Chemical Reaction Engineering 1
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Lecture 23
Importance and Applications of Extrusion Technology in Food Processing

Welcome to the 13th lecture of module four. In this module we are discussing reactor design. Before going to this lecture let us have brief recap on our previous lecture.

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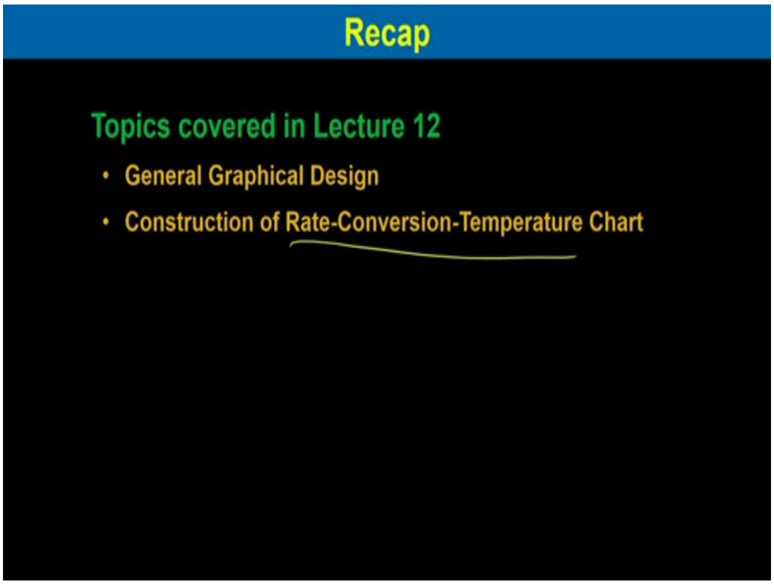

Recap

Topics covered in Lecture 12

- General Graphical Design
- Construction of Rate-Conversion-Temperature Chart

In the last lecture we have covered graphical design procedure for the reactor size and then we have seen how to construct rate conversion and temperature chart. So, rate conversion and temperature chart is basically plot of conversion versus temperature at different rates, which we call it you know Contour plot, where three parameters are plotted in two dimension.

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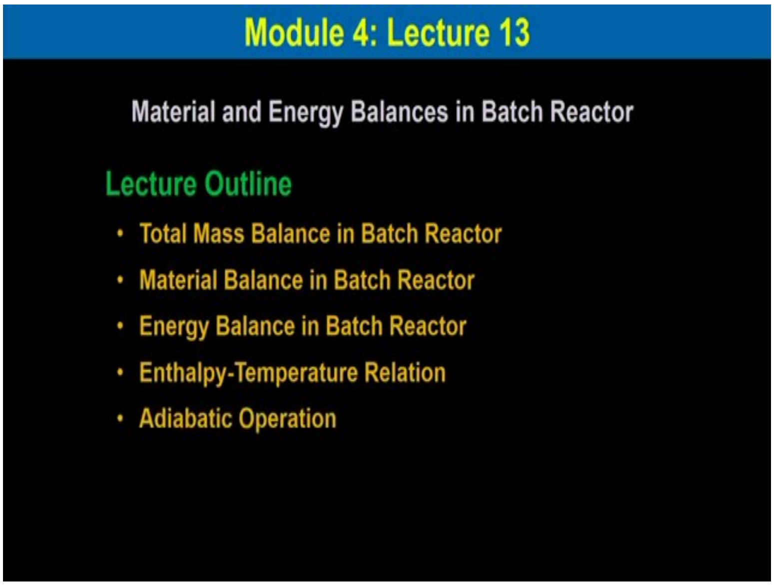

Module 4: Lecture 13

Material and Energy Balances in Batch Reactor

Lecture Outline

- Total Mass Balance in Batch Reactor
- Material Balance in Batch Reactor
- Energy Balance in Batch Reactor
- Enthalpy-Temperature Relation
- Adiabatic Operation

In this lecture, we will consider material and energy balances in batch reactor. The brief lecture outline are as follows. We will consider total mass balance in batch reactor, material balance in batch reactor, then we will consider energy balance in batch reactor, enthalpy, temperature relationship and finally we will consider adiabatic operation.

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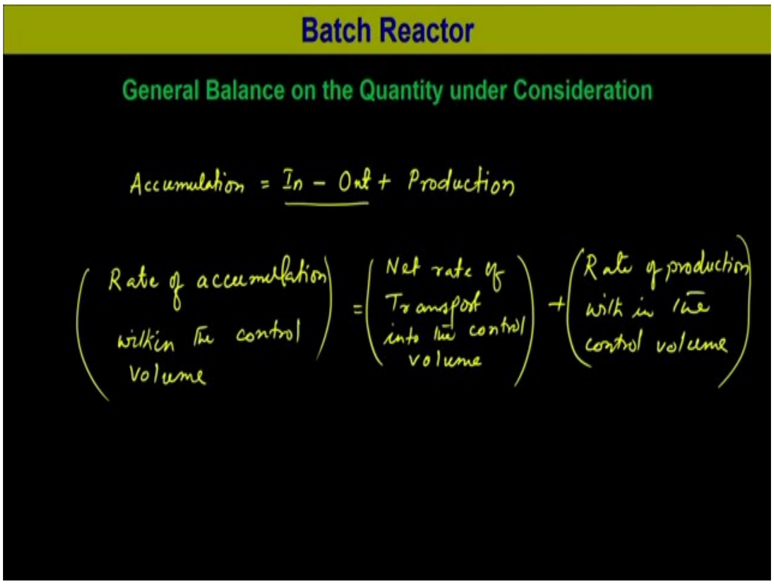

Batch Reactor

General Balance on the Quantity under Consideration

$$\text{Accumulation} = \underline{\text{In} - \text{Out}} + \text{Production}$$

$$\begin{pmatrix}\text{Rate of accumulation}\\ \text{within the control}\\ \text{Volume}\end{pmatrix} = \begin{pmatrix}\text{Net rate of}\\ \text{Transport}\\ \text{into the control}\\ \text{volume}\end{pmatrix} + \begin{pmatrix}\text{Rate of production}\\ \text{with in the}\\ \text{control volume}\end{pmatrix}$$

So, let us start with batch reactor general balance on the quantity under consideration. So, as we have already discussed the reactor design at the beginning of this module, to how to design a batch reactor for a single reaction. And we have considered a generalized transport equations or the balanced equation, like if we consider rate of accumulation of a certain components inside the reactor that means accumulation terms.

So, accumulation would be equal to rate of transport into the control volume that is we can call it in minus rate of transport out of the control volume which is out plus the rate of production within the control volume, so we can write simply production. Now, the transport in and transport out which is a little bit artificial but if we can call together is the net rate of transport into the control volume, then that would be much better.

So, we can write in terms of net rate of transport, so we can write rate of accumulation within the control volume which would be equal to net rate of transport into the control volume plus rate of production within the control volume. So, now, if we consider batch reactor and first we will consider multiple reaction which is happening inside the reactor and we will develop the generalized balance equation, which can be simplified to the single reaction.

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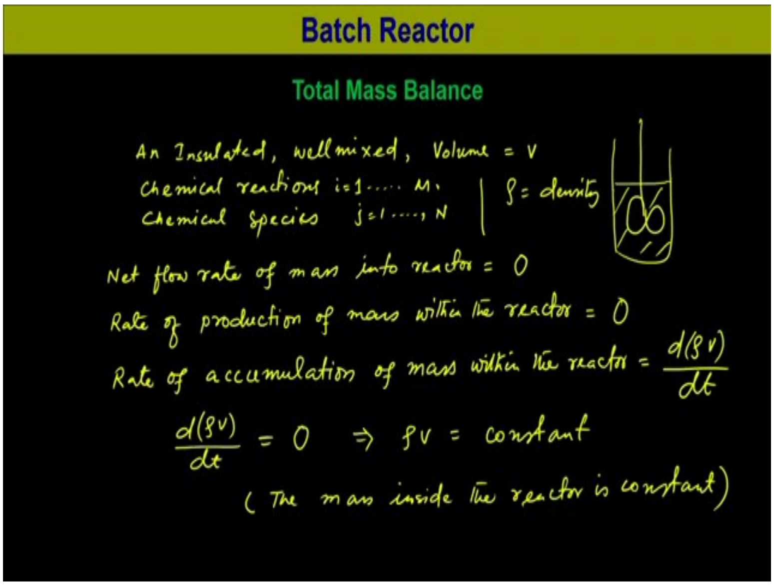

Batch Reactor

Total Mass Balance

An Insulated, well mixed, Volume = V

Chemical reactions $i = 1 \ldots\ldots M$,

Chemical species $j = 1, \ldots, N$

ρ = density

Net flow rate of mass into reactor = 0

Rate of production of mass within the reactor = 0

Rate of accumulation of mass within the reactor = $\frac{d(\rho V)}{dt}$

$$\frac{d(\rho V)}{dt} = 0 \Rightarrow \rho V = \text{constant}$$

(The mass inside the reactor is constant)

So, let us consider an insulated system well mixed batch reactor and volume is equal to V, in which there are M number of chemical reactions, so chemical reactions 1 to M and N number of species. So, chemic chemical species, say J is equal to 1, 2 and here I can say, right, I is equal to 1 to M, J is equal to 1 to N. So, N number of chemical species, M number of chemical reactions are happening inside a batch reactor.

The reactor is well insulated and it is well mixed whose volume is V. Now, if we write the balanced equation total mass balance equation in a batch reactor, we can write, so this is our batch reactor and it is well insulated, where we have incorporated some chemical species and chemical reactants and they will react and forming different species through several chemical reactions.

So, we can write the net flow rate of mass into reactor, so this net flow rate means in and out, so since batch reactor, we used to include the material inside close it and then start it for a certain period of time, so there is no inlet or outlet. So, the net rate of term mass into the reactor would be 0. Now, rate of production of mass within the chemical reactions would be also 0 as we have seen earlier that the mass is conserved in any chemical reactions.

If there is not huge change in energy, like in nuclear reactions where mass change is significant due to the evolution of heat, huge amount of heat. So, in this case, even if we have considered highly exothermic reaction of combustion, and where heat is evolved to a quite significant amount, but the mass change is not so significant because that is with respect to the mass of the chemicals we used is negligible.

So, rate of production of mass within the reactor would be 0. The rate of accumulation of mass within the reactor would be equal to, if V is the volume and if we consider the density ρ is equal to the density of the fluid, then the mass would be ρ V, so the rate of accumulation of mass within the reactor would be $\frac{d(\rho V)}{dt}$, so ρV is the total mass within the reactor and if we write the balanced equation.

So, accumulation would be equal to net rate of mass into the reactor and rate of production of mass within the reactor. So, we can write $\frac{d(\rho V)}{dt}$ is equal to 0, which simply says that the mass inside the reactor each constant or from here we can say that rho V is equal to constant. The mass inside the reactor is constant. So, this is the total material balance equation in a batch reactor. Now, let us do the species mole balance.

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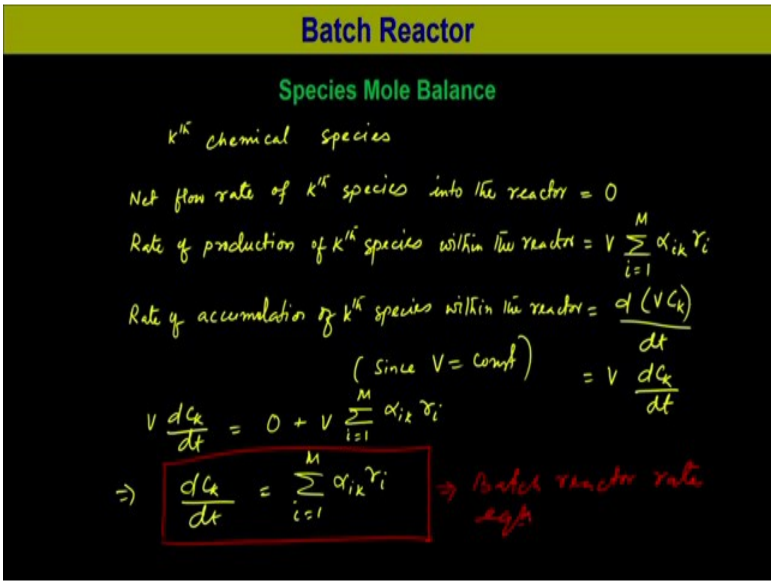

Batch Reactor

Species Mole Balance

k^{th} chemical species

Net flow rate of k^{th} species into the reactor = 0

Rate of production of k^{th} species within the reactor $= V\sum_{i=1}^{M}\alpha_{ik} r_i$

Rate of accumulation of k^{th} species within the reactor $= \frac{d(VC_k)}{dt}$

(Since V = const) $= V\frac{dC_k}{dt}$

$$V\frac{dC_k}{dt} = 0 + V\sum_{i=1}^{M}\alpha_{ik} r_i$$

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

→ Batch reactor rate eqn

Now, if we write for any species say Kth species chemical species, so we will consider Kth chemical species and we can write net flow rate of Kth spieces into the reactor is equal to 0, the rate of production of Kth species within the reactor would be V is the volume of the reactor and there are M number of reactions going on, so I is equal, summation over I is equal to 1 to M alpha ik RI, so the alpha IK is the stoichiometric coefficient of the chemical species. So, this is the rate of production of Kth species within the reactor.

Now, rate of accumulation of Kth species within the reactor, this would be d V into say Ck is the concentration of species K dt and which we can write would be equal to V dCk dt since V is equal to constant, so we are considering constant volume system. So, here V is equal to constant so we can take out the V from the differential sign, so V dCk dt.

So, if we write the balanced equation we would obtain V d Ck dt would be equal to 0 plus V summation over I is equal to 1 to M alpha ik RI. So, from here we can write so V we will cancelled out so it we will get dCk dt would be equal to summation over I is equal to 1 to M alpha ik RI, so this is a familiar batch reactor species balance equation or we can say batch reactor rate equation.

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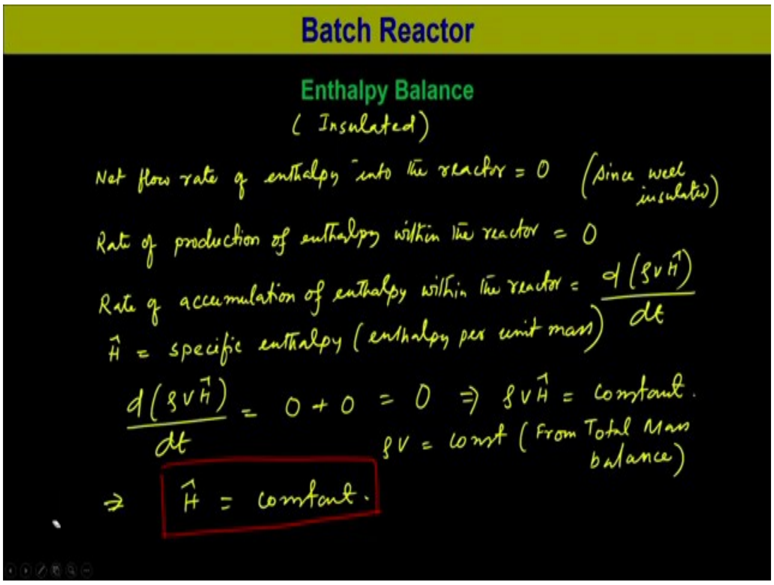

Batch Reactor

Enthalpy Balance

(Insulated)

Net flow rate of enthalpy into the reactor = 0 (Since well insulated)

Rate of production of enthalpy within the reactor = 0

Rate of accumulation of enthalpy within the reactor = $\frac{d(\rho V \vec{H})}{dt}$

$\vec{H}$ = specific enthalpy (enthalpy per unit mass)

$$\frac{d(\rho V \vec{H})}{dt} = 0 + 0 = 0 \Rightarrow \rho V \vec{H} = \text{constant.}$$

ρV = const (From Total Mass balance)

$$\Rightarrow \boxed{\vec{H} = \text{constant.}}$$

So, now, we will consider the enthalpy balance equations we have seen the how to calculate for a single reaction how to calculate the heat of reaction from the thermodynamics and how the heat of reaction is related with temperature we have seen that, So, now, we will consider the enthalpy balance for a particular reactor that is batch reactor and as we have considered the reactor is well insulated.

So, enthalpy balance insulated reactor, so we can write net flow rate of enthalpy into the reactor, this would be 0, since it is well insulated . Then rate of production of enthalpy within the reactor should be 0 and rate of accumulation of enthalpy within the reactor would be d

$\frac{d(\rho V \hat{H})}{dt}$, so $\hat{H}$ is the specific enthalpy that means it is enthalpy per unit mass, ρV is the mass of the fluid or the reactants. And $\hat{H}$ is the enthalpy per unit mass so this is change of enthalpy with respect to time.

So, now, if we write the balance equation we would get $\frac{d(\rho V \hat{H})}{dt}$ would be equal to the net rate of enthalpy into the reactor is 0 and this is also 0, so it would be 0. So, from here we can write $\rho V \hat{H}$ is equal to constant and from the total mass balance we have seen ρV is equal to constant from total mass balance. So, from here we can write H the enthalpy $\hat{H}$, specific enthalpy is constant, so this is not so trivial as it first appear as we are much more concerned about the change in temperature instead of enthalpy.

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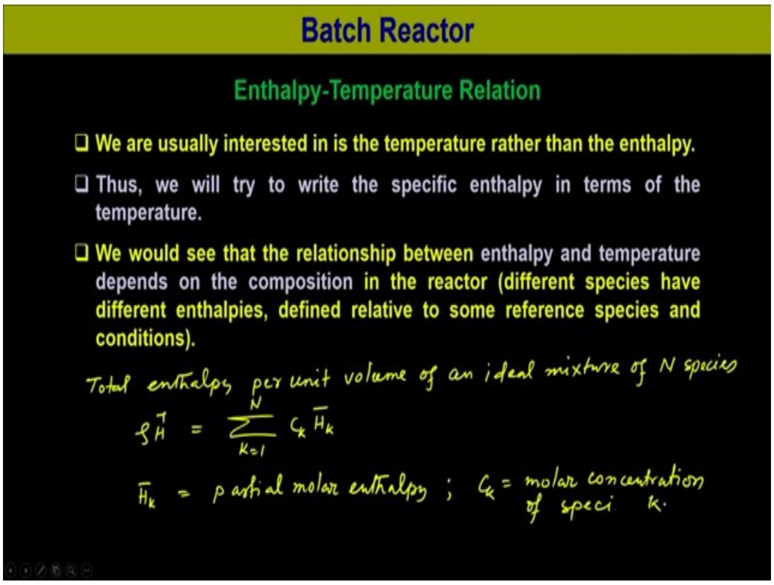

Batch Reactor

Enthalpy-Temperature Relation

- We are usually interested in is the temperature rather than the enthalpy.
- Thus, we will try to write the specific enthalpy in terms of the temperature.
- We would see that the relationship between enthalpy and temperature depends on the composition in the reactor (different species have different enthalpies, defined relative to some reference species and conditions).

Total enthalpy per unit volume of an ideal mixture of N species

$$\rho \hat{H} = \sum_{k=1}^{N} C_k \bar{H}_k$$

$\bar{H}_k$ = partial molar enthalpy ; C_k = molar concentration of speci k.

So, let us see how the enthalpy is related with the temperature, so enthalpy temperature relation. So we are ussually intrested is in the temperature rather than enthalpy and we will try to write the specific enthalpy in terms of the temperature and then we would see that the relationship between enthalpy and temperature will depend on the composition in the reactor, that means different species have different enthalpies, which is defined relative to some reference species and conditions.

So if we write total enthalpy per unit volume of an ideal mixtures of N species, so total enthalpy, per unit volume of an ideal mixture of N species, you can write $\rho \hat{H} = \sum_{K=1}^{N} C_K \overline{H_K}$ here $\overline{H_K}$ is the partial molar enthalpy and Ck is the molar concentration of species k.

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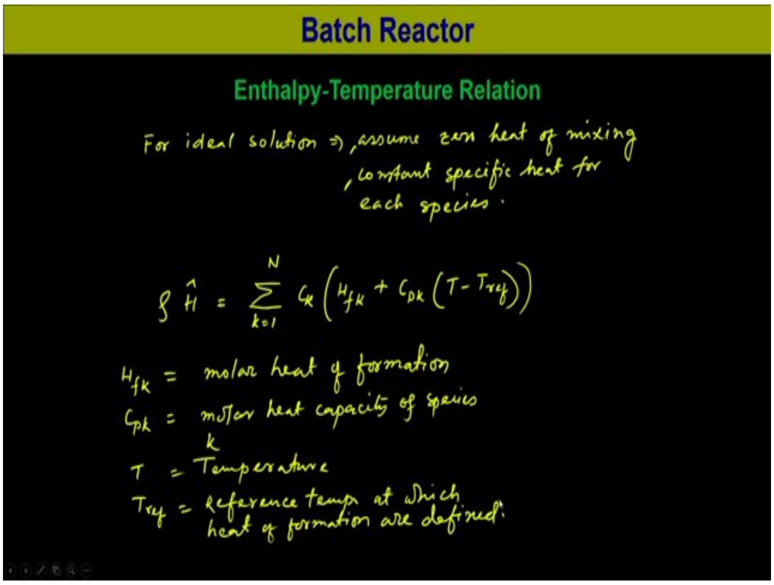

Batch Reactor

Enthalpy-Temperature Relation

For ideal solution ⇒ , assume zero heat of mixing
, constant specific heat for
each species.

$$\rho \hat{H} = \sum_{k=1}^{N} C_k \left(H_{fk} + C_{pk}\left(T - T_{ref}\right)\right)$$

H_{fk} = molar heat of formation
C_{pk} = molar heat capacity of species k
T = Temperature
T_{ref} = reference temp at which heat of formation are defined.

Now, if we consider 0 heat of mixing as we have considered ideal solution, so for ideal solution we can assume 0 heat of mixing and also assume constant specific heat for each species so then we can write in terms of temperature $\rho \hat{H} = \sum_{K=1}^{N} C_K (H_{fK} + C_{pK}(T - T_{ref}))$. Hfk is the molar heat of formation and C_{pK} is the molar heat capacity of species K, species K. C_{pK} is the molar heat capacity of species K, T is the temperature and T_{ref} is a reference temperature at which the heats of formations are defined.

So this relation of enthalpy temperature is a drastic simplification of the no different situations where small change in enthalpy is of great importance, like in case of many gas phase reactions the small change in enthalpy can change no, so gas phase reactions. The enthalpy change is much larger compared to the heat of mixing. So, there should be error due to the assumption of constant specific heat.

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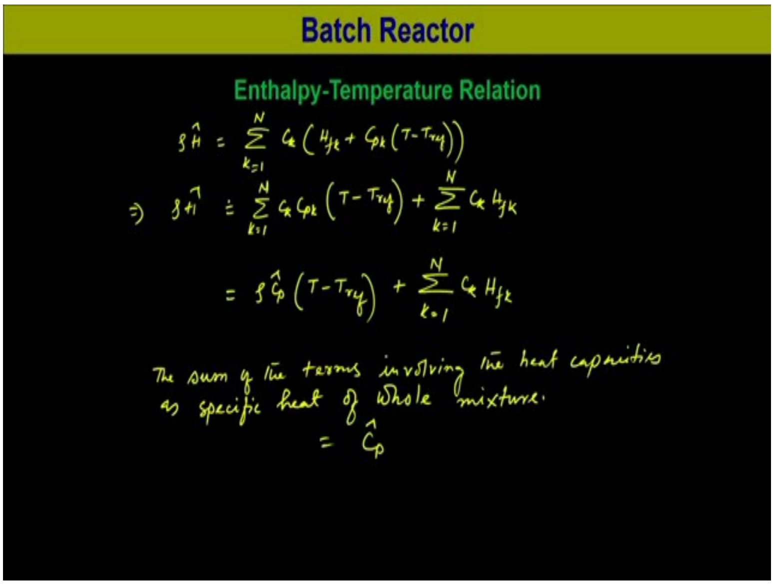

Batch Reactor

Enthalpy-Temperature Relation

$$\rho\hat{H} = \sum_{k=1}^{N} C_k \left(H_{fk} + C_{pk}(T - T_{ref})\right)$$

$$\Rightarrow \rho\hat{H} = \sum_{k=1}^{N} C_k C_{pk}\left(T - T_{ref}\right) + \sum_{k=1}^{N} C_k H_{fk}$$

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

The sum of the terms involving the heat capacities as specific heat of whole mixture.

$$= \hat{C}_p$$

Now, so we have $\rho\hat{H} = \sum_{K=1}^{N} C_K (H_{fK} + C_{pK}(T - T_{ref}))$. Now, if we simplify this, this would be $\rho\hat{H} = \sum_{K=1}^{N} C_K C_{pK}(T - T_{ref}) + \sum_{K=1}^{N} C_K H_{fK}$, so the sum of the term of the heat capacities, we can write the specific heat of the whole mixture because this is from K is equal to 1 to N for N species.

So, we can write, from here we can write this would be = $\rho\hat{C}_p(T - T_{ref}) + \rho\sum_{K=1}^{N} C_K H_{fK}$. So, here we have considered the sum of the terms involving the the heat capacities as specific heat of whole mixture and we call it H $\hat{C}_p$.

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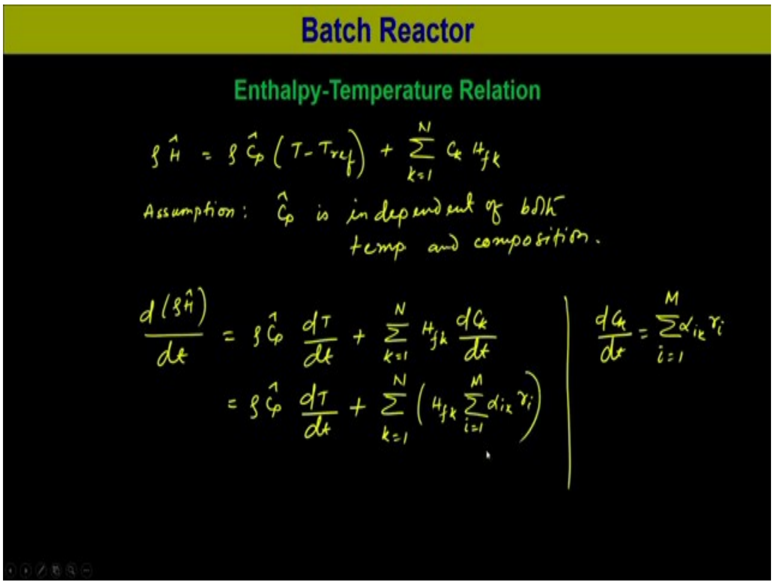

Batch Reactor

Enthalpy-Temperature Relation

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

Assumption : $\hat{C}_p$ is independent of both temp and composition.

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

$$= \rho \hat{C}_p \frac{dT}{dt} + \sum_{k=1}^{N} \left(H_{fk} \sum_{i=1}^{M} \alpha_{ik} r_i \right)$$

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

So, now, if we take the time derivative of it, of this relation, so we have $\rho \hat{H}$ = $\rho \hat{C}_p (T - T_{ref}) + \rho \sum_{K=1}^{N} C_K H_{fK}$. Now, if we take the derivative of this and put into the differential form and assume $\hat{C}_p$ is independent of both temperature and composition, so this is another big assumptions specific heat of the whole mixture is independent of both temperature and composition.

Now, if we take the derivative of this, this would be $\frac{d(\rho \hat{H})}{dt} = \rho \hat{C}_p \frac{dT}{dt} + \sum_{K=1}^{N} H_{fK} \frac{dC_K}{dt}$ which we can write $= \rho \hat{C}_p \frac{dT}{dt} + \sum_{K=1}^{N} H_{fK} \frac{dC_K}{dt}$, k from the species balance, we have obtained $\frac{dC_K}{dt}$ is equal to $\sum_{i=1}^{M} \alpha_{ik} r_i$. So, if we substitute this over here, this would be. $\sum_{i=1}^{M} \alpha_{ik} r_i$

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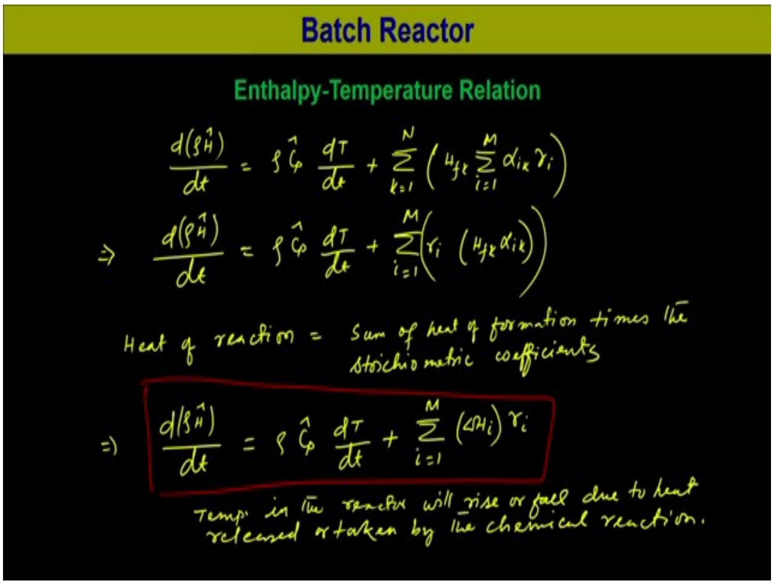

Batch Reactor

Enthalpy-Temperature Relation

$$\frac{d(\rho\hat{H})}{dt} = \rho\hat{C}_p\frac{dT}{dt} + \sum_{k=1}^{N}\left(H_{fk}\sum_{i=1}^{M}\alpha_{ik}r_i\right)$$

$$\Rightarrow \frac{d(\rho\hat{H})}{dt} = \rho\hat{C}_p\frac{dT}{dt} + \sum_{i=1}^{M}\left(r_i\,(H_{fk}\alpha_{ik})\right)$$

Heat of reaction = Sum of heat of formation times the stoichiometric coefficients

$$\Rightarrow \boxed{\frac{d(\rho\hat{H})}{dt} = \rho\hat{C}_p\frac{dT}{dt} + \sum_{i=1}^{M}(\Delta H_i)r_i}$$

Temp. in the reactor will rise or fall due to heat released or taken by the chemical reaction.

Now, we have the $\frac{d(\rho\hat{H})}{dt} = \rho\hat{C}_p\frac{dT}{dt} + \sum_{K=1}^{N}(H_{fK}\sum_{i=1}^{M}\alpha_{ik}r_i)$. Now if we reverse the order of the summation we can write from here, $\frac{d(\rho\hat{H})}{dt} = \rho\hat{C}_p\frac{dT}{dt} + \sum_{K=1}^{N}(H_{fK}\sum_{i=1}^{M}\alpha_{ik}r_i)$, so this will be summation over this.

So, this term the summation over heat of formation H_{fK} times the stoichiometric coefficient for the M number of chemical reactions can be recognized as the heat of reactions, which is the definition of the heat of the reaction, so from the definition the heat of reaction, sum of the heat of formation times the stoichiometric coefficient, this is the heat of reaction, so we can write from here $\frac{d(\rho\hat{H})}{dt}$ would be equal to $\rho\hat{C}_p\frac{dT}{dt}$

So $\frac{d(\rho\hat{H})}{dt} = \rho\hat{C}_p\frac{dT}{dt} + \sum_{K=1}^{M}(\Delta H_i)r_i$, so this relation of energy balance or enthalpy balance simply say that the temperature in the reactor will rise or fall due to heat released or taken by the chemical reaction. So, this relationship will tell whether the temperature of the reactor will increase or it will fall due to the heat released or taken by the chemical reaction.

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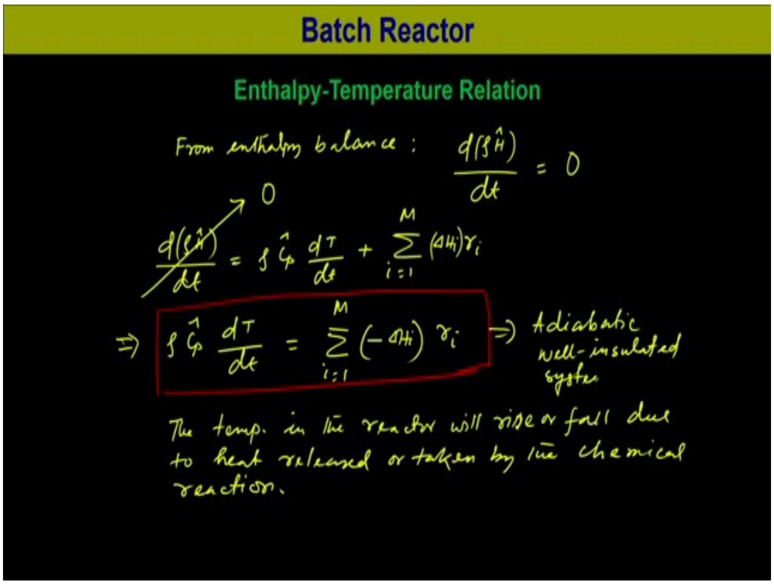

Batch Reactor

Enthalpy-Temperature Relation

From enthalpy balance : $\frac{d(\rho \hat{H})}{dt} = 0$

$$\cancel{\frac{d(\rho \hat{H})}{dt}} \xrightarrow{} 0 = \rho \hat{C}_p \frac{dT}{dt} + \sum_{i=1}^{M} (\Delta H_i) r_i$$

$$\Rightarrow \boxed{\rho \hat{C}_p \frac{dT}{dt} = \sum_{i=1}^{M} (-\Delta H_i) r_i} \Rightarrow$$ Adiabatic well-insulated system

The temp. in the reactor will rise or fall due to heat released or taken by the chemical reaction.

Now, if we write for the adiabatic system the relations which we have developed that is…

Now, from the enthalpy balance we know that $\frac{d(\rho \hat{H})}{dt} = 0$, so if we substitute in this relation

$\frac{d(\rho \hat{H})}{dt} = \sum_{K=1}^{M} (-\Delta H_i) r_i$ this term from the total enthalpy balance, this is 0.

Now if we substitute this is 0 we can write $\rho \hat{C}_p \frac{dT}{dt} = \sum_{K=1}^{M} (-\Delta H_i) r_i$, so this relation simply said that the temperature in the reactor will rise or fall due to heat released or taken by the chemical reaction. Now, this derivation is basically for adiabatic well insulated systems, adiabatic well insulated system.

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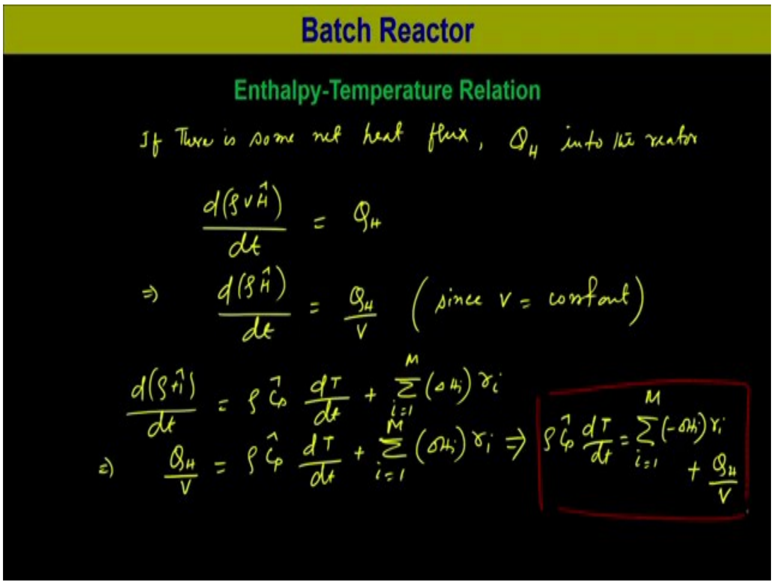

Batch Reactor

Enthalpy-Temperature Relation

If There is some net heat flux, Q_H into the reactor

$$\frac{d(\rho V \hat{H})}{dt} = Q_H$$

$$\Rightarrow \frac{d(\rho \hat{H})}{dt} = \frac{Q_H}{V} \quad (\text{since } V = \text{constant})$$

$$\frac{d(\rho \hat{H})}{dt} = \rho \hat{C}_p \frac{dT}{dt} + \sum_{i=1}^{M} (\Delta H_i) r_i$$

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

Now, if we considered there is some net heat flux to this system, say Q_H, then the energy balance equation, if there is some net heat flux, say Q_H, which is into the reactor. So, the energy balance equation $\frac{d(\rho V \hat{H})}{dt} = Q_H$. Now, since V is constant we can write

$\frac{d(\rho \hat{H})}{dt} = \frac{Q_H}{V}$, since V is constant.

So, in the earlier balanced equation that is $\frac{d(\rho \hat{H})}{dt} = \sum_{K=1}^{M} (-\Delta H_i) r_i$ here this term is $\frac{Q_H}{V}$, so if we substitute here this should be $\frac{Q_H}{V} = \rho \hat{C}_p \frac{dT}{dt} + \sum_{K=1}^{M} (\Delta H_i) r_i$, and from here we can write

$\rho \hat{C}_p \frac{dT}{dt} = \sum_{K=1}^{M} (-\Delta H_i) r_i + \frac{Q_H}{V}$, so this is the equation of the reactor temperature.

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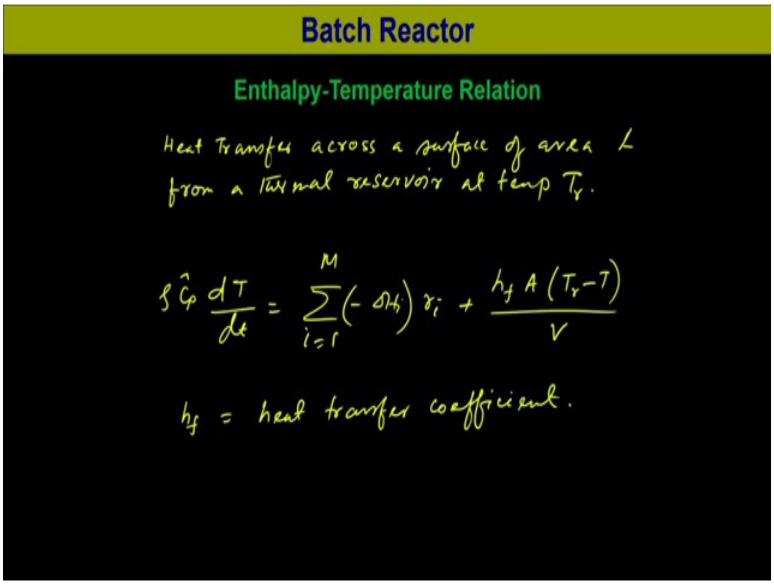

Batch Reactor

Enthalpy-Temperature Relation

Heat Transfer across a surface of area A from a thermal reservoir at temp T_r.

$$\rho \hat{C}_p \frac{dT}{dt} = \sum_{i=1}^{M} (-\Delta H_i) r_i + \frac{h_f A (T_r - T)}{V}$$

h_f = heat transfer coefficient.

Now, if this heat flux is happening across the surface which area is A, so heat transfer across a surface of area A from a from thermal reservoir at temperature T, so we can write this relation $\rho \hat{C}_p \frac{dT}{dt} = \sum_{K=1}^{M} (-\Delta H_i) r_i + \frac{h_f A(T_r - T)}{V}$, so h_f is the heat transfer coefficient.

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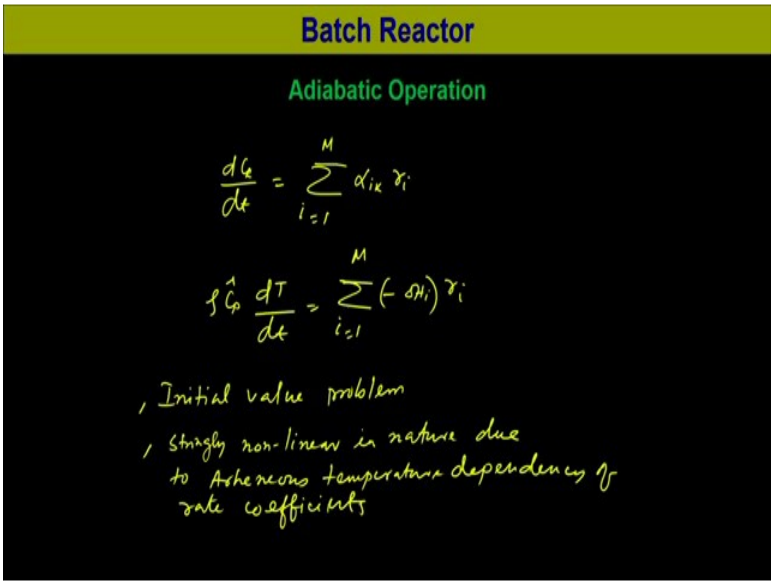

Batch Reactor

Adiabatic Operation

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

$$\rho \hat{C}_p \frac{dT}{dt} = \sum_{i=1}^{M} (-\Delta H_i) r_i$$

, Initial value problem

, Strongly non-linear in nature due to Arrhenius temperature dependency of rate coefficients

So, most of the reactors are non isothermal reactors and this is the important case which we need to consider because for adiabatic reactor when there is no heat in or heat out the adiabatic operation is often desirable because there is little utilities we need to know incorporate and it should be very easy to know operate during its normal operation.

So, as you have seen for the constant volume non isothermal batch reactor we have no two balance equation 1 is 4 this is balanced that is $\frac{dC_k}{dt} = \sum_{i=1}^{M} \alpha_{ik} r_i$ and adiabatic systems we have energy balance $\rho \hat{C}_p \frac{dT}{dt} = \sum_{K=1}^{M} (-\Delta H_i) r_i$, so as we know the rate of the chemical reactions is depends on both the temperature and the concentration.

But this temperature dependency of the arrhenius relation of the rate constant is quite nonlinear in nature, so this is a no case of initial value problems and can be solved as we have no discussed before for the initial value problems for the integration, so this is initial value problem and the equations are strongly nonlinear in nature due to arrhenius temperature dependency of rate cofficients.

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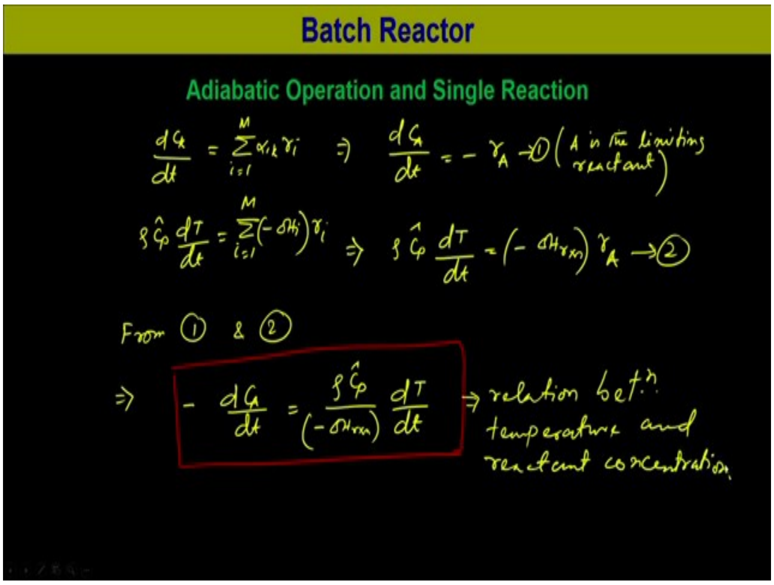

Batch Reactor

Adiabatic Operation and Single Reaction

$$\frac{dC_k}{dt} = \sum_{i=1}^{M} \alpha_{ik} r_i \Rightarrow \frac{dC_A}{dt} = -r_A \rightarrow ① \left(A \text{ is the limiting reactant}\right)$$

$$\rho \hat{C}_p \frac{dT}{dt} = \sum_{i=1}^{M} (-\Delta H_i) r_i \Rightarrow \rho \hat{C}_p \frac{dT}{dt} = (-\Delta H_{rxn}) r_A \rightarrow ②$$

From ① & ②

$$\Rightarrow \boxed{-\frac{dC_A}{dt} = \frac{\rho \hat{C}_p}{(-\Delta H_{rxn})} \frac{dT}{dt}} \Rightarrow \text{relation bet}^{n} \text{ temperature and reactant concentration}$$

Now if we consider single reaction and adiabatic operation so we can write the species balance equation say we have $\frac{dC_k}{dt} = \sum_{i=1}^{M} \alpha_{ik} r_i$ for single reaction we can write, $\frac{dC_A}{dt} = -r_A$ for the reactants, so A is the limiting reactant. Similarly, the temperature relations $\rho \hat{C}_p \frac{dT}{dt} = \sum_{K=1}^{M} (-\Delta H_i) r_i$, this we can write $\rho \hat{C}_p \frac{dT}{dt} = (-\Delta H_{rxn}) r_A$.

Now, from this two relation for the single reaction if we equate rate r_A, so we would obtain from these two relations say this is one and this is two, so from one and two we can get $-\frac{dC_A}{dt} = \frac{\rho \hat{C}_p \frac{dT}{dt}}{(-\Delta H_{rxn})}$. So this gives the this is the relation between temperature and concentration, so relation between temperature and reactant concentration.

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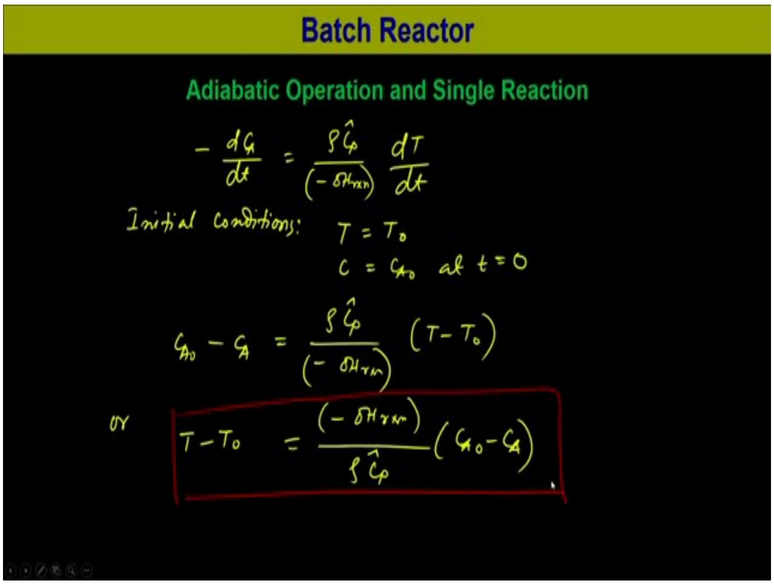

Batch Reactor

Adiabatic Operation and Single Reaction

$$-\frac{dC_A}{dt} = \frac{\rho \hat{C}_p}{(-\Delta H_{rxn})}\frac{dT}{dt}$$

Initial conditions: $T = T_0$

$C = C_{A0}$ at $t = 0$

$$C_{A0} - C_A = \frac{\rho \hat{C}_p}{(-\Delta H_{rxn})}(T - T_0)$$

or $$\boxed{T - T_0 = \frac{(-\Delta H_{rxn})}{\rho \hat{C}_p}(C_{A0} - C_A)}$$

Now, if we integrate this relation, so we have $-\frac{dC_A}{dt} = \frac{\rho \hat{C}_p \frac{dT}{dt}}{(-\Delta H_{rxn})}$, initial conditions $T = T_0$ $C = C_{A0}$ at T is equal to 0, so if we integrate with this this relation we would get $C_{A0} - C_A$ would be equal to $C_{A0} - C_A = \frac{\rho \hat{C}_P}{(-\Delta H_{rxn})}(T - T_0)$ or we can write $T - T_0 = \frac{(-\Delta H_{rxn})}{\rho \hat{C}_P}(C_{A0} - C_A)$.

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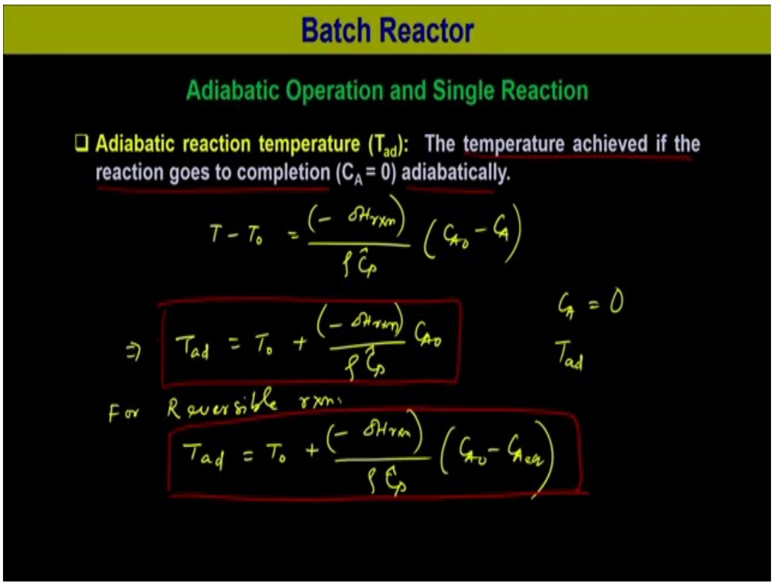

Batch Reactor

Adiabatic Operation and Single Reaction

- ☐ Adiabatic reaction temperature (T_{ad}): The temperature achieved if the reaction goes to completion ($C_A = 0$) adiabatically.

$$T - T_0 = \frac{(-\Delta H_{rxn})}{\rho \hat{C}_p}(C_{A0} - C_A)$$

$$\Rightarrow \boxed{T_{ad} = T_0 + \frac{(-\Delta H_{rxn})}{\rho \hat{C}_p} C_{A0}}$$

$C_A = 0$

T_{ad}

For Reversible rxn:

$$\boxed{T_{ad} = T_0 + \frac{(-\Delta H_{rxn})}{\rho \hat{C}_p}(C_{A0} - C_{Aeq})}$$

Now, from this relation, from this second relation this relation we can derive the adiabatic reaction temperature, the adiabatic reaction temperature T adiabatic if we define this is the temperature which is achieved if the reaction goes to completion that is C_A is equal to 0 adiabatically that means the temperature achieved if the reaction goes to completion adiabatically, so we have $T - T_0 = \frac{(-\Delta H_{rxn})}{\rho \hat{C}_P}(C_{A0} - C_A)$.

So, for adiabatic reaction temperature C_A should goes to completion 0 and T can be written as $T_{ad} = T_0 + \frac{(-\Delta H_{rxn})}{\rho \hat{C}_P} C_{A0}$, now if the reaction is reversible in nature, for reversible reaction we can write $T_{ad} = T_0 + \frac{(-\Delta H_{rxn})}{\rho \hat{C}_P}(C_{A0} - C_{Aeq})$.

So for adiabatic reaction for reversible reaction, the adiabatic reaction temperature would be the temperature at which the reactants attends the equilibrium concentration, so this is very trickier to calculate the adiabatic reaction temperature for the reversible reaction because the equilibrium concentration will change with the temperature. So this is the equation for the single reactions, irreversible reaction.

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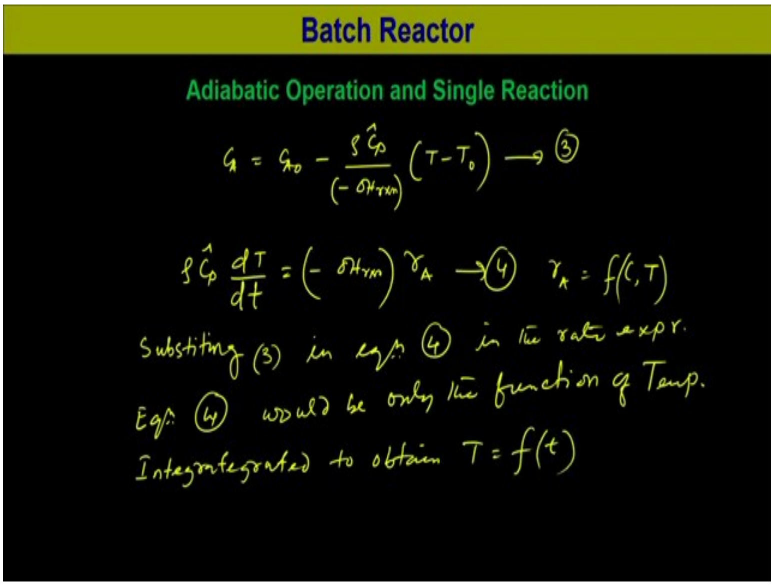

Batch Reactor

Adiabatic Operation and Single Reaction

$$C_A = C_{A0} - \frac{\rho \hat{C}_p}{(-\Delta H_{rxn})}(T - T_0) \longrightarrow ③$$

$$\rho \hat{C}_p \frac{dT}{dt} = (-\Delta H_{rxn})\, r_A \longrightarrow ④ \quad r_A = f(C, T)$$

Substiting (3) in eqn ④ in the rate expr.

Eqn ④ would be only the function of Temp.

Integrated to obtain $T = f(t)$

And for this single reaction the expression is $C_A = C_{A0} - \frac{\rho \hat{C}_P}{(-\Delta H_{rxn})}(T - T_0)$, this is for adiabatic batch reactor single reaction. So, now this can be substituted in the energy balance equation, we know the energy balance equation $\rho \hat{C}_p \frac{dT}{dt} = (-\Delta H_{rxn}) r_A$, so $r_A = f(C,T)$

So, if we substitute this rate equation in case of the concentration, so this relations would be substituting say this is equation three and this is equation four, so if we substitute equation three in equation four in the rate expression then this equation the second equation four will be only the function of temperature. So, equation 4 would be only the function of temperature so this can be integrated to obtain temperature as a function of time, temperature as a function of time.

So, in general, this whole set of equations can be solved numerically to obtain the concentration and temperature profile. So, thank you very much for attending this lecture and we will continue our discussion on the that's the batch reactor balance equations, the reactor design equations both in particularly emphasis should be given on the energy balance equations, and we will continue in our next lecture, thank you.