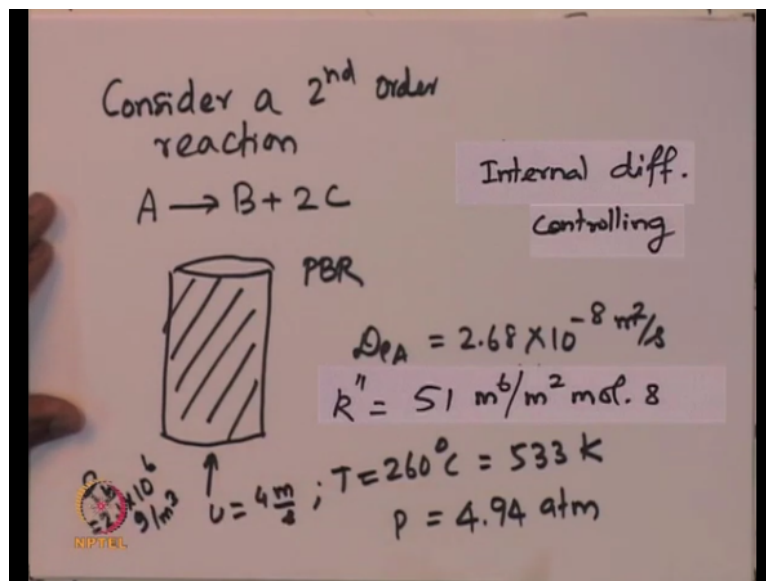


Chemical Reaction Engineering - II
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Lecture - 39
Fluidized Bed Reactor Design I

Friends let us look at an example problem for packed bed reactor design. So consider a second-order reaction.

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Consider a second-order reaction A going to B+2C. So now suppose if this is a tubular reactor, suppose if this is a tubular packed bed reactor, packed bed reactor, it is filled with catalyst and if the gas fluid feed stream is actually flowing at a superficial velocity of 4 meters per second so that is the superficial velocity with which the feed stream is flowing.

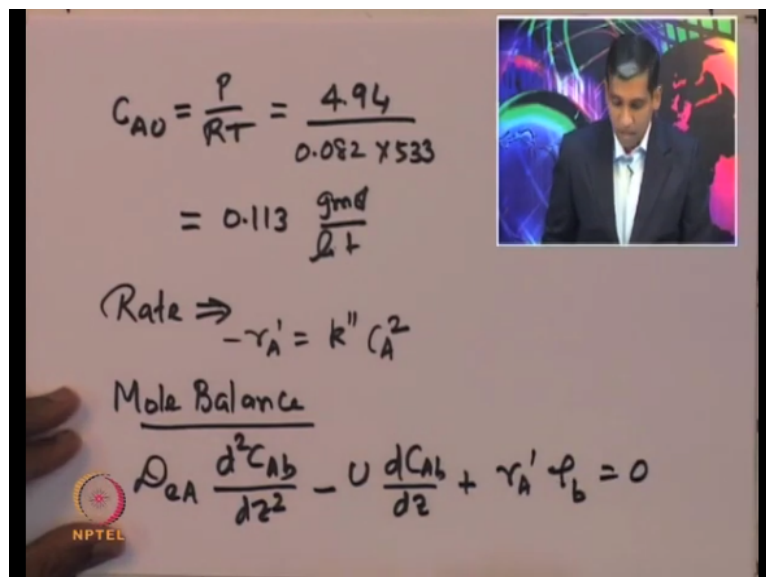
And if the feed temperature is 260 degree C which is equal to 533 Kelvin and if the pressure at which the fluid is flowing into the stream is 4.94 atmospheres and it is undergoing a reaction A giving B+2C and suppose if the diffusivity of the species DeA effective diffusivity is given by 2.68×10^{-8} meter square per second. So that is the diffusivity of the species.

And if the corresponding intrinsic reaction rate, specific reaction rate is 51 meter power 6/meter squared mole second so that is the specific reaction rate and there are other properties

that are given so density of the catalyst particle is about 2.1×10^6 gram per meter cube that is the density of the catalyst.

And then the surface area which is available for the catalytic reaction is 410 meter square per gram of the catalyst. Now so we need to find out what is the pore diffusion if this is supposed to be a strongly internal diffusion controlled, diffusion limited reaction. So we need to design the reactor, find out what is the size of the reactor, etc. So now the first step towards doing this is to find out what is the concentration with which the fluid is actually flowing into the reactor.

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$$C_{A0} = \frac{P}{RT} = \frac{4.94}{0.082 \times 533}$$

$$= 0.113 \frac{\text{gmol}}{\text{L}}$$

Rate $\Rightarrow -r_A' = k'' C_A^2$

Mole Balance

$$D_{eA} \frac{d^2 C_{Ab}}{dz^2} - U \frac{dC_{Ab}}{dz} + r_A' r_b = 0$$

So C_{A0} is the inlet concentration that is equal to P/RT that is the pressure with which the fluid is the species is flowing into the reactor divided by the gas constant R multiplied by divided by the temperature of the fluid stream at the inlet. So that is given by $4.94/0.082 \times 533$, so that comes out to be about 0.113 gram moles per liter. So that is the concentration with which the feed actually enters the reactor.

So now if I look at what is the rate law, the next step is look at the rate law. So we said it is a second-order reaction. So therefore the rate law $-r_A'$ that is equal to the specific reaction constant multiplied by the C_A square which is the second-order reaction and now we can write a mole balance, the mole balance which we have already looked at in the previous lecture.

So the mole balance for such a packed bed reactor will be the axial dispersion coefficient of the reactant species $DeA \cdot d^2 C_{Ab}$ which is the bulk concentration of the species at any location in the reactor $/dz^2 - U \frac{dC_{Ab}}{dz} - \Omega \rho'_A (C_{Ab})^p = 0$ which is the superficial velocity. Let us assume that the superficial velocity remains constant and also that the volume expansion is negligible. So into $dC_{Ab}/dz + r_A \text{ prime} \cdot \text{density of the catalyst}$.

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$$DeA \frac{d^2 C_{Ab}}{dz^2} - U \frac{dC_{Ab}}{dz} - \Omega \rho'_A (C_{Ab})^p = 0$$

$$\Rightarrow DeA \frac{d^2 C_{Ab}}{dz^2} - U \frac{dC_{Ab}}{dz} - \Omega k'' S_a \rho_b C_{Ab}^2 = 0$$

Assume $\left| DeA \frac{d^2 C_{Ab}}{dz^2} \right| \ll \left| U \frac{dC_{Ab}}{dz} \right|$

$$\Rightarrow \frac{dC_{Ab}}{dz} = - \frac{\Omega k'' S_a \rho_b C_{Ab}^2}{U}$$

So now plugging in the rate law which is basically given by the plugging in the rate law we find that we can write the mole balance as the axial dispersion coefficient $DeA \cdot d^2 C_{Ab}/dz^2 - U \frac{dC_{Ab}}{dz} - \Omega \rho'_A (C_{Ab})^p = 0$. If capital omega is the overall effectiveness factor, then the overall rate is given by the overall effectiveness factor multiplied by the corresponding rate evaluated at the surface concentration.

So if the mass transport limitations are negligible because the reaction is now happening at a strongly internal diffusion control, the reaction rate now has to be estimated at the bulk concentration itself. So therefore we can write the rate expression as the effectiveness factor $\omega \cdot \text{the reaction rate evaluated at the bulk concentration } C_{Ab}$ so that is equal to 0. So that is the mole balance.

Now we can rewrite this as into bed density of the catalyst. So plugging in the rate law, we can write this as axial dispersion coefficient $\cdot d^2 C_{Ab}/dz^2 - U \frac{dC_{Ab}}{dz} - \omega k'' S_a \rho_b C_{Ab}^2 = 0$. So that is the mole balance. So plugging in the rate law, we can write this as axial dispersion coefficient $\cdot d^2 C_{Ab}/dz^2 - U \frac{dC_{Ab}}{dz} - \omega k'' S_a \rho_b C_{Ab}^2 = 0$. So that is the mole balance.

That is the mole balance which captures the heterogeneous catalytic reaction which is happening inside the packed bed reactor. Note that the explicit expression for effectiveness factor may not be available and it will be a function of bulk concentration C_{Ab} . Now suppose as before if we assume, if we assume that the rate of diffusion of the species $d^2 C_{Ab}/dz^2$ that if that is significantly smaller compared to the rate of the bulk flow of the species and the corresponding let us assume that the corresponding condition is satisfied.

Then, we can rewrite this mole balance as dC_{Ab}/dz that is equal to $-\omega k'' C_{Ab}^2/U$ which is the specific reaction constant $\omega k'' C_{Ab}^2/U$. So that is the mole balance. For a second-order reaction, the overall effectiveness factor is in general a function of the conversion; however, as a reaction is internal diffusion control we assume overall effectiveness factor to be approximately equal to the internal effectiveness factor.

In fact, it turns out that this is the case for this problem as will be shown shortly. Now we can integrate this expression and we need some boundary conditions to integrate this expression. So suppose the concentration of the species that is actually fed into the reactor at $Z=0$. So $Z=0$ is the inlet to the reactor, at that location the concentration of the species is C_{Ab0} .

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$@ z=0 \Rightarrow C_{Ab} = C_{Ab0}$
 $L = \frac{U}{\omega k'' S_a C_{Ab0}} \left(\frac{1}{1-X} - 1 \right)$
 $X = 81\%$
 $\eta = \left(\frac{2}{n+1} \right)^{1/2} \frac{3}{\phi_n}$ with $n=2$
 ϕ_2

So suppose at $Z=0$, the concentration of the species is equal to C_{Ab0} so that is the boundary condition. With this we can integrate the mole balance and on integration we can find out what is the length of the reactor as a function of conversion. So length of the reactor is U/the

overall effectiveness factor, ρ_b is the bulk density of the catalyst, k is the corresponding specific reaction constant $*C_{Ab0}^{1/1-X-1}$.

So that is the relationship between the length and the corresponding other parameters of the reactor and the conversion. So now suppose if I specify that the conversion has to be 0.81, suppose if the conversion has to be 81% then what is the length of the reactor? What is the length of the reactor that is required to achieve such a conversion? So now what is the first step here?

We need to find out what is the overall effectiveness factor and if we know all the other parameters then we should be able to calculate what is the length of the reactor which is required for that particular to achieve that particular conversion. So therefore now in order to find out the overall effectiveness factor, see overall effectiveness factor is basically a combination of the resistance that is offered by the internal effectiveness factor and the resistance that is offered because of the external mass transport.

So therefore the first step is to calculate the effectiveness factor η and that will be for a general n th order reaction the effectiveness factor is given by $2/n+1$ to the power of $1/2$ \times 3 / the corresponding Thiele modulus with $n=2$, n is basically the second-order reaction. So we have to find out the Thiele modulus corresponding to the second order reaction and by plugging in the Thiele modulus you will be able to find out what is the effectiveness factor for this particular system. So we need to find out what is the Thiele modulus for this reaction system.

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Handwritten mathematical derivation on a whiteboard:

$$\phi_2 = R \sqrt{\frac{k'' S_a \rho_b C_{Ab0}}{D_{eA}}}$$

$$d_p = 0.38 \text{ cm}$$

$$\phi_2 = 2.59 \times 10^7 \leftarrow \text{very large}$$

$$\eta = \left(\frac{2}{3}\right)^{1/2} \frac{3}{2.59 \times 10^7} = 9.47 \times 10^{-8}$$

\Rightarrow Strongly diffusion limited

$$\Omega \approx \eta = 9.47 \times 10^{-8}$$

NPTTEL

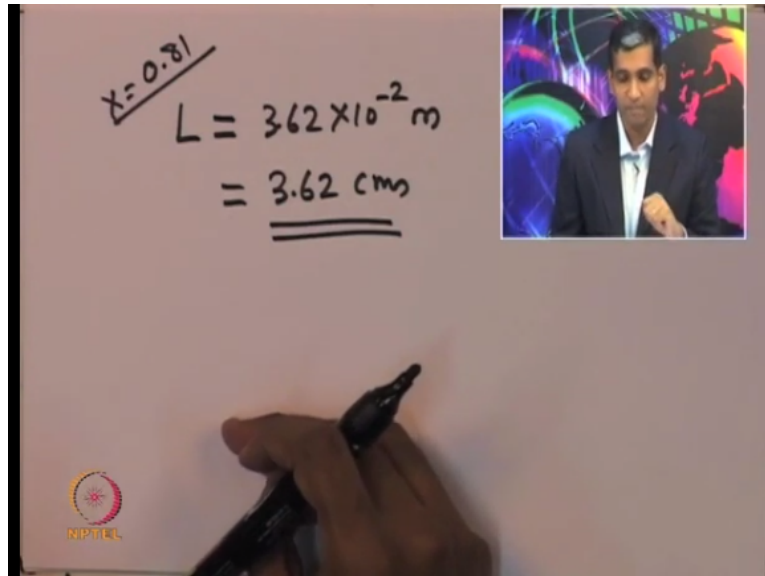
So now the Thiele modulus for a second-order reaction is given by $R \sqrt{k' C_{A0} / D_e}$ which is the length scale or the radius of the spherical catalyst pellet $\times k'$ double prime $\times S_a$ which is the area of the catalyst per gram or surface area of the catalyst available for reaction per gram of catalyst and that is the value of S_a and suppose if multiplied by the density bulk density of the catalyst into C_{A0} which is the concentration of the species at the inlet/the corresponding diffusivity D_e .

Note that Thiele modulus now will be a function of local concentration and therefore a function of position; however, for the parameter values chosen, the Thiele modulus is not very different with respect to position and hence it is evaluated at the inlet concentration. Now if the diameter of the particle that is being used for this particular reaction if that is equal to 0.38 centimeters of the particle that is filled inside the reactors by 0.38 centimeters.

Then, we can calculate the Thiele modulus ϕ^2 and that is equal to 2.59×10^7 to the power of 7. So that is a significantly large quantity, so it is very large which suggests that clearly it is an internal diffusion limited system and now we can calculate what is the effectiveness factor η so that is equal to $2/3$ to the power of $1/2 \times 3/2.59 \times 10^7$ and that is equal to 9.47×10^{-8} .

So the effectiveness factor is extremely small which suggests that it is a strongly diffusion limited. So if it is strongly diffusion limited then the overall effectiveness factor ω will be approximately equal to the internal effectiveness factor itself and so that should be equal to 9.47×10^{-8} . So now plugging in this expression, all the details of overall effectiveness factor etc into the model equation to find out into the expression to that relates the length versus all the other parameters and the conversion.

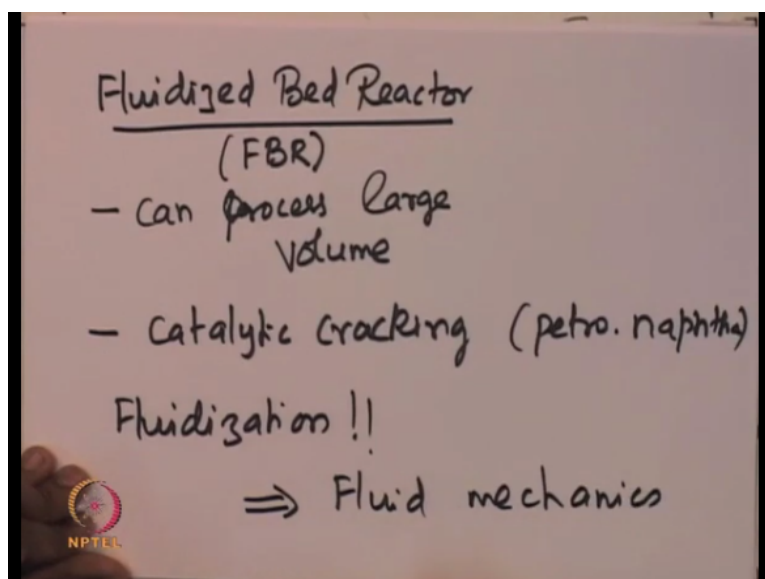
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So we can find out the length of the reactor in which the reaction has to be conducted in order to achieve a conversion of 0.81 is basically given by 3.62×10^{-2} meters. So that is basically 3.62 centimeters. So in order to achieve this conversion for the given set of conditions, the reactor that needs to be used is extremely small.

So it is important to perform such kind of design to get a feel of what should be the dimensions of the reactor in which the corresponding reaction has to be conducted in order to achieve a certain conversion. So now with this we move on to the next aspect where we want to now look at fluidized bed reactors is another type of reactor which is commonly used in industries for many different purposes.

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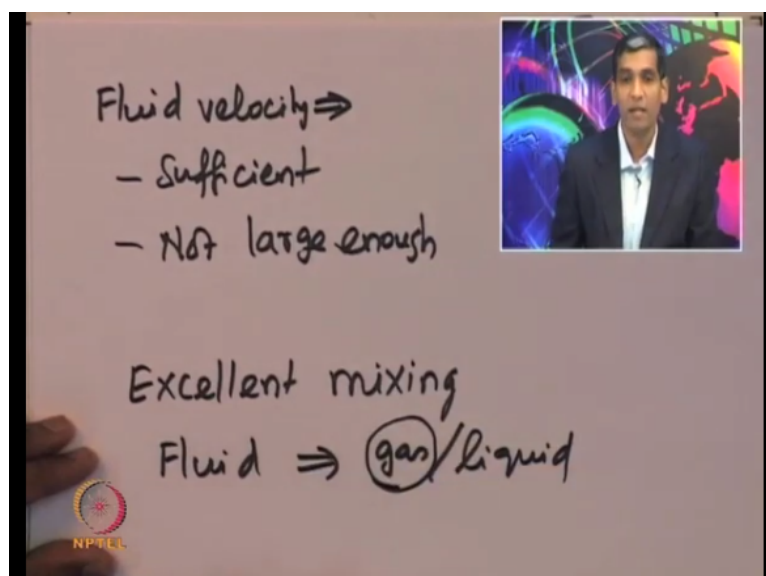
So let us look at the fluidized bed reactor. So hereafter it will be referred to as FBR which is the fluidized bed reactor. Remember PBR is the packed bed reactor, FBR will be the fluidized bed reactor. Now the major advantage of a fluidized bed reactor is that it can process large volume of reactions. So it can actually process can process large volume, so that is an important advantage of using a fluidized bed reactor.

And it is very commonly used in catalytic cracking particularly of petroleum naphtha which is again an important process in petroleum industry. So catalytic cracking is one very common example where fluidized bed reactor is actually being used in the industry settings. So what is fluidization? So fluidization is essentially where a small solid particles are actually suspended in an upward moving flow.

So suppose if there is a tube which; when there is a fluid which is flowing through the tube. Then, the velocity of the fluid is such that these particles which are present inside the reactor which is catalyst particles which are present inside the reactor are actually they get suspended in the fluid as it moves. So this process of getting suspended in the upward moving fluid is what is called as a fluidization process.

So it is the fluidization which is actually a key plays a key role in these kind of reactors. Clearly because fluidization is involved, clearly there is a lot of fluid mechanics which is required in order to model or design such kind of a reactor some aspects of which is what we are going to see in this lecture.

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Fluid velocity \Rightarrow

- Sufficient
- Not large enough

Excellent mixing

Fluid \Rightarrow (gas/liquid)

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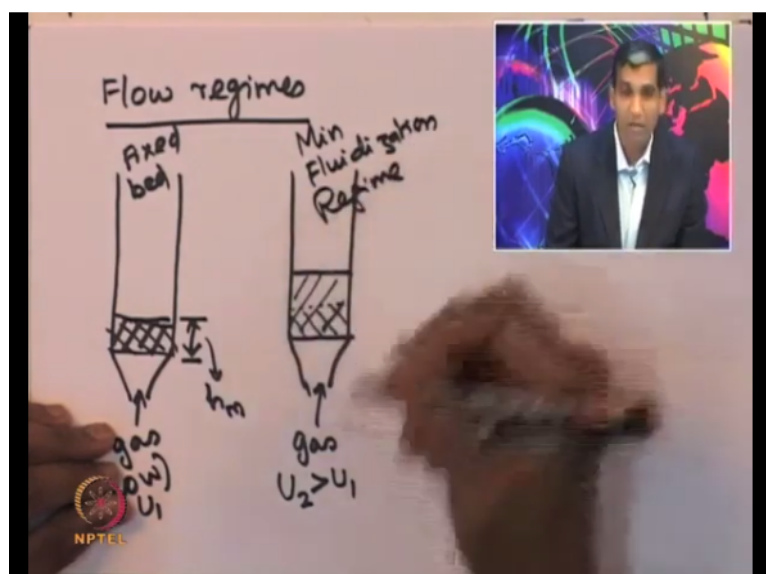
So now the fluid velocity in order for fluidization to occur, the fluid velocity should be such that it is just sufficient to suspend the particles in the fluid stream but not large enough, it should not be large enough to actually take the particles outside the reactor. Remember that these are particles which are present inside the reactor which may be a tube and then there is fluid which is flowing from the bottom of this tube.

And the fluid velocity should be just sufficient in order for these catalyst particles to rise along with the fluid; however, it should not be significantly large enough in order for these particles to be washed away from the tube. So therefore the controlling the fluid velocity is actually an important step in the fluidization process. So another important aspect of the fluidized bed reactor is that it provides excellent mixing.

Because while the fluidization process occurs, these particles are carried by the fluid and it is not fluid velocity is not large enough so that the particles leave but there is a recirculation of these catalyst particles and that causes a vigorous and excellent mixing which is required in many different kinds of reactions. So the fluid that is typically used for fluidization process could actually be a gas or a liquid stream.

It could be either of these two which is commonly used. In this particular discussion, we are going to concentrate mainly assume that it is a gas which is actually fluidizing the catalyst particles. So let us look a little bit more deeply into what is this fluidization process. So there are different kinds of flow regimes which may be attained while the fluidization occurs.

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So let us look at what these flow regimes are. So now suppose if there is a tube here and this is filled with let say catalyst particles, filled with catalyst particles. Now there is a fluid which is actually flowing through this tube. So let say it is a gas, if the velocity is very low if the flow velocity is very small then what happens is that the velocity of the fluid is not sufficient to lift the particles.

That means that these particles they exert a gravity force due to its natural weight while these gas when they actually move through these particles they exert a drag force on the particles. Now if the gravitational force that the solid particles are exerting is significantly larger than the drag force that is that it experiences from the gas which is moving passed in then these particles will not be displaced.

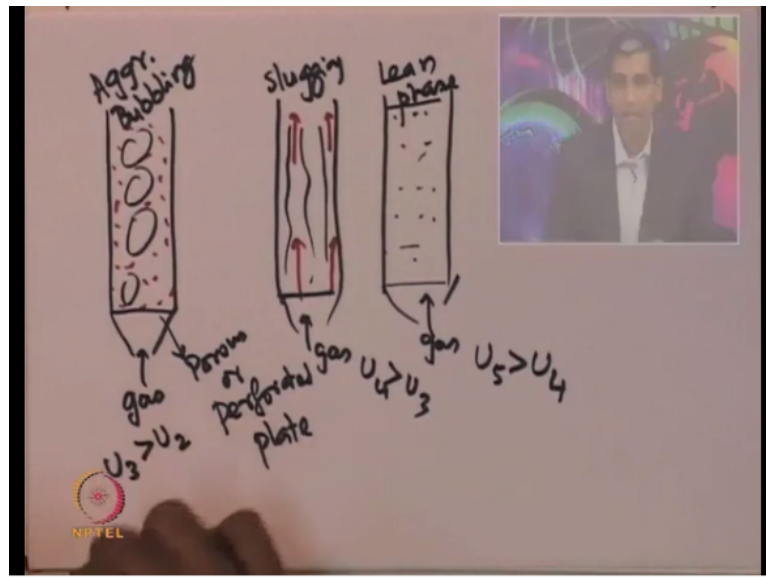
And they will tend to stay as it is and the gas will simply escape from the pores and then leave the reactor. So this kind of an operation where the gas flow rate is extremely small is called the fixed bed operation. It is called the fixed bed operation and the height of the catalyst bed which is present inside the reactor in this fixed bed operation is called the h_m , we refer to that as h_m which is the height up to which the fluid catalyst particles are actually packed in its settled condition.

Now as a next step suppose if we gradually increase the velocity of the gas, suppose if we gradually increase the superficial velocity. So if the superficial velocity of the gas in the fixed bed condition if this is U_1 and suppose if the superficial velocity here is U_2 which is slightly greater than U_1 then what happens is that these fluid particles the drag force that is exerted by the gas stream which is moving pass these particles is now going to be just equal to the gravitational force which is exerted by the particles due to its natural weight.

And so therefore the particles will be fluidized and so the particles will start rising. So here one could see that there will be two phases where there will be some section which is raised and some section which actually stays as packed as it was before. So this kind of a regime is what is called as the minimum fluidization regime. It is called the minimum fluidization regime. So now if I look at the third case where there will be an aggressive bubbling.

Suppose if I further increase the flow rate superficial velocity of the fluid which is actually flowing into the tube.

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So suppose if I increase the superficial velocity, if it is U_3 which is greater than U_2 , if I further increase the superficial velocity then there is going to be aggressive bubbling of the gas, so the gas bubbling starts inside. So there will be aggressive bubbling of the gas and along with it these fluid particles are now going to be suspended around these bubbles. So these bubbles now carry the fluid particles along with it and therefore there will be aggressive bubbling and it is also going to have aggressive amount of mixing of these particles.

And therefore there will be aggressive mixing of the reactant species in the gas stream. So typically there will be a porous or a perforated plate. Typically, there will be a porous or a perforated plate which prevents these particles from going back into the gas stream. So this regime is called the aggressive bubbling regime. Then, the next regime is suppose if you have a tube with gas flowing inside.

And if the superficial velocity is U_4 which is let say greater than U_3 , so the velocity is now slightly greater than what it was in the aggressive bubbling case, then what happens is called the slugging process where the gas is now the gas velocity is significantly higher and the drag force is now going to be significantly higher than the gravitational force which is exerted by the solid particles because of its natural rate.

And that is going to be that inequality is going to be significantly predominant which is going to be predominant than the aggressive bubbling case and so there will be slugs which will be formed where the gas stream is now going to escape through these channels which is present.

So the gas stream is simply going to escape through these channels and so you can see that there will be channels of particles and the gas stream is created inside the tube.

So this process of fluidization is called the slugging process where it happens at a significantly higher velocity and the last regime is called the lean regime. So if there is a gas which is flowing here and if the velocity superficial velocity is U_5 which is greater than the superficial velocity in the case of slugging then there is going to be a lean phase where the particles are suspended with very low density all through the reactors.

So that is called the lean phase. So in this discussion today we are primarily going to look at the fluidization regime and we will not look into the slugging and the aggressive bubbling regimes. Even in the fluidization regime, there will always be some minimal bubbling which will be present and the particles will be carried by these bubbles and so we are going to look at how these particles are carried by bubbles and what fluid mechanics is involved and how can it be used in terms of designing the perfect fluidized bed reactor which is the objective.