Gasdynamics:
Fundamentals and Applications
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Lecture-03
Thermodynamics-01

Let us come to this lecture following the discussions on flow regimes, where we looked at mach numbers and how the fluid flow features vary as mach number changes from very low mach numbers to all the way to very high mach numbers. So, the important point in compressible flows is that the density changes significantly and also other variables like pressure, temperature also change significantly with change in velocity of the flow.

So, the point is that the flow contains significant amount of kinetic energy and when there is changes in velocity then large changes of kinetic energies produced and that interacts with the internal energy of the gas itself producing these changes in temperature, pressure and density. So, because there is such interactions thermodynamics becomes essential in the description of gas dynamic flows.

The understanding here is that you would have already done full courses on thermodynamics and fluid mechanics or fluid dynamics. So, that we do not go into all the details of thermodynamics, but it is essential that you know it very well to understand gas dynamics. Similarly, fluid flow equations you should know well, but we will have a brief review particularly to those concepts which are important for gas dynamics.

So, let us go ahead with thermodynamics, this review of thermodynamics is made into 2 separate lectures. So, first there are some very important concepts that we should sort of clear before we go into other discussions.

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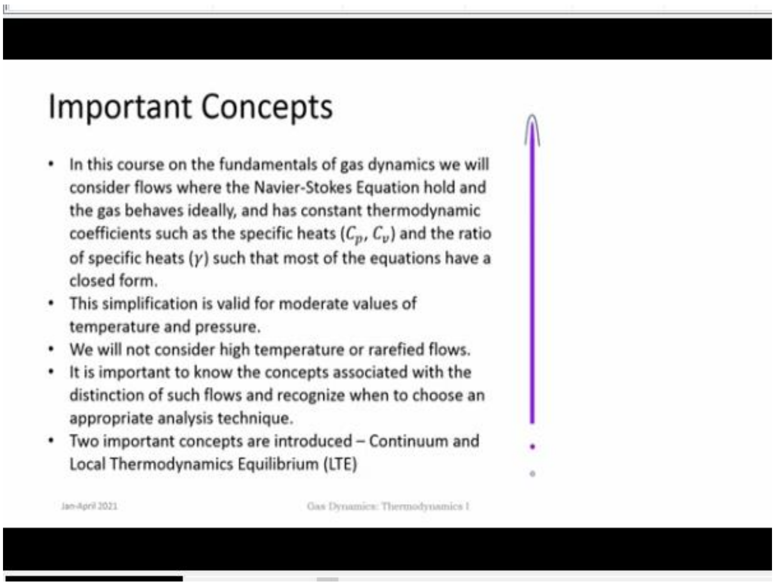

Important Concepts

- In this course on the fundamentals of gas dynamics we will consider flows where the Navier-Stokes Equation hold and the gas behaves ideally, and has constant thermodynamic coefficients such as the specific heats (C_p, C_v) and the ratio of specific heats (γ) such that most of the equations have a closed form.
- This simplification is valid for moderate values of temperature and pressure.
- We will not consider high temperature or rarefied flows.
- It is important to know the concepts associated with the distinction of such flows and recognize when to choose an appropriate analysis technique.
- Two important concepts are introduced – Continuum and Local Thermodynamics Equilibrium (LTE)

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So, the point is that, in this base fundamental course on gas dynamics, we will consider only such kind of flows, which are where the Navier stokes equations hold or the gas behaves as a continuum ideally and has constant thermodynamic properties and coefficients such as the specific heat at constant pressure and constant volume. So, that is what we would do in most of this almost entire of this course.

But, since, we are also talking about various applications of gas dynamics, we should be aware of where these whatever we discuss here, though qualitatively they may be similar, you have to really be careful when applying concepts from what we do in the course to cases where they may not hold good. So, these simplifications that we do in this course are valid for moderate values of temperature and pressure.

And we will discuss to certain extent where they are valid. But we will not consider extremely high temperatures where the physical phenomena will be different or rarefied flows or extremely low dense flows. So, there are such concepts which we need to know so, that we apply the correct analysis technique, when we look at certain problem that you would do in the course of your applications. So, the 2 important concepts are the concept of continuum and the concept of local thermodynamic equilibrium.

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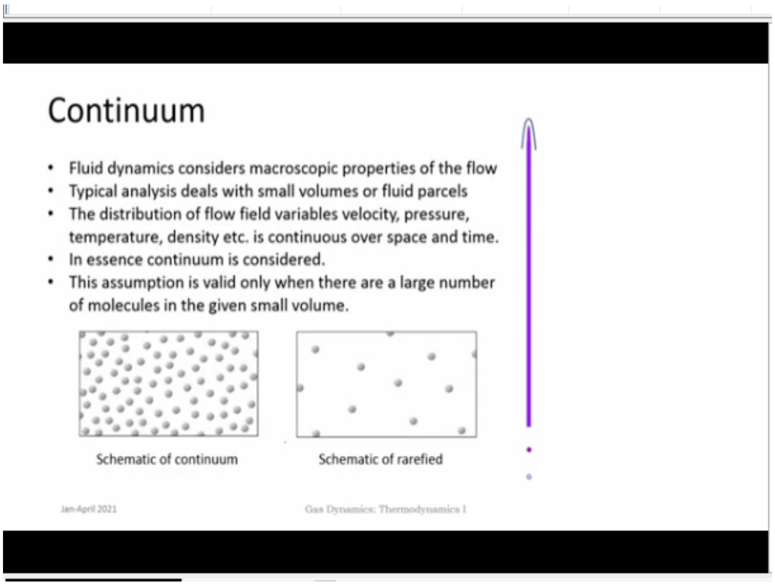

Continuum

- Fluid dynamics considers macroscopic properties of the flow
- Typical analysis deals with small volumes or fluid parcels
- The distribution of flow field variables velocity, pressure, temperature, density etc. is continuous over space and time.
- In essence continuum is considered.
- This assumption is valid only when there are a large number of molecules in the given small volume.

Schematic of continuum

Schematic of rarefied

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So, in continuum, so, fluid dynamics basically considers macroscopic properties of flow, we know that the gases are composed of several molecules and these molecules are always moving around and they are colliding with each other, this is the microscopic view of these matters, but when we look at gaseous flows, we do not consider such microscopic properties and we look at the whole gas to be present as a continuous medium.

So, when doing that we divide them these places into small volumes and we consider the fluid flow equations across many such small volumes or controlled volumes. So, what we do consider is that the distribution of flow field variables like velocity, pressure, temperature, density, it is continuous over space and time So, they are essentially you are considering a continuous description you do not go into places where there is you do not go to the microscopic view of matter.

But this view is valid only if there are extremely significantly large number of molecules in that given small volume that you have considered to analyse the fluid flow. So, if that does not hold good, then you are not in the region of continuum and then you will have to look at other methods to describe the movement of these molecules.

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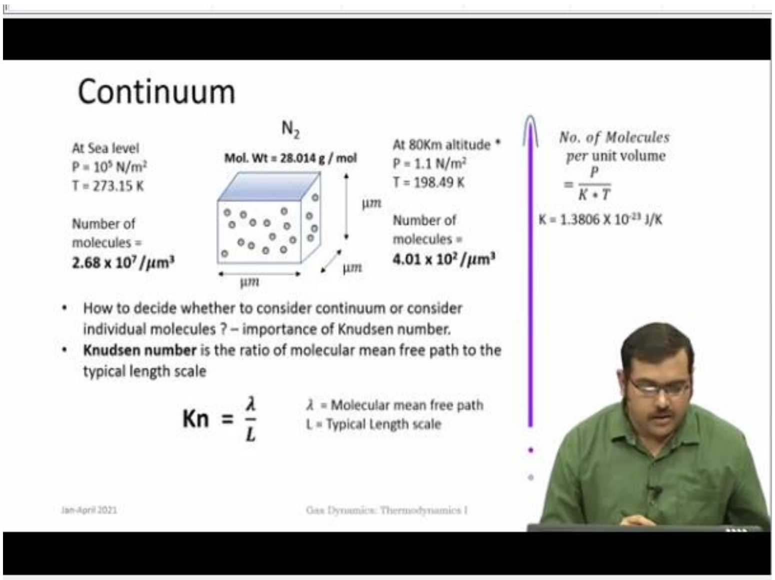

Continuum

N_2

Mol. Wt = 28.014 g / mol

At Sea level
P = 10^5 N/m^2
T = 273.15 K

Number of molecules =
2.68 x 10^7 /μm^3

At 80Km altitude *
P = 1.1 N/m^2
T = 198.49 K

Number of molecules =
4.01 x 10^2 /μm^3

No. of Molecules per unit volume $= \frac{P}{K * T}$

K = 1.3806 X 10^{-23} J/K

- How to decide whether to consider continuum or consider individual molecules ? – importance of Knudsen number.
- **Knudsen number** is the ratio of molecular mean free path to the typical length scale

$$Kn = \frac{\lambda}{L}$$

λ = Molecular mean free path
L = Typical Length scale

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Now, how do we decide whether we are in the continuum regime or we are not in the continuum regime, we need a figure of merit always is a figure of merits will help us. So, that figure of merit is actually the Knudsen number(Kn), the Knudsen number is a ratio of the molecular mean free path(λ) to the typical length scales (L) that will occur in the flow. So, for example, the Knudsen numbers for a sort of typical volume which is considered over here is about cube of 1 cubic micro metre (μm^3) in dimensions.

This is quite a small cube, but, when we consider at sea level which is having about a bar of pressure and temperature is proximately around 273 K which is almost 0^o centigrade. So, you will have the number of molecules is very high, it is about 10^7, but at the same time, if you go to an altitude, which is around 80 km in the earth's atmosphere, their pressure drops down significantly.

Density drops down significantly and number of molecules drops down quite significantly.
So, one needs to consider the Knudsen number and these kind of altitudes are quite routine in considering say movement to space or access to space kind of problems.

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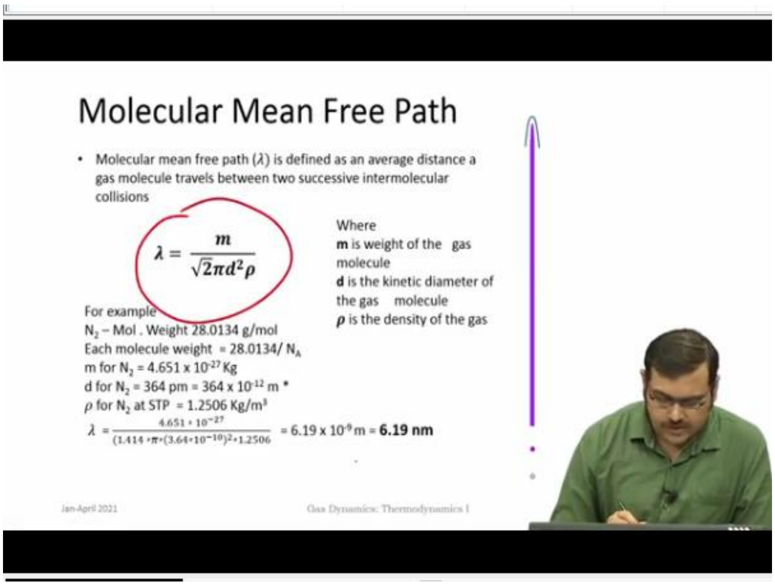

Molecular Mean Free Path

- Molecular mean free path (λ) is defined as an average distance a gas molecule travels between two successive intermolecular collisions

$$\lambda = \frac{m}{\sqrt{2}\pi d^2 \rho}$$

Where
m is weight of the gas molecule
d is the kinetic diameter of the gas molecule
ρ is the density of the gas

For example
N_2 – Mol . Weight 28.0134 g/mol
Each molecule weight = 28.0134/ N_A
m for N_2 = 4.651 x 10^{-27} Kg
d for N_2 = 364 pm = 364 x 10^{-12} m *
ρ for N_2 at STP = 1.2506 Kg/m^3
$\lambda = \frac{4.651 * 10^{-27}}{(1.414 * \pi * (3.64 * 10^{-10})^2 * 1.2506}$ = 6.19 x 10^{-9} m = **6.19 nm**

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So, when you are looking at such problems, then you should be carefully considering what is the Knudsen number and the molecular mean free path can be calculated based on the equations here and a typical number for this at standard temperatures and pressures is in the range of nano meters. So, normally when we consider normal flows, we do not actually look at Knudsen number because we are mostly considering continuum flows. But then there may be situations when this continuum may not be valid.

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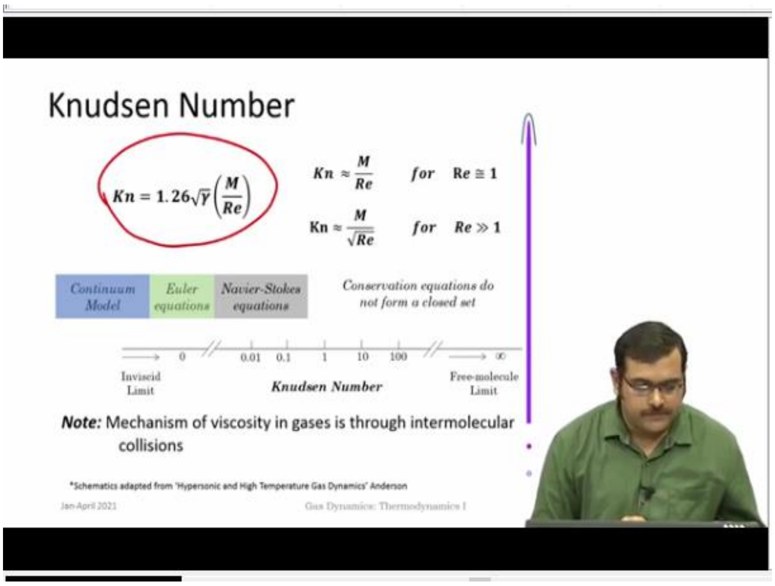

Knudsen Number

$$Kn = 1.26\sqrt{\gamma}\left(\frac{M}{Re}\right)$$

$Kn \approx \frac{M}{Re}$ for $Re \cong 1$

$Kn \approx \frac{M}{\sqrt{Re}}$ for $Re \gg 1$

Note: Mechanism of viscosity in gases is through intermolecular collisions

*Schematics adapted from 'Hypersonic and High Temperature Gas Dynamics' Anderson

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So, Knudsen number can also be related with the mach number(M) and Reynold's number(Re) by this equation. So, it can be related to these fluid flow numbers. So, generally it is considered that when Knudsen numbers (Kn) are small of course, when we are considering continuum, what we are saying is that the small volume that we have considered as for analysis or the control volume for analysis is large enough to contain large number of molecules.

That means, the molecular mean free path (λ) must be much, much less than the typical length scale (L) being considered. And this is true when Knudsen numbers are less than about 0.1. So, less than 0.1. So, small Knudsen numbers mean continuum flow, if Knudsen numbers start becoming larger approach value of 1 and greater than that, then that is not continuum flow. So, there are Navier Stokes equations do not hold good.

And we should really consider other kinds of analysis techniques to do that. So, when looking at gas dynamic flows in various applications carefully look at the Knudsen number. So, that you are sure that you can apply continuum-based analysis for your problem.

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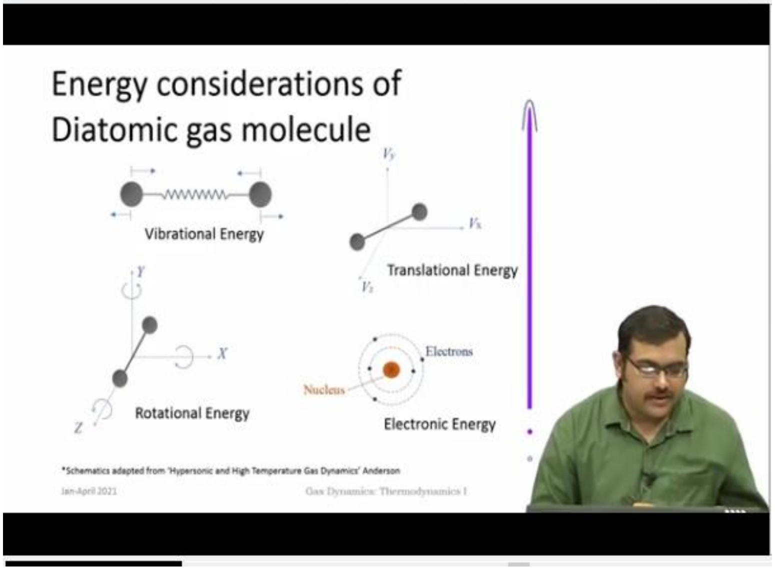

Energy considerations of Diatomic gas molecule

*Schematics adapted from 'Hypersonic and High Temperature Gas Dynamics' Anderson

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The second important concept that comes is this is also related to the microscopic description of matter of gases, which we do not normally describe, but it may become important in certain cases, like when temperatures go really high and this is quite possible in the gas dynamic flows that we consider and that is we have to consider these energy considerations very carefully.

So, from this energy considerations belong to the way gas molecules move and within itself as well as around it and so the energy of the gas molecule can be composed of different modes, they can be due to the motion of the gas molecule in X-Y-Z coordinates, which is the translational energy or if you consider a diatomic molecule, then there are 2 atomic masses there and the they can vibrate among the distances can change and vibrate among themselves or the molecule can rotate among the certain axis.

And the molecule is composed of certain electronic structure and there is an energy associated with that electronic structure. So, there are different modes of energy in a gas molecule.

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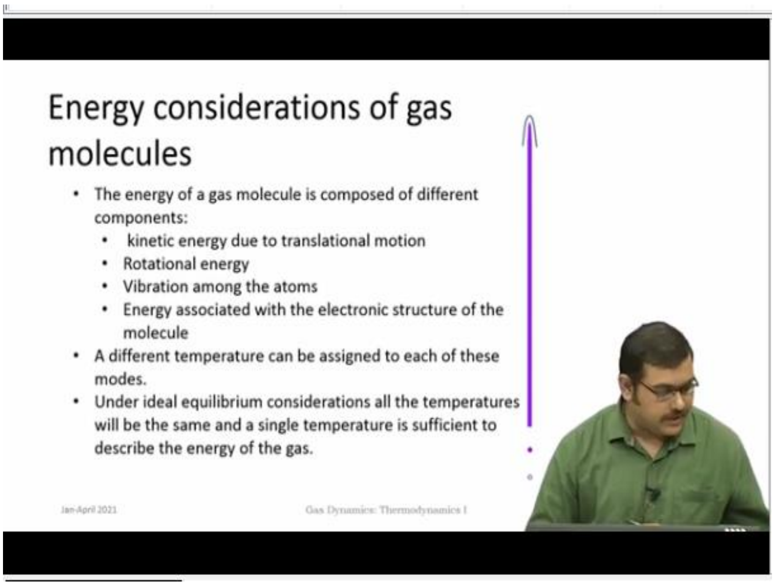

Energy considerations of gas molecules

- The energy of a gas molecule is composed of different components:
  - kinetic energy due to translational motion
  - Rotational energy
  - Vibration among the atoms
  - Energy associated with the electronic structure of the molecule
- A different temperature can be assigned to each of these modes.
- Under ideal equilibrium considerations all the temperatures will be the same and a single temperature is sufficient to describe the energy of the gas.

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And the kinetic energy due to translation, rotational energy, vibration between atoms and also the electronic structure. So, what we call as temperature is actually related to these energies that are there in these different modes. So, if you consider each mode separately then a separate temperature can be defined or assigned to each of these modes, but we do not normally do it because we are considering ideal cases where we are having a lot of molecules.

And they interact the collide with each other and they sort of the energy distributes uniformly among all these different modes. And so we are considering always only a single temperature and that single temperature can be sufficient to describe the energy of the gas or the internal energy of the gas. And in many cases in these compressible flows, particularly at much higher speeds, then temperature can increase so much that other modes of energy become more excited than the remaining. Then we will have differences and the consequence of that is changes to the specific heats of the gases .

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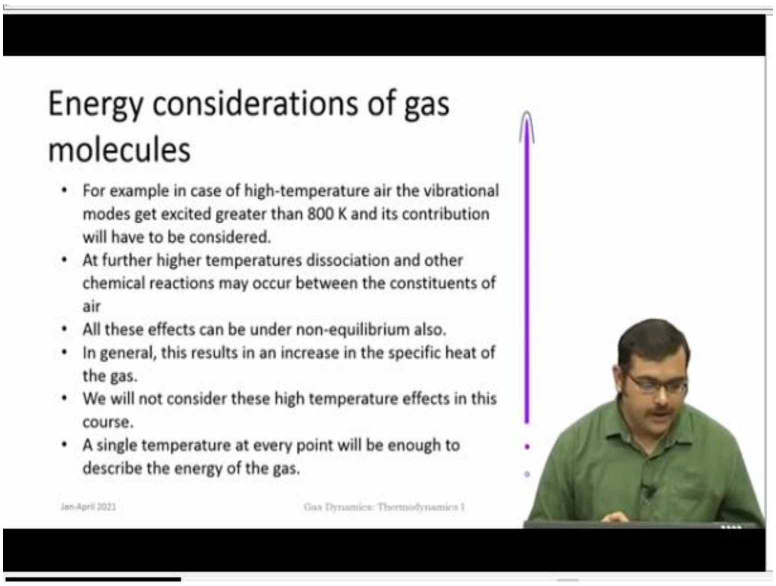

Energy considerations of gas molecules

- For example in case of high-temperature air the vibrational modes get excited greater than 800 K and its contribution will have to be considered.
- At further higher temperatures dissociation and other chemical reactions may occur between the constituents of air
- All these effects can be under non-equilibrium also.
- In general, this results in an increase in the specific heat of the gas.
- We will not consider these high temperature effects in this course.
- A single temperature at every point will be enough to describe the energy of the gas.

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So, and also in certain cases the temperatures can be so high that chemical reactions like dissociation may occur like nitrogen molecule may split up into nitrogen atoms. And if these chemical reactions occur, they can be under non equilibrium conditions also. And so these high temperature effects, we will not consider in this course that is a separate topic in itself. So, in this course, we will say that a single temperature at every point will describe the energy of the gas.

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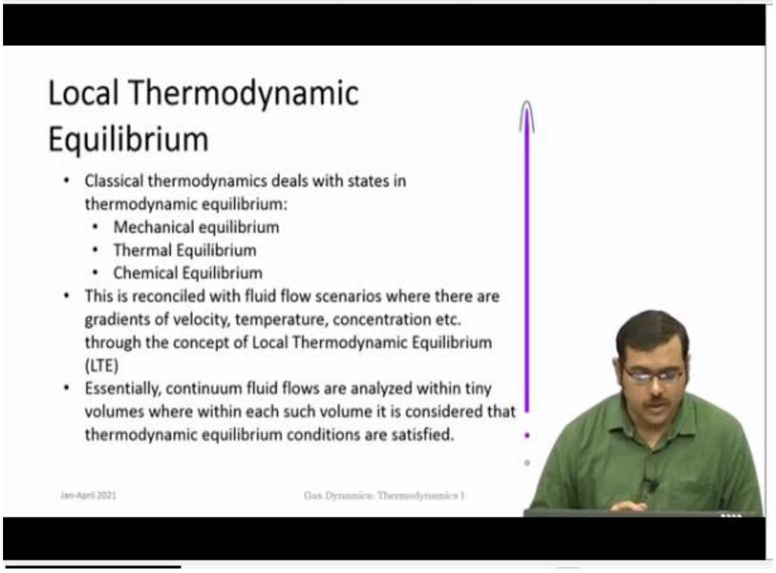

Local Thermodynamic Equilibrium

- Classical thermodynamics deals with states in thermodynamic equilibrium:
  - Mechanical equilibrium
  - Thermal Equilibrium
  - Chemical Equilibrium
- This is reconciled with fluid flow scenarios where there are gradients of velocity, temperature, concentration etc. through the concept of Local Thermodynamic Equilibrium (LTE)
- Essentially, continuum fluid flows are analyzed within tiny volumes where within each such volume it is considered that thermodynamic equilibrium conditions are satisfied.

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So, another important concept that comes here is the local thermodynamic equilibrium. So, if you consider what classical thermodynamics deals with? Classical thermodynamics deals with states that are in thermodynamic equilibrium and thermodynamic equilibrium means that the two states that you are considering state a and state b, they have to be in mechanical equilibrium, thermal equilibrium and chemical equilibrium.

Mechanical equilibrium implies balance of forces, thermal equilibrium comes from the zeroth law of thermodynamics stating that if 2 bodies are in contact and there is no flow of heat, they should be in the same temperature, they should be having the same temperature, they are in thermal equilibrium and chemical equilibrium comes from the fact that there is no change in the composition the molar composition of a mixture and that is chemical equilibrium.

But, when we look at several fluid flow scenarios, globally if you take the whole fluid flow you may see there is lot of changes happening within the flow , there you need to apply certain forces to make the flow move and all such things happen and there is large changes in temperature and pressure and all these happen. So, the equilibrium concept essentially says they are the gradients should be very, very small or negligible.

But fluid flows happen only when there are gradients of pressures and heat transfers happen when there is gradients of temperature. So, we are looking at such a flow. So, how do you reconcile these 2 things with classical thermodynamics with fluid flow is through the concept of local thermodynamic equilibrium. So, where we are fluid flows are always analysed by considering small, tiny volumes.

And we are saying that in each of those particular volumes, very tiny volumes that we are considered thermodynamic equilibrium is valid. So, that is a very local thermodynamic equilibrium and that conditions are valid in that tiny particular volume and then it is interacting with other volumes. So, each of those volumes are in thermodynamic equilibrium.

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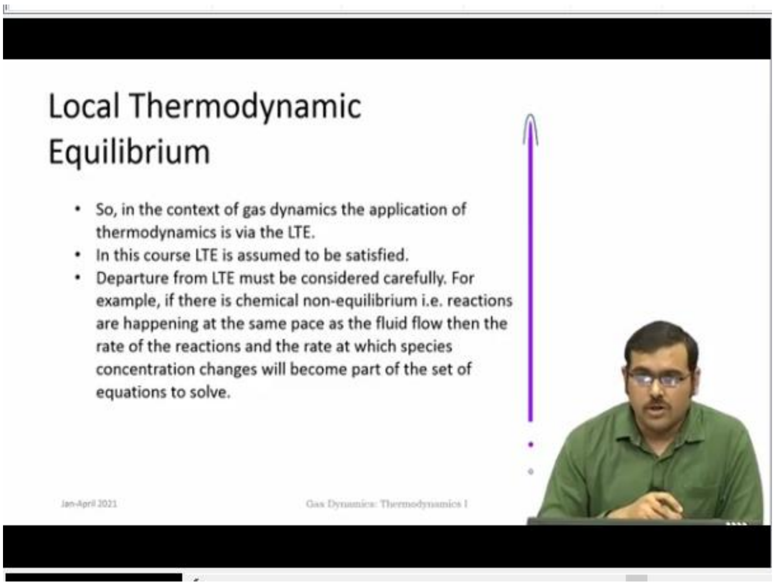

Local Thermodynamic Equilibrium

- So, in the context of gas dynamics the application of thermodynamics is via the LTE.
- In this course LTE is assumed to be satisfied.
- Departure from LTE must be considered carefully. For example, if there is chemical non-equilibrium i.e. reactions are happening at the same pace as the fluid flow then the rate of the reactions and the rate at which species concentration changes will become part of the set of equations to solve.

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So, we are going to deal with cases only where the local thermodynamic equilibrium (LTE) is valid and it is assumed to be satisfied. So, departures from local thermodynamic equilibrium must be considered very carefully, examples are when you have chemical non equilibrium, you have reacting flows and they happen at the same pace as the reactions happen as fast as the fluid flow happens.

Then the species changes as the rates of formation and they change as the flow happens. So, the set of equations that you need to consider will involve separate equations for such species. So, they have to be really considered carefully and, in this course,, we will not consider a departure from local thermodynamic equilibrium.

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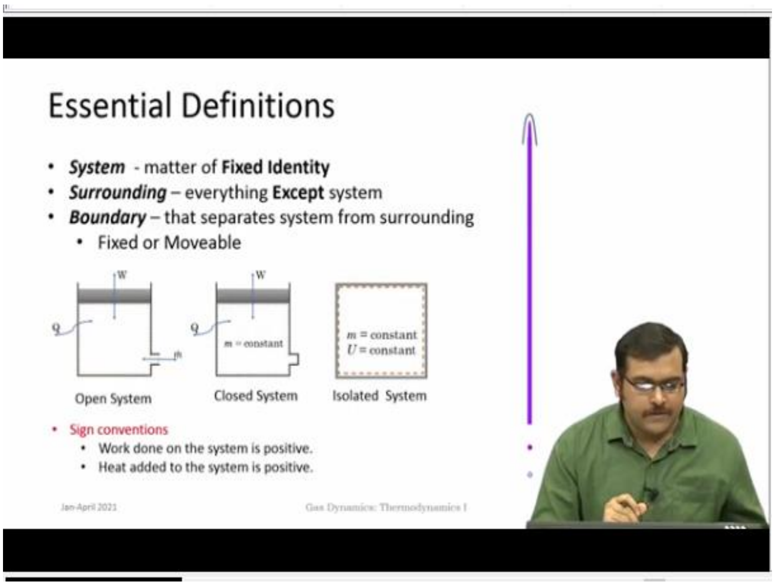

Essential Definitions

- ***System*** - matter of **Fixed Identity**
- ***Surrounding*** – everything **Except** system
- ***Boundary*** – that separates system from surrounding
  - Fixed or Moveable

- Sign conventions
  - Work done on the system is positive.
  - Heat added to the system is positive.

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So, when we will look at now that those 2 important concepts of continuum and local thermodynamic equilibrium have been considered, we are going to consider cases which are in continuum and in local thermodynamic equilibrium. And so, these are essential definitions for thermodynamics, and this is just a recap and for more details you should revise thermodynamics if you have to do so.

So, system is just a matter of that is being considered for analysis and everything other than that is the surrounding and there is you can specify a boundary between the system and the surrounding. There are different kinds of systems you have the open system where you can have exchange of mass into the system. And of course, there is a exchange of heat and work across the boundaries of the system.

While in a closed system there is no exchange of mass it is only work can heat, while if no work or heat is being exchanged and you have an isolated system. So, there are certain sign conventions which are usually followed but when heat or work is added to the system, heat work is done on the system or heat is added to the system it is considered as positive.

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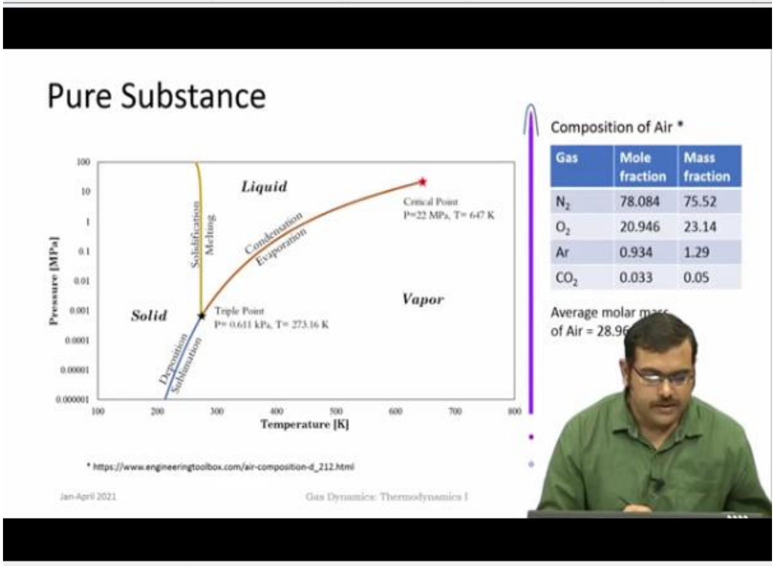

Pure Substance

Composition of Air *

Gas	Mole fraction	Mass fraction
N_2	78.084	75.52
O_2	20.946	23.14
Ar	0.934	1.29
CO_2	0.033	0.05

Average molar mass of Air = 28.96

* https://www.engineeringtoolbox.com/air-composition-d_212.html

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And we consider a pure substance, pure substances substance whose chemical composition remains the same for various changes that happens to the object as it undergoes a process . So, it may change phases like it can go from solid to liquid or liquid to vapour you have different change in phases, but it does not change in chemical composition. Example is just plain water as it changes from ice to water to water vapour and steam you have it all over the this one.

So, but it still remains as H_2O it's chemical composition does not change, why this is important is because we are considering in most of our classes we will consider flows with air as the medium. So, air is our gas and air is a mixture, it is it is not a single molecule like that of water, it has a mixture of molecules which has a nitrogen oxygen as the main components in mole fractions, it is 78% of nitrogen and close to 21% of oxygen.

You have other trace elements like argon and carbon dioxide the rest are very, very small. But this mixture behaves for most of our considerations, it behaves like a pure substance, like we do not really have to consider the individual behaviour of these molecules, but we will consider the average behaviour for air and it has an average molar mass of 28.6 kilograms per kilo mole .

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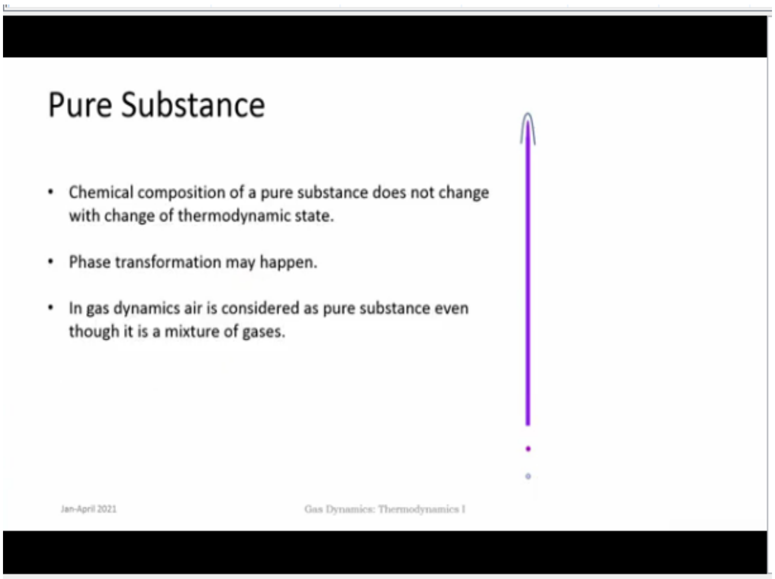

Pure Substance

- Chemical composition of a pure substance does not change with change of thermodynamic state.
- Phase transformation may happen.
- In gas dynamics air is considered as pure substance even though it is a mixture of gases.

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So, for all practical purposes in the course, air is considered as a pure substance throughout the course.

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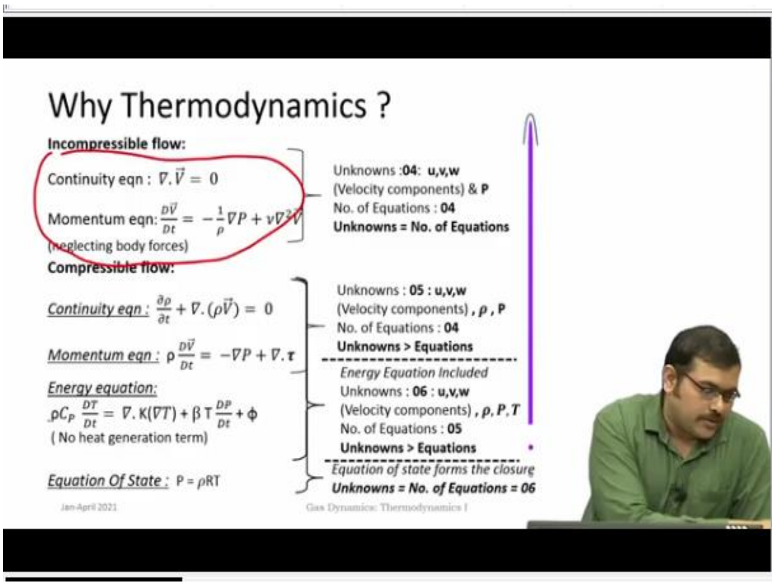

Why Thermodynamics ?

Incompressible flow:

Continuity eqn : $\nabla.\vec{V} = 0$

Momentum eqn: $\frac{D\vec{V}}{Dt} = -\frac{1}{\rho}\nabla P + \nu\nabla^2\vec{V}$

(neglecting body forces)

Unknowns :**04**: **u,v,w** (Velocity components) & **P**
No. of Equations : **04**
Unknowns = No. of Equations

Compressible flow:

Continuity eqn : $\frac{\partial\rho}{\partial t} + \nabla.(\rho\vec{V}) = 0$

Momentum eqn : $\rho\frac{D\vec{V}}{Dt} = -\nabla P + \nabla.\tau$

Energy equation:
$\rho C_P \frac{DT}{Dt} = \nabla.K(\nabla T) + \beta T\frac{DP}{Dt} + \phi$
(No heat generation term)

Equation Of State : $P = \rho RT$

Unknowns : **05 : u,v,w** (Velocity components) **, ρ , P**
No. of Equations : **04**
Unknowns > Equations

Energy Equation Included
Unknowns : **06 : u,v,w** (Velocity components) **, ρ, P, T**
No. of Equations : **05**
Unknowns > Equations

Equation of state forms the closure
Unknowns = No. of Equations = 06

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So, now let us take a look at how if you look at the have a glance at the equations of the flow, how thermodynamics comes into picture when we consider compressible flows? For that, let us just take a comparison between incompressible flow and compressible flow. So, these equations the equations here depict a typical incompressible flow of constant density that means, here density is known and it is not variable, the viscosity is also known.

So, if you take such a case, a typical incompressible fluid flow then you have the 3 components of velocities that are unknown, which is u, v and w and you have pressure which is unknown that is a fourth variable. So, this to describe the fluid flow, you have continuity and momentum equations, they contain in themselves, this momentum equation is a vector equation.

So, it has 3 equations in itself contained within it. So, you have 4 equations. So, if you will see the number of unknowns and number of equations, you have a consistent set you have 3 unknowns of velocity and 1 unknown of pressure and number of equations is also 4. So, to solve these equations, if you are able to solve it, you can do it if you know the boundary conditions and the initial conditions.

Then this it is possible to solve this equation as they are completely consistent and density is known in this case, but if you come to compressible flows, this density is a variable. So, along with the components of velocity and pressure density becomes a variable. So, now you have 5 variables and if you consider only the fluid flow equations, which is continuity and momentum then you will not be able to get a consistent set of equations.

So, this number of equations will be 4, but number of unknowns will be 5. So, you need additional equations. So, these equations come together by adding energy consideration. So, you can have the energy equation . So, when you add energy equation there temperature becomes an equation. So, an additional unknown is added that is temperature. So, now, density, pressure and temperature are unknown.

So, you have totally 6 unknowns with the addition of energy equation, energy equation is a scalar equation. So, this is only a single equation. So, energy equation will add one more equation. So, you have 5 equations. So, you have 6 unknowns and 5 equations means, you need additional equations to still solve this problem and that equation is supplied through the equation of state.

So, both the energy equation by definition of what is enthalpy here it is the enthalpy that comes into picture and the equation of state which is in this case is the perfect gas ideal equation of state$P = \rho RT$, you are bringing in thermodynamics without these equations, it is not possible to solve the compressible flows. So, thermodynamics is an integral part of understanding and analysing compressible flows.

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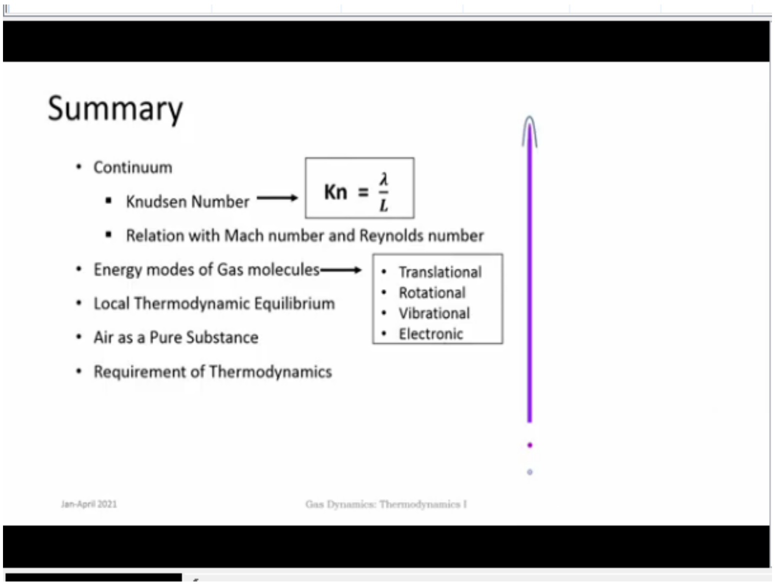

Summary

- Continuum
  - Knudsen Number → $Kn = \frac{\lambda}{L}$
  - Relation with Mach number and Reynolds number
- Energy modes of Gas molecules →
  - Translational
  - Rotational
  - Vibrational
  - Electronic
- Local Thermodynamic Equilibrium
- Air as a Pure Substance
- Requirement of Thermodynamics

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So, we have understood the 2 essential concepts here that is continuum and local thermodynamic equilibrium and the importance of Knudsen number and to know that its value so that when you are doing the analysis, you are priory know whether you are applying the correct equations.

And we have understood how important thermodynamics is to understand compressible flows, we are going to use air as a medium and air is considered as a pure substance in this course. So, thermodynamics essentially deals with understanding the energy exchanges using the laws of thermodynamics, and these laws we will discuss in the next class.