Chemical Reaction Engineering I
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Lecture No. 15
Material and Energy Balances in Plug Flow and Mixed Flow Reactors

Welcome to the 15th lecture of Module 4. In this module we are discussing reactor design. Before going to this lecture let us briefly discuss what we have covered in the last lecture.

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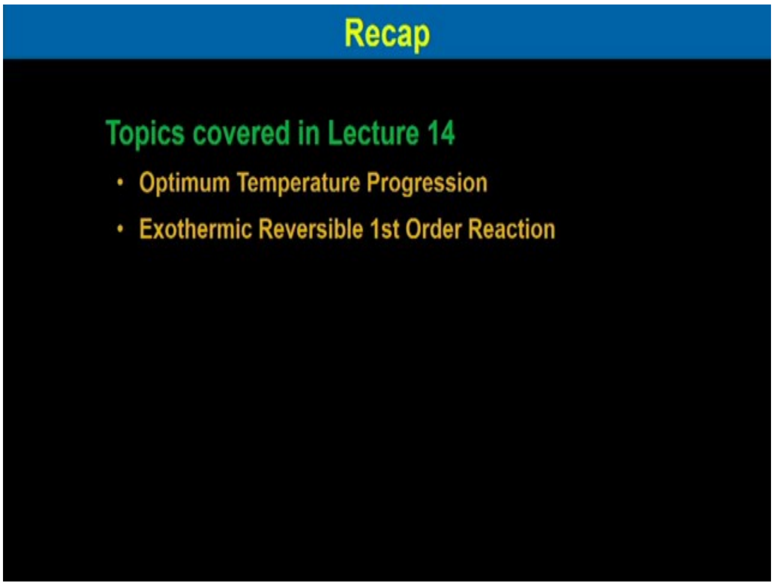

Recap

Topics covered in Lecture 14

- Optimum Temperature Progression
- Exothermic Reversible 1st Order Reaction

In the last lecture we have covered optimum temperature progression in a batch reactor. So we have seen for 3 different cases how to obtain the optimum temperature. We have seen for a case of irreversible single reaction the maximum allowable temperature is the optimum temperature. Even in the case of the reversible endothermic reaction the maximum allowable temperature is also the optimum temperature.

The only case which you have considered where we can find the optimum temperature if you wanted to run at a single temperature, that is for single exothermic reversible reaction, where the change in temperature changes the equilibrium conversion and we have seen how to go about to design the reactor following a, temperature trajectories instead of a single temperature. So we have considered exothermic reversible first order reaction and we have considered the cases.

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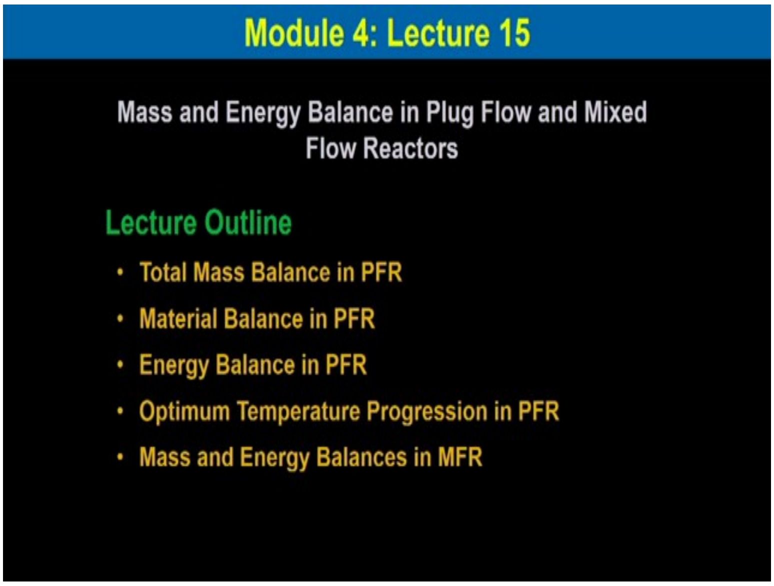

Module 4: Lecture 15

Mass and Energy Balance in Plug Flow and Mixed Flow Reactors

Lecture Outline

- Total Mass Balance in PFR
- Material Balance in PFR
- Energy Balance in PFR
- Optimum Temperature Progression in PFR
- Mass and Energy Balances in MFR

Now in this module, we will consider mass and energy balance in plug flow as well as mixed flow reactors. The lecture outline are as follows. So we will consider total mass balance in plug flow reactor then we will consider material balance in plug flow reactor and particularly energy balance is our interest, when we look for temperature and pressure effects, so energy balance in PFR, then optimum temperature progression in PFR. Then we will consider similar mass and energy balance in mixed flow reactor or CSTR.

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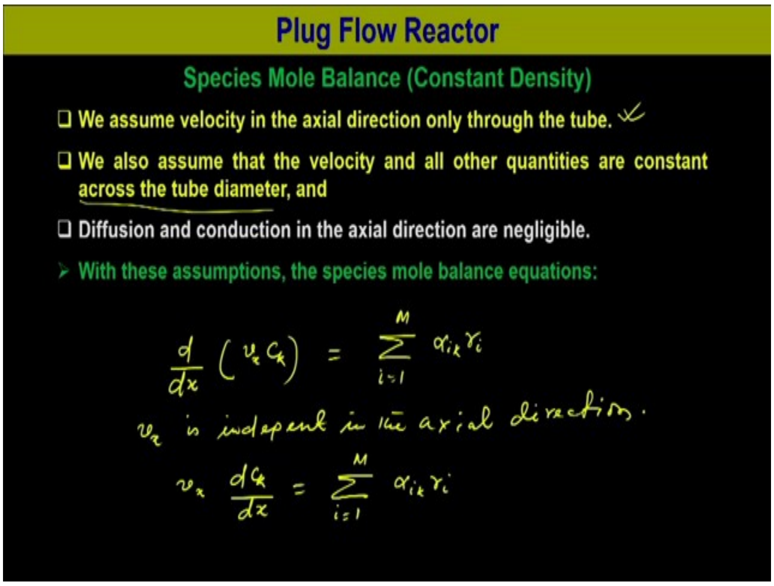


Plug Flow Reactor

Species Mole Balance (Constant Density)

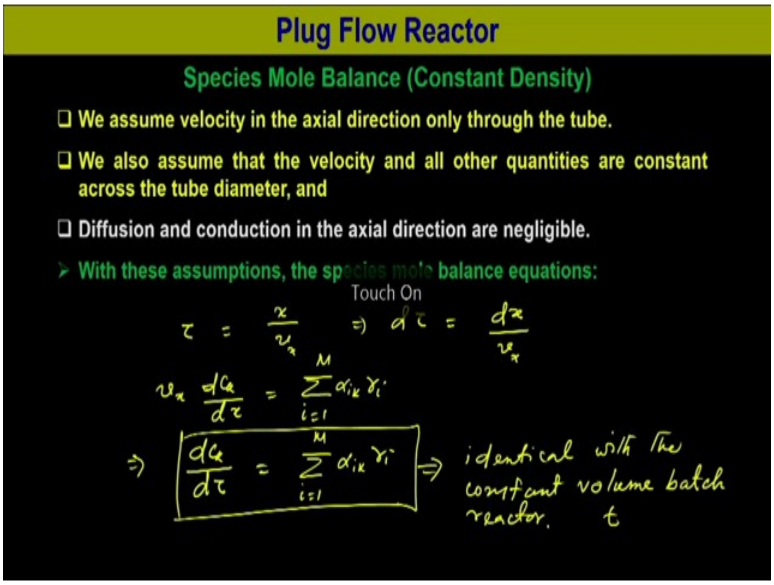
- ☐ We assume velocity in the axial direction only through the tube. ✓
- ☐ We also assume that the velocity and all other quantities are constant across the tube diameter, and
- ☐ Diffusion and conduction in the axial direction are negligible.

➤ With these assumptions, the species mole balance equations:

$$\frac{d}{dx}\left(v_x C_k\right) = \sum_{i=1}^{M} \alpha_{ik} r_i$$

v_x is independent in the axial direction.

$$v_x \frac{dC_k}{dx} = \sum_{i=1}^{M} \alpha_{ik} r_i$$



Plug Flow Reactor

Species Mole Balance (Constant Density)

- ☐ We assume velocity in the axial direction only through the tube.
- ☐ We also assume that the velocity and all other quantities are constant across the tube diameter, and
- ☐ Diffusion and conduction in the axial direction are negligible.

➢ With these assumptions, the species mole balance equations:

Touch On

$$\tau = \frac{x}{v_x} \Rightarrow d\tau = \frac{dx}{v_x}$$

$$v_x \frac{dC_k}{d\tau} = \sum_{i=1}^{M} \alpha_{ik} r_i$$

$$\Rightarrow \boxed{\frac{dC_k}{d\tau} = \sum_{i=1}^{M} \alpha_{ik} r_i} \Rightarrow$$

identical with the constant volume batch reactor. t

So let us start with the species mole balance for constant density plug flow reactor. In this case we assume that the velocity in the axial direction only through the tube. So we consider the plug flow reactor is as a tube and the velocity is only in the axial direction. We also assume that the velocity and all other quantities are constant across the tube diameter and diffusion and conduction in the axial direction are negligible.

So there is negligible diffusion in the axial direction and the conduction in the axial direction. So if we consider that with this assumption we can write the species mole balance as

$$\frac{d}{dx}\left(v_x C_k\right) = \sum_{i=1}^{M} \alpha_{ik} r_i$$

Now if the velocity is independent with the axial direction that is for constant density then, so v_x is independent in the axial direction. So we can take out v_x from the differential equations, from the derivative so we can write

$$v_x \frac{dC_k}{dx} = \sum_{i=1}^{M} \alpha_{ik} r_i$$

Now if we define the residence time that is, so defining residence time

$$\tau = \frac{x}{v_x}$$

x is the length of the tube divided by v_x is the residence time tau. So then we can differentiate

$$d\tau = \frac{dx}{v_x}$$

Now we if we substitute we have these equations of species mole balance,

$$v_x \frac{dC_k}{dx} = \sum_{i=1}^{M} \alpha_{ik} r_i$$

Now if we substitute this things $\frac{dx}{v_x}$ over here this would be

$$\frac{dC_k}{d\tau} = \sum_{i=1}^{M} \alpha_{ik} r_i$$

So this is the species mole balance equation for constant density plug flow reactor and this is identical with the constant volume batch reactor. Only the reaction time in case of batch reactor t is replaced with the residence time tau.

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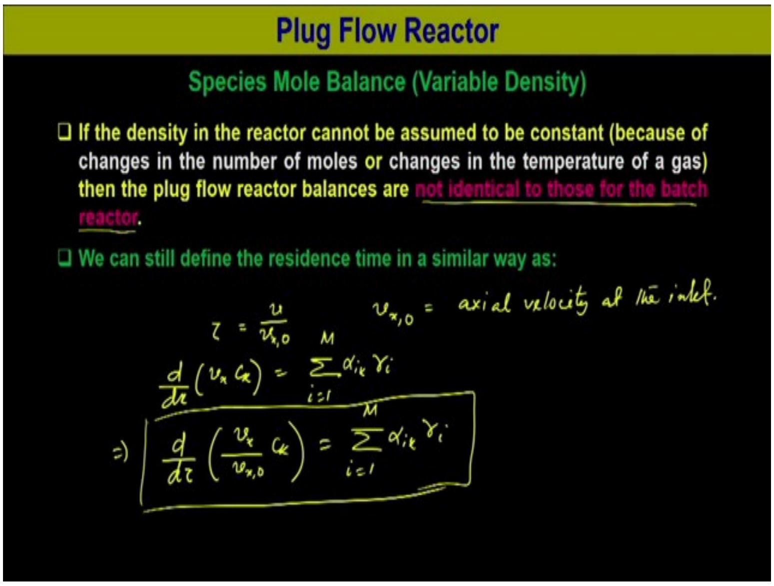

Plug Flow Reactor

Species Mole Balance (Variable Density)

- ☐ If the density in the reactor cannot be assumed to be constant (because of changes in the number of moles or changes in the temperature of a gas) then the plug flow reactor balances are not identical to those for the batch reactor.
- ☐ We can still define the residence time in a similar way as:

$$\tau = \frac{u}{v_{x,0}} \qquad v_{x,0} = \text{axial velocity at the inlet.}$$

$$\frac{d}{d\tau}(v_x C_k) = \sum_{i=1}^{M} \alpha_{ik} r_i$$

$$\Rightarrow \boxed{\frac{d}{d\tau}\left(\frac{v_x}{v_{x,0}} C_k\right) = \sum_{i=1}^{M} \alpha_{ik} r_i}$$

Now if the density in the reactor cannot be assumed to be constant because of the changes in number of moles or in the changes in the temperature of the gas then the plug flow reactor balance are not identical with that of the batch reactor. So for variable density system the species mole balance equations between the plug flow reactor and the batch reactor they are not identical.

But in this case still we can define the residence time in a similar way. Like we can write

$$\tau = \frac{v_x}{v_{x0}}$$

So v_{x0} here is the axial velocity at the inlet then these equations that is

$$\frac{d}{dx}\left(v_x C_k \right) = \sum_{i=1}^{M} \alpha_{ik} r_i$$

This can be written as, with substitution of this τ would be

$$\frac{d}{dx}\left(\frac{v_x}{v_{x0}} C_k \right) = \sum_{i=1}^{M} \alpha_{ik} r_i$$

So this is for variable density system in a plug flow reactor. This is the species mole balance equation.

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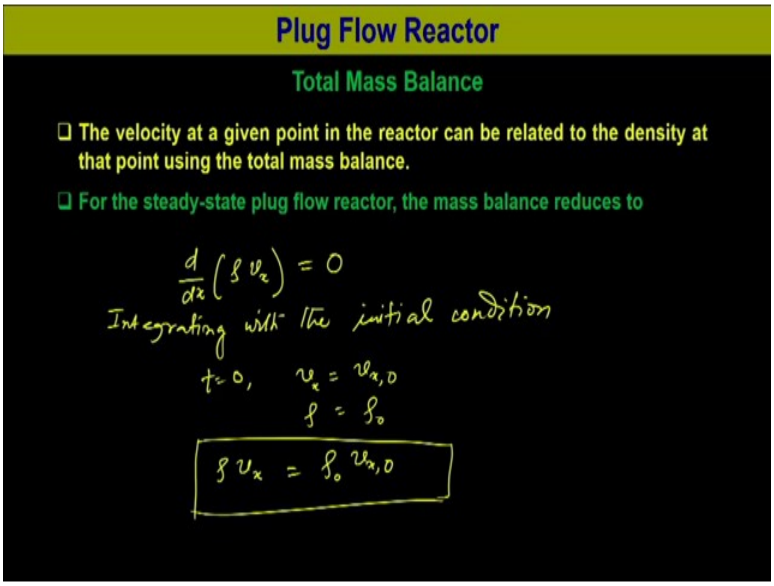


Plug Flow Reactor

Total Mass Balance

- The velocity at a given point in the reactor can be related to the density at that point using the total mass balance.
- For the steady-state plug flow reactor, the mass balance reduces to

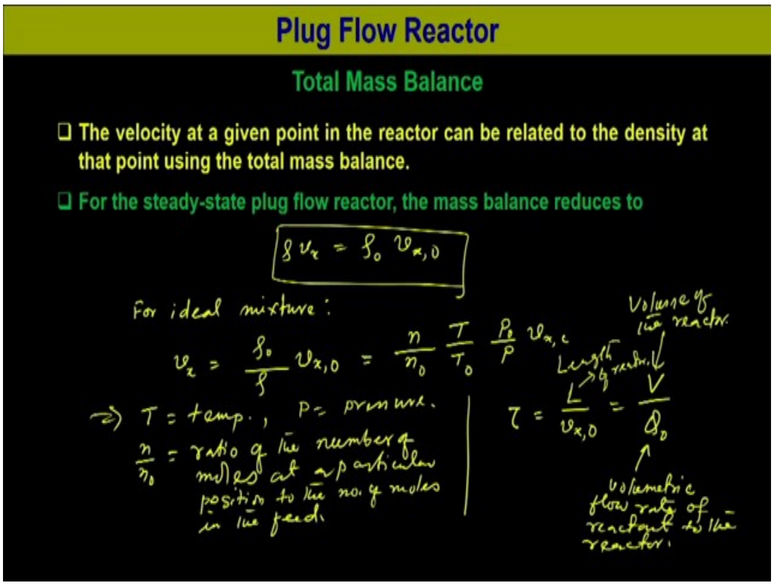
$$\frac{d}{dx}(\rho v_x) = 0$$

Integrating with the initial condition

$t=0, \quad v_x = v_{x,0}$

$\rho = \rho_0$

$$\boxed{\rho v_x = \rho_0 v_{x,0}}$$



Plug Flow Reactor

Total Mass Balance

- The velocity at a given point in the reactor can be related to the density at that point using the total mass balance.
- For the steady-state plug flow reactor, the mass balance reduces to

$$\boxed{\rho v_x = \rho_0 v_{x,0}}$$

For ideal mixture:

$$v_x = \frac{\rho_0}{\rho} v_{x,0} = \frac{n}{n_0}\frac{T}{T_0}\frac{P_0}{P} v_{x,0}$$

$\Rightarrow$ T = temp., P = pressure.

$\frac{n}{n_0}$ = ratio of the number of moles at a particular position to the no. of moles in the feed.

$$\tau = \frac{L}{v_{x,0}} = \frac{V}{Q_0}$$

Length of reactor.

Volume of the reactor.

volumetric flow rate of reactant to the reactor.

Now the total mass balance can be written as the velocity at a given point in the reactor can be related to the density at that point using the total mass balance. So for steady state plug flow reactor, the mass balance reduces to

$$\frac{d}{dx}(\rho v_x) = 0$$

That means if we integrate with the initial conditions at $t = 0, v_x = v_{x0}, \rho = \rho_0$

So if we integrate this we will get

$$\rho v_x = \rho_0 v_{x0}$$

So this is the total mass balance equation.

Now for the plug flow reactor, now the local velocity, so we have

$$\rho v_x = \rho_0 v_{x0}$$

Now the local velocity can be computed using the ideal gas law using local composition and temperature. So if we use the local composition and temperature we can calculate the local velocity. So like for ideal mixture, the velocity we can write

$$v_x = \frac{n}{n_0}\frac{T}{T_0}\frac{P_0}{P}v_{x0}$$

T is the temperature, $\frac{n}{n_0}$ is the ratio of the number of moles at a particular position to the number of moles in the feed, and P is the pressure. Now the most direct measure for the reactor capability to carry out the reaction can be obtained using the local residence time based in the inlet conditions or the inlet flow rate and the reactor volume. So we can write

$$\tau = \frac{L}{v_{x0}} = \frac{V}{Q_0}$$

So Q_0 is the volumetric flow rate of the reactant to the reactor, V is the volume of the reactor and L is the length of the reactor.

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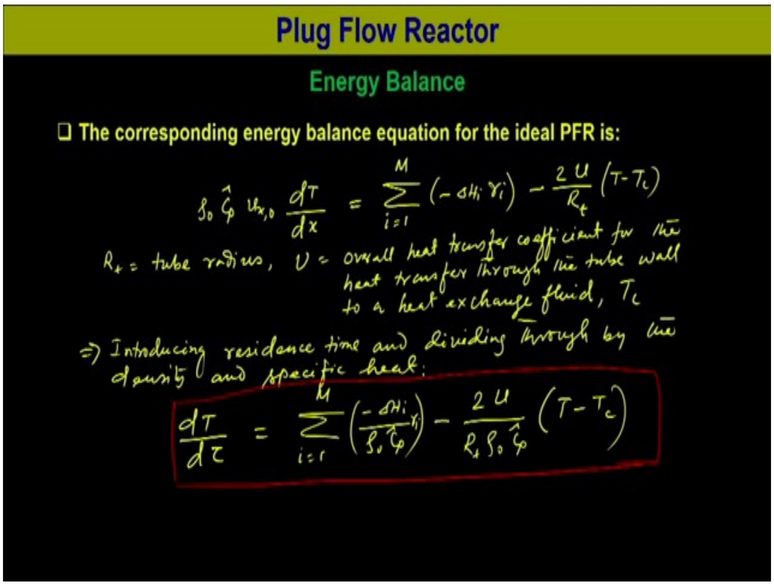

Plug Flow Reactor

Energy Balance

☐ The corresponding energy balance equation for the ideal PFR is:

$$\rho_0 \hat{C}_p u_{x,0} \frac{dT}{dx} = \sum_{i=1}^{M} (-\Delta H_i r_i) - \frac{2U}{R_t}(T - T_c)$$

R_t = tube radius, U = overall heat transfer coefficient for the heat transfer through the tube wall to a heat exchange fluid, T_c

$\Rightarrow$ Introducing residence time and dividing through by the density and specific heat:

$$\boxed{\frac{dT}{d\tau} = \sum_{i=1}^{M}\left(\frac{-\Delta H_i}{\rho_0 \hat{C}_p} r_i\right) - \frac{2U}{R_t \rho_0 \hat{C}_p}(T - T_c)}$$

Now we can write the corresponding energy balance equation for the ideal PFR as

$$\rho_0 \hat{C}_P v_{x0} \frac{dT}{dx} = \sum_{i=1}^{M} (-\Delta H_i r_i) - \frac{2u}{R_t}\left(T - T_c\right)$$

So here R_t is the tube radius, U is the overall heat transfer coefficient to the, for the heat transfer through the tube wall. So this heat transfer is through the tube wall to a heat exchange fluid maintained at temperature Tc.

So this heat flux could take many other form depending on the heat transfer area and the tube diameter and all. So the other terms are the typical density heat capacity and velocity we have defined earlier. If we introduce here the residence time then we can write this relation as, so introducing residence time and dividing through, by the density and specific heat so we can obtain

$$\frac{dT}{d\tau} = \sum_{i=1}^{M} \left(\frac{-\Delta H_i r_i}{\rho_0 \hat{C}_P} \right) - \frac{2u}{R_t \rho_0 \hat{C}_P}\left(T - T_c\right)$$

So this is the basic energy balance equation. This is basic energy balance equation for the plug flow reactor. So this is almost identical with the energy balance equation of the batch reactor, the only difference is the form of the heat transfer through the wall. And this is valid for non-constant density and constant density as well.

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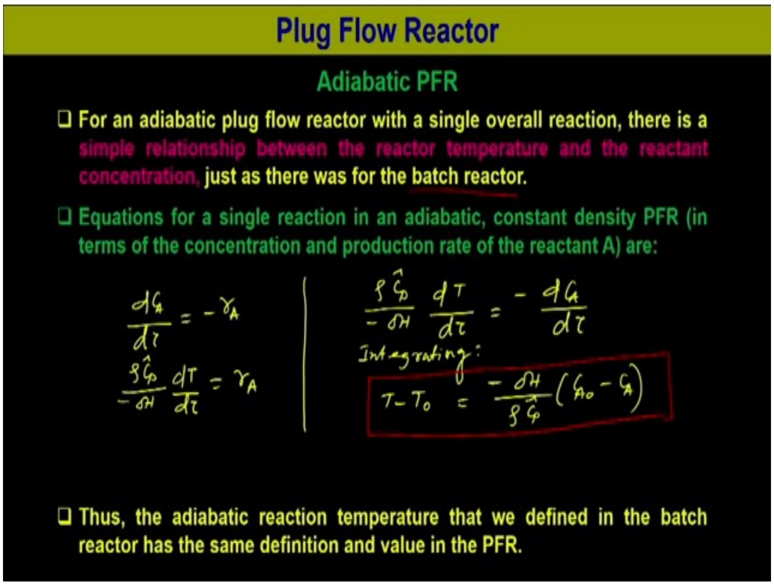

Plug Flow Reactor

Adiabatic PFR

- ☐ For an adiabatic plug flow reactor with a single overall reaction, there is a simple relationship between the reactor temperature and the reactant concentration, just as there was for the batch reactor.
- ☐ Equations for a single reaction in an adiabatic, constant density PFR (in terms of the concentration and production rate of the reactant A) are:

$$\frac{dC_A}{d\tau} = -r_A$$

$$\frac{\rho \hat{C}_P}{-\Delta H} \frac{dT}{d\tau} = r_A$$

$$\frac{\rho \hat{C}_P}{-\Delta H} \frac{dT}{d\tau} = -\frac{dC_A}{d\tau}$$

Integrating:

$$\boxed{T - T_0 = \frac{-\Delta H}{\rho \hat{C}_P}\left(C_{A0} - C_A\right)}$$

- ☐ Thus, the adiabatic reaction temperature that we defined in the batch reactor has the same definition and value in the PFR.

But if we consider adiabatic plug flow reactor, for an adiabatic plug flow reactor with a single overall reaction there is a simple relationship between the reactor temperature and the reactant concentration. Just we have done for the batch reactor. Equations for a single reaction in a adiabatic constant density PFR in terms of the concentration and production rate of the reactant A we can write

$$\frac{dC_A}{d\tau} = -r_A$$

And energy balance equation should be reduced to

$$\frac{\rho \hat{C}_P}{-\Delta H_i}\frac{dT}{d\tau} = r_A \frac{\rho \hat{C}_P}{-\Delta H_i}\frac{dT}{d\tau}$$

So from these two relation we can equate the rate of chemical reactions and we can write

$$\frac{\rho \hat{C}_P}{-\Delta H_i}\frac{dT}{d\tau} = -\frac{dC_A}{d\tau}$$

And if we integrate we can obtain a simple relationship between temperature and concentration. So

$$T - T_0 = \frac{-\Delta H_i}{\rho \hat{C}_P}\left(C_{A0} - C_A \right)$$

So this is the relation as we have obtained for the batch reactor, same relations we can obtain here between the temperature and the concentration for a single reaction. Thus adiabatic reaction temperature that we defined in the batch reactor has the same definition and value in case of the plug flow reactor. So we are not introducing that part over here on the adiabatic reaction temperature.

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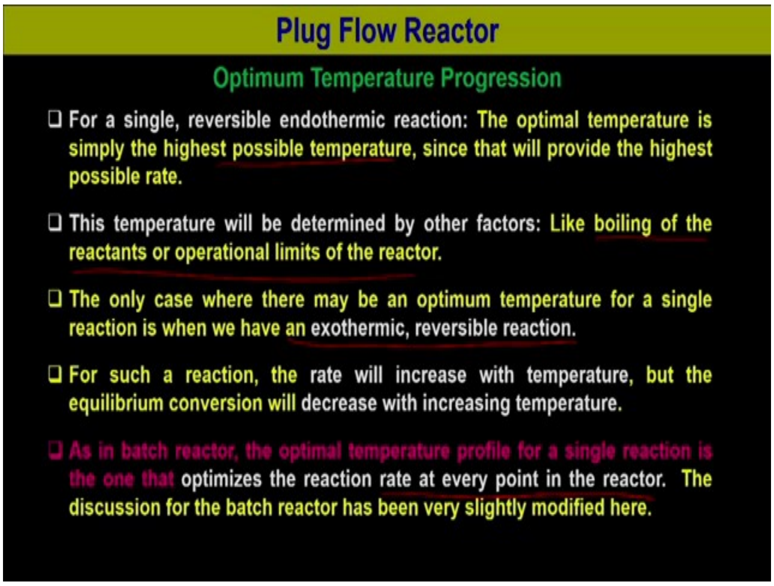

Plug Flow Reactor

Optimum Temperature Progression

- For a single, reversible endothermic reaction: The optimal temperature is simply the highest possible temperature, since that will provide the highest possible rate.
- This temperature will be determined by other factors: Like boiling of the reactants or operational limits of the reactor.
- The only case where there may be an optimum temperature for a single reaction is when we have an exothermic, reversible reaction.
- For such a reaction, the rate will increase with temperature, but the equilibrium conversion will decrease with increasing temperature.
- As in batch reactor, the optimal temperature profile for a single reaction is the one that optimizes the reaction rate at every point in the reactor. The discussion for the batch reactor has been very slightly modified here.

Now the optimum temperature progression, in case of batch reactor we have discussed how the temperature, optimum temperature progression would change. It is similar to the batch reactor temperature progression phenomena. So obtaining the optimum single temperature or temperature profile in a PFR is also very similar what we have found for the batch reactor. If we plan to operate the reactor isothermally at a single temperature, then there may be an optimum temperature to select. For a single irreversible reaction, in this case the optimal temperature is simply the highest possible temperature since that will provide the highest possible rate.

This temperature how we can determine, it will be determined by the boiling of the reactants or the operational limits of the reactor. That will tell what is the maximum permissible limit for the reaction to maintain. Now for a single reversible endothermic reaction the optimum temperature is also simply the highest possible temperature since that will produce the highest possible rate and that will be determined again under the same conditions of boiling of the reactants or operational limits of the reactor. The only case where there may be an optimum temperature for a single reaction is when we have an exothermic reversible reaction.

So for an exothermic reversible reaction we can have optimum single temperature or a temperature progression. For such a reaction, the rate will increase with temperature but the equilibrium conversion will decrease with increase in temperature. As in batch reactor the optimal temperature profile for a single reaction is the one that optimizes the reaction rate at every point in the reactor. The discussion of batch reactor has been slightly modified and discussed over here.

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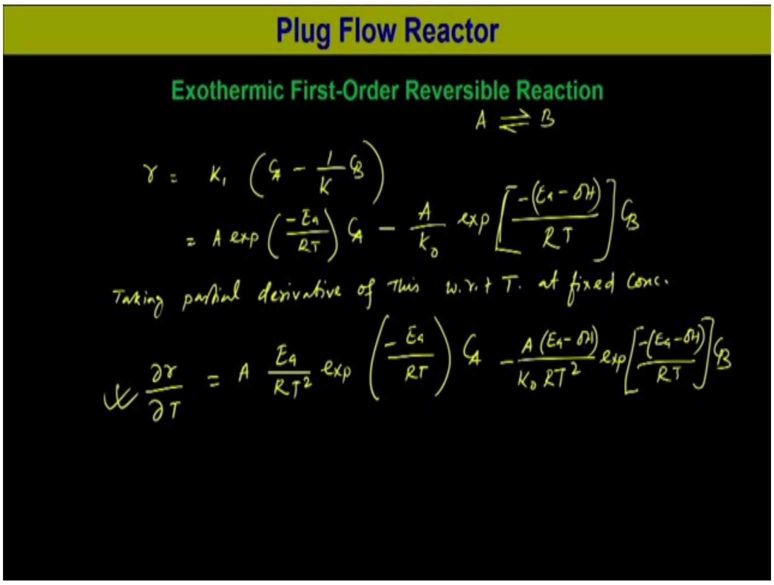


Plug Flow Reactor

Exothermic First-Order Reversible Reaction

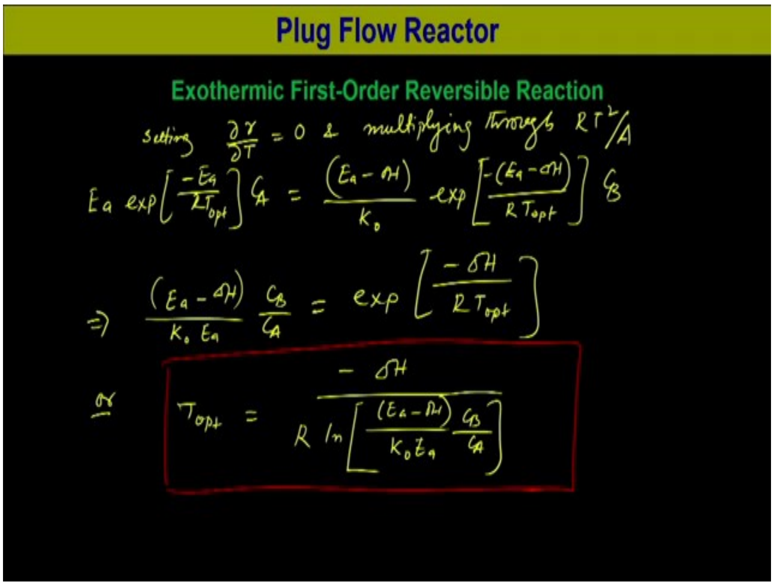
$A \rightleftharpoons B$

$$r = K_1\left(C_A - \frac{1}{K}C_B\right)$$

$$= A\exp\left(\frac{-E_a}{RT}\right)C_A - \frac{A}{k_0}\exp\left[\frac{-(E_a-\delta H)}{RT}\right]C_B$$

Taking partial derivative of this w.r.t T. at fixed Conc.

$$\frac{\partial r}{\partial T} = A\frac{E_a}{RT^2}\exp\left(\frac{-E_a}{RT}\right)C_A - \frac{A(E_a-\delta H)}{K_0RT^2}\exp\left[\frac{-(E_a-\delta H)}{RT}\right]C_B$$



Plug Flow Reactor

Exothermic First-Order Reversible Reaction

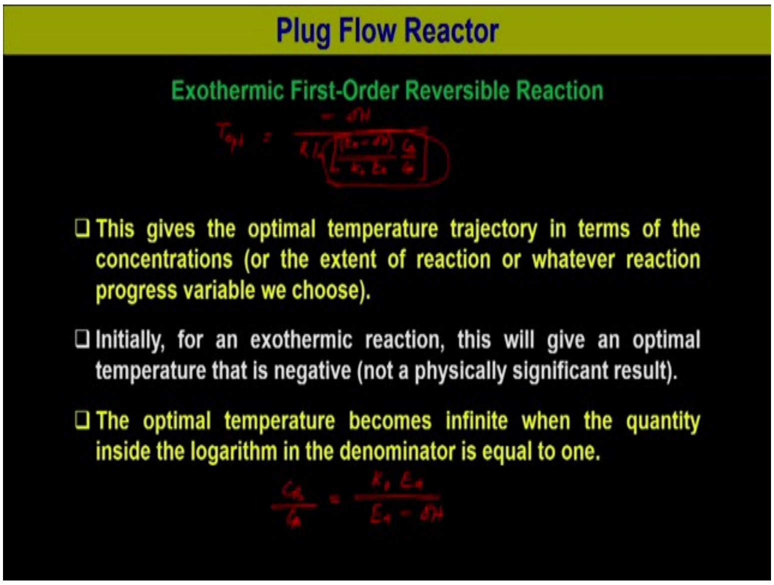
setting $\frac{\partial r}{\partial T} = 0$ & multiplying through RT^2/A

$$E_a\exp\left[\frac{-E_a}{RT_{opt}}\right]C_A = \frac{(E_a-\delta H)}{K_0}\exp\left[\frac{-(E_a-\delta H)}{RT_{opt}}\right]C_B$$

$$\Rightarrow \frac{(E_a-\delta H)}{K_0E_a}\frac{C_B}{C_A} = \exp\left[\frac{-\delta H}{RT_{opt}}\right]$$

or

$$\boxed{T_{opt} = \frac{-\delta H}{R\ln\left[\frac{(E_a-\delta H)}{K_0E_a}\frac{C_B}{C_A}\right]}}$$



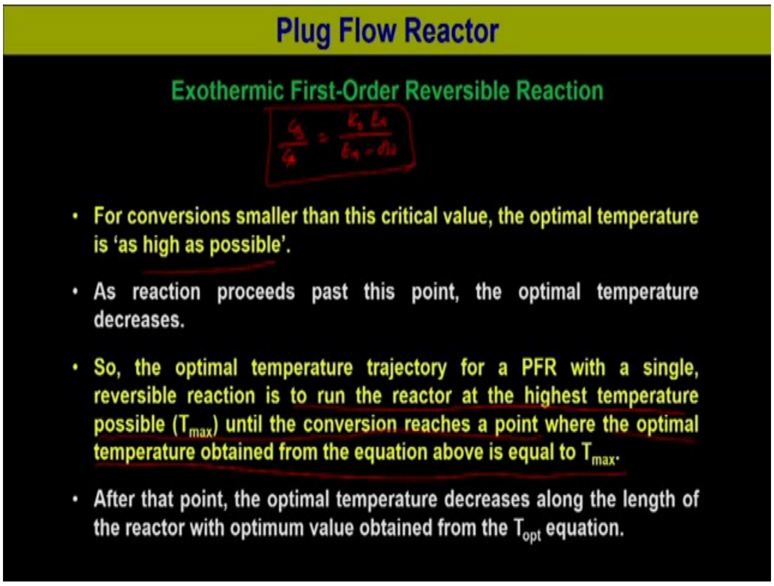
Plug Flow Reactor

Exothermic First-Order Reversible Reaction

$$T_{opt} = \frac{-\Delta H}{R \ln \boxed{\left[\frac{(E_a-\Delta H)}{k_0 E_a}\frac{C_B}{C_A}\right]}}$$

- ❑ This gives the optimal temperature trajectory in terms of the concentrations (or the extent of reaction or whatever reaction progress variable we choose).
- ❑ Initially, for an exothermic reaction, this will give an optimal temperature that is negative (not a physically significant result).
- ❑ The optimal temperature becomes infinite when the quantity inside the logarithm in the denominator is equal to one.

$$\frac{C_B}{C_A} = \frac{k_0 E_a}{E_a - \Delta H}$$



Plug Flow Reactor

Exothermic First-Order Reversible Reaction

$$\boxed{\frac{C_B}{C_A} = \frac{k_0 E_a}{E_a - \Delta H}}$$

- For conversions smaller than this critical value, the optimal temperature is 'as high as possible'.
- As reaction proceeds past this point, the optimal temperature decreases.
- So, the optimal temperature trajectory for a PFR with a single, reversible reaction is to run the reactor at the highest temperature possible (T_{max}) until the conversion reaches a point where the optimal temperature obtained from the equation above is equal to T_{max}.
- After that point, the optimal temperature decreases along the length of the reactor with optimum value obtained from the T_{opt} equation.

So let us consider single first order reversible reaction.

$$A \rightleftharpoons B$$

So we can write

$$r = k_1\left(C_A - \frac{1}{K}C_B\right)$$

So A to B reversible reaction. So we can use the Arrhenius reactions of the rate constant and the equilibrium constant at

$$= A\exp\left(\frac{-E_a}{RT}\right)C_A - \frac{A}{k_0}\exp\left(-\frac{(E_a-\Delta H)}{RT}\right)C_B$$

Now if we take the partial derivative with respect to temperature at a fixed concentration then we can write, so taking partial derivative of this with respect to temperature at fixed concentration; so we can write

$$\frac{\partial r}{\partial T} = A\frac{E_a}{RT^2}\exp\left(\frac{-E_a}{RT}\right)C_A$$

So we can write

$$\frac{\partial r}{\partial T} = -\frac{A}{k_0}\frac{\left(E_a - \Delta H\right)}{RT^2}\exp\left(-\frac{\left(E_a - \Delta H\right)}{RT}\right)C_B$$

So this is the partial derivative and now if we set this

$$\frac{\partial r}{\partial T} = 0$$

multiplying both sides by $RT^2\!\big/\!A$ we can obtain

$$E_a\exp\left(\frac{-E_a}{RT_{opt}}\right)C_A = \frac{\left(E_a - \Delta H\right)}{k_0}\exp\left(-\frac{\left(E_a - \Delta H\right)}{RT_{opt}}\right)C_B$$

Now if we rearrange this we can write

$$\frac{\left(E_a - \Delta H\right)}{k_0 E_a}\frac{C_B}{C_A} = \exp\left(\frac{\left(-\Delta H\right)}{RT_{opt}}\right)$$

This also we can write as

$$T_{opt} = \frac{-\Delta H}{R\ln\left[\frac{\left(E_a - \Delta H\right)}{k_0 E_a}\frac{C_B}{C_A}\right]}$$

So this is the expression for optimum temperature in a plug flow reactor. So the equation is

$$T_{opt} = \frac{-\Delta H}{R\ln\left[\frac{\left(E_a - \Delta H\right)}{k_0 E_a}\frac{C_B}{C_A}\right]}$$

So this is the expression. So this expression gives the optimum temperature trajectories in terms of the concentration or the extent of reaction or whatever reaction progression variable we choose. So this will give the optimum temperature how it will progress in a plug flow reactor. Initially if we look into, for the exothermic reaction as we discussed for the batch reactor as well, this will give an optimum temperature which is negative because ΔH is negative for exothermic reaction. So that is not physically meaningful results.

The optimum temperature becomes infinite when the quantity inside the algorithm, inside the logarithm in the denominator is equal to 1. That means when this term becomes 1 then the optimum temperature becomes infinite. So that means the term

$$\frac{C_B}{C_A} = \frac{k_0 E_a}{E_a - \Delta H}$$

So when this equal to this then these terms become unity inside the logarithm. So

$$\frac{C_B}{C_A} = \frac{k_0 E_a}{E_a - \Delta H}$$

For conversion smaller than this critical value the optimum temperature is as high as possible. So if the conversion is smaller or compared to this critical value where it will become, the term inside the logarithm become 1, till that point the optimum temperature we should keep as high as possible.

As the reaction proceeds past this point the optimum temperature decreases. So initially we should keep as high as temperature possible, then decrease the temperature as the conversion will increase. So the optimum temperature trajectories for a PFR with a single reversible reaction to run the reactor at highest temperature possible until the conversion reaches a point where the optimal temperature obtained from the above equation is T_{max}. After that point the optimal temperature decreases along the length of the reactor with optimum value obtained from the T optimum equation.

So we have derived the equations for, to obtain the optimum temperature which gives the optimum temperature progression. So initially we need to keep the temperature at the inlet of the reactor is as high as possible because at that point the conversion is low and so we need to have as fast as the reaction is possible. So the reactions complete with a smaller time and then we decrease the temperature, as we the reactant goes through the reactor length as it passes through the length of the reactor. So then optimum temperature from time to time we can obtain from the optimum temperature profile equation.

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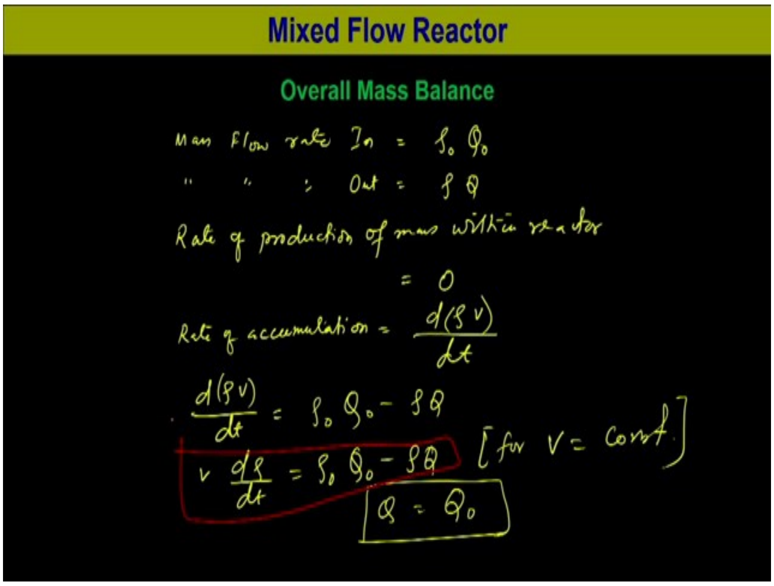
Mixed Flow Reactor

Overall Mass Balance

Mass Flow rate In $= \rho_0 Q_0$

" " : Out $= \rho Q$

Rate of production of mass within reactor $= 0$

Rate of accumulation $= \frac{d(\rho v)}{dt}$

$\frac{d(\rho v)}{dt} = \rho_0 Q_0 - \rho Q$

$v \frac{d\rho}{dt} = \rho_0 Q_0 - \rho Q$ [for $v =$ const.]

$Q = Q_0$

So now let us consider ideal mixed flow reactor, overall mass balance. As we have discussed earlier that for the mixed flow reactor because of the homogenous mixing of the content of the reactor, the concentration is uniform everywhere inside the reactor. So there is no special distribution of the concentration inside the reactor. So the steady state mass balance equation for CSTR is a, is an algebraic equation. So if we consider CSTR, the mass flow rate into the reactor is $\rho_0 Q_0$, mass flow rate out is ρQ and rate of production or mass within reactor is equal to 0. So the rate of accumulation would be equal to $\frac{d(\rho v)}{dt}$ and all these terms are having the usual meaning and significance. So the overall mass balance equation should be

$$\frac{d(\rho v)}{dt} = \rho_0 Q_0 - \rho Q$$

Now if the reactor volume is constant, for constant volume we can take out v outside. So we can write

$$\mathrm{v}\frac{d\rho}{dt} = \rho_0 Q_0 - \rho Q \text{ for [v = constant]}$$

That is for v is equal to constant. Now if assume the density ρ_0 that is the density of the fluid is same as the density inside the reactor at any time then we can simply write $Q = Q_0$, so this is the overall mass balance relation.

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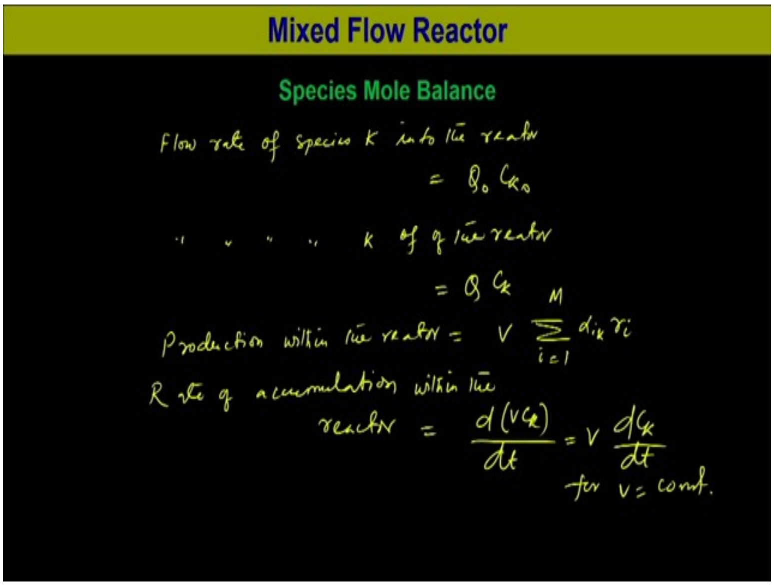


Mixed Flow Reactor

Species Mole Balance

Flow rate of species k into the reactor

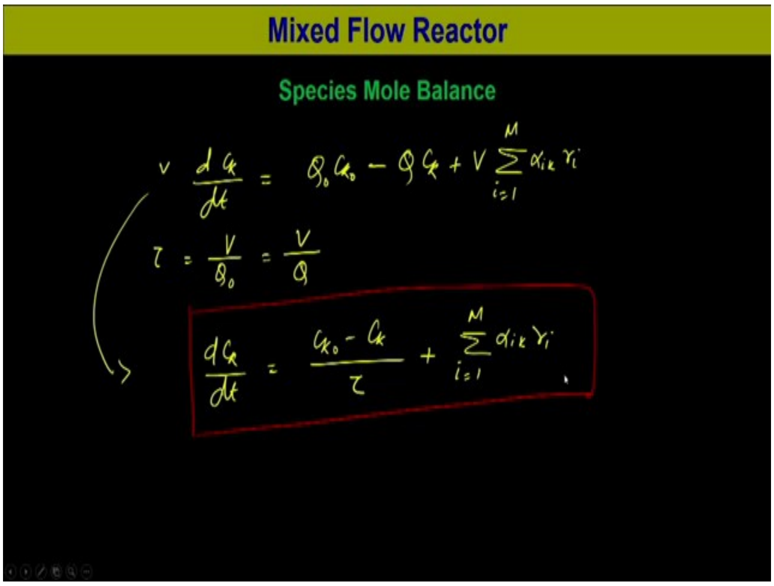
$$= Q_0 C_{k0}$$

" " " " k of of the reactor

$$= Q C_k$$

Production within the reactor $= V \sum_{i=1}^{M} \alpha_{ik} r_i$

Rate of accumulation within the reactor $= \frac{d(VC_k)}{dt} = V\frac{dC_k}{dt}$ for V = const.



Mixed Flow Reactor

Species Mole Balance

$$V\frac{dC_k}{dt} = Q_0 C_{k0} - Q C_k + V\sum_{i=1}^{M} \alpha_{ik} r_i$$

$$\tau = \frac{V}{Q_0} = \frac{V}{Q}$$

$$\boxed{\frac{dC_k}{dt} = \frac{C_{k0} - C_k}{\tau} + \sum_{i=1}^{M} \alpha_{ik} r_i.}$$

Now if you consider mole balance, this is mole balance we can, for a particular species k we can write the species mole balance as flow rate of species k into the reactor is equal to $Q_0 C_{k0}$

Flow rate of species k out of the reactor is equal to QC_k. Now the production within the reactor, that is due to the chemical reaction, it would be equal to v and if multiple reaction is happening it would be $v\sum_{i=1}^{M}\alpha_{ik}r_i$

and the rate of accumulation within the reactor, that would be

$$\frac{d(vC_k)}{dt} = v\frac{dC_k}{dt} \text{ for v = constant}$$

So now if we write the overall balance equation we can write

$$v\frac{dC_k}{dt} = Q_0 C_{k0} - QC_k + = v\sum_{i=1}^{M}\alpha_{ik}r_i$$

If the density inside the reactor is same as that of the (outside), that of the feed then we can define the residence time

$$\tau = \frac{v}{Q_0} = \frac{v}{Q}$$

So then this equation we can write as

$$\frac{dC_k}{dt} = \frac{C_{k0} - C_k}{\tau} + \sum_{i=1}^{M}\alpha_{ik}r_i$$

So this is the species mole balance equation under the conditions of the constant density.

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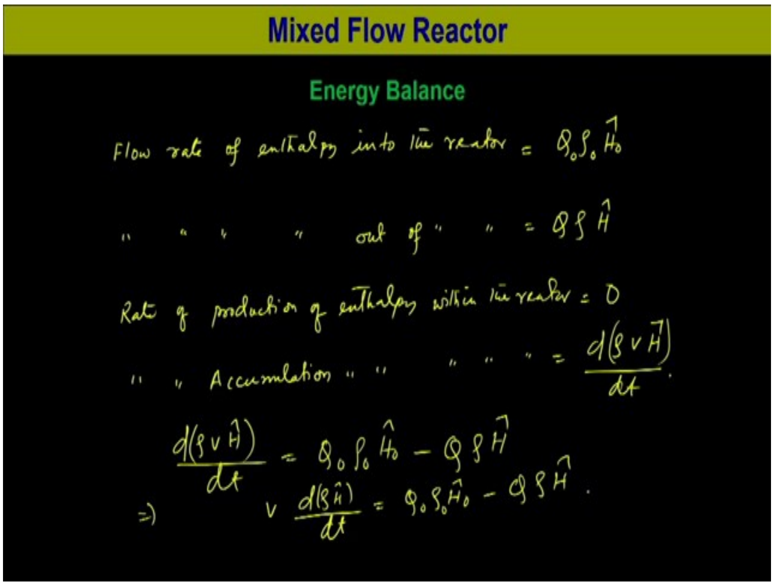

Mixed Flow Reactor

Energy Balance

Flow rate of enthalpy into the reactor = $Q_0\rho_0\hat{H}_0$

" " " " out of " " = $Q\rho\hat{H}$

Rate of production of enthalpy within the reactor = 0

" " Accumulation " " " " " = $\frac{d(\rho v\hat{H})}{dt}$.

$$\frac{d(\rho v\hat{H})}{dt} = Q_0\rho_0\hat{H}_0 - Q\rho\hat{H}$$

$$\Rightarrow v\frac{d(\rho\hat{H})}{dt} = Q_0\rho_0\hat{H}_0 - Q\rho\hat{H}.$$

Now we can write the energy balance equation for flow rate of enthalpy into the liquid, into the reactor, so flow rate of enthalpy into the reactor would be $Q_0\rho_0\Delta H_0$. Flow rate of enthalpy out of the reactor would be $Q\rho\Delta H$, and rate of production of enthalpy within the reactor would be 0. Rate of accumulation of enthalpy within the reactor would be equal to $\frac{\rho V\Delta H}{dt}$. So if we write the balance equation from here, it would be

$$\frac{d(\rho V\Delta H)}{dt} = Q_0\rho_0\Delta H_0 - Q\rho\Delta H$$

For constant volume system this would be

$$\mathrm{V}\frac{d(\rho\Delta H)}{dt} = Q_0\rho_0\Delta H_0 - Q\rho\Delta H$$

Now if there is no heat transfer through the wall but the reactant which is coming inside the reactor and the enthalpy is going out with the product which is going out from the reactor.

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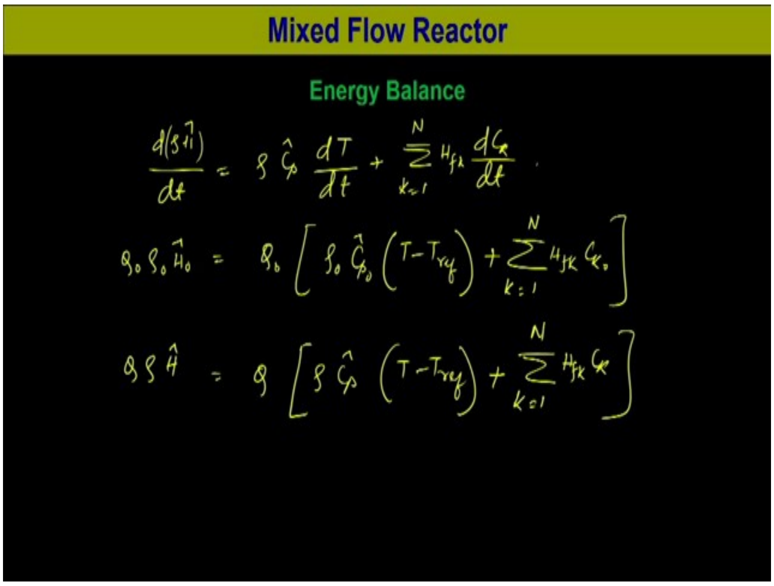

Mixed Flow Reactor

Energy Balance

$$\frac{d(\rho \hat{H})}{dt} = \rho \hat{C}_p \frac{dT}{dt} + \sum_{k=1}^{N} H_{fk} \frac{dC_k}{dt} .$$

$$Q_0 \rho_0 \hat{H}_0 = Q_0 \left[\rho_0 \hat{C}_{p_0} \left(T - T_{ref} \right) + \sum_{k=1}^{N} H_{fk} C_{k0} \right]$$

$$Q \rho \hat{H} = Q \left[\rho \hat{C}_p \left(T - T_{ref} \right) + \sum_{k=1}^{N} H_{fk} C_k \right]$$

So we can write similarly in case of the batch reactor we have done, we can write

$$\frac{d(\rho \Delta \hat{H})}{dt} = \rho \hat{C}_P \frac{dT}{dt} + \sum_{k=1}^{N} H_{fk} \frac{dC_k}{dt}$$

So we can get the enthalpy temperature relationship. Now we can write, under steady state conditions we can write this relation would be

$$Q_0 \rho_0 \hat{H}_0 = Q_0 \left[\rho_0 \hat{C}_{P0} \left(T - T_{ref} \right) + \sum_{k=1}^{N} H_{fk} C_{k0} \right]$$

Similarly, we can write

$$Q \rho \hat{H} = Q \left[\rho \hat{C}_P \left(T - T_{ref} \right) + \sum_{k=1}^{N} H_{fk} C_k \right]$$

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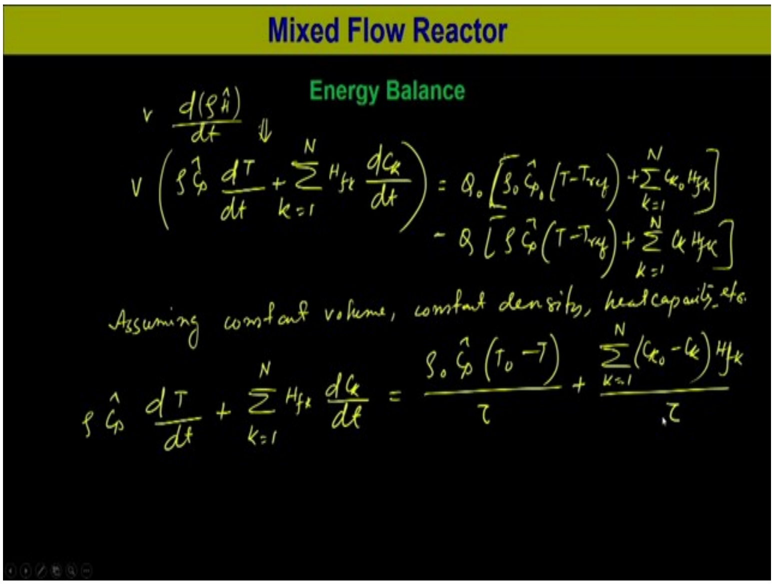

Mixed Flow Reactor

Energy Balance

$$V \frac{d(\rho \hat{h})}{dt} \Downarrow$$

$$V\left(\rho \hat{C}_p \frac{dT}{dt} + \sum_{k=1}^{N} H_{fk}\frac{dC_k}{dt}\right) = Q_0\left[\rho_0 \hat{C}_{p0}(T-T_{ref}) + \sum_{k=1}^{N} C_{k0}H_{fk}\right] - Q\left[\rho\hat{C}_p(T-T_{ref}) + \sum_{k=1}^{N} C_k H_{fk}\right]$$

Assuming constant volume, constant density, heat capacity etc.

$$\rho\hat{C}_p \frac{dT}{dt} + \sum_{k=1}^{N} H_{fk}\frac{dC_k}{dt} = \frac{\rho_0\hat{C}_{p0}(T_0-T)}{\tau} + \frac{\sum_{k=1}^{N}(C_{k0}-C_k)H_{fk}}{\tau}$$

Now if we substitute these three terms in the energy balance equation we can write V is equal to, so So this is nothing but

$$V\left(\rho\hat{C}_P\frac{dT}{dt}+\sum_{k=1}^{N}H_{fk}\frac{dC_k}{dt}\right)$$

So this term can be written as this, then if we substitute the other two terms this would be equal to

$$V\left(\rho\hat{C}_P\frac{dT}{dt}+\sum_{k=1}^{N}H_{fk}\frac{dC_k}{dt}\right)=Q_0\left[\rho_0\hat{C}_{P0}(T-T_{ref})+\sum_{k=1}^{N}H_{fk0}C_{k0}\right]-Q\left[\rho\hat{C}_P(T-T_{ref})+\sum_{k=1}^{N}H_{fk}C_k\right]$$

Now if we assume constant volume, constant density and constant heat capacity; so assuming constant volume, constant density, heat capacity, etcetera. we can write

$$\rho\hat{C}_P\frac{dT}{dt}+\sum_{k=1}^{N}H_{fk}\frac{dC_k}{dt}=\frac{\rho_0\hat{C}_{P0}(T-T_0)}{\tau}+\frac{\sum_{k=1}^{N}(C_{k0}-C_k)H_{fk}}{\tau}$$

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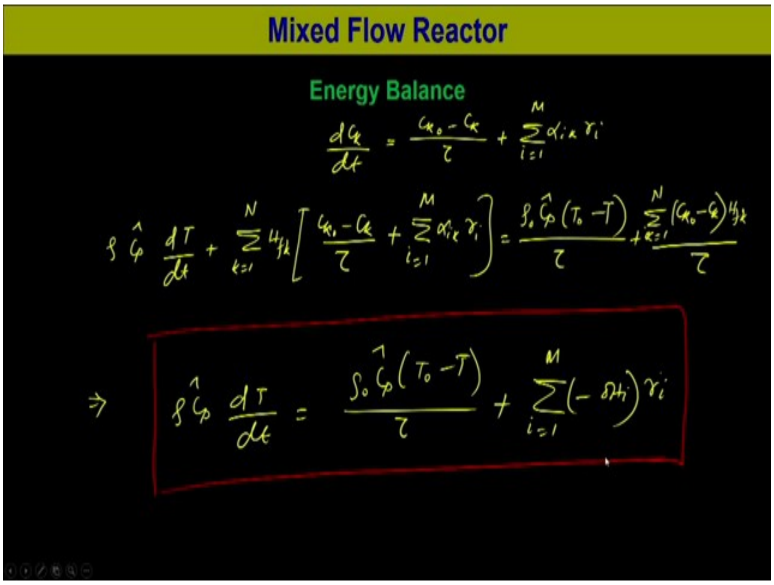

Mixed Flow Reactor

Energy Balance

$$\frac{dC_k}{dt} = \frac{C_{k0} - C_k}{\tau} + \sum_{i=1}^{M} \alpha_{ik} r_i$$

$$\rho \hat{C}_p \frac{dT}{dt} + \sum_{k=1}^{N} H_{fk}\left[\frac{C_{k0} - C_k}{\tau} + \sum_{i=1}^{M} \alpha_{ik} r_i\right] = \frac{\rho_0 \hat{C}_p (T_0 - T)}{\tau} + \frac{\sum_{k=1}^{N} (C_{k0} - C_k) H_{fk}}{\tau}$$

$$\Rightarrow \boxed{\rho \hat{C}_p \frac{dT}{dt} = \frac{\rho_0 \hat{C}_p (T_0 - T)}{\tau} + \sum_{i=1}^{M} (-\Delta H_i) r_i}$$

Now if we substitute the derivative in this expression that is $\frac{dC_k}{dt}$ we have derived earlier, if we substitute that, that is basically

$$\frac{dC_k}{dt} = \frac{C_{k0} - C_k}{\tau} + \sum_{i=1}^{M} \alpha_{ik} r_i$$

If you substitute in the earlier equations we would obtain

$$\rho \hat{C}_P \frac{dT}{dt} + \sum_{k=1}^{N} H_{fk}\left[\frac{C_{k0} - C_k}{\tau} + \sum_{i=1}^{M} \alpha_{ik} r_i\right] = \frac{\rho_0 \hat{C}_P (T - T_0)}{\tau} + \frac{\sum_{k=1}^{N} (C_{k0} - C_k) H_{fk}}{\tau}$$

Now from the both sides the term $\frac{\sum_{k=1}^{N} (C_{k0} - C_k) H_{fk}}{\tau}$ we will cancel from both sides, and using the definition of the heat of reaction, this relations will reduce to

$$\rho \hat{C}_P \frac{dT}{dt} = \frac{\rho_0 \hat{C}_P (T - T_0)}{\tau} + \sum_{i=1}^{M} -\left(\Delta H_i\right) r_i$$

So this is the energy balance equation for the CSTR. Now if the reactor is not adiabatic there would be heat flux through the wall.

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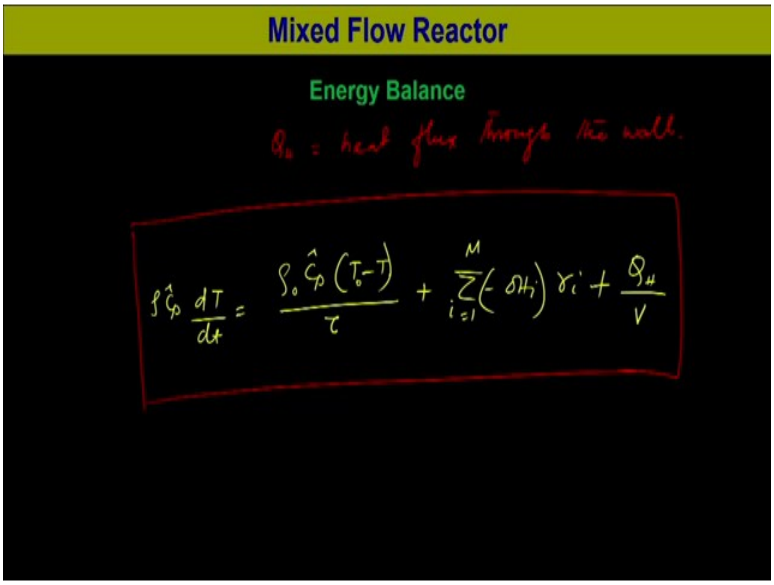

Mixed Flow Reactor

Energy Balance

Q_H = heat flux through the wall.

$$\boxed{\rho \hat{C}_p \frac{dT}{dt} = \frac{\rho_0 \hat{C}_p (T_0 - T)}{\tau} + \sum_{i=1}^{M} (-\Delta H_i)\, r_i + \frac{Q_H}{V}}$$

So if there is heat flux through the wall say Q_H in that case this would be added into the energy balance equation and you would obtain

$$\rho \hat{C}_P \frac{dT}{dt} = \frac{\rho_0 \hat{C}_P (T - T_0)}{\tau} + \sum_{i=1}^{M} \left(-\Delta H_i\right) r_i + \frac{Q_H}{V}$$

So this is for non-adiabatic systems where there is a heat flux through the wall.

So thank you very much for attending this lecture and we will continue our discussion on the reaction design and particularly the energy balance equation for the CSTR where we would see so many interesting phenomena happens when we have a single reaction. We will discuss those phenomena for the, basically that is called the steady state multiplicity of the CSTR or continuous mixed flow reactor, thank you.