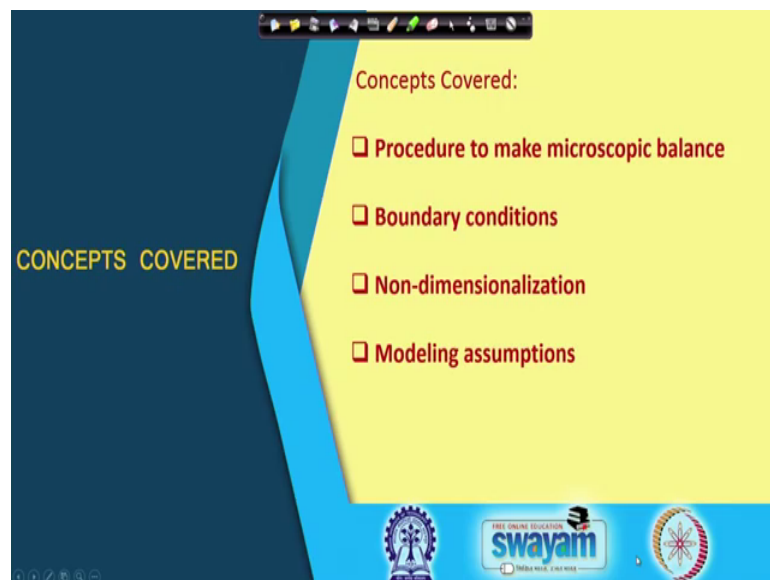


Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture – 30
Microscopic Balances – VII

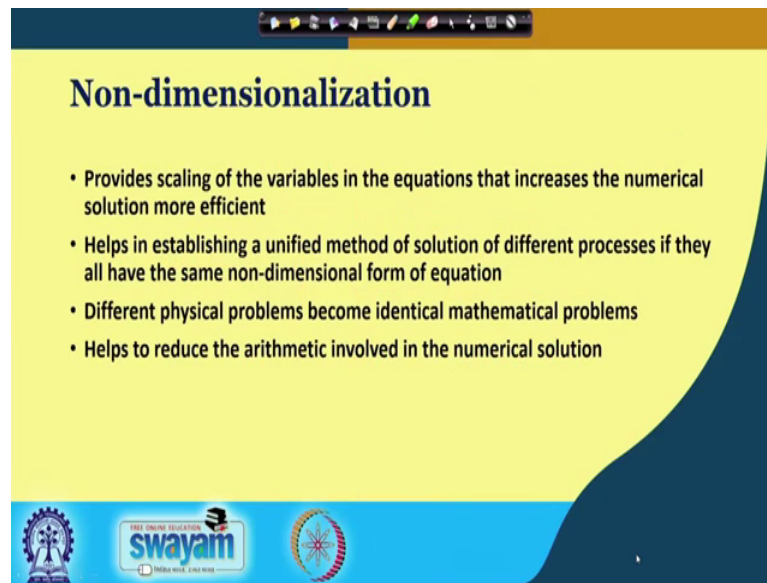
Welcome. After knowing about the various types of modeling assumptions and looking at how we can get the model equations from a full 3D unsteady state equation. Today we shall be looking into the another aspect that is of the non-dimensionalization. So, first let us understand that what is the significance of non-dimensionalization.

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Now, many a times we have known that we find the equations which are not in a dimensional form that is there is no as such any unit associated with any of the terms of the particular equation. And in that case, you will find that we are having many times some numbers, which we call the non-dimensional numbers based on which we made such solutions.

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Non-dimensionalization

- Provides scaling of the variables in the equations that increases the numerical solution more efficient
- Helps in establishing a unified method of solution of different processes if they all have the same non-dimensional form of equation
- Different physical problems become identical mathematical problems
- Helps to reduce the arithmetic involved in the numerical solution

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And there are methods to find out the non-dimensional numbers which I shall not be talking about and which are taught separately under transport phenomena and fluid mechanics. What I shall be dealing with is that how to non-dimensionalize the model equations, and when we the non-dimension of the model equations we obtain certain non-dimensional numbers and after this non-dimensionalization is done.

So, first let us understand why do we need to non-dimensionalize. It is not mandatory, but it is suggested that to the extent possible one when after you have deduced the model equations which are in the dimensional form. If possible, make it non-dimensional before you go for the solution of these equations and the advantages of converting the dimensional form to non-dimensional form will be now listed. First is that it provides some scaling of the variables in the equations that increases the numerical solution more efficient.

So, when you are non-dimensionalize enough equations you find that many of the terms may not be relevant for the given situation. So, you find that sometimes you will end up simplifying the original equation and that way you find that your numerical solution also becomes more efficient then the another advantage is that, it helps in establishing a unified method of solution of different processes if all of them have the same non-dimensional form. It is especially true when you go for the transport phenomena processes.

Now, even though apparently the momentum transfer, the heat transfer, the mass transfer look different. But when you see the model equations you can easily find that there is a similarity in the mathematical representations of all these apparently different type of processes. Now, when this is the case then you can obviously, say that the mathematical techniques used for the solution of these equations will also be the same. So, when you are making these numbers non-these equations non-dimensional, you will find that you have the equations, they have the similar structure, ok, and with the similar type of the non-dimensional numbers.

When I say similar type, it means that that every time we are not getting same non-dimensional numbers. For example, Reynold's number may be appearing in the momentum balance, in the energy balance, in the mass balance but for example, your were some other numbers like the Prandtl number, the Sherwood number these are pertaining to either the heat transfer or the mass transfer respectively.

So, you will find that such kind of analogous number like the Sherwood number which appears in the mass transfer equation has an analogous a number that is Nusselt number in the heat transfer. Similarly, the Prandtl number which is there in the heat transfer equations we have an analogous number in the mass transfer at the Schmidt's number, ok. So, in that fashion you will find that the, you will find analogous numbers are appearing in various transport phenomena equations in terms of the energy balance, momentum balance, and mass balance, ok.

So, when these kind of things happen you find that even though the numbers may look different, but the form of the equations remain the same and you can deduce the similar conclusions from all these apparently different types of equations. So, that is why the theories become unified, ok. And next, the different physical problems began identical mathematical problems.

So, we are able to reduce the apparently different types of physical problems into similar type of mathematical problems, and this way we are able to reduce the arithmetic involved in the numerical solution. It means that suppose you solve for some momentum balance equations, and under similar condition if you have a mass transfer or heat transfer; you will find the form of the equations remain the same. So, whatever solutions

you have obtained for the momentum balance equation will also be applicable for the mass balance or the heat balance.

So, I shall not be going into the solution of this but we shall be looking into some examples of how to non-dimensionalize a given an equation which were obtained from momentum balance, energy balance or the mass balance.

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Example


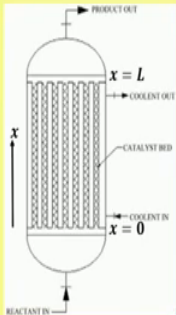
- Consider the steady-state operation in packed bed reactor. A reaction takes place in the bed. Assuming plug flow, only axial diffusion of the species is considered. Mass balance for a such system is given by:

$$\frac{d}{dx} \left(D \frac{dc}{dx} \right) + R(c) = 0$$

Where c is the species concentration, D is the diffusivity, x is the axial direction, L is the height of the reactor, and $R(c)$ is the rate of reaction, that is a function of the concentration c .

Let us assume a second-order reaction, that is, $R(c) = -kc^2$

Where k is the reaction rate coefficient.



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So, here is one simple example. In this case we are having a steady state operation of an packed bed reactor about the packed bed reactor I explained you how it works and what is meant by packed bed reactor in my earlier lecture. So, I will not be going into a detail of the operation of a packed bed reactor.

So, here we have a packed bed reactor and in this some reaction takes place and here we see that reactant is going from the bottom and it is coming out from the products are coming out from the top. And here for the mathematical analysis we have shown the axis that is the x axis, which is having the origin at the base of the particular catalytic bed and on this top, we have the length of the catalytic bed or the packing. So, it is mentioned that we assume plug flow.

So, as I explained to you earlier that when we make this plug flow assumption, we get a one-dimensional flow, and in this case, we will be having the axial flow and there will be axial diffusion is considered. That means, there will be a gradient or the distribution of

the composition or the component concentration along the axial direction along the flow direction. So, because of this gradient there will be a diffusive flow, ok.

So, the this that is why we say that there will be axial diffusion and due to plug flow assumption in the radial direction there will not be any gradient, that is we are taking the radial mixing complete mixing in the radial direction. And mass balance for such a system reduces to this.

Now, you see that when we are doing this this particular plug flow assumption then we find that there will not be any variation with respect to the y , m , r and θ direction because we are taking axisymmetry. So, only thing we shall be having will be in the axial direction, ok. And we are talking about the diffusive term, so this is a diffusive term and we also shall be having the source term and because we have assumed this to be a steady state operation. So, there is no time derivative in the mass balance equation, ok. So, we this this is the diffusive term which is coming from the balance and this is the source term which is also appearing due to the reactions of the particular components.

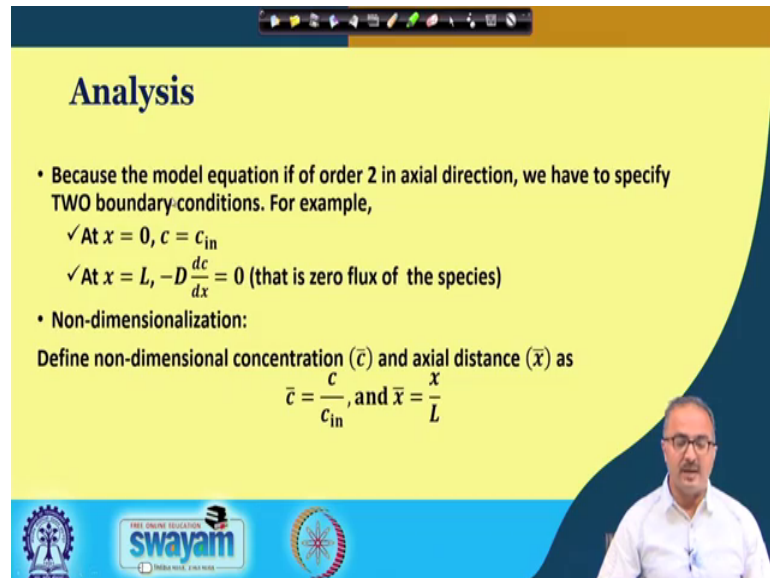
So, here we have explained all the notations used in this particular analysis and for the reaction rate that is assumed that it is a second order reaction so that the rate of reaction is given in terms of this, like we are given in terms of the square of the concentration. Now, here the negative sign shows that there particular component is being consumed. Now, if a particular component is generated then we put a positive sign, ok. So, that is the significance of the sign being for the reaction rate.

And k is the reaction rate constant. As I told you in the previous class that the reaction rate constant may be obtained from the Arrhenius type equation, ok. An Arrhenius type equation is used if there is a change in the temperature. That means what? That if we consider this reaction to be having a thermal effect also because of exothermic or endothermic effects, then we will also write one energy balance equation, and from the energy balance equation we shall be able to obtain the temperature distribution along the flow direction.

So, for the sake of simplicity and for the sake of demonstrating how we go for non-dimensionalization? I have just considered the mass balance equation, but you can extend it very easily for the energy balance equation and non-dimensionalize it, ok. So,

for the time being we are taking this particular k to be constant without loss of any generality.

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Analysis

- Because the model equation is of order 2 in axial direction, we have to specify TWO boundary-conditions. For example,
 - ✓ At $x = 0$, $c = c_{in}$
 - ✓ At $x = L$, $-D \frac{dc}{dx} = 0$ (that is zero flux of the species)
- Non-dimensionalization:
Define non-dimensional concentration (\bar{c}) and axial distance (\bar{x}) as
$$\bar{c} = \frac{c}{c_{in}}, \text{ and } \bar{x} = \frac{x}{L}$$

Now here we have that because in this equation we have this double derivative, ok, so we need two boundary conditions as I explained to you in my earlier lecture. So, because of this we need two boundary condition and two boundary conditions are like one we put at the inlet. And for example, at the inlet we specify the composition or concentration of the particular species, so we are writing the concentration is equal to some c_{in} . And then we are writing for the other end that is the x equal to L to the height of the particular packed bed reactor we are putting the flux to be 0.

As I told you earlier that these are not restrictive you can have in this particular case you may have this particular c as a function of time t , ok. It need not be constant it may be varying with time at the inlet, ok. And similarly, here it need not be 0 it may have some finite value, ok. This will depend on the particular situation at hand.

And now, let us go for the non-dimensionalization of this of this equation. Now, for that let us define two non-dimensional parameters like one is \bar{c} another is \bar{x} . Now, this \bar{c} is defined as the ratio of the actual concentration to the inlet concentration, and similarly the \bar{x} is defined as a ratio of the axial position divided by the total length of the particular reactor. Now, in this case you see that many times when we do this kind of non-dimensionalization, we also get another advantage in

terms of the domain of the particular non-dimensional parameter. Here you can see is this that we know that the c whether if the c is the raw material concentration the maximum c could be only c_{in} , it cannot exceed that, ok.

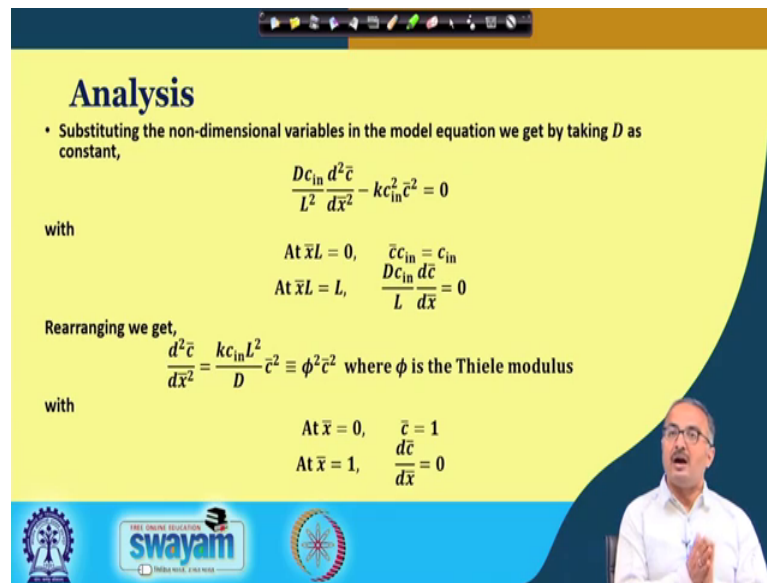
And if this whole raw material is getting consumed then this c will be reduced to 0. That means, for this particular c over bar will be now restricted between 0 and 1. Similarly, when you look at x over bar what you find that with at the starting x is 0 and at the end of the reactor that x is equal to L . In that way you find that x over bar also has a domain it is between 0 and 1.

And how does it help? This kind of situation is called normalization; that means, we are normalizing the particular variable; that means, we are restricting the values between 0 and 1. And that way whenever we are trying to get the solution of the equations, we have a check that we know that in terms of the non-dimensional variables we cannot have any solution which is less than 0 or more than 1.

That means, if we are getting some solution which is showing this kind of things happening but we are getting more than 1 or less than 0 in terms of the non-dimensional numbers we know that we have done something wrong. So, this kind of non-dimensionalization should be done very discretely to the extent possible we want we would define the things in a manner that they are non-dimensionalized and also at the same time normalized.

Please understand it is not always possible to get normalized non-dimensional numbers, some many times it so happens that there is no bound after we non-dimensionalize it. So, if to the extent possible we will try to get normalization but if it is not possible it is, ok, ok. But incidentally, in this case we find that the non-dimensional parameters are also normalized.

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Analysis

- Substituting the non-dimensional variables in the model equation we get by taking D as constant,

$$\frac{Dc_{in}}{L^2} \frac{d^2\bar{c}}{d\bar{x}^2} - kc_{in}^2\bar{c}^2 = 0$$

with

$$\begin{aligned} \text{At } \bar{x}L = 0, \quad \bar{c}c_{in} &= c_{in} \\ \text{At } \bar{x}L = L, \quad \frac{Dc_{in}}{L} \frac{d\bar{c}}{d\bar{x}} &= 0 \end{aligned}$$

Rearranging we get,

$$\frac{d^2\bar{c}}{d\bar{x}^2} = \frac{kc_{in}L^2}{D} \bar{c}^2 \equiv \phi^2 \bar{c}^2 \text{ where } \phi \text{ is the Thiele modulus}$$

with

$$\begin{aligned} \text{At } \bar{x} = 0, \quad \bar{c} &= 1 \\ \text{At } \bar{x} = 1, \quad \frac{d\bar{c}}{d\bar{x}} &= 0 \end{aligned}$$

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Now, after defining the non-dimensional numbers we again go back to the parent equation and there we are now going to put the non-dimensional parameters replacing the dimensional parameters.

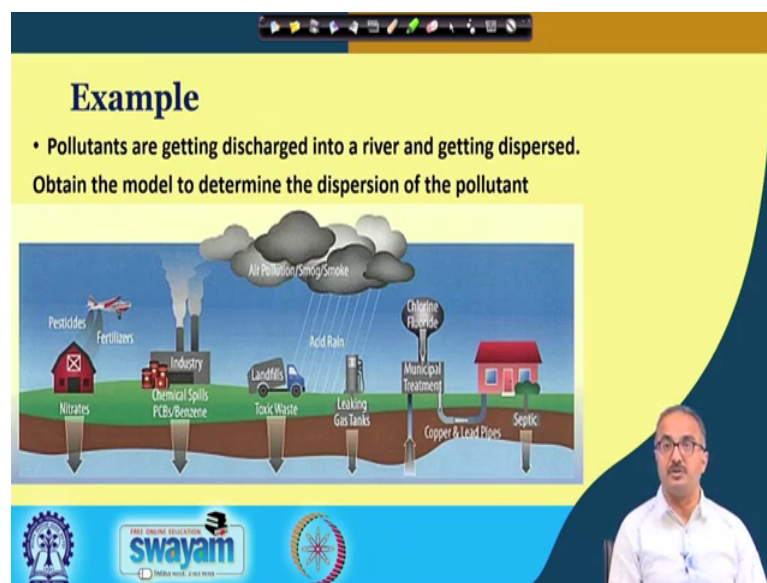
And in this case what we are doing we assuming that the diffusivity is constant so that we can take it out of the differential. And then when we take it out of the differential and we put the dimensional parameters in terms of the non-dimensional parameters we have this particular equation. After you obtain this equation it is now simply a way of mathematical manipulation to get the non-dimensional form of the mass balance equation. And please remember that you when you non-dimensionalize you not only non-dimensionalize the balance equation, also you non-dimensionalize the boundary conditions and initial conditions as the case may be.

So, here also we are putting the dimensional form of the boundary conditions in terms of the non-dimensional numbers. So, here we obtain this non-dimensional form of the boundary conditions, ok. And after you do the manipulations, we obtain this but this particular equation that is for the mass balance equation and these equations we got for the boundary conditions. And when as I told you earlier that when you are non-dimensionalizing you land up with some non-dimensional numbers, and here we have one non-dimensional number that is phi and this phi is called the Thiele modulus, ok.

And this Thiele modulus gives us the relative importance of the reaction rate and the dispersion of the component; that means, for that how fast because we need that whenever their reaction is happening, because of that there is a change in the composition. At the same time because of dispersion also because they due to the gradient in the concentration within the particular reactor there will also be a change in the composition, so which of these two reaction or the dispersion are playing the major role, ok. So, that is given by the Thiele modulus, ok.

So, this is how we are having this, the particular rate of reaction this mass balance equation in terms of the Thiele modulus when we are non-dimensionalizing it, ok. And this is now I will stop up to these equations we are not going into the solution of this particular equations, ok.

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Next, we come to a very common example in which we find that many a times we are quite nowadays quite concerned with the environmental pollution. And you know that environmental pollution may be happening due to some land pollution, due to water pollution, due to air pollution. We have also noise pollution; we have thermal pollution but as far as transport phenomena based analysis is concerned we will be talking about the air pollution or the water pollution where there is some dispersion of some pollutants, ok. So, we are talking in those terms. And we can even talk of thermal pollution where we can use the energy balance equation. So, here in this example I shall be talking about

the pollution which with respect to the mass balance that is done some species is getting dispersed and this species is the pollutant, ok.

And you know that in this particular schematic figure what I have shown, the various ways the air pollution and water pollution may happen. Here you can see that from the various industries the effluent gas that comes out that will take that may have some very different types of a components, in those components are some compounds of sulfur or nitrogen etcetera and they will be now getting into the atmosphere and this emitted air may also contain suits that is unburned solid particle or some burnt ashes. They will also be there in this particular emitted gases, and due to these presence of the particulate gases you will find that this water will condense all these particulate matters and they will form smog.

Especially you see these smogs, in the winter in many of the cities and this causes a big problem because it reduces the visibility and causes accidents. So, this you keep hearing from time to time in the news, ok. And this is nothing but the dispersion of various types of pollutants in the air, ok. And that is why you find that nowadays we are talking so much about the reduction of the environmental pollution.

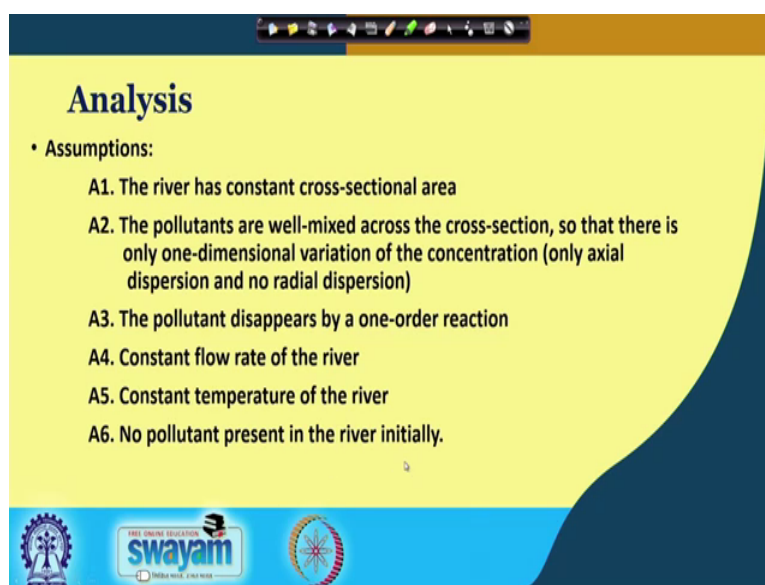
Next is the water pollution. Now, water can also get polluted in various ways I have shown you some of the ways water may get polluted, right from the industries many pesticides or many bad chemicals are being ejected into the rivers or some water bodies from the industries. For example, laser industry, a textile industry, dyes are coming out, from these paints are coming out of this and they are going into the river and they are polluting the river.

Then, we have some pesticide from fertilizer plants, we are getting many pesticides or herbicides which are coming into the river, then from various landfills that we are whenever we have some pits we put some landfill to construct some may be some other things, the buildings on those landfills. And the landfills themselves may have many toxic matter in them and they also ultimately seep through the ground and they go into the water bodies and they also cause the land pollution, ok. And perhaps you know that in many places we have the arsenic pollution, the water that comes out that has a lot of arsenic and that causes many kind of diseases to us, ok.

And then we have some kind of leaking gas plants, then from municipal treatment also from our household applications we are getting many minerals and other things into the water body. And here you can see that from the smog or from the air pollution due to air pollution we are getting acid rain because these nitrogen oxides sulfur oxides, they form some acids in contact with the water. So, these are the various ways these positions are occurring.

Now, our concern is this how we can apply our these balance equations to know that how the pollutants are getting dispersed into the atmosphere. So, for this particular problem we have taken only river pollution and we are seeing that some pollutants are getting discharged into the river and getting dispersed. So, we have to obtain the model to determine how the pollutants are getting dispersed into the river.

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Analysis

- Assumptions:
 - A1. The river has constant cross-sectional area
 - A2. The pollutants are well-mixed across the cross-section, so that there is only one-dimensional variation of the concentration (only axial dispersion and no radial dispersion)
 - A3. The pollutant disappears by a one-order reaction
 - A4. Constant flow rate of the river
 - A5. Constant temperature of the river
 - A6. No pollutant present in the river initially.

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For the sake of simplicity, I have considered only one species but you can extend it for multi species. So, here we make some assumptions, to just give you a feeling that how we can model it.

So, first assumption is that we consider that river to be to have some constant cross-sectional area. This assumption may be taken if our domain of study is a given region, ok, in that region we may because a river may not be having too much of change in the cross-sectional area, from one end to the other end. So, we can obtain we can assume safely that it is having a constant cross-sectional area.

Then pollutants are well mixed across the cross section. So, that there is only one-dimensional variation of the concentration; that means, we are assuming that across the river cross section there is a pollutant the pollution or getting well mixed, and so that there is the pollutant concentration is changing only in the flow direction, and not across the river.

Then, pollutant disappears by some first order reactions there is one order reaction is there, there they are getting dispersed by that there is some reaction is occurring and they get dispersed. So, then we have constant flow rate of the river, then constant temperature of the river. These constant, it means it is not that the river changes its flow rate very frequently, ok. So, for a given for finite time period we may considered that the river has a constant flow rate.

And thermal, thermally also in generally many a times we find that because it has a large thermal capacity, ok. So, even though we might be adding some kind of hot streams into the river or might we might be having adding some cold stream to the river but because of the high thermal capacity of the river we say that it is acting as a sink and a an ideal sink is one which does not change its temperature, ok, from that point of view we assume that the river is at a constant temperature. So, that for the given period of time there is no change in the temperature and we may need not we did not consider the energy balance. And we also assumed that no pollutant is present in the river initially that kind of gives us the initial condition for this analysis.

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Analysis

- Since flow is one-dimensional and constant, momentum balance is not written
- Since temperature is constant, energy balance is not written
- Since pollutant concentration changes along the flow direction, component material balance is written as

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial z^2} - u \frac{\partial c}{\partial z} - kc$$

Where c is the pollutant concentration (kg/m^3), k is the reaction rate constant (s^{-1}), D is dispersion coefficient (m^2/s), u is the river velocity

- Initial condition $c(z, 0) = 0$
- Boundary condition $c(0, t) = c_{\text{in}}, \quad \left. \frac{\partial c}{\partial z} \right|_{(L,t)} = 0$

So, since the flow is one-dimensional and constant, so momentum balance is not written. So, we are not concerned about the momentum balance. Then as I said the temperature is constant, so we are also not writing the energy balance. So, only thing we are writing is the mass balance because the pollutant concentration is changing along the flow direction. So, again if you can see the total equal mass balance equation in three-dimensional steady state you find that we are retaining the unsteady state term and then we are keeping the diffusion of the term, ok.

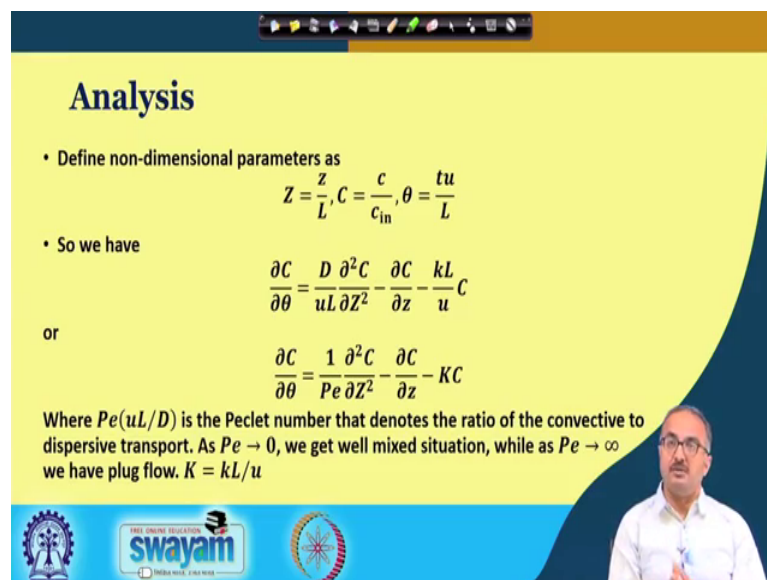
And this is coming due to the one-dimensional flow of the river and is a convective term and this last term is the source term as the pollutant is getting is disappearing due to some first order reaction. So, that is how we are obtaining we are reducing the three-dimensional unsteady state a mass balance equation in a one-dimensional unsteady state equation, ok. After this, what we do? That I have also given you the units of the radius, SI units of the various parameters here ok. Now, you see that initial condition as proposed in the problem that we are taking that initially there is no pollutant present. So, we are putting that at time t equal to 0 for all z the constant is 0.

Next to be the boundary condition now you can you see that you say second order equations, so we need two boundary conditions. So, at the initial that means, within the domain of study and the control volume we choose that the start of the control volume we take that there is certain concentration of the pollutant; that means, as if some

pollutant is getting ejected from some source, and that is some particular concentration. So, that source concentration is coming over here. Again, I may mention that this may be a function of time.

And at the other end of the control volume we are having the 0 flux; that means, we are saying that as if it is coming to a constant value, ok. So, now, you see that in this case we are having these two types of boundary condition, first type is again I am going to say that this is the boundary condition of our type one or the Dirichlet boundary condition and the second one is a Norman-Boundary condition. Again, without loss of generality we can take it to be 0, you may also take it to be some finite value, depending on the situation.

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Analysis

- Define non-dimensional parameters as

$$Z = \frac{z}{L}, C = \frac{c}{c_{in}}, \theta = \frac{tu}{L}$$
- So we have

$$\frac{\partial C}{\partial \theta} = \frac{D}{uL} \frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z} - \frac{kL}{u} C$$
- or

$$\frac{\partial C}{\partial \theta} = \frac{1}{Pe} \frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z} - KC$$

Where $Pe(uL/D)$ is the Peclet number that denotes the ratio of the convective to dispersive transport. As $Pe \rightarrow 0$, we get well mixed situation, while as $Pe \rightarrow \infty$ we have plug flow. $K = kL/u$

Now, once you have done this now what we do? We now define some of the non-dimensional variables now here you see that by capital Z is a non-dimensional axial position which we put by z by L, ok, and this is the C is the non-dimensional concentration this is c by c in as I explained earlier. And in this case, I have to define a non-dimensional time, ok. And this non-dimensional time is nothing but the actual time divided by the time it takes for traversing the length L, with the speed u.

So, that is this L by you can see say time unit. So, this L by u is nothing but the time it takes for the one volume of this water to traverse from 0 to l, ok. So, that is how we are

getting this is a characteristic time and with this theta we are defining a non-dimensional time, ok.

Now, instantly as you can see that capital Z and capital C are both also normalized; however, theta is not normalized, ok. Theta will start from 0 and it keep on increasing, that is we can keep on extending our time in future, and that is obvious. And since we are not we are not solving for time is an independent variable. So, we are not really bothered about the normalization of the time, ok.

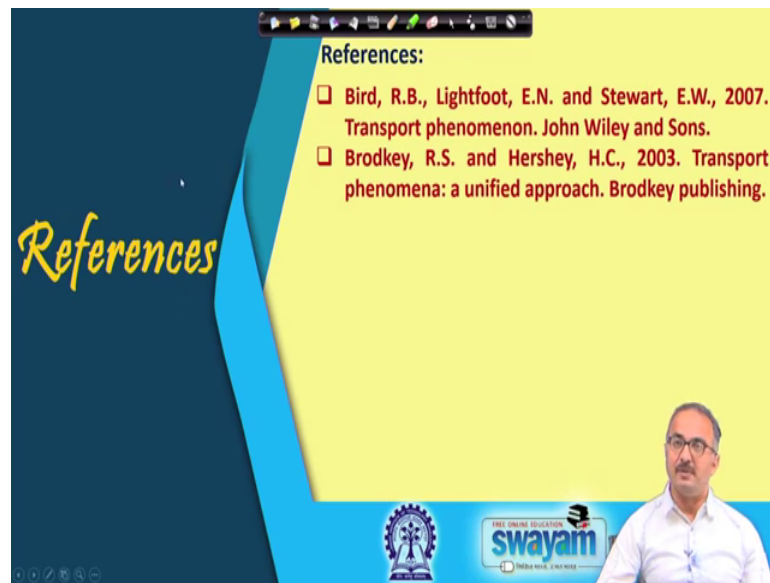
So, here we have now after putting all these numbers we get this particular equation. And in this equation, you can easily see that this particular D by uL, this is given by some non-dimensional number and this non-dimensional number is the Peclet number, ok. And this Peclet number denotes the ratio of the convective to the dispersive transport; that means, how much of this particular component is getting dispersed due to the concentration gradient and how much of it is going because of the convective flow, ok.

So, now you see that as these Peclet number tends toward 0, tends towards 0 means as if the convective flow is much much less than the dispersive flow then it means that there is a well-mixed because when is a very very fine mixed then we know that the diffusive quotient is very very high, ok.

That means, when different is very very high with respect to the convective flow; that means, the mixing will also be very thorough. So, when the D is much much higher than the convection then we find that Peclet number goes to 0. On the other hand, when the diffusivity is very very less when compared to the convection, we find that the Peclet number tends to infinity and that gives us a plug flow situation, ok.

So, these are the two extreme conditions, for the Peclet number. So, here we obtain this equation in terms of Peclet number, and another one other this a non-dimensional rate constant we find here in terms of the capital K. So, this is how we are able to reduce these equations further for non-dimensional equation from the dimensional equation.

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More elaboration of these principles and theories may be found in these particular references.

Thank you.