Environmental Air Pollution

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Lecture No. 29

Air Quality Modeling – 2

I was just looking at the notes yesterday that somebody has copied.

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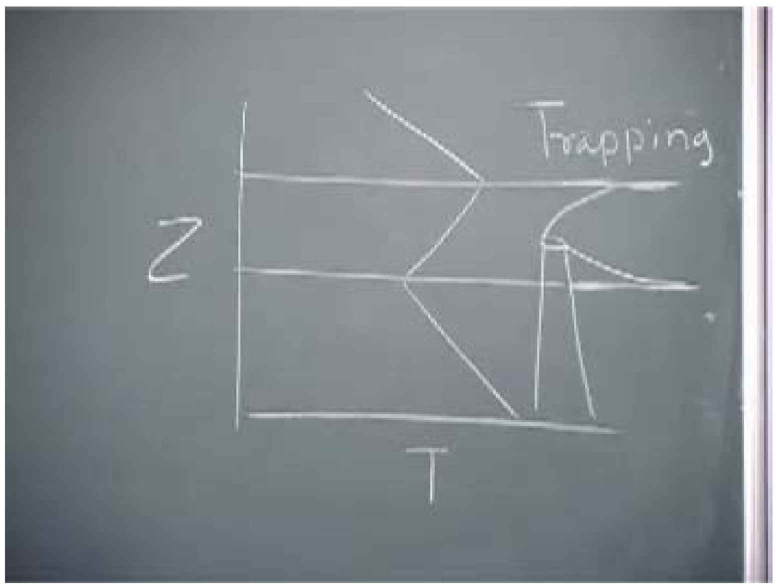

[00:27] some small thing. If you go back to your notes, is that what we said or we said something else? [01:11] Did we say it this way? Yes sir. Right, no confusion about it because… obviously… but this is not correct, this is not correct. Do you think this is correct?

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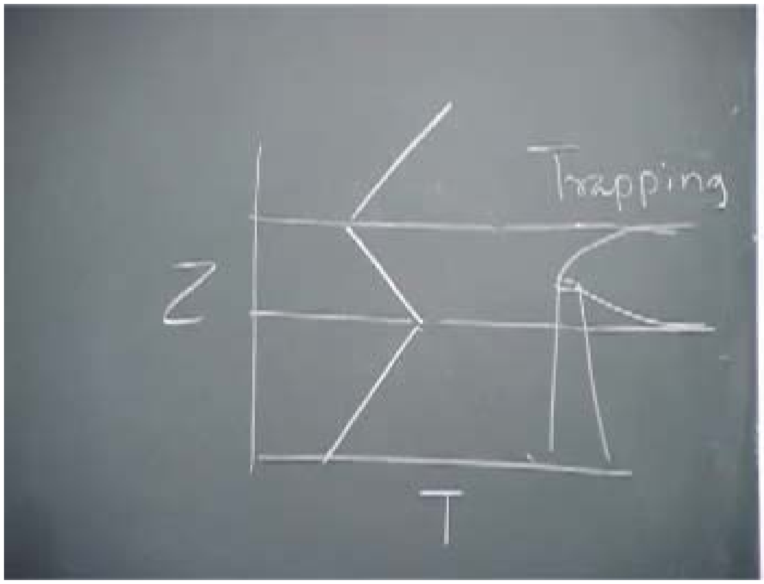

This is not correct because for this to be correct, it has to be inversion here, dispersion permitted here and again…. Does this make more sense? This makes more sense. You see here since this is inversion (Refer Slide Time: 02:18), no dispersion can take place here; there is again elevated inversion (Refer Slide Time: 02:22), so there is no dispersion that can take place here; here (Refer Slide Time: 02:28), you see either the conditions are neutral or unstable, so the dispersion will take place in that little layer that is left. For the trapping, the atmospheric conditions in terms of the temperature and the height would have an elevated layer on top and ground-based inversion – inversion on top and inversion at the bottom. Is that clear now? We were discussing about the modeling part because we have understood, we have studied at least to a small extent what is meteorology and what is atmospheric phenomena. I will do it again – about the box model.

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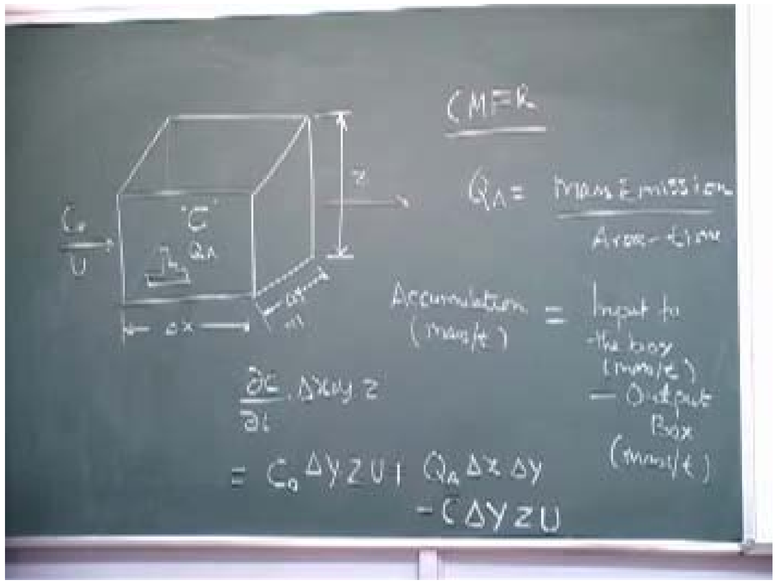

You have a box and the wind may be blowing like this and it is going like this and I am calling this as delta x, this as delta y and I am calling this as z and I assume delta y to be unity because I can have many boxes and if things are similar… so the condition across or in the cross-wind direction… this is the wind direction (Refer Slide Time: 04:19), it will always be the same in the cross-wind direction. We said there were some emissions that might take place inside the box and we call that as Q_A and the wind that is blowing in the box, which may be a part of city or you can divide a city into many boxes. Here is the initial concentration – the concentration outside the box, let us say C_0 and wind speed is U. Then we want to find out the concentration inside the box, which may be typically your city. To find out this, what we set was accumulation in the box equals to input to the box minus output from box and units since we are doing mass balance, it should always be mass per time, mass per time, mass per time.

So accumulation I can write as… I will directly write in differential form del C by del t. I have to get the units to mass per time so what do I multiply here (Refer Slide Time: 06:04)? The volume of…? The box, sir. The volume of the box, right? We are inside the box, so y times z equals the input of the box, one is this input (Refer Slide Time: 06:23), so this will be concentration C_0 times the area, the cross-sectional area – that is y times z or delta Y times Z times wind speed. What else is the input? Q_A and let me define Q_A

equal to mass emission of whatever the pollutant is per unit area per unit time. So Q_A. What do I do? Multiply by the… [07:34] the surface area of the box – that is delta x times delta y and output. I am assuming the box to be a completely mixed reactor. So what do I do? Minus. Suppose the final concentration in the box is C and the box you are modeling as CMFR – completely mixed flow reactor, so then, what I can do is C times delta Y Z times U – this is what I can write. What do I do if I say that the pollutant inside the box is somehow decaying or reacting with time? That is possible because some pollutants within this box can go undergo some kind of transformation or change, so what do I need to add here? What we will do is we will do this analysis first and we can also add another term where some decay of the pollutant is going on. Let us do this one for the time being.

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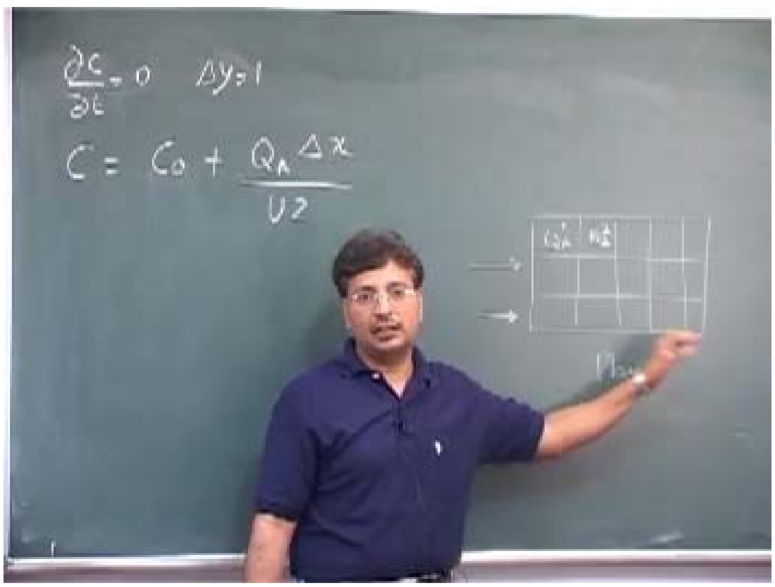

If you simplify this and put at steady state… goes to 0 and if you can give me the expression and I put delta y equal to 1, then the expression which we wrote yesterday was C_0 plus Q_A delta x by U Z. Is that what we got last time? Things look simple but they have lot of applications. You can divide the whole city into grids. I am making a plan of the city. Suppose the wind is blowing like this (Refer Slide Time: 10:24), Q_A may vary from Q_A one, Q_A two and so on and so forth; wind is blowing, so whatever is the concentration C, that becomes C_0 for the next block and that way you can solve it continuously, the concentration here, here, here, here, here (Refer Slide Time: 10:50).

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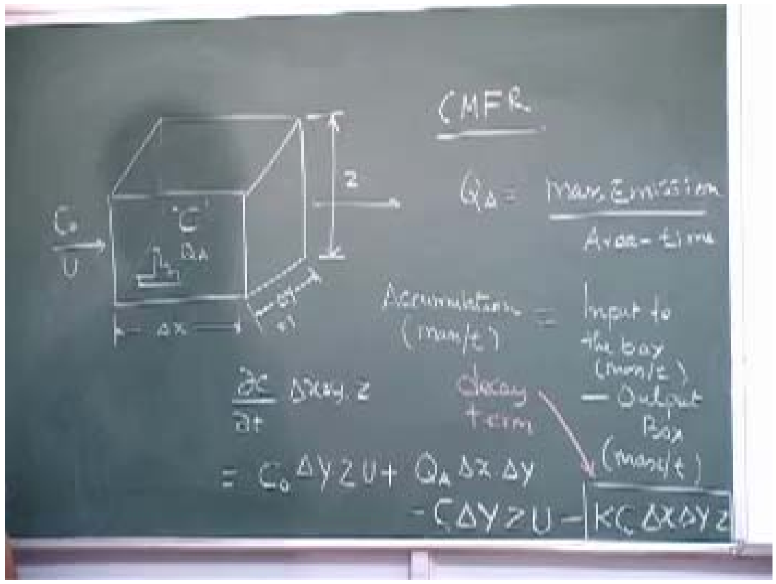

Before we make some example, suppose the same pollutant was decaying in the box, it means the output is just not only because of the wind that is kind of cleaning the box but there is a decay. The rate constant for decay is let us say K – you have done that before, the decay rate constant the pollutant, whatever that pollutant is, it means concentration will decrease. What do I write if decay constant is K? K C. K C, all right K C. Is that all? [11:41] Times…? delta V. delta V. What is delta V? [11:49] [11:53] K C, what do I write? [11:59] [12:02] Volume. Volume, correct. I am saying this thing is decaying, so you have minus K C, we have to get the same dimension – mass per unit time and K has units that is decay constant is always time inverse, so C by T in a way, so I must multiply this with volume. Does everyone agree with me? We are also considering the decay of the pollutants so i can say delta x times delta V times Z – this is the decay term (Refer Slide Time: 13:02) and you can still simplify the equation and you will get some answer.

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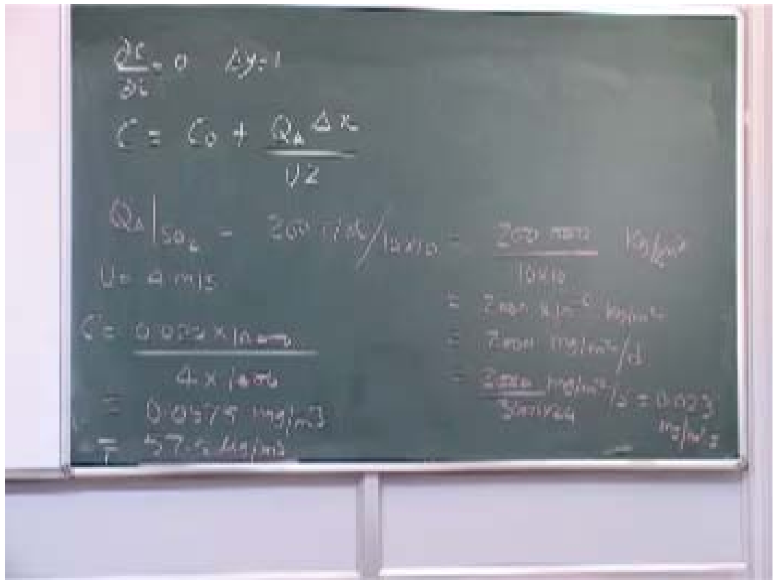

I will do a very simple example – a kind of realistic thing that we had. It was estimated that Q_A of SO_2 in Kanpur was of the order of let us say 200 hundred tons per day. This was the total in the city, so you divide the city area let us say by 10, by 10, so that comes out to be 200 – that is kg, kilometer per square. With simple this thing when the concentration was estimated and that concentration came out to be much less than what was the measured concentration. If you want, we can do this calculation quickly. Just help me in doing this calculation. This is kilometer square – do not forget. I can say 200. [14:32] 2,000 and if that is kilometer per meter square with 10 to the power of minus… —6, 6, this is kg per meter square. I can say 200, so kg I can convert into…? Grams. Grams, so that will be 10 to the power of —3 milligram, 10 to the power —6 gone, so it is so much milligrams per meter square. Let us do it in milligrams: 2,000 milligrams per meter square per day. Suppose this is the emission that we are talking about, let us also do this one in terms of seconds, 200,000 milligrams per meter square and for this, I have the calculator, so I will do that – 2,000 divided by 3,600. [15:52] Oh yes, there has to be 24 too. Suppose this is the number and wind speed was let us say 4 meters – that is the average wind speed. Supposing that I can simply find out C, suppose initial concentration outside Kanpur I assume to be 0, so the Q_A is 0.023 times delta X – that is the length of the city I can take, that is equal to… that many meters divided by 4 meters per second divided by the mixing height – I can take that as 1,000 meters, that is typical, that we discussed, so Z equals 1,000. How much does this give you? This goes off, this goes off (Refer Slide Time: 17:16) and this will be 2.5, so I will give you the exact number; in terms of microgram per meter cube, this will be…? 57. 57, so you expect average concentration of sulfur dioxide in Kanpur to be about 57.5 micrograms per meter cube. Is this part clear?

The idea is not simply doing the calculation part. You always deal with the actual things as a field engineer and you should make some sense out of it. Then we compared this number with the measurements done in Kanpur for several years and we found that average concentration that was measured in Kanpur at some five different locations were always around… it varied between 15 to 25. Suppose the actual concentration is 15 to 25. What would it say is either this number is incorrect (Refer Slide Time: 18:50) or what could have gone wrong. Then, we checked this number over and over again, compared with various cities and we thought this number was very good. We are almost getting just the half of this one (Refer Slide Time: 19:06). We are talking very broad estimates – we have not done any kind of sophisticated modeling nor are we talking about great deal of numerical models and using the computers.

If this was 57.5 – I am telling you the real example – the measured values were 15, 20, 15, 20 for many years. Then obviously what we thought… immediately you think maybe the measurement of sulfur dioxide is not correct because mathematics is probably all right, we then checked the methods and the methods were all all right, then we thought what could possibly go is that maybe this thing is happening (Refer Slide Time: 19:49). Then, research was done here and then we said along with sulfur dioxide, what can happen to sulfur dioxide with your atmospheric chemistry? What will happen to sulfur dioxide? Go into sulfates – that is the first primary reaction. Then along with this one, sulfate measurements were done and then sulfate measurements were almost twice the value of sulfur dioxide – again, I am talking at the broad scale, not very fine scale – and that told us there is something else happening. One of the reasons of not getting the sulfur dioxide at the average levels… we are not talking about specific, we are not talking about a particular day, but we said there was something wrong and then we found this particular thing was important and that is how we found that the sulfate levels were higher and in fact at most of the places in northern India, sulfur dioxide is very quickly converted into sulfates whatever the reactions are. So you apply this thing.

The other application can be… suppose the reaction was not important, then you can say this is not properly done (Refer Slide Time: 21:03) or you can also find out… suppose if this was higher and this term was giving lower (Refer Slide Time: 21:10), it means the pollution is coming from outside. Simple application. You should always think – not only about getting the numbers and doing things but as to how you can apply at the broad level. When you at least know the broad picture, then you can go to the finer details slowly. Here, we have not considered any turbulence – it is just completely a mixed flow reactor. Let us slightly go into some specific thing now.

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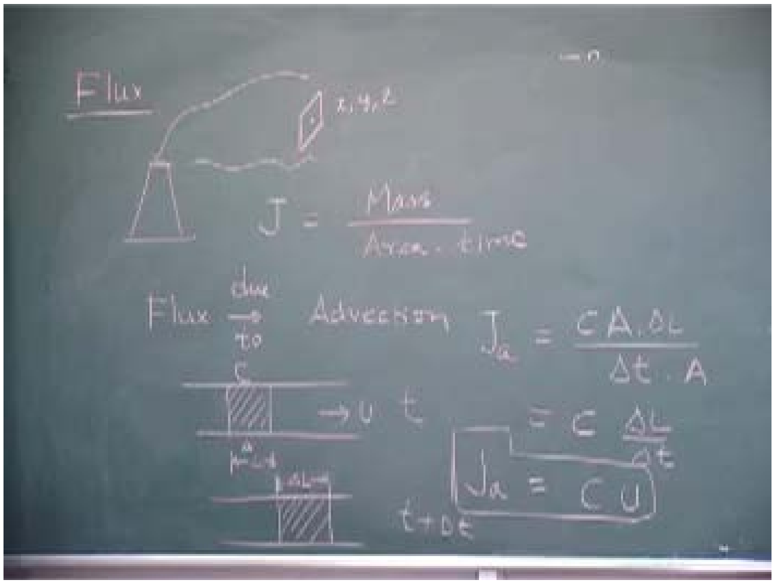

I want to talk to you about flux, pollutant flux because we are going to use this a lot. How do we define the flux? Suppose this is a chimney, I am just giving you an example, and the pollutants are traveling. If I have let us say a block, not only a block let us say I have a strip and the point here is let us say x, y and z. If I have to define the flux J, this is nothing but mass of the pollutant per unit area that is the area into time. Now, the one thing you want to define, another thing is flux due to advection. Suppose there is a pipe.

We are just going through the definitions right now and you are looking at the strip that has concentration C at time t, this length is L and after some time, the distance traveled t plus delta t and this length… let us call this as delta L really (Refer Slide Time: 23:41), delta L and I want to find out the C, so let us see the mass.

Let us say I want to find out the flux due to advection. What is the word advection I am using? When there is a flow, then there is advection; when there is no flow, there is no advection. It is the advection part. What can I do about write the flux due to advection is concentration times I can write the volume, so that will become my mass per unit time. What will volume be? Suppose the cross-sectional area is A, so A times delta L. Did I get the mass? Suppose the velocity is U. I can divide this by delta t. Is this the flux? Mass per unit or this is not the flux as yet. So what do I do? Multiply by A. Do you agree with me that this is the flux?

If this is the flux, A cancels out, this will be equal to C times U, so this is one information that we need to remember because we will be using this information sometimes. So flux due to advection is the mean concentration times the wind speed. If C is changing with respect to time, things will be different – then we have to have the derivatives. If U is changing with respect to time, then things will be different. We have just considered one direction – that is why we have to take only the one direction wind; if the directions were different.… The problem with air pollution as we will see is always three-dimensional. Water pollution you can probably modulate with a two-dimensional thing, ground water flow you can modulate with one dimension – it is just one dimension going down, but in air we will use the three-dimensional thing. We will see slowly as we move, we will go to three-dimensional thing. The next thing that we would want to talk about is the… we will leave this one there but we will use it at some point.

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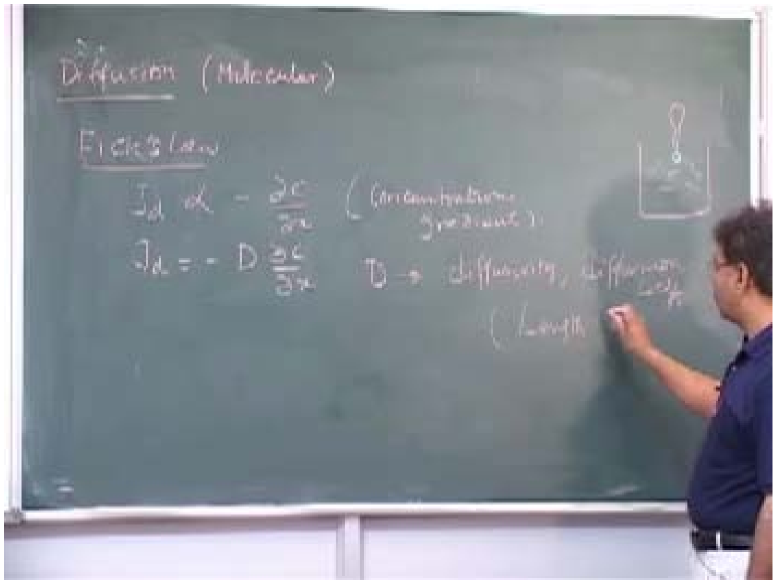

I will write about the diffusion part. Let us say for simplicity we talk only about the molecular diffusion, molecular diffusion. Do you remember the Fick's law? By molecular diffusion, what I really mean, if I can give you simple example, you have the water filled here and you have a dropper and you drop ink, let us say and after some time, you see the ink is getting diffused. In this case, the Fick's law says the diffusion or the flux is J, what name did we give it? A – that was for advection. For diffusion, let us call this as d.

With time, the flux is reducing, so that is proportional to minus of concentration gradient – that is the Fick's law. This J_d, constant of proportionality, we are just talking one dimension – do not forget about this and D as you will remember from the earlier classes is called the molecular diffusivity or diffusion coefficient. Well, molecular is anyway we are talking about… this is the diffusivity or diffusion coefficient. What will be the units of D? Please tell me, because many students forget the units of D. Quickly derive so that you are sure about it. [29:34] Meters per…? [29:39] Meters per time, meter square per time. [29:42]. Meter square time square? You tell me, I will write the number. [29:48] Length square per time – do not forget that.

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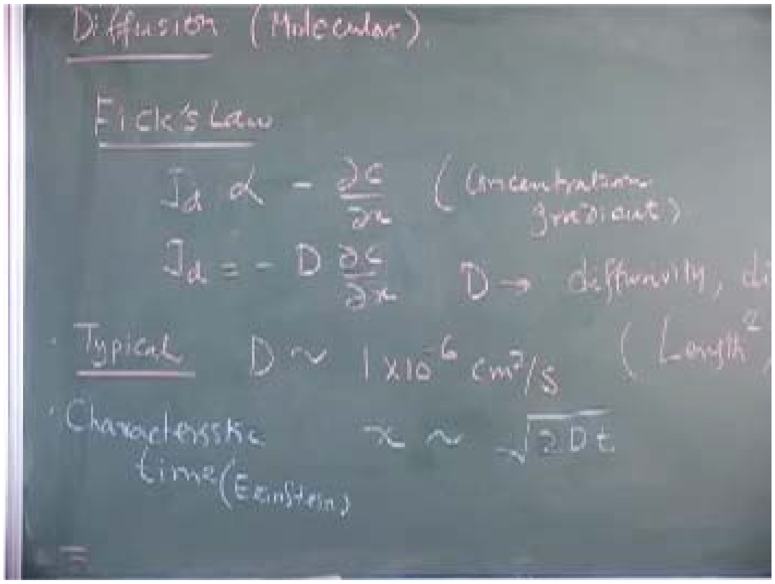

Characteristic value of the molecular diffusion depends on the substances we are talking about, it depends on the medium in which it is getting transported, it depends on the characteristics or the properties of the substance that is being diffused. A typical characteristic value in the air, typical for particles, typical value of D is of the order of.… Let me check the number. That looks good. Again, you have noted this one down, so I will remove this. Another simple example: suppose… this value of… Let us also define another thing: characteristic time for the molecular diffusion. This was given by Albert Einstein. He said that the typical distance of the diffusion, how far the thing will go is of the order of 2 times Dt. Again, what are we talking about? Do not forget: we are not jumping anywhere else but we are just talking about molecular diffusion right now. I just worked out a very hypothetical example.

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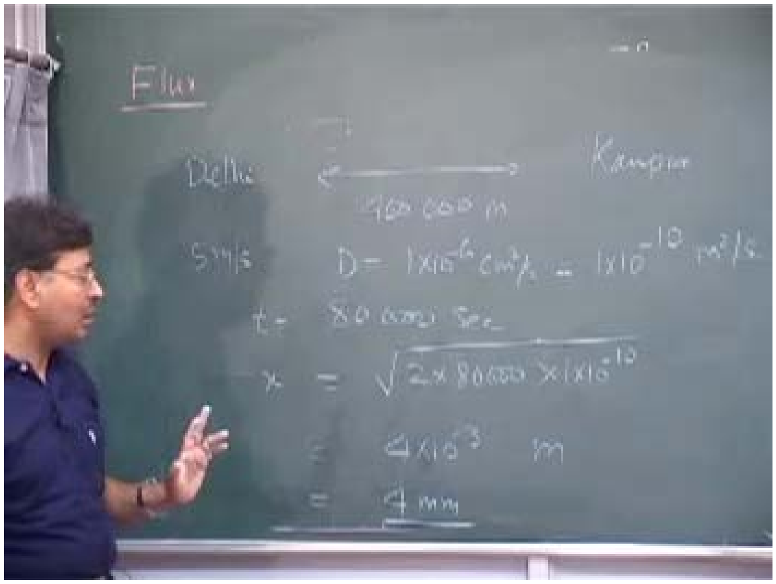

Suppose from Delhi a non-reactive pollutant is going and coming to Kanpur and the wind speed as 5 meters per second. Suppose this wind speed is maintained and the distance I took as 400 kilometers or you can say 400,000 meters. Suppose only the molecular diffusion was taking place and your D, take that as 1 into 10 to the power of —6 centimeter square per second or if you want to convert this into meters then what will this value be? 10 meter square per second. I want to find out what is the characteristic distance the particle will disperse, so if there was a flue that was going on, how much the pollutants will disperse from their mean position – that is what we want to find out.

Again, a very hypothetical unrealistic example but then we want to conclude something at the end of this one, so what do I do? What I need is the time. I can find out the time that will be taken for the pollutants to travel from Delhi to Kanpur and of course you can do that. I will try to give you the number and that time came out to be, correct me if I am wrong, as 80,000 seconds. Correct. The steam t was 80,000 seconds and now I have everything what I need there. x, the mean dispersion that will take place in the X direction of course, we are just assuming one direction – that came out to be 2 times D is here what and since I brought my calculator, I might as well do it. How much? 4 into 10 to the power —3. [34:55] Somebody said 4 into 10 to the power —3. Well, we are assuming that to be correct, but this you can correct even if it is wrong, it does not matter, so that is in meters. That will be equal to 4 millimeter? 4 millimeter.

If this was the situation, I think we cannot live on this earth because if the pollutant travelled and then only the mean distance it travelled was only let us say 4 mm, it means that something more is happening. So the molecular diffusion gives us the basis, it gives us the argument to develop but then it is not the molecular diffusion alone that takes place in the atmosphere. Then, this theory is fine when you are talking about the small system where molecular diffusion is the only effective but you will see here molecular diffusion cannot be effective in this case in our atmosphere as to.…

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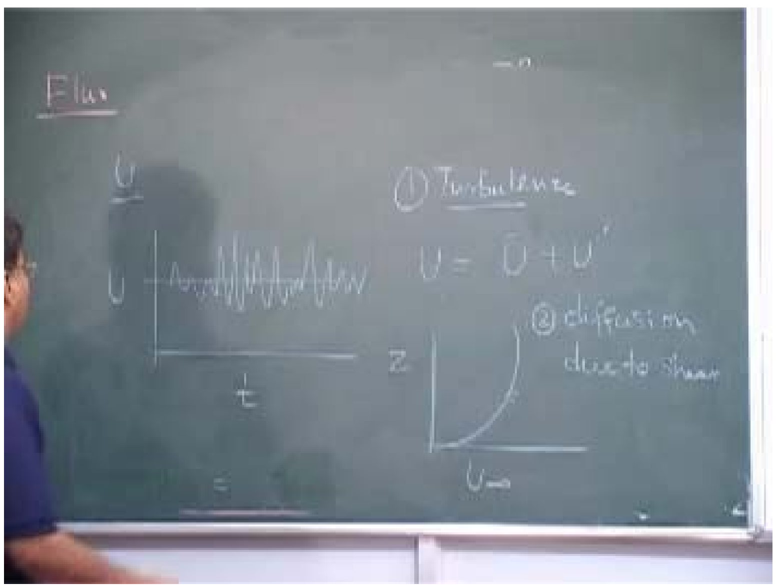

The basic thing U is never fixed. Always, there are fluctuations. If I have to plot the U with time, you might have the average velocity like this, so that U at any time, any instant time is U bar plus… that is U bar plus the plus or minus whatever the fluctuations may be in terms of this one. That is the situation that is existing. Another thing what we know is this will create not the steady state conditions, this will add to the diffusion parts, so diffusion will be much more.

Another thing that I can tell you is the wind profile will be like this in the atmosphere. This is your Z and then what we are plotting this side is U. At any instant point we take, the velocity just above that point is different and velocity just below that point is different. So there is always a shear, so there will be shear diffusion in addition to what we are talking about. Shear diffusion or diffusion due to shear that is [37:49]. Now, what you want say is there is one part, one diffusion is because of turbulence, so this (Refer Slide Time: 38:10) is because of the turbulence. If there was no turbulence, then you get the straight line, so the turbulence. Second thing is diffusion. If I have the turbulence and diffusion, I might still be you can use the Fick's law because this will still be this thing, but what will change is the D because D will no more be molecular diffusion in the atmosphere, but it could be a combination of molecular diffusion plus turbulence diffusion or the diffusion due to shear. That is what we have to consider in our next calculation; whatever we do, we should say….

If you really want to find out what will happen to the pollutants when they travel from Delhi to Kanpur, they are not going to disperse just by 4 mm or whatever number that we got but it will be much more. Let us say we utilize this knowledge. If you say this D will vary, then with your knowledge of class, two classes, what will this D depend on? What determines the turbulence in the atmosphere? Mixing height. Mixing height is one thing and the other thing… mixing height because of the wind pattern. [39:38] What is that thing which we have spent so much of time understanding and that influences the turbulence? [39:48] Radiation, solar radiation. Solar radiation, but then that solar radiation we have measured in what terms? Atmospheric…? Stability. Stability, so you say here the D will be a function of atmospheric stability. See sometimes, we want to learn not in terms of quantitative but we should get the feel qualitative; that is what is more concept – to get the qualitative sense of the thing. Mathematics can be done, mathematics is there in the books but then, we want to see… because this theory is pretty well developed, everyone knows about this one, so the D will be function of the atmospheric turbulence and atmospheric turbulence as the air pollution person or the meteorologists we say the indication or indicator of the turbulence is the atmospheric stability where we spend of so much time learning the atmospheric stability. Then we want to start something new but I think time stops us here. Unless you have a question, we will stop the class here and meet in the next class because I want to derive I am sure you must have heard about…

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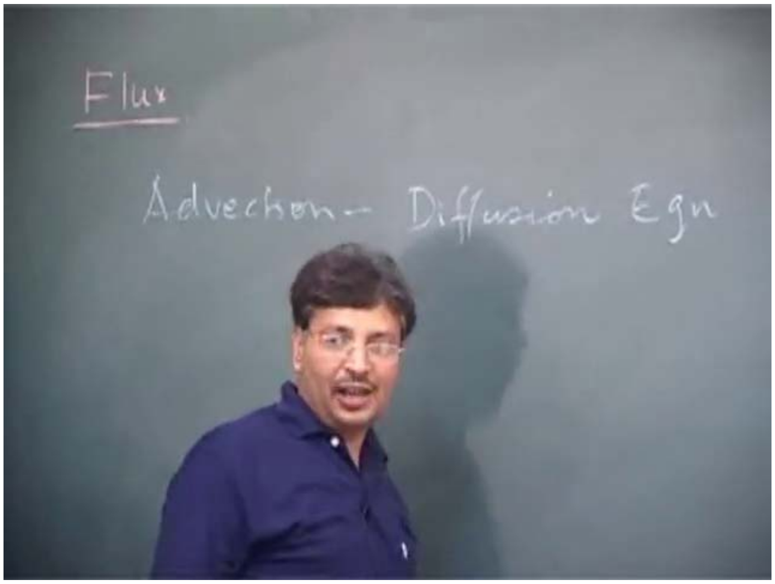

It will take little time, so I will draw some boxes, we will stop it there.