cause of any transport be it momentum heat or species. Now, when we have change difference between the temperature pressure or concentration at two different points it is the gradient, which is going to cause molecular transport of heat mass or momentum between these two points, between these two surfaces. So, these gradients are the driving forces for any kind of transport and if you could increase the gradient then the overall the then the transport phenomena of that specific type will get enhanced.

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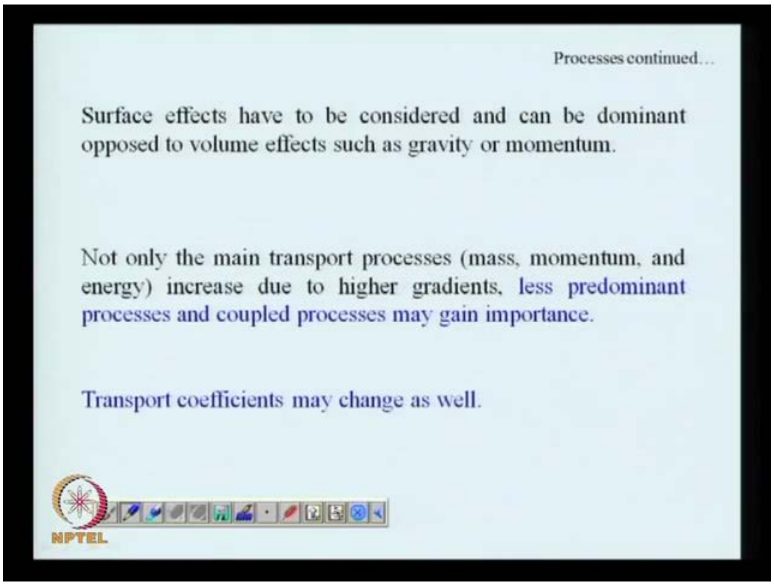

Processes continued…

Surface effects have to be considered and can be dominant opposed to volume effects such as gravity or momentum.

Not only the main transport processes (mass, momentum, and energy) increase due to higher gradients, less predominant processes and coupled processes may gain importance.

Transport coefficients may change as well.

So, the capital x in here they do not the property, which can be measured it could be pressure it could be temperature or it could be the concentration of the species. So, this property this gradient of d x over a certain distance x would tell us the magnitude of this transport process. So, if you can increase the gradient the corresponding transfer flux may increase and as a result of which the equilibrium state will be achieved faster compared to the previous case where the gradient was smaller.

Now, the direct implication of this is that we need to consider the surface effects, which can be dominant in microscale and not only the main transport process is will increase due to higher gradients less predominant processes and coupled processes may gain importance. Additionally, the transport coefficients that we know of the value of diffusivity or thermal conductivity may change when the system size is reduced. So, these are the effects which one needs to be considered. So, in the next slide we are going to see the effect of this coupled processes. The processes, which could be neglected in a macroscale process and how, they become more prominent at microscale process.

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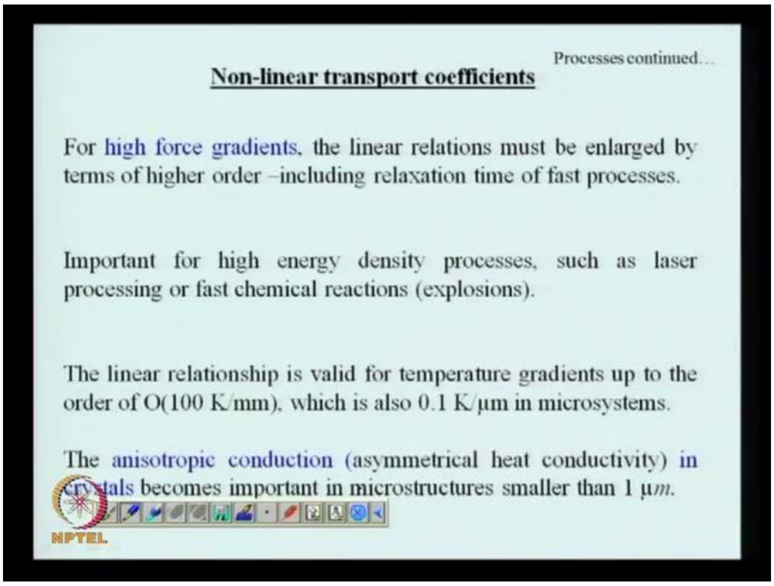

Processes continued…

Non-linear transport coefficients

For high force gradients, the linear relations must be enlarged by terms of higher order –including relaxation time of fast processes.

Important for high energy density processes, such as laser processing or fast chemical reactions (explosions).

The linear relationship is valid for temperature gradients up to the order of O(100 K/mm), which is also 0.1 K/μm in microsystems.

The anisotropic conduction (asymmetrical heat conductivity) in crystals becomes important in microstructures smaller than 1 μm.

And when we talk about the coefficients we know that the coefficients we assume them to be a constant over a certain operational range, if the temperature etcetera. Remain constant but for high force gradients the linear relations, which are applicable for macroscopic systems. For example, Newton’s law or Fourier’s law needs to be expanded in order to in and in higher order terms are to be incorporated, which signifies the relaxation time for first processes. So, any high energy density process such as laser processing or fast chemical reactions for example, which may happen in explosions you need to add additional terms you need to provide additional terms in the flux relation so, as to explain the process.

Now, we know that for a temperature difference of hundred kelvin per millimetre the linear relationship is valid. Now, hundred degree kelvin temperature change over one millimetre is quite large we do not come across such high temperature gradients in macro processes, but when we convert this into microsystems this refers to the about point one kelvin per micron. Now, there are certain processes in which at the microscale this kind of temperature gradients are common place there they will they you will find such temperature gradients taking place in microdevices.

So, whenever, that happens the linear relationship for the transport coefficients in this case the thermal conductivity, which we generally, consider for macrosystems will need to be expanded by including higher order terms. So, the processes not only have changes like the unimportant rather unimportant processes become important, but the relations will also change, when you go from macro to microscale. In the dependence of the of dependence of thermal conductivity for example, on the crystal structure is also with also has also become important for example, if we think about conduction in a crystylise crystalline substance.

Then it may, so happen, that at small scale the thermal conductivity is at different directions different planes of the crystals are different. So, an isotropic conduction thermal on anisotropic heat conduction in crystals need to be incorporated into Fourier’s law. So, as to find out, the total amount of conductive heat transfer in such small systems.

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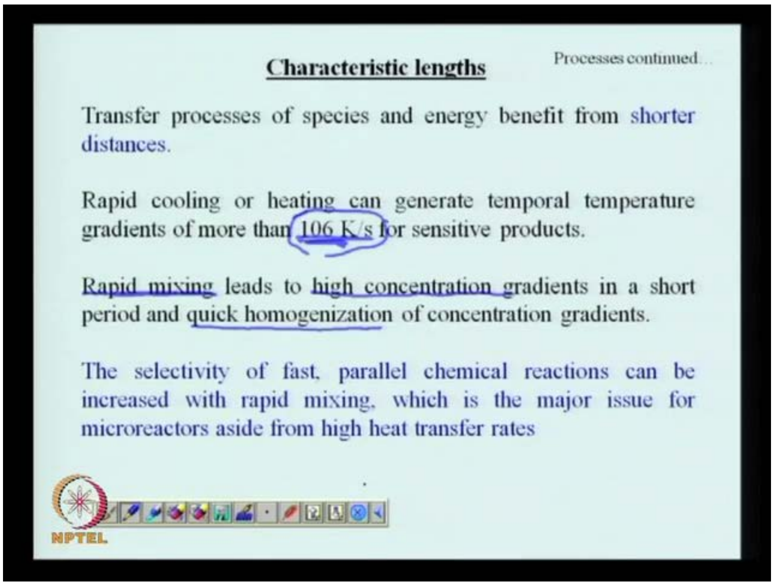

Processes continued...

Characteristic lengths

Transfer processes of species and energy benefit from shorter distances.

Rapid cooling or heating can generate temporal temperature gradients of more than 106 K/s for sensitive products.

Rapid mixing leads to high concentration gradients in a short period and quick homogenization of concentration gradients.

The selectivity of fast, parallel chemical reactions can be increased with rapid mixing, which is the major issue for microreactors aside from high heat transfer rates

So, the thermal conductivities at different crystal planes so, a tensor equation has to be written incorporating the thermal conductivities of the crystal at all possible planes and that has to be used in the thermal heat conduction equation. Now, we also have to think about the characteristic lengths, where the we know that transport processes benefit from shorter distances. And we can have rapid cooling or heating since the process is faster and we get this much it is about this much of temperature gradient for sensitive products. So, we have rapid mixing that is something, which we need to take into account rapid heat transfer giving rise to thermal giving rise to gradients. Where the linear relationship of the transport properties transport relations need to be expanded.

And we get a situation in which the concentration gradient that one can obtain would be very high like compare, because like the temperature gradient. Here is high the concentration gradient could also be very high. And you this would lead to rapid transport such that this is going to give rise to quick homogenisation. So, if you are dissolving a substance in a microdevice, then the high concentration gradients. Since, the concentration changes over a very short distance this would give rise to and quick dissolution of the substance. And the concentration gradient high concentration gradient ensures that the system comes to equilibrium at a faster rate compared to the macrosystem.

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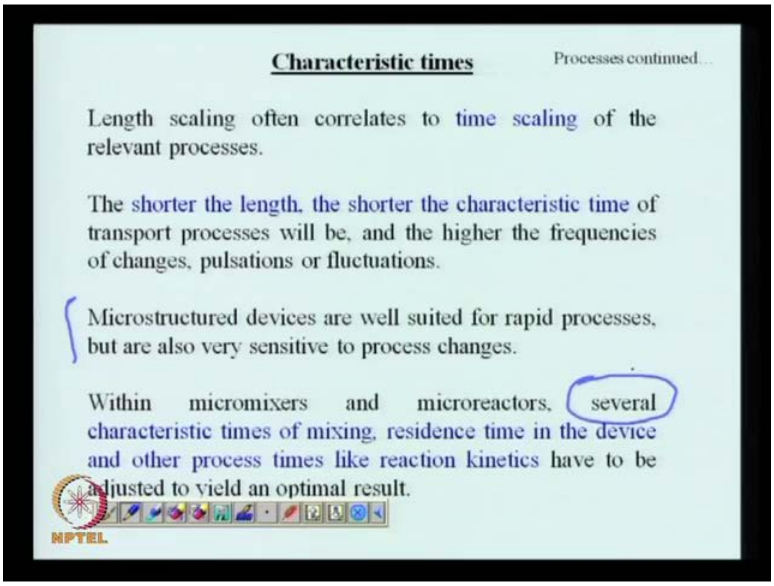

Characteristic times

Processes continued...

Length scaling often correlates to time scaling of the relevant processes.

The shorter the length, the shorter the characteristic time of transport processes will be, and the higher the frequencies of changes, pulsations or fluctuations.

Microstructured devices are well suited for rapid processes, but are also very sensitive to process changes.

Within micromixers and microreactors, several characteristic times of mixing, residence time in the device and other process times like reaction kinetics have to be adjusted to yield an optimal result.

Now, the selectivity of fast parallel chemical reactions as we have seen before it can be increased with rapid mixing and this is one of the major advantages this can be tuned to become one advantage of micro reactors. Now, length scaling often correlates with time scaling of the relevant processes, in generally speaking the shorter the length and the shorter would be the characteristic time. So, if we think about dissolution of a substance or once one component getting diffused into another component or two liquids flowing side by side. And due to diffusion there is going to be some sort of over lapping or some sort of mixing taking place at the boundary of these two immiscible solids.

Then the time scale of mixing for a microdevice due to the shorter length of transport the time scale is going to be faster much a lot faster than the macroscopic systems. So, this is definitely one of the biggest advantages of microdevices, where the transport length is small the transport time is small the overall system reaches equilibrium at a time at a time much before than that takes place in a macro device. So, by tuning these the processes one can suppress undesirable reactions in a specific reaction undesirable side reaction and can promote the reaction that one would like to have.

So, the microstructure devices are well suited for rapid processes, but they are also quite sensitive to any change in the process conditions. So, this has to be kept in mind as well so, but at the same time we may have several characteristic times of mixing of residence time in the device and one has to adjust the other processes to yield an optimum result.

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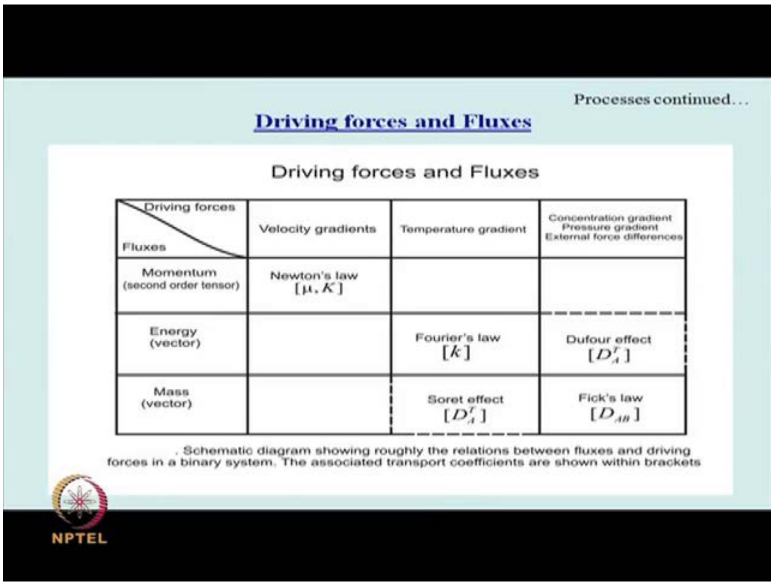

Processes continued…

Driving forces and Fluxes

Driving forces and Fluxes

Driving forces / Fluxes	Velocity gradients	Temperature gradient	Concentration gradient Pressure gradient External force differences
Momentum (second order tensor)	Newton's law $[\mu, K]$		
Energy (vector)		Fourier's law $[k]$	Dufour effect $[D_A^T]$
Mass (vector)		Soret effect $[D_A^T]$	Fick's law $[D_{AB}]$

. Schematic diagram showing roughly the relations between fluxes and driving forces in a binary system. The associated transport coefficients are shown within brackets

Now, this figure is this table is quite interesting to look at. Now, when we were discussing about macro processes we all know that velocity gradients is the root cause of momentum transfer. And the relation, which connects momentum transport with the velocity gradient that is the fluxes and the driving forces, would be Newton's law, when we know that, if there is a temperature gradient existing in the system energy transport is going to take place which is a vector quantity. So, Fourier's law provides the relationship between the driving force temperature gradient and the energy.

On the other hand, when we talk about mass the change the reason for mass transfer is concentration gradient or some sort of a pressure some sort of a gradient, which is created and this is this is governed by Fick's law. So, this these three laws and these three processes we are familiar with that is Newton’s law Fourier’s law and Fick’s law tell us the magnitude of momentum transfer transport energy and mass transport. There are two other effects, which one needs to be taken into account, which are shown here as dufour effect and soret effect.

Now, it has been found it has been seen that the, if we create a temperature gradient in between two points on in a medium then that will give rise to temperature gives rise to mass transport between point one and point two. So, mass transfer not only takes place as a result of concentration gradient it can also take place as a result of temperature gradient and this effect is known as the soret effect. And the diffusion coefficient corresponding to temperature induced mass transport is denoted by the soret coefficient d a t, which is a function of temperature.

Similarly, if we have a concentration gradient in between two places then that may also give rise to energy gradient and this is known as the dufour effect. Normally, the temperature gradients or the concentration gradients necessary to have this kind of heat transfer this kind of mass transfer on heat transfer are very large. So, we do not come across the we do not realize the effectiveness or the or realize the presence of these effects in macrosystems. But in microsystems as the gradients keep on increasing at high value of the gradients these effects start to play an increasingly important role.

So, when we think about mass transfer we not only should look at what is the concentration gradient and thereby use Fick’s law that is used a normal diffusion coefficient denoted by D A B. But we also have to see, what is the temperature gradient in between the two points? Where such mass transfer is taking place so, both the value of D A T and the value of a D A B needs to be taken into account and the relative importance of concentration dependent concentration gradient dependent mass transport and temperature gradient needed temperature gradient control mass transport both will have to be taken into account. And the relative magnitude of each of these will have to be considered and the right expression to be used for microsystems.

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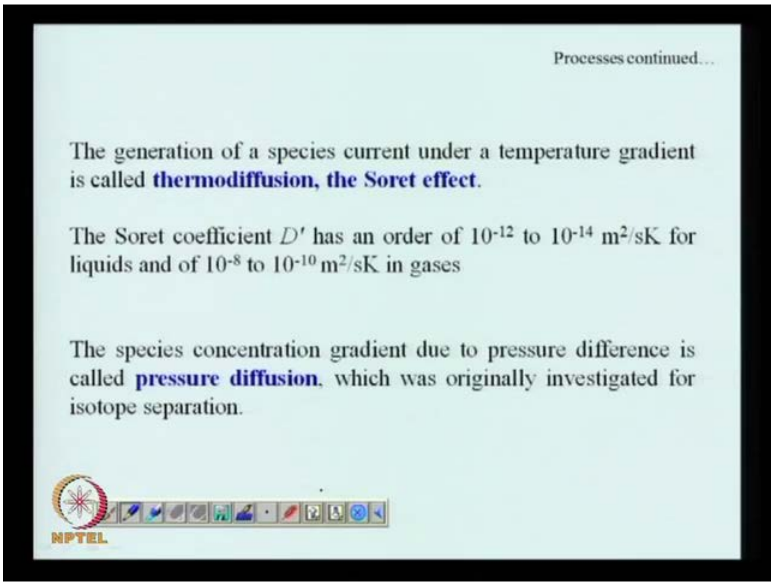

Processes continued…

The generation of a species current under a temperature gradient is called **thermodiffusion, the Soret effect**.

The Soret coefficient D' has an order of 10^{-12} to 10^{-14} m^2/sK for liquids and of 10^{-8} to 10^{-10} m^2/sK in gases

The species concentration gradient due to pressure difference is called **pressure diffusion**, which was originally investigated for isotope separation.

The same applies for energy transport by temperature gradient as well as by other gradients. Now, when you look at the values of these diffusion coefficients for example, D A T and D A B you will you know that you will never come across a situation in microsystems, where the where you have enough temperature gradient present in the system such that these two processes become comparable. So, let us see what are the what are the values are for example, the soret coefficient is of the order of 10 to the power minus 12 to 10 to the power minus 14 for liquids and 10 to the power minus 8 to 10 to the power minus 10 for gases.

So, this shows the values are quite small compared to the corresponding effect of macroscale and you need not use them in macrosystems. But in microsystems due to the enhanced value of the gradients the species transport or the heat transport by such processes become important. So, this again, shows the interdependence of heat and mass transfer in microsystems, because of the presence of temperature induced mass transfer and concentration induced heat transfer. So, the process becomes much more complicated, when you go to microscale and these additional effects, which were not present in macrosystems become progressively important.

So, this is something, which needs to be looked into and one should be careful about using the species equation or the energy transport equation and they may have to add or they may have to include additional terms to account for the enhanced heat or mass transfer in microscale devices.

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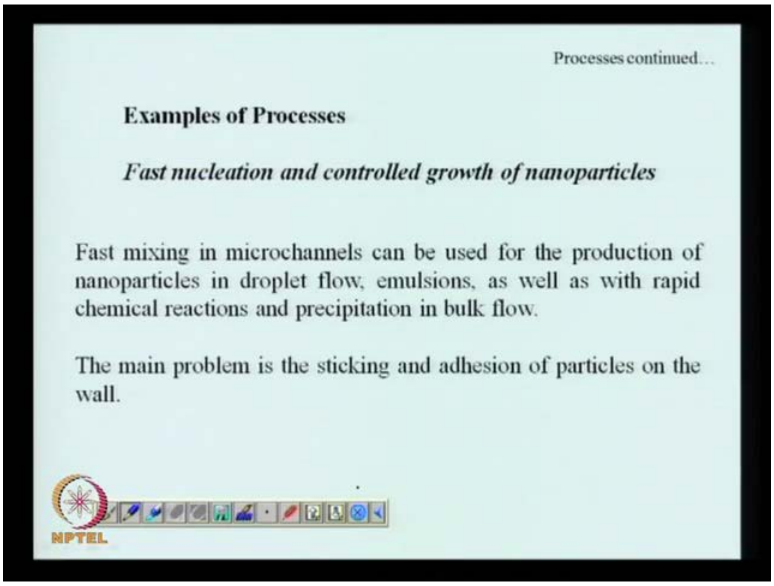

Processes continued…

Examples of Processes

Fast nucleation and controlled growth of nanoparticles

Fast mixing in microchannels can be used for the production of nanoparticles in droplet flow, emulsions, as well as with rapid chemical reactions and precipitation in bulk flow.

The main problem is the sticking and adhesion of particles on the wall.

So, these are definitely advantages the presence of these effects can be an advantage in terms of higher transport, but at the same time one has to be careful about modelling such a process. But incorporating the these effects on one hand and the nature of the coefficients the values of these transport coefficients they will also be different, because of the presence of high temperature or concentration gradients in microsystems. So, next we would see some of the examples of processes where such, enhanced rates are possible.

And the presence of these enhanced rates has lead to interesting applications for example; nucleation fast nucleation of nanoparticles in small devices in fast mixing in microchannels can be used for the production of nanoparticles in flow of droplets as well as rapid chemical reaction and precipitations in bulk flow. But the main problem of production of our general production of nanoparticles or any particles in flow for example, in a microchannel would be that once the particles are formed the tendency of the particles would be to go towards the wall stick to the walls and just create a nucleation point for further accumulation of particles around that. And thereby form a bigger particle or a cluster of particles that will start to effect the flow and they will increase the heat transfer.

So, these, kind of sticking of particles to the side walls would enhance the pressure drop necessary to make the liquid flow in such microchannels and in the way in extreme cases this may even clock the entire nano entire channel. So, precipitation of rather the formation of nanoparticles though would be, can be effected in a much more efficient way in microdevices. But the precipitation of such particles accumulation agglomeration and sticking of such particles are particle assembly to the side walls can be detrimental to the overall operation of such devices. And once clocked or once such particles form or deposit on the on the microchannel for example, it would be very difficult to completely clean such a surface and to reuse it.

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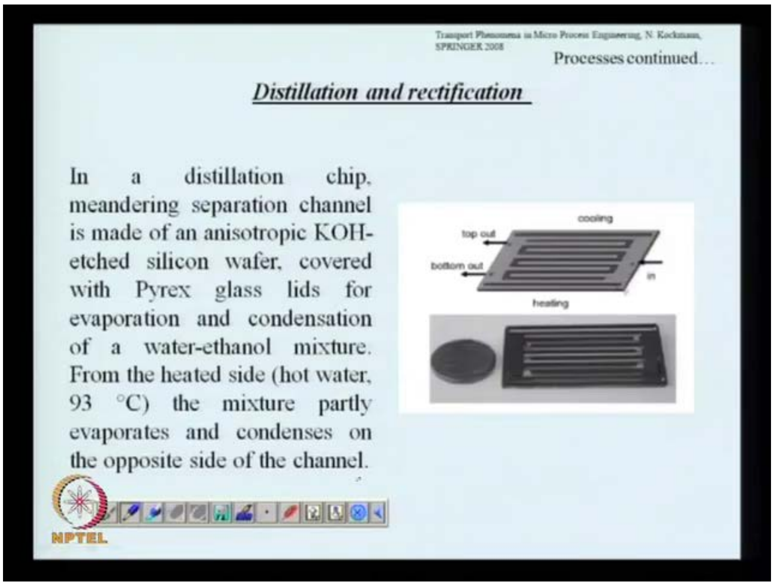

Transport Phenomena in Micro Process Engineering, N. Kockmann, SPRINGER 2008

Processes continued…

Distillation and rectification

In a distillation chip, meandering separation channel is made of an anisotropic KOH-etched silicon wafer, covered with Pyrex glass lids for evaporation and condensation of a water-ethanol mixture. From the heated side (hot water, 93 °C) the mixture partly evaporates and condenses on the opposite side of the channel.

So, this creates additional problem for repeated use of such devices for generation of subsequent generation of nanoparticles. So, these are the drawbacks of the devices that one has to be very careful about. The next example that we see is an interesting example, it is about distillation and rectification taking place on a single chip. So, here, if you look that we have silicon vapour, where using anisotropic K O H treatment, which you are familiar with that the K O H essentially H is silicon depending on the crystal plane it encounters.

So, that is why it is called anisotropic etching; that means, in one specific direction the etching will be a lot faster compared to the other direction. So, as a result of which you can get nice shapes the most common one being a v groove. So, the etching rate in the direction in the perpendicular direction is a lot faster than the etching rate at this sides. Whenever, they come and come and meet the crystal another crystal plane the etching stops as a result of which the etching is self stopping, when the two crystal planes meet and you get nice v shaped channels etched on silicon vapour. So, the anisotropic etching property of K O H hot K O H has been used with on silicon vapor to create a number of channels using certain mask, which has been so, it is a photolithography technique.

So, using such a technique a device has been made where there are channels and in one channel in through the channels there would be a heated water ethanol mixture. And the temperature from the heated side the mixture will evaporate and it is going to condense on the opposite side of the channel. So, the rectification takes place, because of evaporation of ethanol from the ethanol water mixture and then subsequent condensation of the higher concentration methanol at the top of the at the cold side of this channel. So, here you can see the advantages everything takes place in a very small device.

So, the attainment of equilibrium the one that happens, on a declination column using bubble cap tray here you have a very tiny channel and through, which a mixture of ethanol and water is flowing. And you are having evaporation or you are having close to you are having boiling and the ethanol come out the vapour and the liquid are in. So, such a close proximity that equilibrium is going to be reached very quickly very effectively. And then you condense the vapour, which has been formed on the other side of the channel and thereby you can now create a condition in which you will have proper enrichment that is you are going to get the higher concentration of ethanol at one side and higher concentration of water on the other side.

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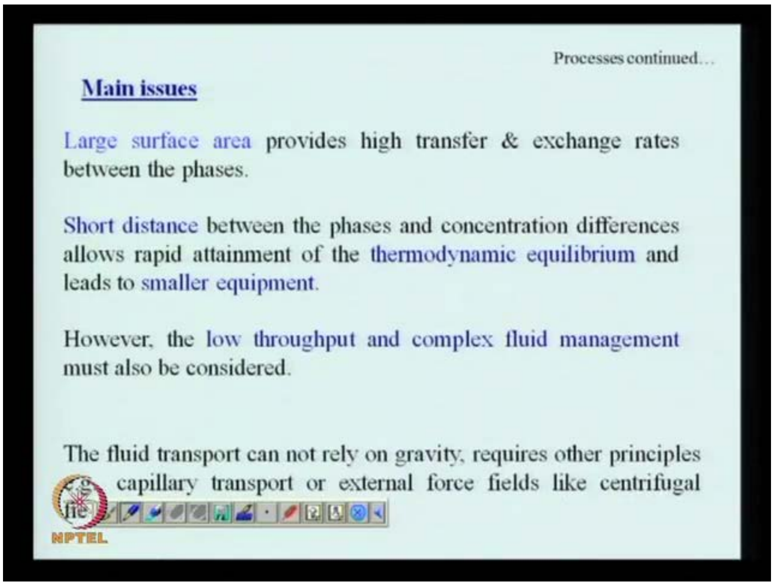

Processes continued…

Main issues

Large surface area provides high transfer & exchange rates between the phases.

Short distance between the phases and concentration differences allows rapid attainment of the thermodynamic equilibrium and leads to smaller equipment.

However, the low throughput and complex fluid management must also be considered.

The fluid transport can not rely on gravity, requires other principles capillary transport or external force fields like centrifugal

So, such distillation and rectification devices are becoming more common in practice, but there are certain problems, which needs to be addressed to as I mentioned the large surface it is providing high values of transfer and the exchange rates are also quite fast. The short distances ensures the thermodynamic equilibrium is reached very quickly, but the main problem is the amount of liquid it can handle, which is the low throughput and how do you manage different liquids and vapour, which are flowing through maze of such channels on a tiny device. And you also have to ensure that also have to think about that you cannot have an gravity like in normal discretion columns.

So, a gravity makes the vapour flow up and the liquid is going to come down and there is going mix mixing between the two. As we know that in microdevices the body force the importance of body force is rather small and therefore, we have to think of other ways for the liquid and the vapour to move. And the same time since, it is going to be a pressure driven flow on such a small systems then how do we ensure that there is no leakage between two adjacent channels. So, that is another technological fabrication challenge that one has to think about in order to in order to have such devices developed a for various applications.

So, low throughput complex fluid management systems prevention of leakage these and the additional forces necessary for the fluid to flow and come in contact with each other are the bottle nicks that are still there that there has been increasing effort to overcome these difficulties to. So, that this becomes more common.

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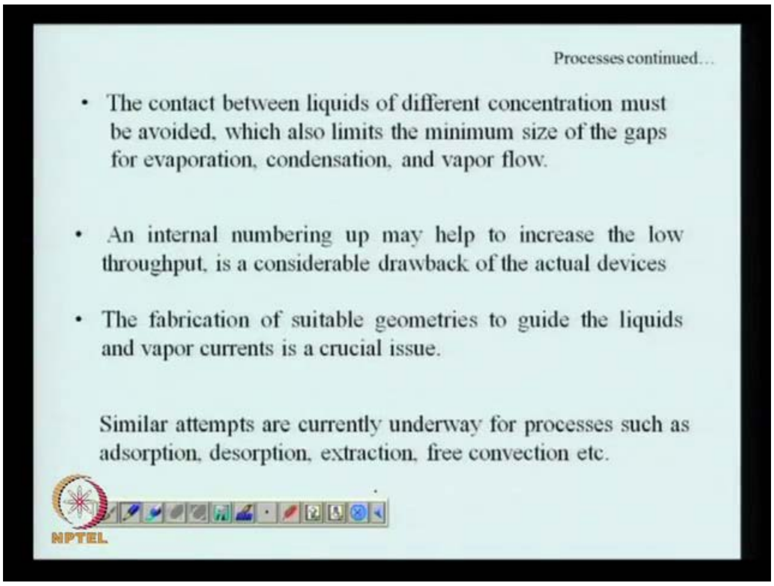

Processes continued…

- The contact between liquids of different concentration must be avoided, which also limits the minimum size of the gaps for evaporation, condensation, and vapor flow.
- An internal numbering up may help to increase the low throughput, is a considerable drawback of the actual devices
- The fabrication of suitable geometries to guide the liquids and vapor currents is a crucial issue.

Similar attempts are currently underway for processes such as adsorption, desorption, extraction, free convection etc.

Now, one way to address such thing is can we do internal numbering up. So, internal numbering up can help to increase the low throughput, but the moment you do internal numbering then the proper distribution equal distribution of liquid into many channels is another fabrication issue is another problem that has to be looked into. So, we also have to have suitable geometries embedded into the construction embedded into the channels itself such that the liquids and vapors are guided properly. So, that the liquids will go in a specific direction and the vapors will go condense at another point and the entire process keeps on moving.

So, there are definitely problems, which are there which needs to be solved before this gets wider application, but similar efforts also underway for adsorption other processes other mass transfer processes such as adsorption, desorption, extraction free convection and so on. And we will see some applications of that for example, if you think of free convection.

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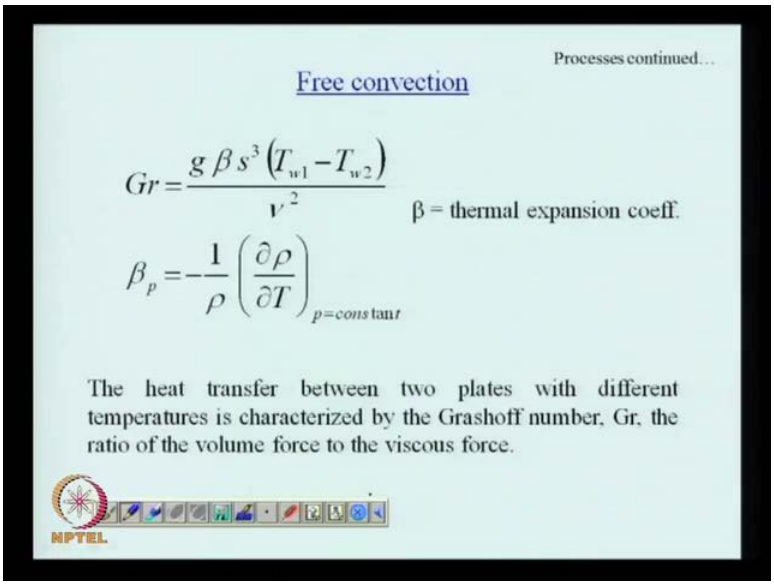

Processes continued…

Free convection

$$Gr = \frac{g\beta s^3 (T_{w1} - T_{w2})}{\nu^2}$$

β = thermal expansion coeff.

$$\beta_p = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{p=constant}$$

The heat transfer between two plates with different temperatures is characterized by the Grashoff number, Gr, the ratio of the volume force to the viscous force.

Now, we all know, what is free convection is that when there is a temperature gradient temperature difference between one packet of fluid and an adjacent packet of fluid. The then the density of the hotter fluid will become less and it is going to rise due to buy and see and to be replaced by cooler fluid from the surrounding. So, if we have a hot surface and fluid let us say air in contact with it. So, air near the surface will automatically rise hot air near the surface it automatically rise to be replace to buy cold air from the surrounding. So, in the subsequent two more two slides we would see whether the effect of free convection is relevant is important in microscale devices.

Now, we all know that in a free convection the two dimensional less numbers, which are important a Grashof number, which the expression for which is shown over there and the Grashof number is nothing but like this balancing force and we have this beta, which is the thermal expansion coefficient. So, it is the expansion different expansion of the gases and the corresponding changes in density at a constant temperature, which is going to cause the fluid to rise and Grashof number is characteristic of the flow, which is nothing but the ratio of the volume force to the viscous force.

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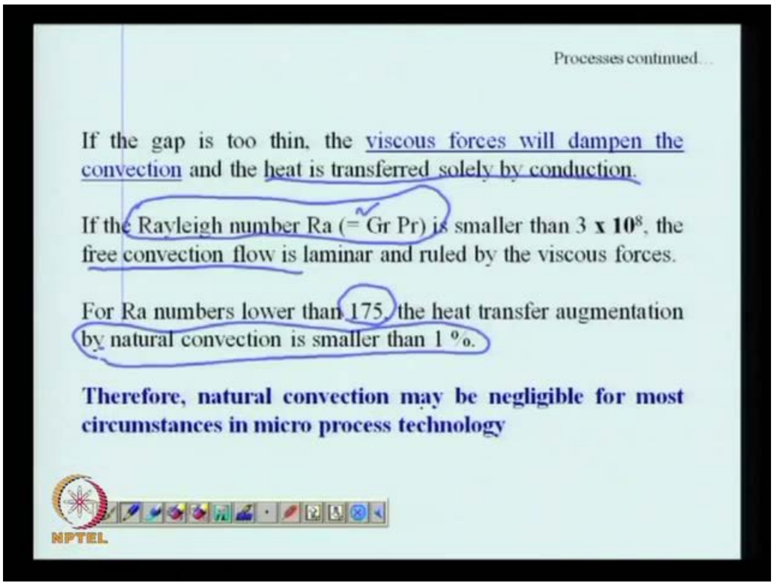

Processes continued…

If the gap is too thin, the viscous forces will dampen the convection and the heat is transferred solely by conduction.

If the Rayleigh number Ra (= Gr Pr) is smaller than 3 **x 10**^{8}, the free convection flow is laminar and ruled by the viscous forces.

For Ra numbers lower than 175, the heat transfer augmentation by natural convection is smaller than 1 %.

Therefore, natural convection may be negligible for most circumstances in micro process technology

So, this tells us the about the dimensionless number Grashof number, which governs such a process. So, now, the gap if the gap is too thin now in if we have so, if your Grashof number, which is the balancing force by viscous force. So, if the gap between two plates is very thin then any balancing driven flow created inside a micro channel will be dampled by viscous forces, if the two layers if the two sides two surfaces are very close to each other. Whereas, if you think of this room then, if the wall is cold then the then the air near the near the wall does not feel the presence of the wall at the other end of the room where as in a micro device the two sides are.

So, close to each other that even, if the air is becoming lighter, it may not rise through the thin gap due to the presence of viscosity due to the forces exerted by the viscosity of such gases. So, viscous forces are going to dampen the convection and the heat then is transferred solely by conduction. So, if you have two plates and at different temperature with air in between and in normal condition the air should rise and there would be some sort of convection process, which is going to extract heat from the hot and deliver it to the cold. But since, the viscous forces predominate and the Grashof number is such that there is no rise of the fluid in between the two plates. So, we have a static layer of fluid in between two hot plates and the only mode by, which energy can get transferred from the hot plate to the cold plate would by conduction only.

So, another number, which tells us whether the free conduction flow is laminar or it is turbulent, is the Rayleigh number, which is the product of Grashof into Prandtl number. Now, since the Grashof number is low Rayleigh number is going to be smaller than 3 into 10 to the power 8. So, you this is obvious that in such a small device due to the presence due to the importance of viscous forces the flow is going to be laminar it is going to be entirely ruled by viscous forces. And in fact, the Rayleigh number is going to be about two hundred or so about and if that is the case, then the heat transfer augmentation by natural convection is going to be smaller than 1 percent of the total heat transfer. So, this tells us that for most of the cases, involving free convection in micro devices the effect of free convection or natural convection can safely be neglected.

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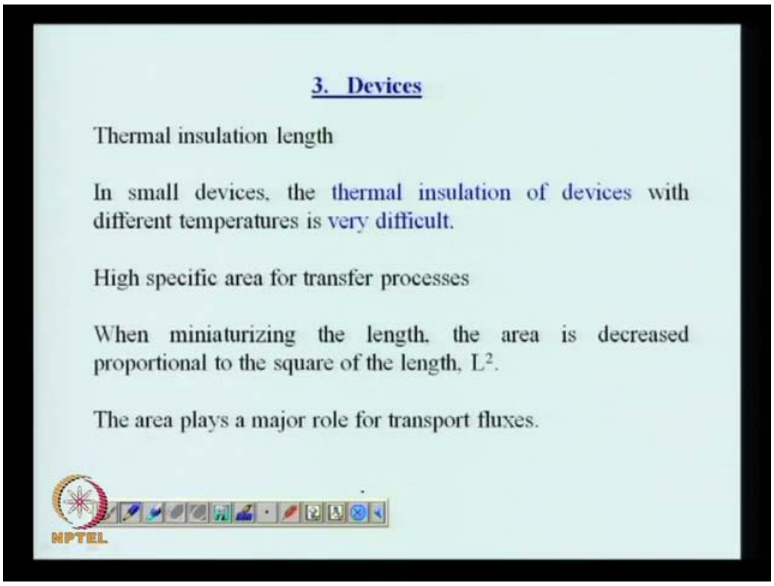

3. Devices

Thermal insulation length

In small devices, the thermal insulation of devices with different temperatures is very difficult.

High specific area for transfer processes

When miniaturizing the length, the area is decreased proportional to the square of the length, L^2.

The area plays a major role for transport fluxes.

So, natural convection is negligible for micro process technology. Now, what are the other factors that one needs to look at while, thinking about or making such devices, one is definitely going to be the thermal insulation length. We know that, we for example, in a micro heat pipe one of the major problem is the presence of the parasitic heat fluxes, which are there in the system, because if we have a channel made and let us say the channel is made of silicon. So, we not only have flow of liquid from the hot side to the from the cold side to the hot side and then the evaporation is going to take place, which is going to extract heat. And then that heat the fluid the vapor is going to come back and condense at the hot end thereby releasing the amount of energy.

So, this kind of free stream mechanism is the cause of the high transport transfer rate of this devices, but you also have, but the channel is going to take channel is going occupy a small fraction of this solid area solid mass the rest of this rest of this are going to be just only silicon. So, there is a possibility that the heat instead of going through going with the liquid through the channel can also pass through the large areas available for silicon. So, I can have conduction through silicon from the hot side to the cold side as a result of which these, parasitic heat transfer can reduce the overall efficiency of heat transfer of micro devices.

So, the thermal how do we insulate a very small section from another section from if we cannot insulate it then the high transport high temperature gradient is going to cause enough transport enough heat transfer in between the two. For example, the destination chip, that we have seen in the previous figures think about these are the three adjacent layers. So, I am going to have hot ethanol air ethanol water mixture coming in and then it flows like this. Now, unless we maintain the temperature gradient properly then we are not going to have any rectification, but since this channels are very close to each other.

Then, if I cannot incubate these two properly then everything is there is going to be temperature homogenization effect as result of enhanced heat transfer, which is detrimental to the overall transport overall efficiency of any such device. So, how do we thermally insulate it is extremely difficult. The advantage is it has high surface area for transport processes the when we miniaturize anything the area is decreased with the proportional to the square of the length. And this l square the proportional dependence on l square this is playing major role for the enhanced transport fluxes in such devices.

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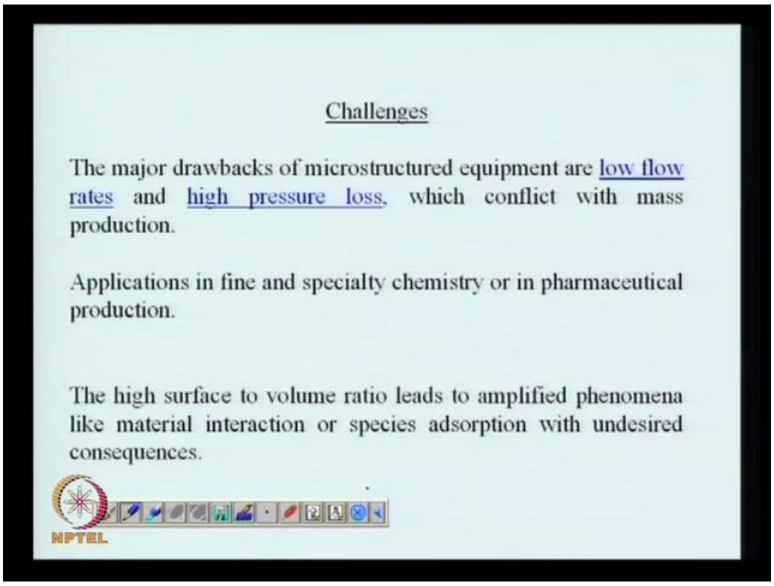

Challenges

The major drawbacks of microstructured equipment are low flow rates and high pressure loss, which conflict with mass production.

Applications in fine and specialty chemistry or in pharmaceutical production.

The high surface to volume ratio leads to amplified phenomena like material interaction or species adsorption with undesired consequences.

So, what are the challenges that we have; obviously, low flow rates low throughputs and high pressure loss. So, this is in conflict with mass production of any material. So, since we cannot make large quantities of something in such devices. So, the material, which is fit for production in such devices, would be fine and specialty chemicals, which are otherwise difficult to make, which are where there are other problems, where it is highly exothermic where there are side reactions undesirable side reactions, which needs to be curdled.

So, these are the and where the final product is very costly and it has to be it can be prepared it needs to be prepared in small quantities only, if such are the product, if such is a product then microchannel or work in microdevices production in microdevices would be beneficial would be relevant.

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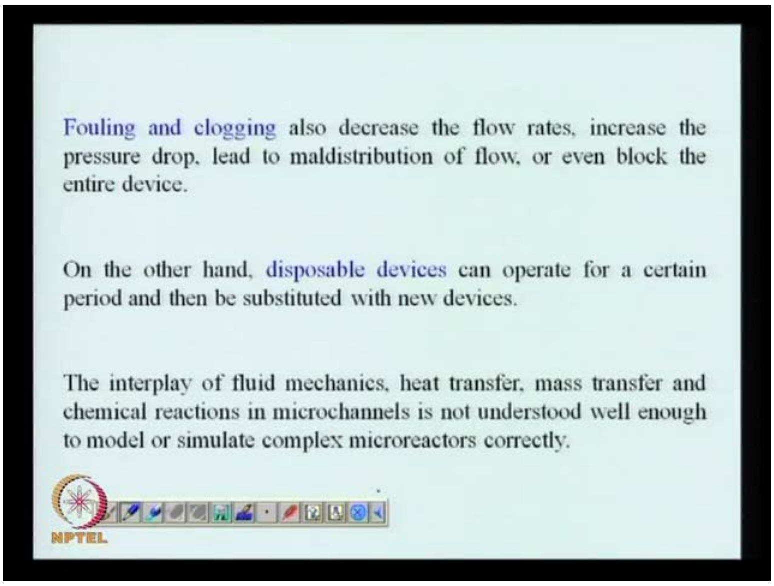

Fouling and clogging also decrease the flow rates, increase the pressure drop, lead to maldistribution of flow, or even block the entire device.

On the other hand, disposable devices can operate for a certain period and then be substituted with new devices.

The interplay of fluid mechanics, heat transfer, mass transfer and chemical reactions in microchannels is not understood well enough to model or simulate complex microreactors correctly.

And the high surface to and another thing that we have read is that the high surface to volume ratio may lead to amplified phenomena like material interaction or species adsorption and this may have undesirable consequences as well. The fouling and clogging also decreases the flow rates it may increase the pressure drop and distribution of the flow can become hampered and the reusability of the devices are also put to question. But the trend in now therefore, to use disposable devices that can operate in a certain number of times and then they can be substituted with new devices. So, this is another approach though as with increasing ease of production of these microdevices. Since, the fabrication techniques are becoming more simpler so mass production of this devices are becoming easier.

Once we can produce such devices in large quantities then; obviously, the shift would be to from reuse to disposing those devices after few uses. So, that is the current trend, which where the we are making disposable microfluidic devices for specific applications. And finally, the interplay of fluid mechanics heat transfer mass transfer and chemical reactions in microchannels is still not understood in to such an extent such that we can design device and fabricate a device for a specific application. So, it is an open area of research which needs lot of attention from all sides to understand the understand and to utilize the plus points of such things.

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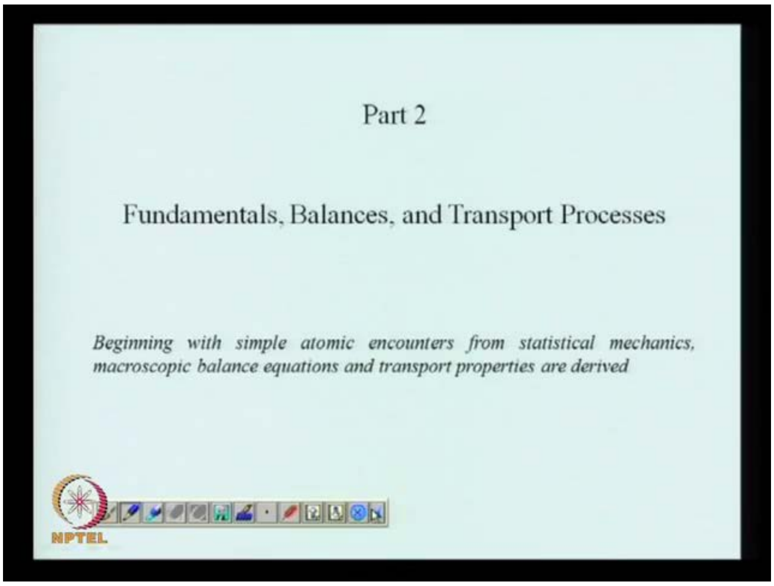

Part 2

Fundamentals, Balances, and Transport Processes

Beginning with simple atomic encounters from statistical mechanics, macroscopic balance equations and transport properties are derived

Now, we come to the part two of this course, where we are going to concentrate more on the fundamentals the balances and the transport processes. The goal is that starting with simple atomistic atomic encounters from statistical mechanics some macroscopic macroscopic balance equations and transport properties how we can write fundamental equations that describes the transport processes in microdevices.

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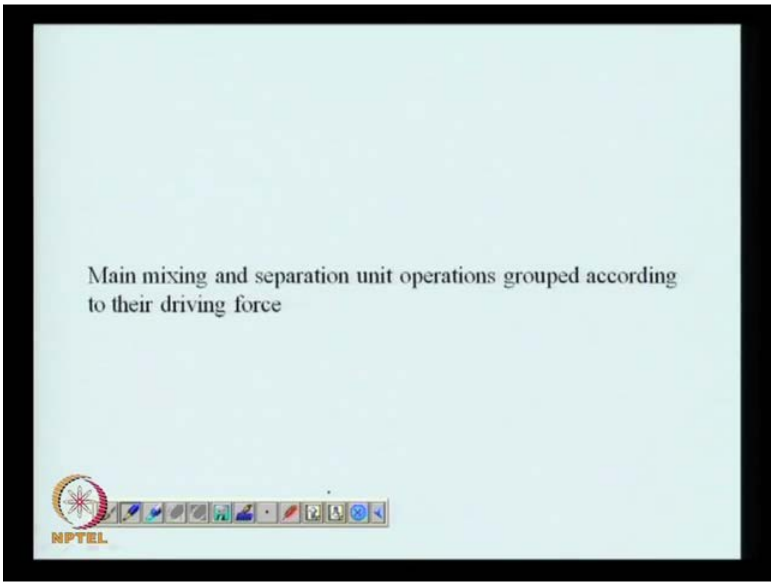

Main mixing and separation unit operations grouped according to their driving force

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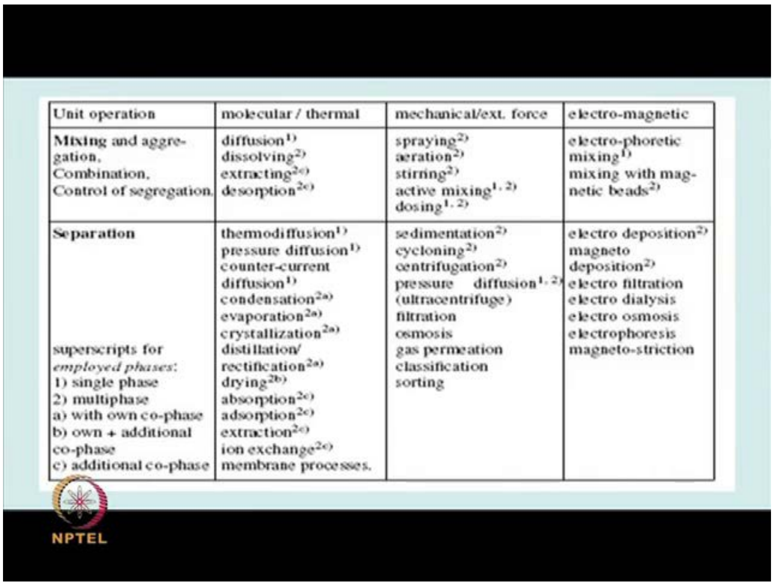

Unit operation	molecular / thermal	mechanical/ext. force	electro-magnetic
Mixing and aggregation, Combination, Control of segregation.	diffusion$^{1)}$ dissolving$^{2)}$ extracting$^{2c)}$ desorption$^{2c)}$	spraying$^{2)}$ aeration$^{2)}$ stirring$^{2)}$ active mixing$^{1,2)}$ dosing$^{1,2)}$	electro-phoretic mixing$^{1)}$ mixing with magnetic beads$^{2)}$
Separation superscripts for *employed phases*: 1) single phase 2) multiphase a) with own co-phase b) own + additional co-phase c) additional co-phase	thermodiffusion$^{1)}$ pressure diffusion$^{1)}$ counter-current diffusion$^{1)}$ condensation$^{2a)}$ evaporation$^{2a)}$ crystallization$^{2a)}$ distillation/ rectification$^{2a)}$ drying$^{2b)}$ absorption$^{2c)}$ adsorption$^{2c)}$ extraction$^{2c)}$ ion exchange$^{2c)}$ membrane processes.	sedimentation$^{2)}$ cycloning$^{2)}$ centrifugation$^{2)}$ pressure diffusion$^{1,2)}$ (ultracentrifuge) filtration osmosis gas permeation classification sorting	electro deposition$^{2)}$ magneto deposition$^{2)}$ electro filtration electro dialysis electro osmosis electrophoresis magneto-striction

So, we are mainly going to look at the mixing and separation unit operations. And the next, figure next table groups these operations according to their driving forces I will skip this portion just let us just you take one example. Now, if you think about mixing and aggregation and if you think on the molecular level, then diffusion is a root cause and there could be some thermal component to it as well, when it think about mechanical then the mixing can be achieved by spraying or there can be electrophoretic mixing as well.

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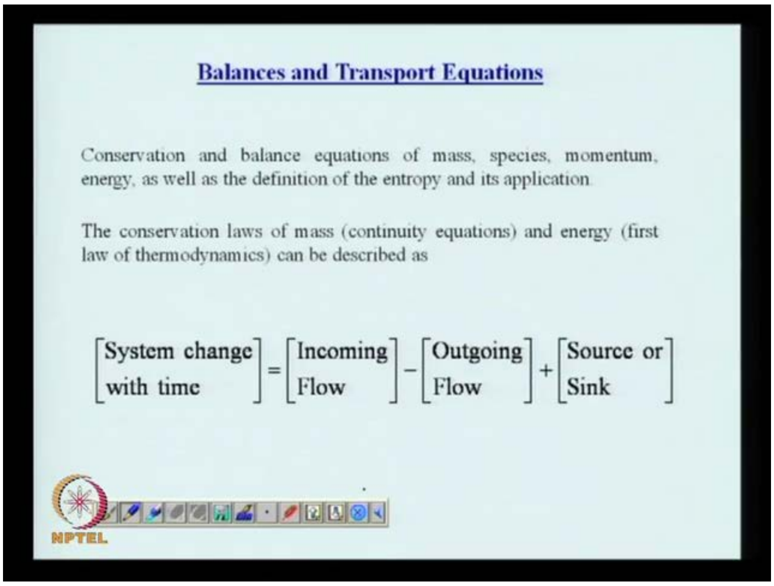

Balances and Transport Equations

Conservation and balance equations of mass, species, momentum, energy, as well as the definition of the entropy and its application.

The conservation laws of mass (continuity equations) and energy (first law of thermodynamics) can be described as

$$\begin{bmatrix}\text{System change}\\ \text{with time}\end{bmatrix} = \begin{bmatrix}\text{Incoming}\\ \text{Flow}\end{bmatrix} - \begin{bmatrix}\text{Outgoing}\\ \text{Flow}\end{bmatrix} + \begin{bmatrix}\text{Source or}\\ \text{Sink}\end{bmatrix}$$

So, this table essentially lists the processes the unit operations the molecular and thermal reasons the mechanical forces that are necessary and other electromagnetic forces. So, you can go through these to learn more about the importance of different forces in such operations. But we are going to concentrate on the balance and the transport equation. Now, we are very much familiar with this type of equations, where systems change in the change in any property of this system it could be the mass of the system. And the change in the mass of the system with time is a result of net flow that is incoming flow outgoing flow plus, if there is any generation inside the system itself.

So, if we have a chemical reaction taking place inside such a system and a species a is being consumed. Then the conservation equation simply tells us that the rate of change of species a inside the control volume would be equal to the net rate of heat addition sorry net rate of addition of species a through the boundaries. Now, through the boundaries the species maybe can be added as a result of conviction or as a result of diffusion as a result of convictive processes. That means, with the flow some species a may come into the system or there maybe conductive fluxes exits across the boundaries as a result of concentration gradient. So, net addition of a to the control volume by conviction and conduction plus generation or depletion of species a by reaction taking place inside the control volume. So, that is the general form of any conservation equation.

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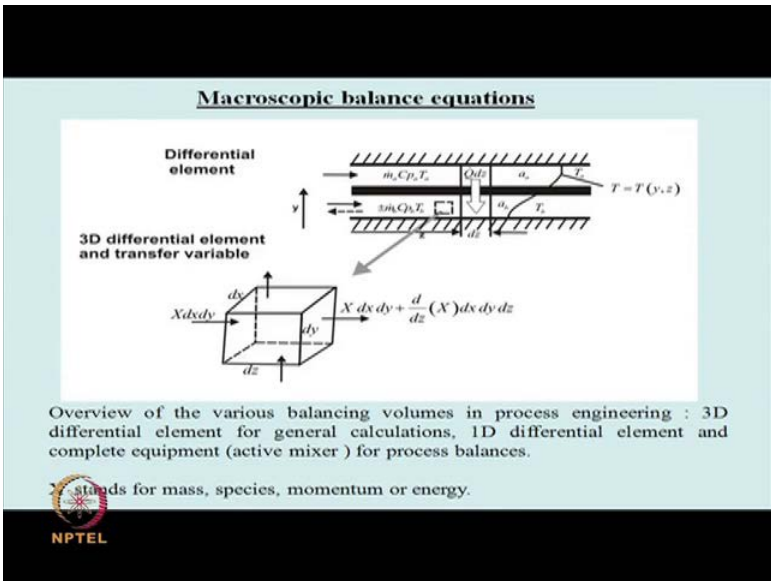

Macroscopic balance equations

Differential element

3D differential element and transfer variable

Overview of the various balancing volumes in process engineering : 3D differential element for general calculations, 1D differential element and complete equipment (active mixer) for process balances.

X stands for mass, species, momentum or energy.

So, we would also like to start with that conservation equation, where the system change with time is a result of all this now there are several ways by, which you can generate a macroscopic balance equation. You can take a control volume and find out the ways by, which something is being added to the control volume it could be convection, it could be conduction and the way it goes out of it and there could be some amount of generation of energy generation of a species in such a system. Or in the other words you can look at a differential channel element and make heat balances such that you have let us say one hot fluid, which is flowing this is the solid boundary. And you have another fluid, which is a cold fluid, which is moving in the other direction and then you have heat transfer across this from the hot to the cold.

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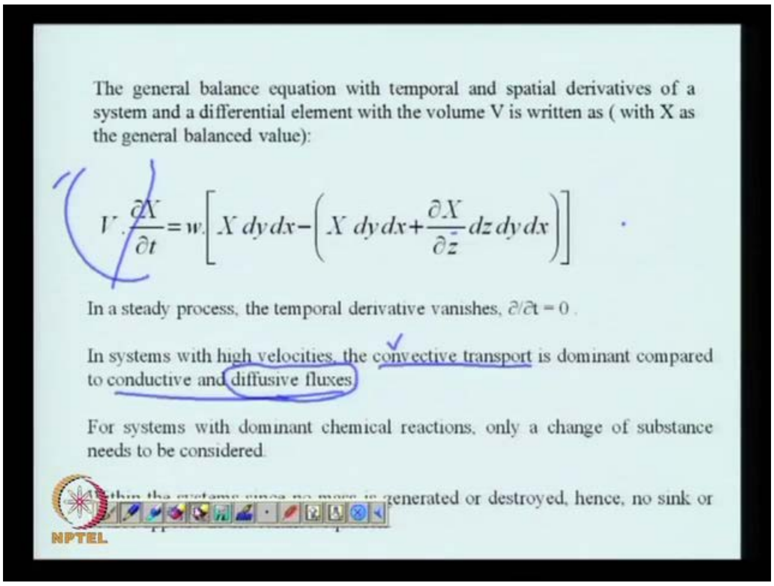

The general balance equation with temporal and spatial derivatives of a system and a differential element with the volume V is written as (with X as the general balanced value):

$$V.\frac{\partial X}{\partial t} = w.\left[X\,dy\,dx - \left(X\,dy\,dx + \frac{\partial X}{\partial z}dz\,dy\,dx\right)\right]$$

In a steady process, the temporal derivative vanishes, $\partial/\partial t = 0$.

In systems with high velocities, the convective transport is dominant compared to conductive and diffusive fluxes

For systems with dominant chemical reactions, only a change of substance needs to be considered

[illegible] generated or destroyed, hence, no sink or

So, you can take a control volume you can take a control volume defined by certain distance and therefore, find out what is the total heat that is being added to such a system. So, this if we can think that it is just a one d process then it is an one d differential we can take as a one d differential element and make such balances. So, whatever, we have described. So, far the general equation is the temporal variation temporal special derivative of a system within and a differential element can be written in this following form, which is just the property and the variation temporal. I mean and the special variation of that property is going to be equal to the temporal variation of the quantity itself. So, if it is a steady state process then this is going to be equal to zero and this is simply in minus out plus or minus generation is going to be equal to zero.

So, that is the standard form, which we are mostly concerned with. So, in systems with high velocities the convictive transport is going to be dominant and if it is a system with low velocity, but high gradient then conductive and diffusive fluxes are going to govern. So, one has to think, which one is going to be important in most in many bulk flow cases in many macro cases. For flow systems the conductive transport will predominate whereas, in microsystems the most the likely chance is that the diffusive fluxes are going to predominate and the effect of convictive transport is rather small. But one has to look at these processes each of this process separately to see what is going to be the predominant case in this.

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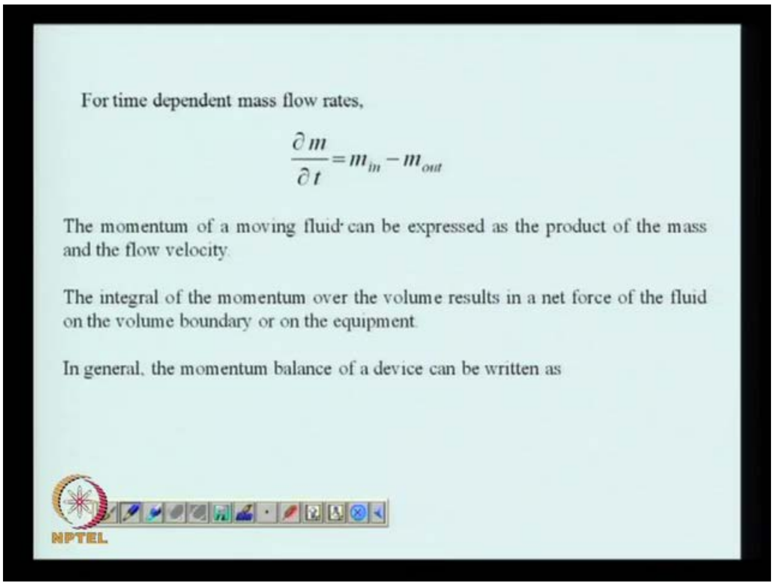

For time dependent mass flow rates,

$$\frac{\partial m}{\partial t} = m_{in} - m_{out}$$

The momentum of a moving fluid can be expressed as the product of the mass and the flow velocity

The integral of the momentum over the volume results in a net force of the fluid on the volume boundary or on the equipment

In general, the momentum balance of a device can be written as

So, if we have time dependent mass flow rates then it is in minus out and the momentum of the fluid can also be expressed as a result of the product of the mass and flow velocity and we know that this has resulted. If we think about the conservation of linear conservation of momentum then that would give rise to equation of motion and a special form of the equation of motion is navier stokes equation. So, you would see what are the terms that would be important in navier stokes equation and flow for flow in very long channels how it can be modified.

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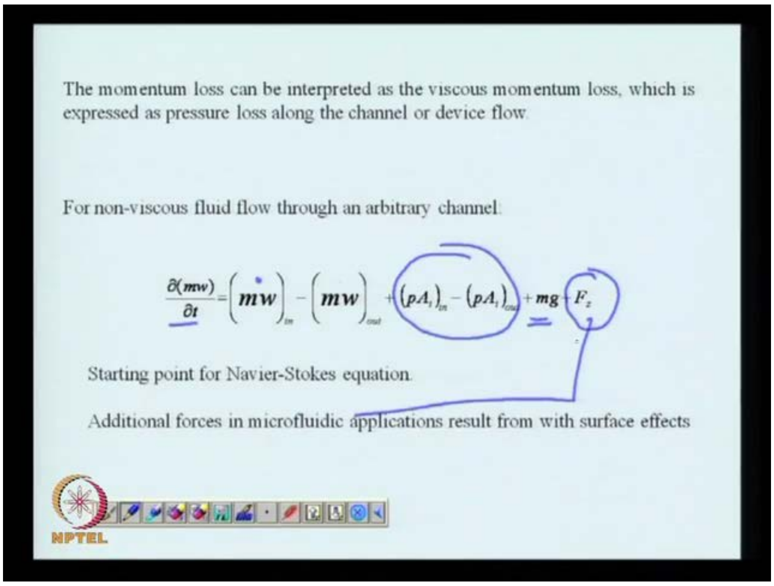

The momentum loss can be interpreted as the viscous momentum loss, which is expressed as pressure loss along the channel or device flow.

For non-viscous fluid flow through an arbitrary channel:

$$\frac{\partial(mw)}{\partial t} = \left(\dot{m}w\right)_{in} - \left(mw\right)_{out} + \left(pA_1\right)_{in} - \left(pA_1\right)_{out} + mg + F_z$$

Starting point for Navier-Stokes equation.

Additional forces in microfluidic applications result from with surface effects

So, these are I will skip part of it now if we think of non-viscous flow in an arbitrary channel then the momentum change rate time rate of change of momentum. Is a momentum that is coming in, the momentum that goes out with the flow the pressure the surface forces, which are acting in the form of pressure the body force and any additional force any other force, which is there in this. So, this is essentially the starting point of navier stokes equation and this results to additional forces in microfluidic of applications, which could be due to different surface forces.

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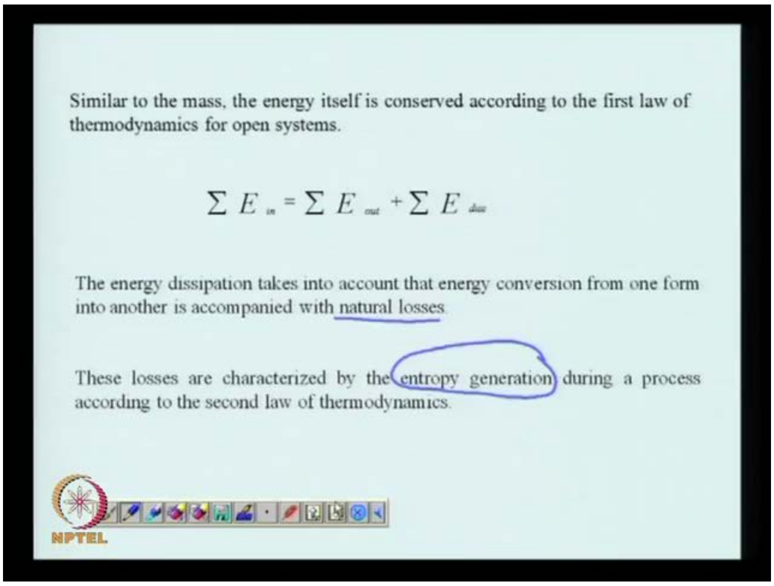

Similar to the mass, the energy itself is conserved according to the first law of thermodynamics for open systems.

$$\sum E_{in} = \sum E_{out} + \sum E_{diss}$$

The energy dissipation takes into account that energy conversion from one form into another is accompanied with natural losses.

These losses are characterized by the entropy generation during a process according to the second law of thermodynamics.

So, similar mass one can the energy is also conserved and the energy dissipation will take into account the energy conservation from one to another and which is accompanied by natural loses. So, whenever, energy gets converted to another form of energy there would be some loses, which cannot be recouped. And in fact, the conversion of energy from one form to another during such a process the magnitude of that energy which dissipates is essentially tells us how efficient the process is. So, that is something one has to look at. So, these loses are characterized by entropy generation and the more the entropy generation the less efficient would the process be and one so one has to device a design the devices in such a way such that the entropy generation would be kept to a minimum.

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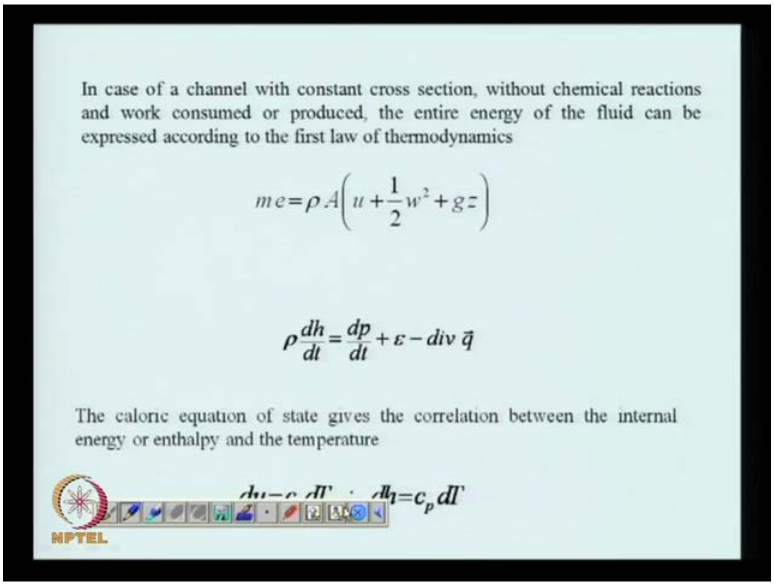

In case of a channel with constant cross section, without chemical reactions and work consumed or produced, the entire energy of the fluid can be expressed according to the first law of thermodynamics

$$me=\rho A\left(u+\frac{1}{2}w^2+gz\right)$$

$$\rho\frac{dh}{dt}=\frac{dp}{dt}+\varepsilon-div\,\vec{q}$$

The caloric equation of state gives the correlation between the internal energy or enthalpy and the temperature

$$du=c_v dT \quad ; \quad dh=c_p dT$$

Now, this in the case of a channel with a constant cross section the energy from the first law of thermodynamics energy is going to be some of the internal energy the kinetic energy and the gravitational energy. So, this form of equation is quite well known to us where this epsilon stands for the dissipation.

So, this is the dissipation function and this is essentially the temperature gradient induced conductive flow of heat into the control volume.

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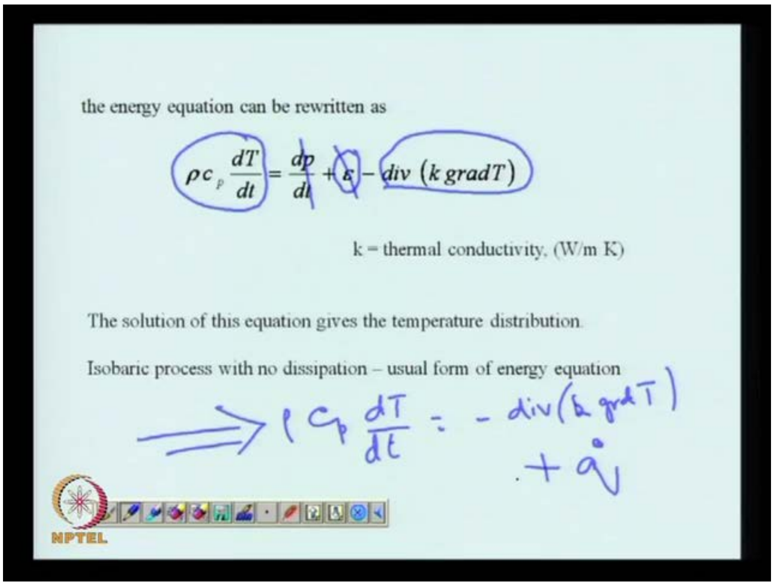

the energy equation can be rewritten as

$$\boxed{\rho c_p \frac{dT}{dt}} = \cancel{\frac{dp}{dt}} + \cancel{\varepsilon} - \boxed{div\,(k\, grad T)}$$

k = thermal conductivity, (W/m K)

The solution of this equation gives the temperature distribution

Isobaric process with no dissipation – usual form of energy equation

$$\Longrightarrow \rho c_p \frac{dT}{dt} = - div(k\, grad T) + \dot{q}$$

So, if we use the caloric equations of state this would look like this energy equation can written in the form that we are aware of so, if it is an so, we have the left hand side, which is the convictive flow of energy. The last term on the right hand side is the conductive transport of energy. And it is an isobaric process the epsilon in this is the dissipation function where any transport of energy any flow is associated with entropy generation.

So, this dissipation function is denoted by epsilon. So, here k is a thermal conductivity and the solution of this equation is gives us the temperature distribution in any substrate. So, if it is an isobaric process with no dissipation then these two terms will not be there and what we will simply have would be rho c p d t over time is going to equal to divergence of k grad t. So, this is the form of the energy equation with which we are mostly familiar, if it is a system with generation of heat. Then this q dot would denote the amount of heat, which is generated per unit volume of the system.

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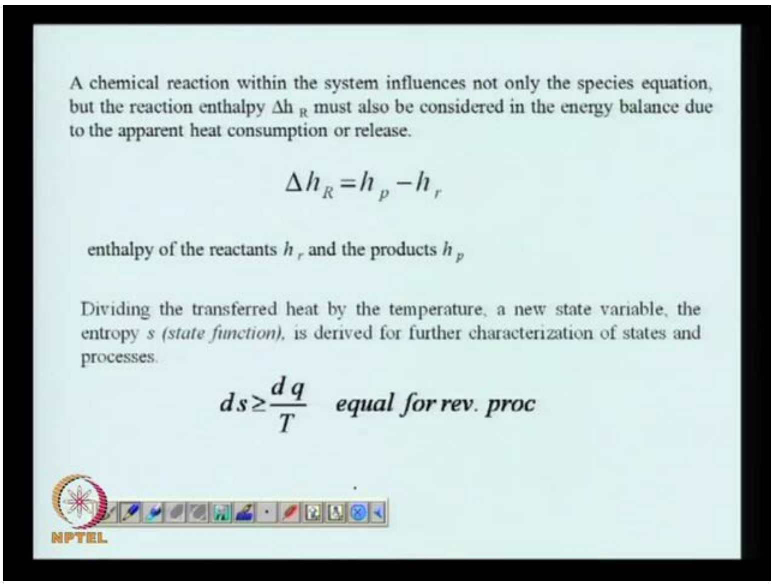

A chemical reaction within the system influences not only the species equation, but the reaction enthalpy Δh_R must also be considered in the energy balance due to the apparent heat consumption or release.

$$\Delta h_R = h_p - h_r$$

enthalpy of the reactants h_r and the products h_p

Dividing the transferred heat by the temperature, a new state variable, the entropy s *(state function)*, is derived for further characterization of states and processes.

$$ds \geq \frac{dq}{T} \quad \textit{equal for rev. proc}$$

So, this is the normal form of energy equation. Now, if we the total amount of heat that is transferred is in a reaction system is given by this. So, if we divide the total amount heat transferred divided by the temperature we get the definition of entropy.

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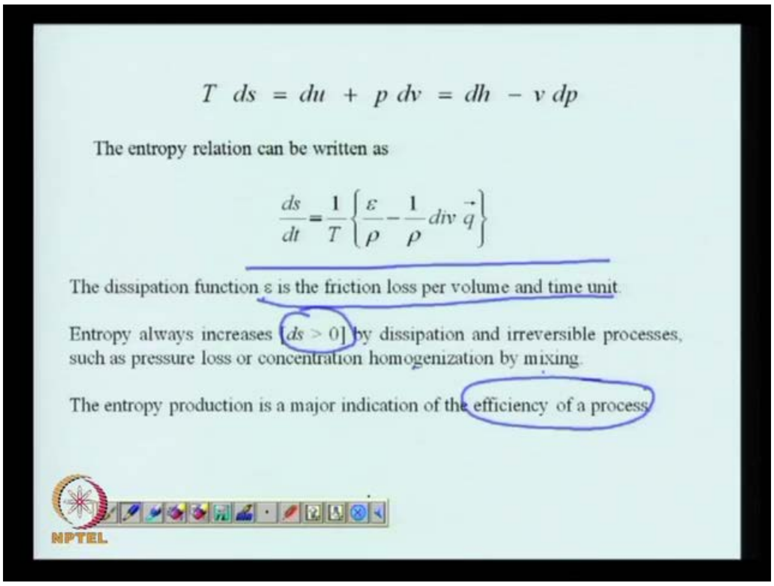

$$T\ ds = du + p\ dv = dh - v\ dp$$

The entropy relation can be written as

$$\frac{ds}{dt} = \frac{1}{T}\left\{\frac{\varepsilon}{\rho} - \frac{1}{\rho} div\ \vec{q}\right\}$$

The dissipation function ε is the friction loss per volume and time unit.

Entropy always increases $(ds > 0)$ by dissipation and irreversible processes, such as pressure loss or concentration homogenization by mixing.

The entropy production is a major indication of the efficiency of a process.

So, in any such process, if we skip this part the dissipation function epsilon is a friction loss per unit volume and time unit. So, this epsilon is an in shorter form this epsilon is connected with entropy generation in the process. So, entropy always increases by dissipation and in any irreversible process such as pressure loss or concentration homogenization by mixing.

So, if the value of this dissipation is large, if the value of the energy generation is large that simply denotes that the system is more system is not very efficient. So, the entropy production is a major indication of the efficiency of the of a process. So, the design should be such that the entropy generation is going to can be to a minimum and for an example, if you have a sudden expansion in the flow area and the liquid was flowing through a small conduit and suddenly it expands to a large area. So, in case of such case in such cases for example, in throttling we need to minimize throttling.

So, in order to preserve in order to minimize entropy generation in a system similarly, if there is a sharp bend in the system then the dissipation the head loss would be much more and the entropy generation would be more and the process becomes less efficient. So, any design has to be thought about has to be analyzed to see how much of head loss how much of energy generation that is taking place.

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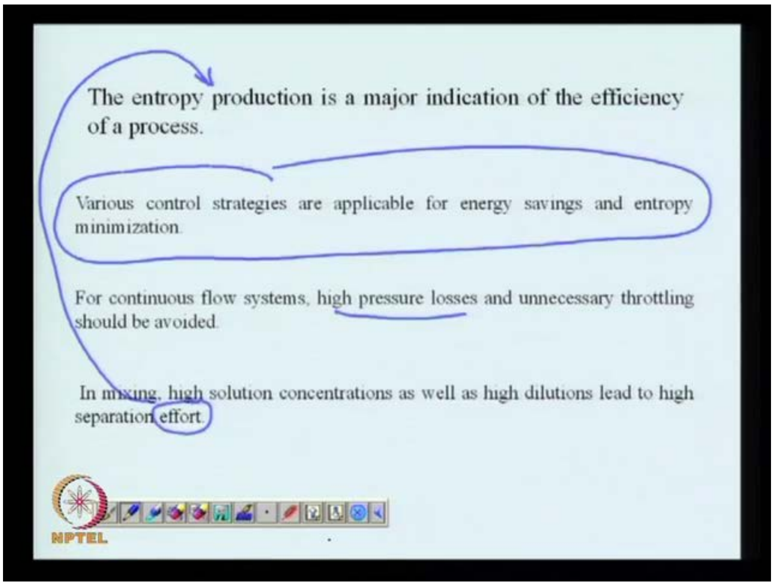
The entropy production is a major indication of the efficiency of a process.

Various control strategies are applicable for energy savings and entropy minimization.

For continuous flow systems, high pressure losses and unnecessary throttling should be avoided.

In mixing, high solution concentrations as well as high dilutions lead to high separation effort.

So, sudden expansion contraction sudden change in the flow path are certain examples, which need to be avoided in order to maximize the efficiency of the process. And various control strategies are applicable for energy saving and entropy minimization and these are some of the examples, that I have already mentioned the additional ones that for if you have a continuous flow system the pressure losses should kept to a minimum. And we need to minimize unnecessary throttling as I have already explained and if you are thinking about mass transfer operations, then high solution concentrations and high dilutions.

These are to be kept to a to a minimum as if you want to concentrate a solution to a very high value or if you would like to dilute something, if you want to get a highly diluted solution these are going to involve larger efforts and any effort is going to give rise to entropy production thereby reducing the efficiency of the process. So, in microsystems these are going to be even more important, because as we know that in microsystem the viscous forces will predominate. And this energy dissipation the dissipation energy dissipation is a function is a strong function of the viscous processes taking place at the interface.

So, for highly systems in which the viscous forces predominate the chances of viscous dissipation would be much more even though the flow velocity is very small. So, for high for low for so we are getting going to get more dissipation even for a slow moving fluid, if the slow movement of the fluid takes place in a microsystem. We all can visualize in a high speed flow in a macrodevice giving rise to entropy generation and thereby reducing the efficiency of the process more frictional head more head would be lost due to friction. But in small systems since it is governed by viscous forces since the gradient is large and very simplest in the very simplified form this dissipation function is proportional to the viscosity and is proportional to the gradient velocity gradient square.

So, since it is proportional to the velocity gradient square and we know that in microfluidic systems the gradient the value of the velocity gradient is large. So, the head lost the dissipation due to fluid friction even for slow flow can be large in microfluidic systems. So, viscous dissipation or any kind of dissipation needs to be carefully examined in microfluidic devices. So, all the equations that we have seen or we are going to see would be valid many of them would be valid, if continuum limit I maintained in a microdevice. But the effect or the contribution of dissipation function corresponding rise in entropy and therefore, reduction in the efficiency of the process needs to be looked into very very carefully.

So, that is what I would like to conclude today that we would for example, in any heat transfer device also since it involves a large gradients similar to large velocity gradients the large temperature gradients will also give rise to a higher entropy generation in microscale devices. So, these are the, so the that is the peculiarity of the process and the device that we have to be careful about. Thank you.