Sustainable Materials and Green Buildings
Professor B. Bhattacharjee
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Indian Institute of Technology Delhi
Lecture 28 - Emission Models and Testing

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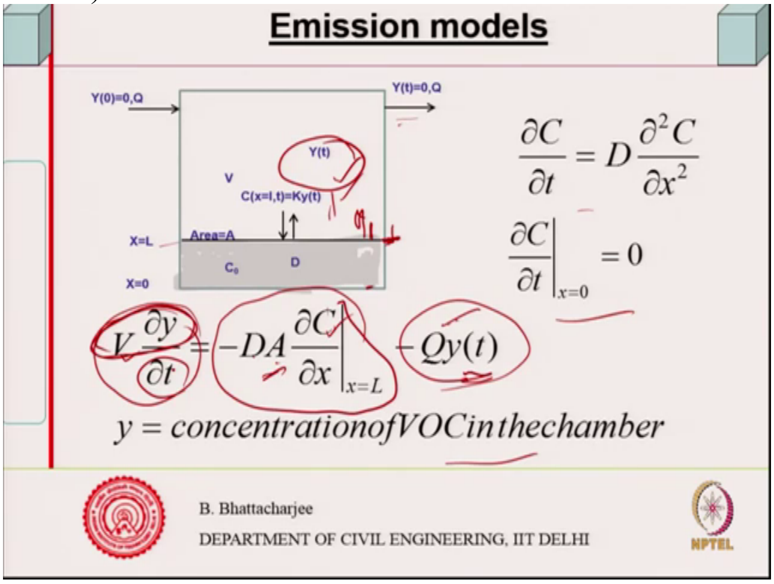

Emission models

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

$$\left.\frac{\partial C}{\partial t}\right|_{x=0} = 0$$

$$V\frac{\partial y}{\partial t} = -DA\left.\frac{\partial C}{\partial x}\right|_{x=L} - Qy(t)$$

$$y = concentrationofVOCinthechamber$$

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So we will continue with the emission models, right. Now this is what we said that you can actually, y is a concentration of VOC in the chamber, C 0 is the concentration here, C l is the concentration here, right? So this change in the concentration multiplied by the volume, concentration is particulate matter per metre cube, right, multiplied this is a, so this divided by the rate of change of concentration in this volume. This is the, you know, there is no volatile coming in from outside, there is some quantity that will be going outside. So if the flow rate is meter cube per unit time, at any time this is constant, we are saying the ventilation rate is constant. So, Y t whatever will go out, will go out with the concentration of the room.

So if Q is the flow per unit time, that multiplied, because it will be in meter cube per second that multiplied by the concentration give how much is going out and how much is coming in to it is because at x equals to L concentration is C, so this is the flux which is entering here per unit area multiplied by the area because this is from Fick's law, D dc dx, del C dx is a flux which is entering at x equals to L where L is the thickness of the whatever layer I am considering. Either it could be a carpet or if it is a paint then bottom of the paint and top of the paint or thickness which could be very small but you know, so depending upon that so at this point whatever the flux that should be entering here and that minus whatever is going out is a change in rate of change of concentration here is y. So that is how we can model.

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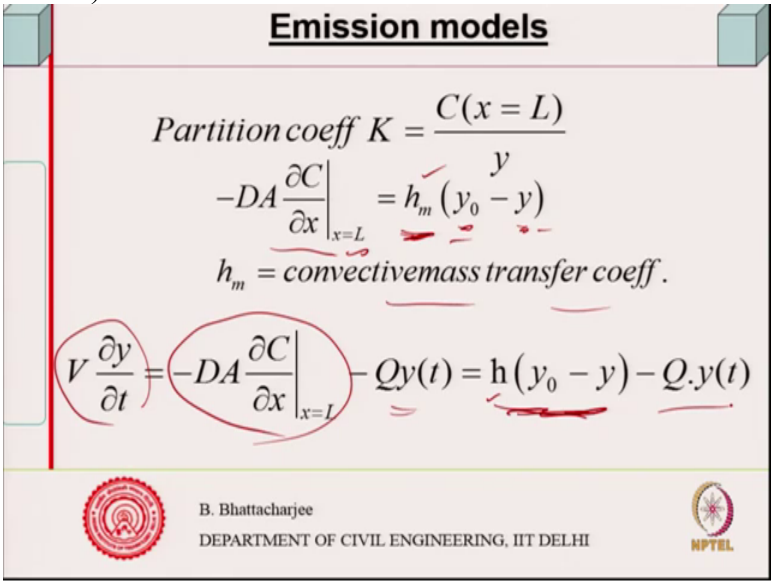

Emission models

$$\text{Partition coeff } K = \frac{C(x=L)}{y}$$

$$-DA\frac{\partial C}{\partial x}\Big|_{x=L} = h_m(y_0 - y)$$

h_m = convective mass transfer coeff.

$$V\frac{\partial y}{\partial t} = -DA\frac{\partial C}{\partial x}\Big|_{x=L} - Qy(t) = \mathrm{h}(y_0 - y) - Q.y(t)$$

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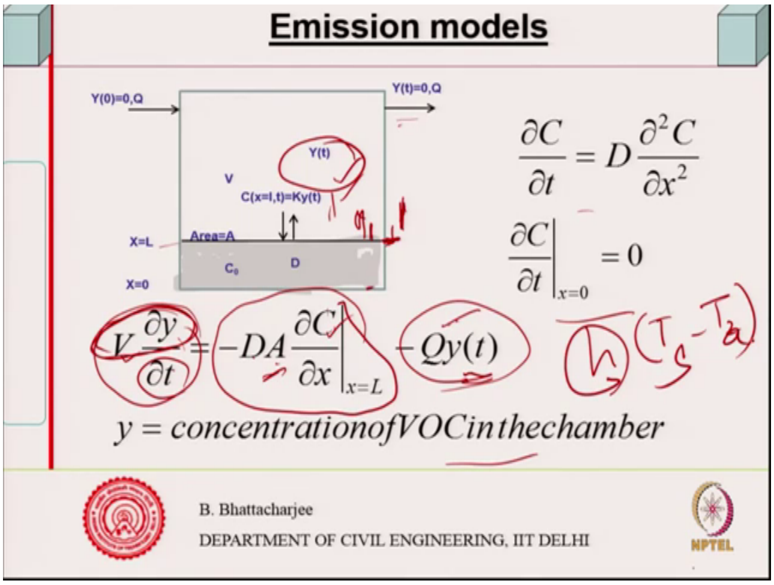

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$$h(T_s - T_a)$$

y = concentration of VOC in the chamber

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Now we call something called partitioning coefficient K which is C x L, C equals at C concentration at L divided by y 0 minus y, right. Now what is y 0? y0 is whatever is coming in, fresh, very fresh air, no volatile at all and y is the room, y is there in the room y 0 minus y. So this is you see this is a, this from surface to from surface to here, surface to here, I can, it is something like a convective heat transfer. The amount of flow from surface to here or amount of you know the volatile that is going in will be a function of the concentration differential itself.

Analogy to heat convection, rate of heat transfer is convective heat transfer is proportional to h convective heat transfer coefficient T1 minus T2 where T1 is you know, T s minus T air temperature, surface to air temperature.

So there is, as the temperature difference decreases flow also decreases, as the concentration difference decreases flow decreases. So we are trying to write similar sort of thing and from analogy at the boundary the flux will be equals to at x equals to L, there is a convective transfer coefficient that is what we are saying, y 0 minus y, so this is the concentration at the air itself and this is what is coming in from outside. So V dy dt this I can replace by, you know, this I can write as h y 0 minus y because y 0 is what is coming in minus y is what is there, the difference is there. So if I know this coefficient, so this is this I can replace by this particular one and write it in this manner.

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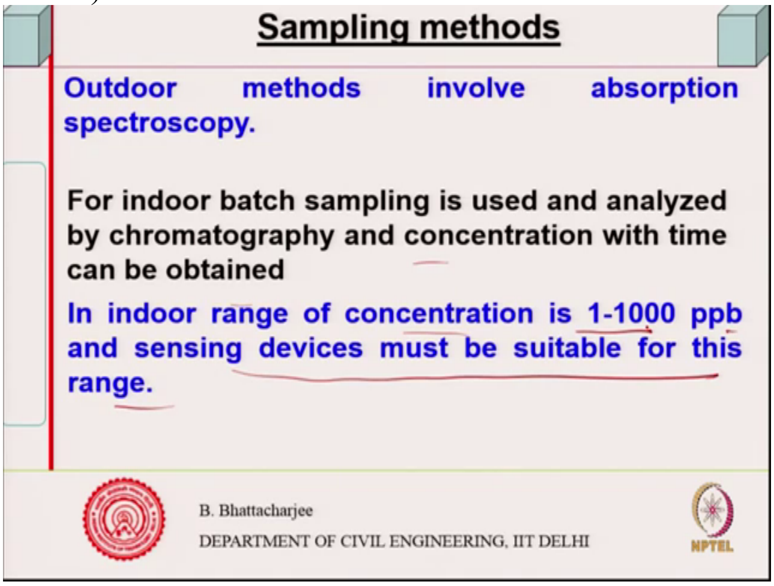

Sampling methods

Outdoor methods involve absorption spectroscopy.

For indoor batch sampling is used and analyzed by chromatography and concentration with time can be obtained

In indoor range of concentration is 1-1000 ppb and sensing devices must be suitable for this range.

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What is done? Sampling is done. Outdoor method involve basically absorption spectroscopy, so they take sample of air and then they measure them using absorption spectroscopy, right. For indoor back sampling is used, so from time to time you take out the sample analyze it, chromatography is one which analyzes the, you know gas concentration of the gases. So gas chromatography they call it, so they will measure and concentration with time we can obtain, so we can obtain the concentration with time inside by taking sampling, right and then testing them in chromatographs.

In indoor range of concentration is 1 to 1000 parts-per-billion and sensing devices must be suitable for this range because it is very small. So you should use such techniques to find out the concentration, because the concentration is very very small in terms of parts per billion. So, you know, so there is a range.

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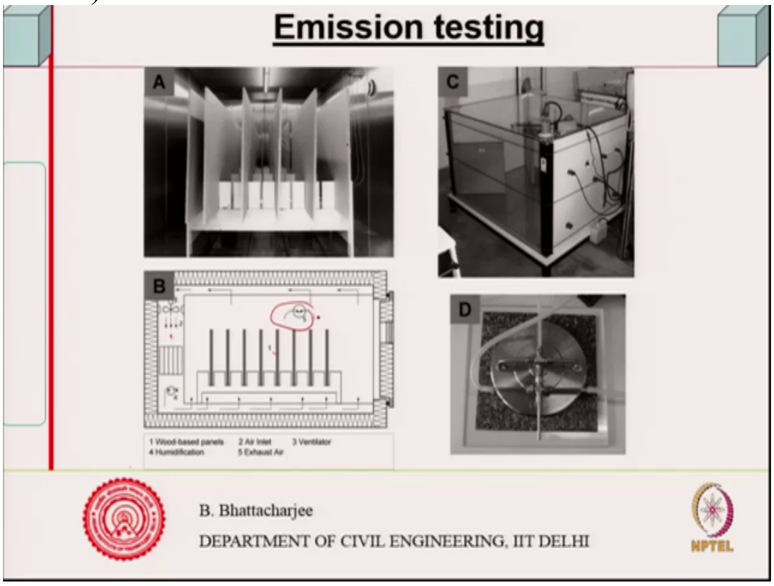

Emission testing

1 Wood-based panels 2 Air inlet 3 Ventilator
4 Humidification 5 Exhaust Air

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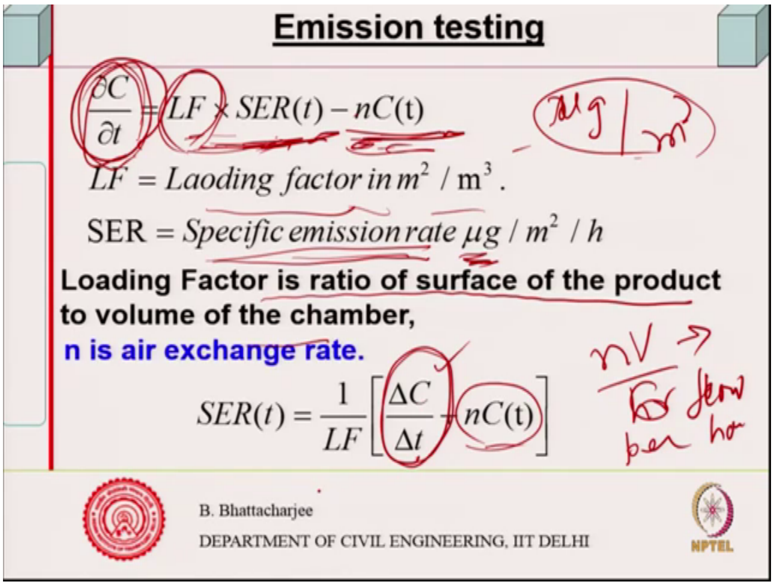

Emission testing

$$\frac{\partial C}{\partial t} = LF \times SER(t) - nC(t)$$

μg / m³

LF = Laoding factor in m^2 / m^3.

SER = Specific emission rate $\mu g / m^2 / h$

Loading Factor is ratio of surface of the product to volume of the chamber,

n is air exchange rate.

nV →
for flow
per hr

$$SER(t) = \frac{1}{LF}\left[\frac{\Delta C}{\Delta t} + nC(t)\right]$$

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So this is how the testings are done, testings are done like this, right, this is your this is basically you have a ventilator, so we looked into the room itself, you can measure. But then for testing purpose same thing, you have a volume where you put this your materials and then allow air to come in, fresh air to come in and go and the same, similar kind of models you can use, right.

So these are your supposing it is your board, these are your boards for where you have the which can generate volatile organic compound. So one is the wood based panels let us say, these are the panels for which I want to measure. So if it is a painting I want to measure, maybe I will have paint on them. Number of them actually then, 2 is air inlet, so where is 2, there must be a fan somewhere air inlet. This is 4, this is 2, so there is a fan, this will bring in air, this brings in air. And air flows like this, 3 is ventilator, 3 is ventilator, right, 3 is ventilator and 4 is humidification, you might do some humidification using a humidifier that is you spray some water moisture, so maintain the right kind of humidity.

And 5 is exhaust, there is a exhaust fan which will take out. So basically you have a system which is you know sort of insulated from all outside. You have the panels mounted, right and you have a ventilating system through which you actually allow air to come in, might humidify to maintain the right kind of humidity that is and there is an exhaust which will take it out, right, which will take it out.

So then rate of change of concentration is a function of what we call loading factor, metre square per metre cube, I will come to that what is loading factor actually, it is actually related to the panel themselves. And specific emission rate what I am interested in. So where loading factor is the ratio of surface to the product, surface of the product to volume of the chamber. For example, if you put in that many number of panels surface areas are known, sum total of the surface area divided volume of this whole chamber, that is what is loading factor, so loading factor of the panel themselves, loading factor for the panel themselves.

So loading factor how much meter square per meter cube I know? So 1 meter cube I am taking, multiplied by the specific emission rate microgram per meter square per hour, so this will give me in terms of micrograms per hour for the whole volume minus C t, the concentration at any time, so rate of change of you know rate of change of n is a number of air changes actually, n will be number of air changes, did I mention this? n is the air exchange rate, number of air exchange rate, right exchange rate, what is that? How many times the volume of the room gets replaced in one hour, so we call it air change, we call it air change, you know.

So if the volume is V, n V per hour, you know n V with the Q, flow per hour in one hour. So one hour you will have n into V of the room and this was already meter cube, this is loading factor is related to per meter cube divided by I have already divided with room volume, so this is simply the volume of the room will go out because both sides volume of the room I have already divided by and here n V is the Q in meter cube per hour where volume of the room, n is the number of air change per hour.

So n into C t concentration changes because that is what is going out of the rate of flow, so if the concentration within the room is C t, number of times in one hour how much volume will go? n V into C t, that is what we will go out and but this is we are talking in terms of per meter cube. So therefore this also you should talk in terms of 1 meter cube, so if I consider 1 meter cube volume then n C t is the number of you know n C t is the what will go out, C t is the concentration at time t and n C t is the n into 1 is the rate of flow metre cube that is going out. Since this is in terms of microgram per meter cube, I mean the concentration could be in microgram per meter cube, so this is meter cube that is going out in 1 hour. So that is how, so this will give you the quantity that is going out at any time, this is the specific emission rate at any time and this is the loading factor, so this is emission. This is what is going out, remaining will go on changing the concentration with time within the room, right.

So SER therefore one can write from this, rate of change of dc dt n C t, so if you do a measurement now change in the concentration with time within the room, same I mean not room, within this within this space, this one, so we will measure the concentration. You might do sampling and then continuously go on measuring sampling or continuous step-by-step sampling of that to be done and this could be measured in a chromatograph to find out a particular type of emission, could be HCO or whatever you are interested in and you know, so you can find out rate of change, C values you can find out as a function of time. And if you find out C value as a function of time, you know, this then dc dt can also be found out.

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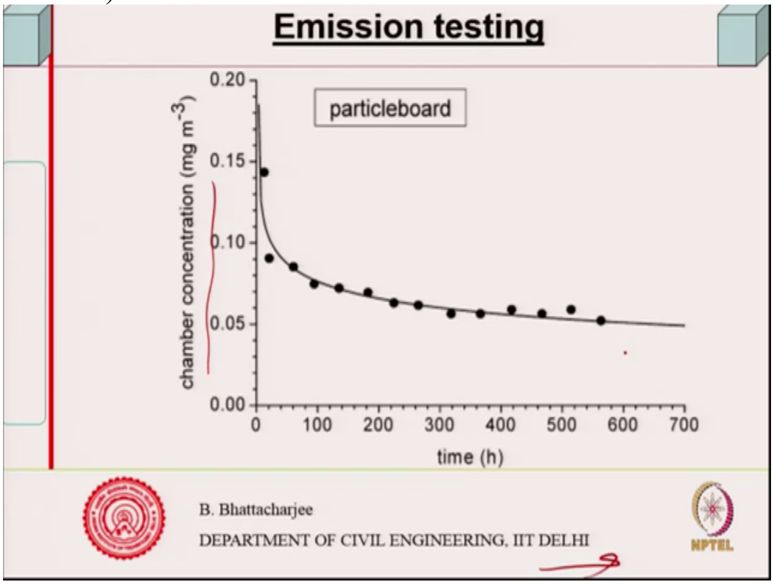

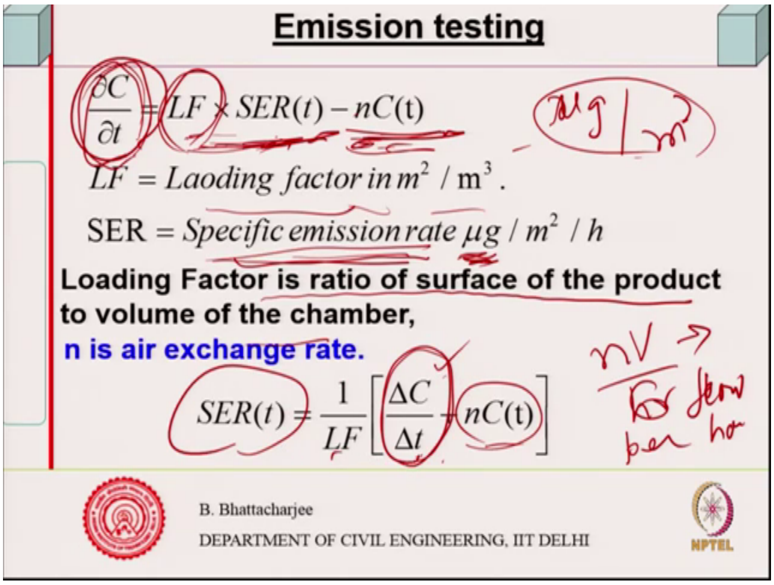

Emission testing

$$\frac{\partial C}{\partial t} = LF \times SER(t) - nC(t)$$

$\mu g / m^3$

LF = Laoding factor in m^2 / m^3.

SER = Specific emission rate $\mu g / m^2 / h$

Loading Factor is ratio of surface of the product to volume of the chamber,

n is air exchange rate.

$$SER(t) = \frac{1}{LF}\left[\frac{\Delta C}{\Delta t} + nC(t)\right]$$

$nV \rightarrow$ for flow per hr

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Because you will find out you know, so you will find out a curve like this. Okay, I will come to this later on but first let me go to this. So you will find out time versus chamber concentration in appropriate unit, this is shown in milligram per meter cube or microgram per meter cube whatever it is for some particle board. So therefore C at any time you can find out, dc dt at any time you can find out because these are the points, you have fitted a curve to this. So both C and dc dt you can find out and therefore dc dt both can be found out. So rate of finite form delta C by delta t one can find out and if you know the loading factor then specific emission rate as it is a function of time that you can find out, specific emission rate.

So the model first thing is why did I explain you the Fick's diffusion law, because it is based on Fick's diffusion law, the second order differential equation actually you are not using much here but that is what is a Fick's diffusion law. I have used it elsewhere also, then we talked about kind of a model that can be there, that means mass balance is what we are looking on. If something is coming in, the air is coming in and same rate of air is going out through exhaust and inlet, I know the rate that is going in and coming in, right and then volatiles will be emitted out from the surfaces.

It could differ if the thick surface at x equals to 0 and x equal to L, at x equals to 0 they will be on concentration, at the surface there will be another concentration, so flux at the surface is known to us, that will add to the VOC in the chamber and air that is coming in will take away some of it. Whatever is remaining will go on increasing the concentration into the room. Therefore this model you can apply to a chamber and estimate the specific emission rate in terms of microgram or milligram or whatever it is meters per hour, right. So that is the equation then turns out to be.

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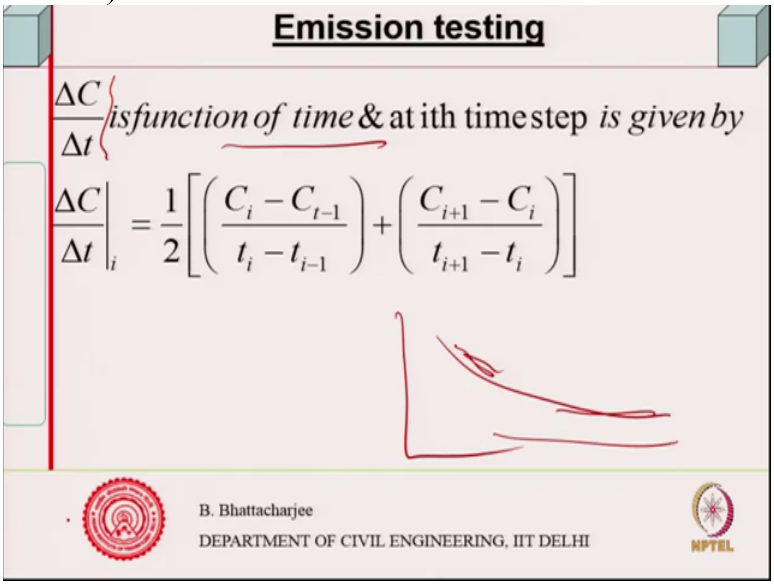

Emission testing

$\frac{\Delta C}{\Delta t}$ is function of time & at ith timestep is given by

$$\left.\frac{\Delta C}{\Delta t}\right|_i = \frac{1}{2}\left[\left(\frac{C_i - C_{t-1}}{t_i - t_{i-1}}\right) + \left(\frac{C_{i+1} - C_i}{t_{i+1} - t_i}\right)\right]$$

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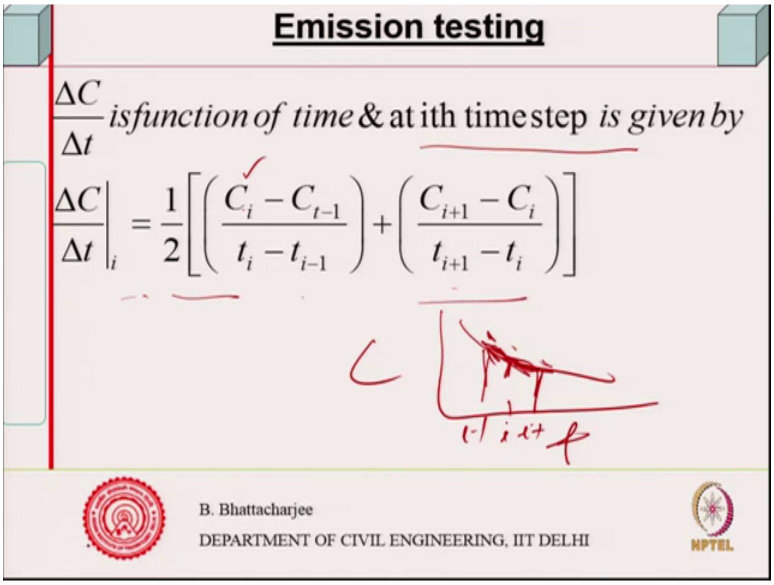

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Let us look a little bit more. Supposing dc dt is a function of time, that is what we have seen because it will be curve like this, this slope is also changing the values are also changing, C is changing and dc dt because it is parabolic. If it was linear, dc dt would have changed but it is not linear because we have also said that it is a function of the difference in the concentration, that is what we try to get a convective transfer coefficient.

So at ith time therefore one can find out like this between two points, you know at ith time because it is a plot time versus C. So at C i, C i minus 1 and C i plus 1, so this is i, i plus 1, i minus 1, so you can take dc dt at this point as a central difference, C i minus this so this is this, you know, we are interested in the slope. So it is a central difference, we are taking half of this and half of this average, so average of this slope and average of this slope. So there is C i minus C i minus, t minus 1 sorry C and similarly this i minus 1, t i minus 1, et cetera, et cetera. And this is the plus side and average we are taking. So you can find out this once you know we have measured the concentration with time.

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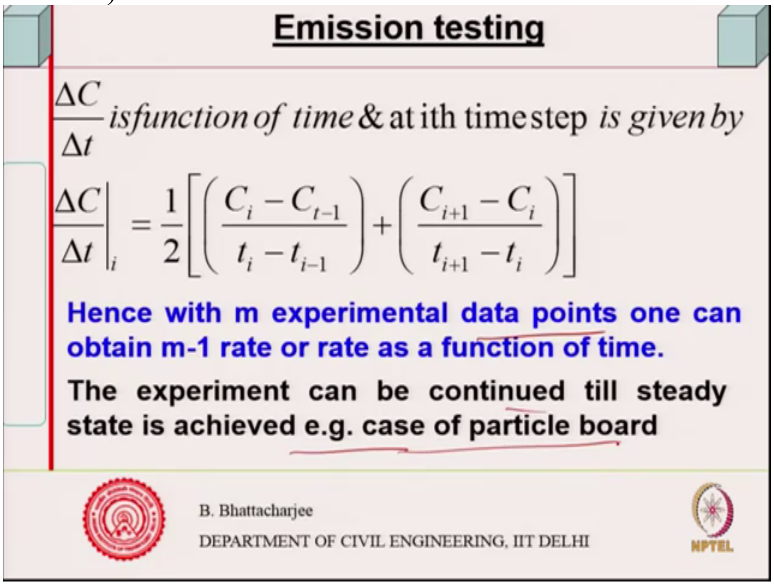

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$\frac{\Delta C}{\Delta t}$ *is function of time* & at ith time step *is given by*

$$\left.\frac{\Delta C}{\Delta t}\right|_i = \frac{1}{2}\left[\left(\frac{C_i - C_{t-1}}{t_i - t_{i-1}}\right) + \left(\frac{C_{i+1} - C_i}{t_{i+1} - t_i}\right)\right]$$

Hence with m experimental data points one can obtain m-1 rate or rate as a function of time.

The experiment can be continued till steady state is achieved e.g. case of particle board

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And with experimental data points one can obtain m minus 1 rate or rate is a function of time as well, so you can find the rate also as a function of time and the experiment can be continued till steady state is achieved because after sometime it will tend to be steady and this once that is achieved okay, you need not continue further. So therefore the rate of emission in the, you know, during initial hours that would be known to you.

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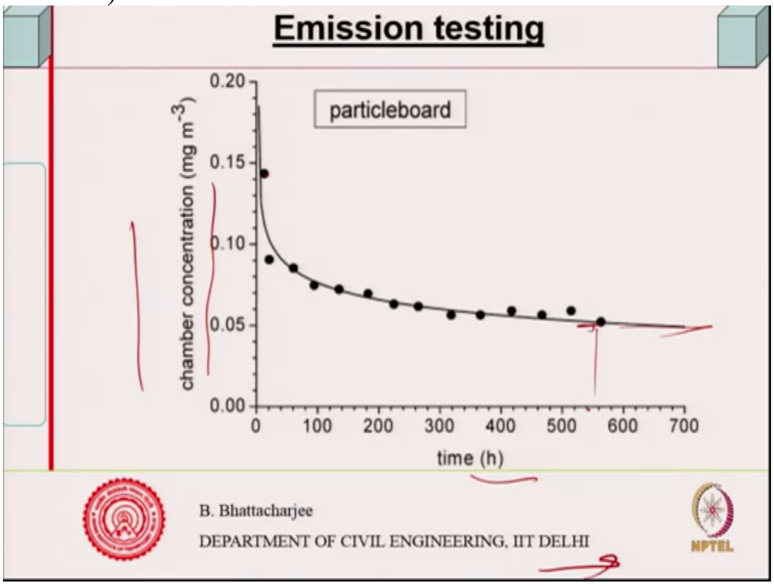

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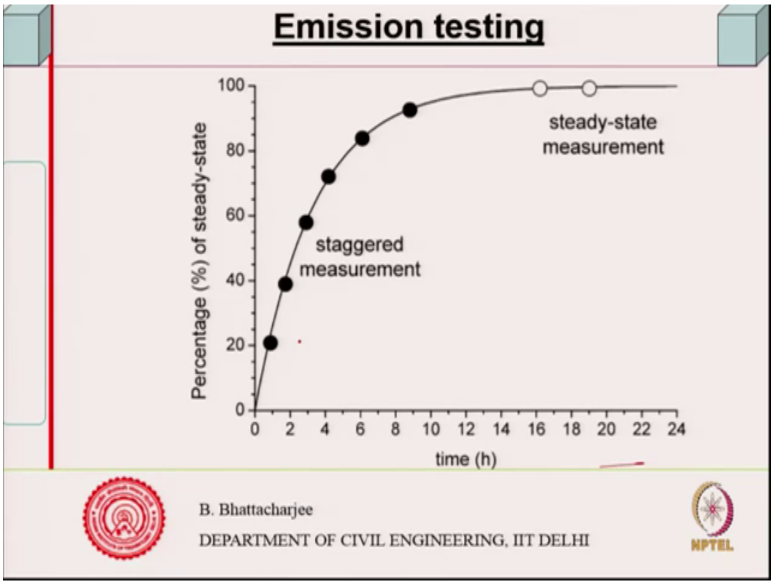

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So this is the type of curve for particle board this is shown, right. Time versus chamber concentration, so this is the C versus t time t curve and DC versus percentage of steady, percentage of steady state is reached after let us say 24 hours or something like that. So this is the steady state and in the beginning this value is very small, then by you know 500 or 600 hours or something like that depending upon the material, so steady state one can depend upon where you are reaching, staggered measurements, so it is you know percentage of steady state rate one can find out. So for example, initially very little then this percentage of steady state concentration one can find out.

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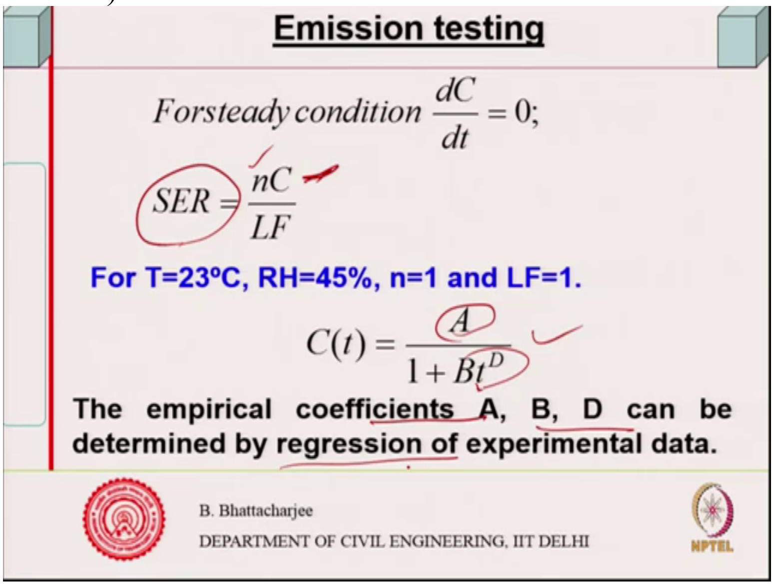

Emission testing

$$For\,steady\,condition\ \frac{dC}{dt} = 0;$$

$$SER = \frac{nC}{LF}$$

For T=23°C, RH=45%, n=1 and LF=1.

$$C(t) = \frac{A}{1 + Bt^{D}}$$

The empirical coefficients A, B, D can be determined by regression of experimental data.

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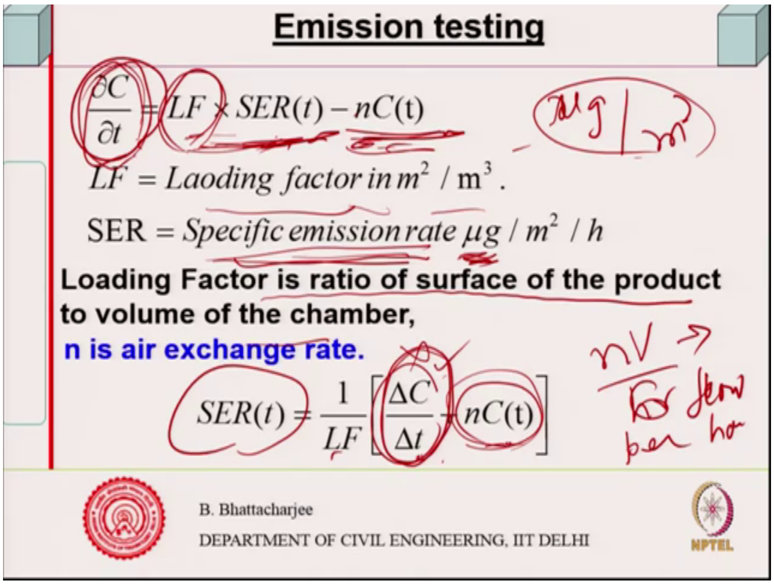

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μg / m³

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Loading Factor is ratio of surface of the product to volume of the chamber,

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nV →

for flow per hr

$$SER(t) = \frac{1}{LF}\left[\frac{\Delta C}{\Delta t} + nC(\mathrm{t})\right]$$

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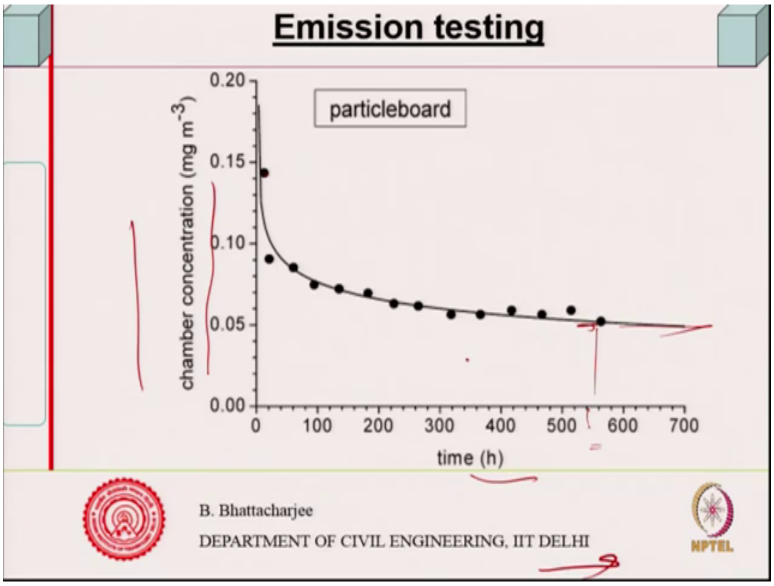

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So for steady state dc dt is equals to 0. So SER is equal to n C by LF loading factor because this term will be equals to 0, this term is equal to 0, this term is equal to 0, you know, this is this term is equal to 0, this is 0, so 1 by LF n C t. So if you know the steady state value, which is not changing with time steady state value constant, steady state value dc dt, so n C, this is the steady state value, after sometime it will reach to this level.

So the emission rate, specific emission rate can be found out in this manner for measurements. Loading factor you know, the number of air changes you know, C you know, and generally C t can be C t can be of this form of curve because you know, this is an exponentially decreasing curve. So one can fit, various kinds of curve could be fitted but people have tried to fit in something like this. That means when t equals to 0 concentration is A and as t increases this reduces, right. And when t is equals to Infinity, C t becomes, basically t is equals to infinity, C t will become you know, it will tend to become 0, it will tend to become 0, right? It will tend to become 0, okay.

So at t equals to 0, t is equals to 0, at t equals to 1, of course one can find out but does not matter. This is a form of curve people use, so empirical coefficient A, B, D can be determined from regression of experimental data, right? So this is what people have done as far as emission rate is concerned.

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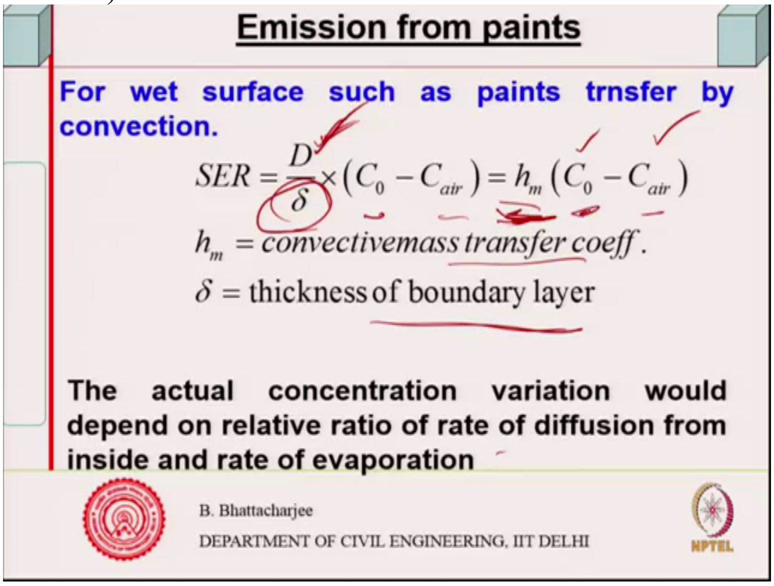

Emission from paints

For wet surface such as paints trnsfer by convection.

$$SER = \frac{D}{\delta} \times (C_0 - C_{air}) = h_m (C_0 - C_{air})$$

h_m = convectivemass transfer coeff.

δ = thickness of boundary layer

The actual concentration variation would depend on relative ratio of rate of diffusion from inside and rate of evaporation

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And specific emission rate if thickness of the boundary layer is delta then this h m also we can obtain because C in the air and C 0 at the surface one can find out, D is the diffusion coefficient. Effective thickness of the boundary layer one can obtain, we do similar things in heat transfer also.

So from analogy of heat transfer, convective heat transfer coefficient can be related to equivalent surface conductance, here we are talking in terms of an equivalent thickness of boundary layer D C 0 C air et cetera, et cetera. So for wet surface such as paints transfer is by convection largely, for wet surface evaporation will occur and the vapor could move by convective heat transfer because you know temperature difference could be there. Evaporation is occurring, the temperature is lower at the surface. Since evaporation is occurring it will absorb latent heat of evaporation, so what we call in case of relative humidity what we call wet bulb temperature, so this will be in wet, its temperature will be lower, right? So heat might be transferred in this manner, but vapour will be transferred outside.

So this, you know surface the paints the convective heat transfer might takes place, I mean convective mass transfer might take place and actual concentration variation would depend upon relative ratio of rate of diffusion from inside and rate of evaporation that is occurring. So how much it is diffusing? If the diffusion rate is faster then evaporation rate, then they will be high concentration there and in fact, then you know the concentration changes because h m is fixed, C 0 is higher now. Now, so more flux SER will also increase.

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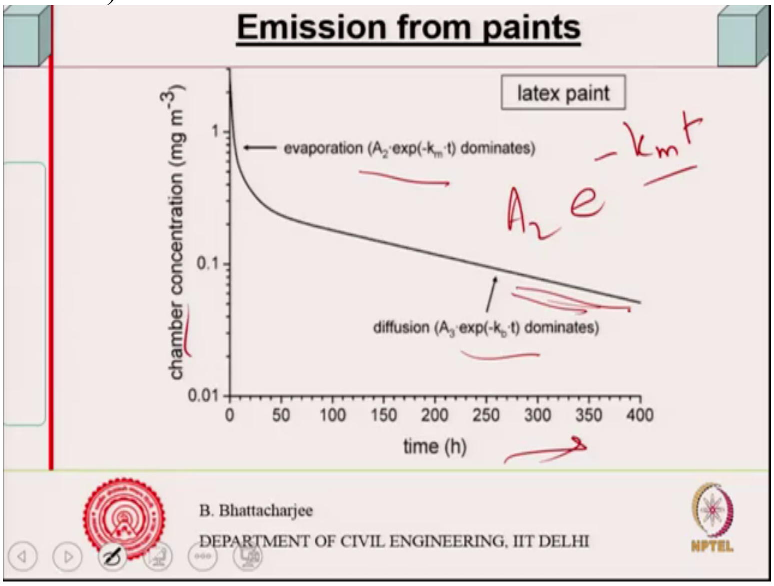

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So this is what it is from paint, latex paint. If you look at latex paint time chamber concentration, time and chamber concentration and one can evaporation is A 2 e 2 to the power, you know it is something like A 2 e to the power minus k m into t, that would dominate during this phase lot of evaporation and later on diffusion process would dominate. So evaporation more, so therefore the concentration is not reducing, you know, the concentrate time concentration is I mean evaporation is occurring and concentration changes are occurring. Later on it has a tendency it would generally e to the power A 3 exponential k 0 that would dominate where diffusion process is occurring. So that is how that is what is related to emission from paints, that is how we measure and what we are interested in SER, the specific especially in steady state situation later or even in initial situation.

So how much volatile organic compound it emits during those period of time, so when you look into some of those, some of those rating system like lead et cetera, we will see how this is taken into account in those cases because the one which are you know, they must be within permissible limit and if you do not use such materials which have got higher emission rate, you get points, right? So look into that when you look into those ones, I think that finishes our discussion on VOC emission part.