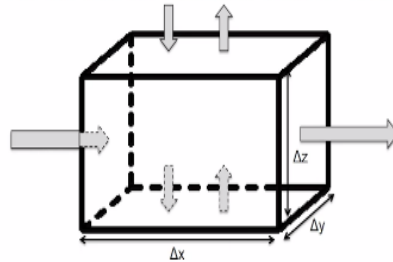


**Environmental Quality: Monitoring and Analysis**  
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**Lecture-39**  
**Dispersion Model Parameters - Part 1**

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Box Models for Pollutant Transfer in Air



Processes in the Box:

- a) Advection (or bulk flow) – velocity
- b) Dispersion
- c) Reaction
- d) Exchange from/to air from bottom surface (land/water)
- e) Transfer/Exchange with upper atmosphere



So, we were looking at box models for pollutant transfers in air. So, essentially this is generic box model for air. The processes that we are considering in the box include advection, dispersion, reaction exchange and all that, ok.

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## Box model in air



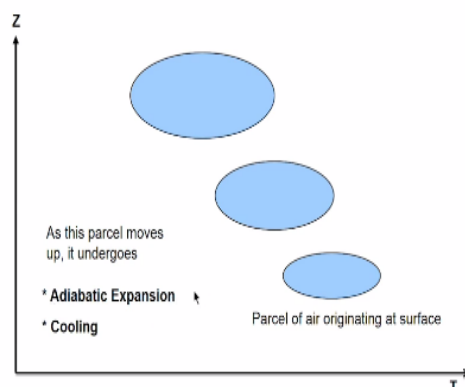
- The height of air layer is not well defined in the box for consideration of this well-mixed layer
- The vertical layer is determined by a concept of a mixing height
- Mixing height is determined by a concept called Stability
- Stability is a function of temperature gradients in the lower atmosphere



So, the specific problem for air is that the height is not very well defined, so we look at what is called as a mixing height and mixing height depends on concept called stability and stability is function of temperature in the lower atmosphere.

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## Atmospheric Stability



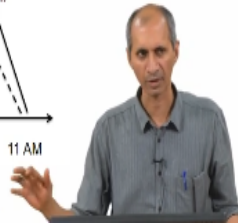
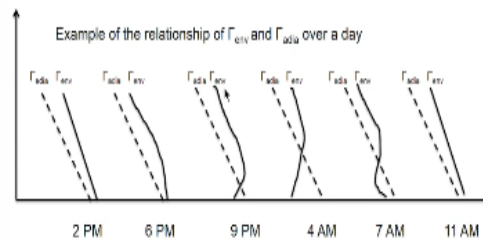
Stability is the behavior of an air parcel when it originates somewhere in the near the earth surface and then it travels upwards and then what happens to it, so the ideal case of that is called an Adiabatic Expansion or cooling as it goes up.

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## Atmospheric Stability



- Environmental Lapse rate,  $\Gamma_{env}$  is the gradient of temperature with height that exists in the natural environment
- $\Gamma_{env}$  changes with time of day, season and location



So, atmospheric stability is the behavior of a parcel in conjunction with this environment whatever is there, environmental lapse rate or the temperature gradient in the environment that exists at any point in time. So this figure shows the change of environmental gradient, one example, this may not happen all the time, it depends on the place and time, the season. But the adiabatic lapse rate from a particular process stays there, it doesn't change, wherever it is released or whatever is the temperature of the exhaust, the adiabatic lapse rate doesn't change.

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## Atmospheric Stability



- $\Gamma_{adia, dry} = -dT/dz = g/C_p = -0.0098 \text{ C / m}$
- Dry Adiabatic Lapse Rate,  $\Gamma_{adia, dry}$
- Environmental Lapse Rate,  $\Gamma_{env}$
- Comparison of  $\Gamma_{adia, dry}$  and  $\Gamma_{env}$  determines the stability condition



The lapse rate represented by Gamma, the adiabatic lapse rate is given as -0.0098 centigrade per kilo per meter or 9.8 centigrade per kilometer this is the adiabatic lapse rate. This is the dry adiabatic lapse rate

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### Dry Adiabatic Lapse Rate

$\rho g dZ = dP \dots (1)$ <i>From the first law of thermodynamics</i> $dQ + dW = dU \dots (2)$ <i>Since it is adiabatic, <math>dQ = 0</math></i> $dW = dU$ $-PdV = mC_v dT \dots (3)$ $d(PV) = PdV + VdP \dots (4)$ $-PdV = VdP - d(PV) \dots (5)$ $PV = nRT$ $d(PV) = nRdT \dots (6)$ <i>Using eqn 5, 6 in 3</i> $VdP - nRdT = mC_v dT$ $VdP = (nR + mC_v)dT$ <i>dividing by m</i>	$VdP = (nR + mC_v)dT$ <i>dividing by m</i> $\frac{1}{\rho} dP = \left( \frac{R}{M_v} + C_v \right) dT$ $\frac{1}{\rho} dP = C_p dT$ $dP = -\rho g dZ$ $-\frac{1}{\rho} \rho g dZ = C_p dT$ $\frac{dT}{dZ} = -\frac{g}{C_p}$  $g = 9.8 \text{ m/s}^2$ $C_p \text{ for dry air} = 1000 \text{ J/kg-K}$ $\Gamma_{\text{adia, dry}} = -dT/dz = g/C_p = -0.0098 \text{ } ^\circ\text{C/m}$
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and this is the derivation of that, it's there in many textbooks, nomenclature varies, but you can go through this. It is basically two things one is the definition of static pressure

$$\rho g dZ = dP$$

And first law of thermodynamics which means it is an adiabatic process,

$$dQ + dW = dU$$

Since it is adiabatic process,  $dQ = 0$ .

$$dW = dU$$

so it's minus of  $PdV$  equals  $mC_v dT$  just based on ideal gas law and all that.

You can go through the derivations fairly straight forward and then use the definitions of  $C_p$ ,  $C_v$  and all that and we come to this point

$$VdP = (nR + mC_v)dT$$

and then we come down here, we'll get

$$\frac{dT}{dZ} = -\frac{g}{C_p}$$

$C_p$  is the specific heat of dry air. So, if you insert these values here, you get - 0.0098 and this also has assumptions that when the parcel is moving up, there is no heat transfer it happens very quickly, so there is no heat transfer that's the assumption of adiabatic process. That it is insulated,

so there is no effect of there is no heat transfer from the surrounding thing there's only buoyancy effect that is all. So, the density is changing based on the this thing.

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## Dry Adiabatic Lapse Rate



Potential temperature,  $\theta$

$$\theta = T_0 = T_1 \left( \frac{P_0}{P_1} \right)^{\frac{\gamma}{\gamma-1}}$$

Potential temperature is the temperature of an air parcel at temperature  $T_1$  and Pressure  $P_1$  if it is moved to a Pressure  $P_0$ . Typically,  $P_0$  is sea level pressure ( $\sim 1013$  mb)

Consequently, stability can be defined as

$$\begin{aligned} \frac{d\theta}{dz} &< 0, \text{ unstable} \\ \frac{d\theta}{dz} &= 0, \text{ neutral} \\ \frac{d\theta}{dz} &> 0, \text{ stable} \end{aligned}$$



There is another term called potential temperature is defined like this  $\theta = T_0$ . This is the temperature corrected to particular pressure, so the pressure with reference to sea level pressure. So, it's a temperature of an air parcel at temperature  $T_1$  and pressure  $P_1$ , if it is moved to pressure  $P_2$ . So, it is similar, it is corrected temperature for pressure. So, just like  $dt$  by  $dZ$  you can also call  $d\theta/dZ$  and the definitions are given.  $\theta$  is the more normalized way of handling it, in many textbooks you will see  $\theta$  rather than temperature, but for practical considerations and temperature gradient is what you will be looking at, when you look at heat flux. So, you look at lapse rate this way or this way the the temperature gradient immediately will tell you whether it is an inversion or not an inversion and what is the value of it, with reference to that.

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## Atmospheric Dispersion



And we also looked at this concept of mixing height, mean mixing height as the place where the intersection of the environmental lapse rate and adiabatic lapse rate happens. And we also defined that this is the plume the boundary of the this thing so you can say within this a lot of things happen plume may go in and out but there is something called as a time averaged plume.

So, if you keep looking at it for a long period of time, there is shape that the emission takes and that's called as the plume.

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## Plume Shapes from a High Chimney



Coning:  
Thermal: Neutral  
Mechanical: Moderate to strong Winds

Classic plume shape – with both  $z$  and  $y$  dispersion equally important. The plume assumes the shape of a cone approximately with the center vertex at the source.

Stack Plume Characteristics Depend on Two Main Factors:

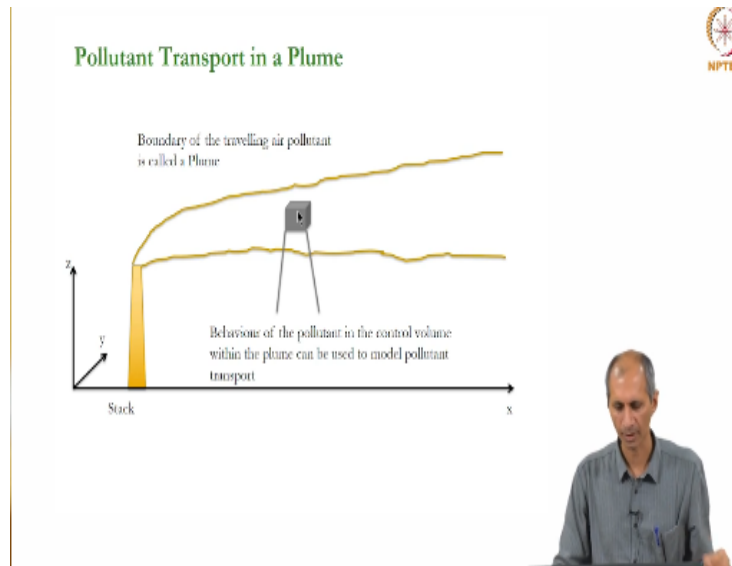
- a) Turbulence (Mechanical)
- b) Thermal (Convection)



And we looked at different shapes from this thing. So this is redrawn again to explain some of the things for each of the different types of plume shapes that can. This is a limited set of plume shape,

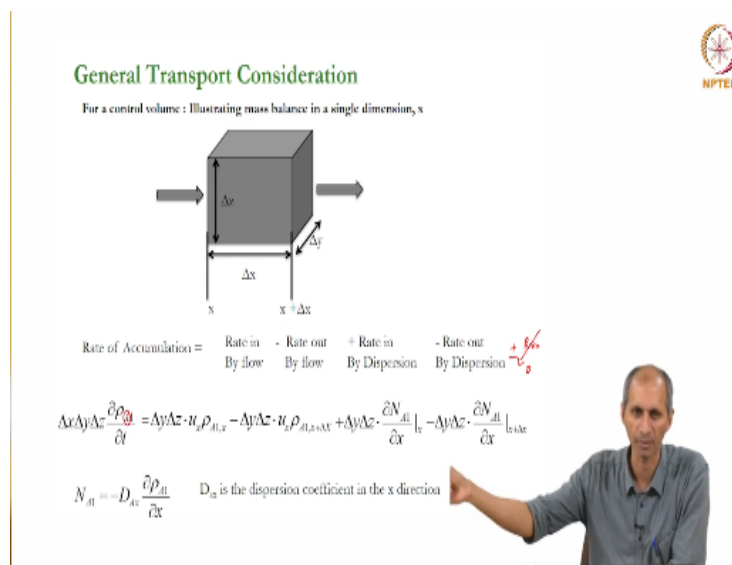
you can have a large number of plume shape based on various combinations of the environmental lapse rate and the plume and the source height and all that so this is one set of conditions, but if you know the basic fundamental aspects behind it you can predict what is kind of, what is the plume shape that you can expect for a given situation. So, there are different kinds of plume shapes that that you can expect.

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So last time when we were looking at we were looking at the pollutant transport, our goal is to be able to predict concentration as function of place and time  $x$ ,  $y$ ,  $z$  and time. So, we look at one control volume within the plume, it is where the pollutant is moving and we try to model it.

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So, we did this last class, we will go over this one again. So, if you take this box which has dimensions of  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$ , we have this term here rate of accumulation equals rate of in by flow or rate out by flow, rate in by dispersion, rate out by dispersion. So, these are the processes we have identified before we write the equation, we have to figure out, we have to determine what are the processes that we are considering in this system.

So, the transport model can have anything the generalized transport model will also have a reaction, will also have adsorption, will also have deposition all these things will happen this multi-phase model but we are not doing that here we are looking at only  $\rho_{A1}$ , so  $\rho_{A1}$  is vapour phase concentration only, ok and we are not even looking at  $\rho_{31}$  which is particulate matter we are only looking at  $\rho_{A1}$ .

So, but this gives you an idea as if you want to do a very complicated model you start here. In this thing you add processes here, so I can add other processes here in this equation and then from here you derive the differential equation that you need to solve. The solution of differential equation is a different issue that's a mathematical part, to make the mathematics solution easier we make more assumptions and make it, you know, easier and all that.

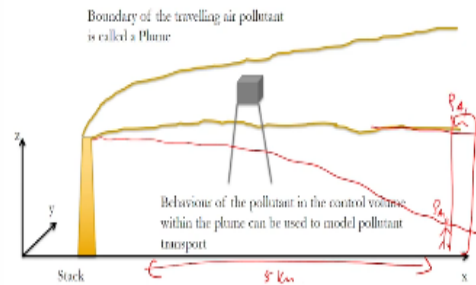
So that's a different section so, from this class point of view you need to be able to write this equation and then somebody else can solve it. That is not an issue, it's ok. You need to understand what are these processes and how they happen whether they are important or not, ok. So, rate of accumulation rate by flow, so what we mean by flow is the wind is bringing it and taking it out away. Dispersion is the different process.

Dispersion is happening because of buoyancy, because of the convection, wind driven convection and anything else so these two are the processes which we have said, so you can add other reactions and all that here, but in this case we are going to assume this reaction to be 0, ok. You write the balance always for one component so in this case, we are writing it for this particular A in the phase that we are interested in, the vapour phase only because this is the phase we are interested in calculating exposure at some point.

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## Pollutant Transport in a Plume



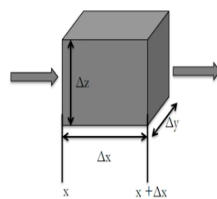
What we are interested in this case is that say, I am interested in this person standing here on the ground and what is the concentration that is you are being exposed to, ok, so from this point of view I would like to know if this plume is going to travel to this person standing at a distance of 5 kilometers or someplace, some distance or if there is a building here and this building somebody is living in this building is there is the plume is going to intersect it what is going to be the concentration at here, so these kind of things is what we are interested in calculating.

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## General Transport Consideration



For a control volume : Illustrating mass balance in a single dimension, x



Rate of Accumulation = Rate in By flow - Rate out By flow + Rate in By Dispersion - Rate out By Dispersion

$$\Delta x \Delta y \Delta z \frac{\partial \rho_{A1}}{\partial t} = \Delta y \Delta z \cdot u_x \rho_{A1,x} - \Delta y \Delta z \cdot u_x \rho_{A1,x+\Delta x} + \Delta y \Delta z \cdot \left( \frac{\partial N_{A1}}{\partial x} \right)_x - \Delta y \Delta z \cdot \left( \frac{\partial N_{A1}}{\partial x} \right)_{x+\Delta x}$$

$$N_{A1} = -D_{Ax} \frac{\partial \rho_{A1}}{\partial x} \quad D_{Ax} \text{ is the dispersion coefficient in the x direction}$$



So, in this equation, we write this rate of dispersion.  $\frac{\partial N_{A1}}{\partial x}$  is a flux term, this is flux multiplied by area. So, this flux here is given by

$$N_{A1} = -D_{Ax} \frac{\partial \rho_{A1}}{\partial x}$$

we are gonna drop the suffix A because we are considering only A in next few slides, no other component here, so it's just Dx this is a Fick's law, this is an equation that is based on Fick's law. Those of you who are not familiar with Fick's law, we will come back to it later after this section.

But it is a very generic law for diffusion it's a very common kind of equation that we see this form of this equation for any flux, ok. So, for now take it from me that this is the structure of this particular term we come back to the fundamentals of that later.

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**General Transport Consideration**

$$\Delta x \Delta y \Delta z \frac{\partial \rho_{A1}}{\partial t} = \Delta y \Delta z \cdot u_x \rho_{A1,x} - \Delta y \Delta z \cdot u_x \rho_{A1,x+\Delta x} + \Delta y \Delta z \cdot \left( \frac{\partial N_{A1}}{\partial x} \right)_{x_1} - \Delta y \Delta z \cdot \left( \frac{\partial N_{A1}}{\partial x} \right)_{x_2}$$


$N_{A1} = -D_x \frac{\partial \rho_{A1}}{\partial x}$ 
 $D_x$  is the dispersion coefficient in the x direction
 $\rho_{A1}$  is a scalar


Dividing by  $\Delta x \Delta y \Delta z$  and setting limit of  $\Delta x \rightarrow 0$ , results in

$$\frac{\partial \rho_{A1}}{\partial t} = \frac{\partial}{\partial x} \left( D_x \frac{\partial \rho_{A1}}{\partial x} \right) - u_x \frac{\partial \rho_{A1}}{\partial x}$$

Extending this to dispersion in y and z directions as well

$$\frac{\partial \rho_{A1}}{\partial t} = D_x \frac{\partial^2 \rho_{A1}}{\partial x^2} + D_y \frac{\partial^2 \rho_{A1}}{\partial y^2} + D_z \frac{\partial^2 \rho_{A1}}{\partial z^2} - u_x \frac{\partial \rho_{A1}}{\partial x}$$





So, we take that equation and start adding all this and dividing by delta x, delta y, delta z, setting the limits of all of them to 0, so first thing what we are doing here is we are only doing it for x, we have not done it for any other things. This equation will become too big write for all components for writing for x only I am writing this so I will get this, similarly if I extend this to y and z as well.

So when we are writing this previous equation, we are only writing the rate in by flow is only in x direction, we know that already there is no pressure driven flow in the y and the z direction, so only x but these two terms (Rate in by dispersion and rate out by dispersion) can be in all three phases. So that is what we are writing here we are writing this extended term, so we will write these terms in all three dimensions.