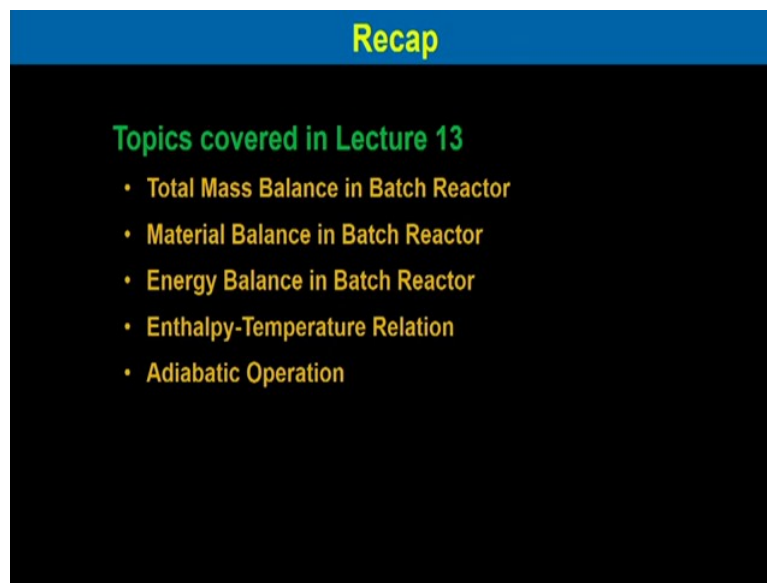


Chemical Reaction Engineering I
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Lecture No. 14

Optimum Temperature Progression in Batch Reactor

Welcome to the 14th lecture of module 4. In this module we are discussing reactor design. And we have started with last couple of lectures we have done. We are working on the temperature and pressure effect. So before going to this lecture let us have brief recap on our previous lecture.

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Recap

Topics covered in Lecture 13

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

In the last lecture we have covered total Mass balance in Batch Reactor. Material Balance in Batch Reactor and then we have done with Energy Balance in Batch Reactor. So although we have done the batch reactor design earlier at the beginning but here we have considered mainly for energy balance. Then we have seen the temperature and enthalpy relation, how enthalpy and temperature they are related. And we have considered Adiabatic operations where we have developed equation to calculate the Adiabatic reaction temperature.

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Module 4: Lecture 14

Optimum Temperature Progression in Batch Reactor

Lecture Outline

- Optimum Temperature Progression
- Exothermic Reversible 1st Order Reaction

So in this lecture we will start with Optimum Temperature Progression in Batch Reactor. As we have seen in the last lecture if we operate the reactor adiabatically for exothermic reaction the temperature adiabatic reaction temperature will change as the reaction proceeds but if either exothermic or endothermic the temperature of the system will change either it decrease or it increase. So over the reactions it proceeds the temperature will change in case of the adiabatic reaction. But if we wanted to operate the reactor at a particular temperature that means we want to operate the reactor in isothermal way then we will have Optimum Temperature Progression for that. And we will see for Exothermic Reversible First-Order Reaction with an example how the optimum temperature can be determined.

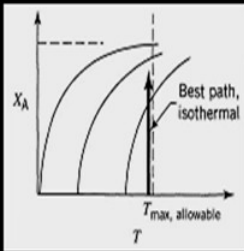
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Batch Reactor

Optimum Temperature Progression

□ For a single, irreversible reaction:
The optimal temperature is simply the highest possible temperature, since that will provide the highest possible rate.

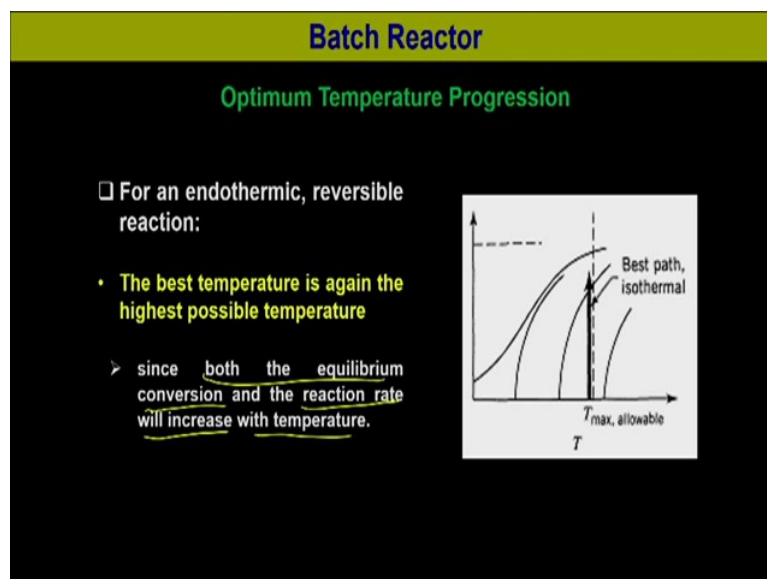
□ This temperature will be determined by other factors: Like boiling of the reactants or operational limits of the reactor.



So optimum temperature progression for a single reaction. If we have single reaction and that is irreversible reaction, the optimum temperature is simply the highest possible temperature since that will provide the highest possible rate. So if we have a single reaction either exothermic or endothermic. In both cases as we increase the temperature the reaction rate will increase. And also the conversion will increase because it is irreversible reaction. So the maximum allowable temperature would be the optimum temperature in case of a single reaction irreversible reaction. But the maximum allowable temperature will be determined by other factors like how much temperature the reactor can withstands or at that temperature whether the product degrades.

So we have to run below the temperature product or reactant that degrades at that temperature. So the maximum allowable temperature will be determined by the property of the reactor, stability and the product or reactant stability and also economics of the system. This temperature show will be determined by boiling of the reactants and operational limits of the reactor. So you can see the conversion versus temperature plot which is obtained from Levin spill at different temperature how the conversion changes or increases and the maximum allowable temperature where you need to optimize your maximum conversion if you want to get and if that temperature is allowed with respect to the boiling of the reactants or the operational limits of the reactor then we can decide that optimum temperature.

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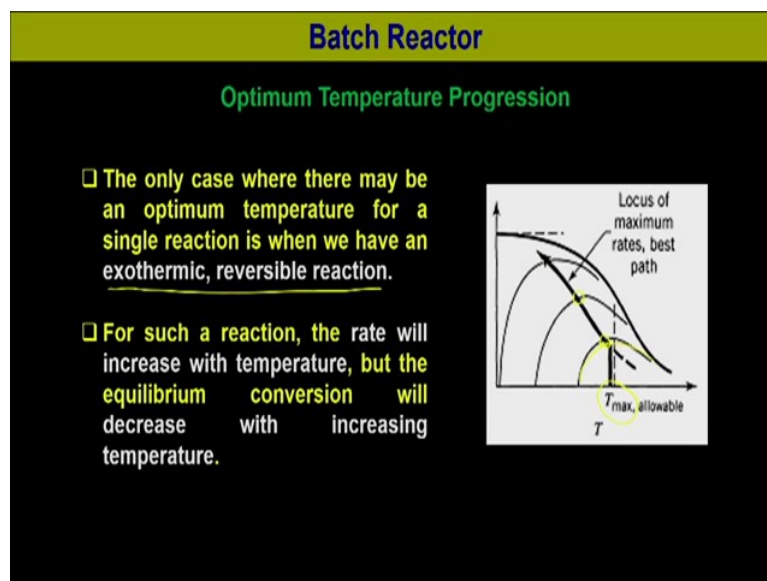
Another case for an endothermic reaction but reversible reaction. For this case what will happen because it is reversible and endothermic. So as we increase the temperature the reaction rate will increase and because it is endothermic in nature and reversible so your

equilibrium conversion will also increase. So the best operation is again the highest possible temperature.

So in this case also similar to the single reaction irreversible reaction. We have seen that the maximum allowable temperature is the optimum temperature in this case as well for endothermic reversible reaction the best temperature is again the highest possible temperature. Since both the equilibrium conversion and the reaction rate will increase with temperature.

So for endothermic reversible reaction both equilibrium conversion as well as the reaction rate with increasing temperature. So that is why the maximum allowable temperature would be the optimum temperature for endothermic reversible reaction. Again in this case the maximum allowable temperature will be determined by the factors which we have discussed that is the boiling of the reactants or the operational limit of the reactor.

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The only case where there may be optimum temperature for the single reaction is when we have exothermic reversible reaction. So if we have exothermic reversible reaction in that case we have a optimum temperature to operate. For such a reaction the rate will increase with temperature but the equilibrium conversion will decrease with increase in temperature. So we have to optimize the temperature in such a way that we will get maximum conversion with minimum time.

So you can see the maximum allowable temperature over here is the T_{max} which is shown over here taken from Levin spill and the rate of the reaction how it is changing, this is the rate

path and maximum rate path and this line is the equilibrium path. So if we can maximize the rate at different temperature then we can achieve the maximum conversion in minimum time. So we will go with an example exothermic first-order reversible reaction.

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Batch Reactor

Exothermic First-Order Reversible Reaction

$$A \xrightleftharpoons[k_{-1}]{k_1} B$$

$$r = k_1 C_A - k_{-1} C_B = k_1 \left(C_A - \frac{1}{K} C_B \right), \quad K = \frac{k_1}{k_{-1}} \text{ eq. const.}$$

start with a pure A $\Rightarrow C_{A0}$

From stoichiometry: $C_B = C_{A0} - C_A$

$$k_1 = A \exp\left(\frac{-E_a}{RT}\right)$$

$$K = K_0 \exp\left(\frac{-\Delta H}{RT}\right)$$

So let us consider this example



$$r = k_1 C_A - k_{-1} C_B$$

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

So this is the forward rate constant is k_1 , the reverse rate constant is k_{-1} and $C_A C_B$ these are the concentration of component A and B, K is the equilibrium constant, capital K is the equilibrium constant.

So this is basically

$$K = \frac{k_1}{k_{-1}}$$

if we start with a pure A that means concentration of A at the beginning is C_{A0} . So from stoichiometry we can write

$$C_B = C_{A0} - C_A$$

Now the forward rate constant and the equilibrium constant we can write in terms of the Arrhenius relation. So the Arrhenius relation for forward reactions

$$k_1 = A \exp\left(-\frac{E_a}{RT}\right)$$

And equilibrium constant capital

$$K = k_0 \exp\left(-\frac{\Delta H}{RT}\right)$$

If we substitute k_1 and K equilibrium constant this Arrhenius relation in this equation rate equation, we would obtain.

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Batch Reactor

Exothermic First-Order Reversible Reaction

$$r = k_1 \left(C_A - \frac{1}{K} C_B \right) = k_1 \left[C_A - \frac{1}{K} (C_{A0} - C_A) \right]$$

$$C_B = C_{A0} - C_A = k_1 \left[C_A - \frac{1}{K} C_{A0} + \frac{1}{K} C_A \right]$$

$$= k_1 \left(1 + \frac{1}{K} \right) C_A - \frac{k_1}{K} C_{A0}$$

$$\Rightarrow -\frac{dC_A}{dt} = k_1 \left(1 + \frac{1}{K} \right) C_A - \frac{k_1}{K} C_{A0}$$

$$\Rightarrow \frac{dC_A}{dt} = -k_1 \left(1 + \frac{1}{K} \right) C_A + \frac{k_1}{K} C_{A0}$$

$$= -A \exp\left(\frac{-E_A}{RT}\right) \left[1 + \frac{1}{K_0 \exp\left(\frac{-D_H}{RT}\right)} \right] C_A$$

$$+ \frac{A \exp\left(\frac{-E_A}{RT}\right)}{k_1 \exp\left(\frac{-D_H}{RT}\right)} C_{A0}$$

$$\left. \begin{array}{l} k_1 = A \exp\left(\frac{-E_A}{RT}\right) \\ K = K_0 \exp\left(\frac{-D_H}{RT}\right) \end{array} \right\}$$

So we have

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

So we will substitute C_B we know

$$C_B = C_{A0} - C_A$$

So if we C_B over here this would be

$$r = k_1 \left[C_A - \frac{1}{K} (C_{A0} - C_A) \right]$$

So if we multiply this would be

$$r = k_1 \left[C_A - \frac{1}{K} C_{A0} + \frac{1}{K} C_A \right]$$

And if we rearrange this would be

$$r = k_1 \left(1 + \frac{1}{K} \right) C_A - \frac{k_1}{K} C_{A0}$$

This is C_A , so this is equal

$$= k_1 \left(1 + \frac{1}{K} \right) C_A - \frac{k_1}{K} C_{A0}$$

Now if we write

$$r = -\frac{dC_A}{dt} = k_1 \left(1 + \frac{1}{K} \right) C_A - \frac{k_1}{K} C_{A0}$$

So from here we can write

$$-\frac{dC_A}{dt} = k_1 \left(1 + \frac{1}{K} \right) C_A - \frac{k_1}{K} C_{A0}$$

Now we have

$$k_1 = A \exp\left(-\frac{E_a}{RT}\right) \text{ and } K = k_0 \exp\left(-\frac{\Delta H}{RT}\right)$$

So if we substitute over here this would be

$$-\frac{dC_A}{dt} = -A \exp\left(-\frac{E_a}{RT}\right) \left(1 + \frac{1}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)} \right) C_A - \frac{A \exp\left(-\frac{E_a}{RT}\right)}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)} C_{A0}$$

So this is the concentration versus temperature relation. So with respect to time.

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Batch Reactor

Exothermic First-Order Reversible Reaction

> If we want to find the optimal single temperature at which to run the reaction, then the temperature is constant with respect to time.

> In that case, we can integrate the rate equation for the concentration of A to get

$$\frac{C_A}{C_{A0}} = \frac{1}{1+K} \left[1 + K \exp\left(-k_1 \left(1 + \frac{1}{K}\right)t\right) \right]$$

$$= \frac{1}{1 + K_0 \exp\left(\frac{-\Delta H}{RT}\right)} \left[1 + K_0 \exp\left(\frac{-\Delta H}{RT}\right) \exp\left[-A \exp\left(\frac{-E_a}{RT}\right) \left(1 + \frac{1}{K_0 \exp\left(\frac{-\Delta H}{RT}\right)}\right)t\right] \right]$$

So from this relation if we wanted to find a single optimum temperature, if we want to find the optimum single temperature at which to run the reaction then the temperature is constant with respect to time. So the earlier equations we have seen that the change in concentration with respect to time and it has a relation with the temperature. But if we wanted to run the reactor at a single optimum temperature that means the temperature is constant with respect to time. So in that case we can integrate the earlier equation, the rate equation for concentration of A to get say we have

$$\frac{C_A}{C_{A0}} = \frac{1}{1+K} \left[1 + K \exp\left(-k_1 \left(1 + \frac{1}{K}\right)t\right) \right]$$

So we can rearrange that if we can integrate the earlier equation we would obtain the concentration profile like this at a constant temperature.

So we can now, since the temperature is constant and we have integrated, we can now substitute K which is a function of temperature here and we would obtain

$$\frac{C_A}{C_{A0}} = \frac{1}{1 + k_0 \exp\left(-\frac{\Delta H}{RT}\right)} \left[1 + k_0 \exp\left(-\frac{\Delta H}{RT}\right) \exp\left(-A \exp\left(-\frac{E_a}{RT}\right) \left(1 + \frac{1}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)}\right)t\right) \right]$$

So this is the relation if we substitute K and small k_1 that is forwarded constant with a Arrhenius relation we would obtain the concentration profile like this. Or alternatively what

we can do, we can fix the time required to obtain a particular conversion. So this relation we can just rearrange to calculate the time required for a particular conversion. So represented in terms of the concentration.

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Batch Reactor

Exothermic First-Order Reversible Reaction

$$t = \frac{1}{k_1 \left(1 + \frac{1}{K}\right)} \ln \left[\frac{1}{\frac{C_A}{C_{A0}} \left(1 + \frac{1}{K}\right) - \frac{1}{K}} \right]$$

$$= \frac{1}{A \exp\left[-\frac{E_a}{RT}\right] \left[1 + \frac{1}{K_0 \exp\left(-\frac{\Delta H}{RT}\right)}\right]} \ln \left[\frac{1}{\frac{C_A}{C_{A0}} \left[1 + \frac{1}{K_0 \exp\left(-\frac{\Delta H}{RT}\right)}\right]} - \frac{1}{K_0 \exp\left(-\frac{\Delta H}{RT}\right)} \right]$$

So if we do that we would obtain

$$t = \frac{1}{k_1 \left(1 + \frac{1}{K}\right)} \ln \left[\frac{1}{\frac{C_A}{C_{A0}} \left(1 + \frac{1}{K}\right) - \frac{1}{K}} \right]$$

Now if we substitute K and k_1 we would have

$$t = \frac{1}{A \exp\left(-\frac{E_a}{RT}\right) \left(1 + \frac{1}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)}\right)} \ln \left[\frac{1}{\frac{C_A}{C_{A0}} \left(1 + \frac{1}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)}\right) - \frac{1}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)}} \right]$$

So this we would obtain if we want to get a time required for a particular conversion.

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Batch Reactor

Exothermic First-Order Reversible Reaction

- To find the optimal temperature for isothermal operation, we either want to minimize C_A for a fixed reaction time or we want to minimize the reaction time for a fixed outlet concentration of A.
- In each case, we take the partial derivative of the quantity we are trying to minimize with respect to temperature (holding the other quantity constant), set it equal to zero, and solve for the temperature.
- An analytical solution for the optimum temperature can readily be obtained, but it is fairly long and messy.
- If you are interested, it is straightforward to solve the equations using Maple or Mathematica.

Now to find the optimum isothermal operation we either want to minimize C_A for a fixed reaction time or we want to minimize the reaction time for a fixed outlet concentration. So either of these 2 we need to consider, so either minimize C_A for a fixed reaction time or minimize reaction time for a fixed outlet concentration, these 2 things we can do. So in each case what we need to do, we take the partial derivative of the quantity we want to minimize with respect to temperature and holding the other quantity constant.

That means if we wanted to minimize the concentration we will take partial derivative of concentration with respect to temperature keeping the time constant or in other case we can take partial derivative of time with respect to temperature keeping the outlet concentration constant and then we need to set it equal to 0 and solve for the temperature. An analytical solutions for the optimum temperature can readily be obtained but it is fairly long and messy. So one can use the, you know software available like if we can use Mathematica, Maple or Matlab this solution is very easy to solve and very straightforward.

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Batch Reactor

Exothermic First-Order Reversible Reaction

- If we can arbitrarily control the temperature of the reactor, then we may wish to select an optimal temperature trajectory rather than a single temperature.
- Intuitively, it makes sense that for a reversible exothermic reaction, we would want to initially have a relatively high temperature (to achieve a high reaction rate) and at higher conversions, we would want to decrease the temperature to avoid equilibrium limitations.
- It can be shown that for a single reaction, the maximum conversion in minimum time is achieved simply by maximizing the rate at each point in time.
- This seems obvious, but in the case of multiple reactions it is no longer necessarily true.

Now instead of finding a fixed optimum temperature that is at one temperature to run the reactions reversible exothermic reaction this that is sometimes not possible to obtain the highest conversion in minimum time. So it is better to use the arbitrary temperature control, we can control arbitrarily the temperature and we may select optimum temperature trajectories rather than a single temperature.

Optimum temperature trajectories means you are, we are not considering a single optimum temperature to run the reactor, the temperature will gradually change depending on our requirement to optimize the conversion and the reaction time. So intuitively it makes sense that for a reversible exothermic reaction what we wanted to do, initially we need to have relatively high temperature because the conversion is low.

So we can very quickly achieve a good conversion with a minimum time. So if we have high-temperature the reaction rate would be faster and it will give the conversion higher in a smaller time. As the conversion increases at higher conversion we would want to decrease the temperature to avoid the equilibrium relations. Since it is exothermic reversible reaction as the conversion will increase it will be limited by the equilibrium relations. That we can avoid if we decrease the temperature at higher conversion.

In that case we will optimize the temperature trajectories depending on our requirements. So it can be shown for a single reaction the maximum conversion in minimum time can be achieved simply by maximizing the rate at each point of time. This seems obvious but in case of multiple reactions it is no longer necessarily true. So this will be done for a single reversible reaction we can maximize the rate at different point of time and we can achieve

maximum conversion with minimum time. But for multiple reactions these may not be necessarily valid.

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Batch Reactor

Exothermic First-Order Reversible Reaction

$$r = k_1 \left(C_A - \frac{1}{K} C_B \right) = A \exp\left(\frac{-E_a}{RT}\right) C_A - \frac{A}{k_0} \exp\left(\frac{-(E_a - \Delta H)}{RT}\right) C_B$$

Taking partial derivative with respect to temp. at fixed concentration:

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

Now if you consider single reversible exothermic reaction and rate we know

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

Which is equal to

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

So if we substitute k_1 and K with the Arrhenius relation and then if we rearrange this relation we would obtain this expression.

Now if we take partial derivative with respect to T at a fixed concentration. So taking partial derivative with respect to temperature at fixed concentration. So you would obtain

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

So this is the partial derivative of rate with respect to temperature at a fixed concentration.

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Batch Reactor

Exothermic First-Order Reversible Reaction

Setting $\frac{\partial r}{\partial T} = 0$ and multiplying both sides by $\frac{RT^2}{A}$:

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

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

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

Now if we set this equal to 0, we would obtain setting $\frac{\partial r}{\partial t} = 0$ and multiplying both sides by

$\frac{RT^2}{A}$. So you would obtain

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

So here as we are optimizing the rate, so the temperature which we obtain is the optimum temperature. So we can write RT_{opt} .

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

Or we can write

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

So this temperature T_{opt} ,

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

So this gives the optimum temperature trajectories in terms of the concentration or the extent of reaction when the, no reaction progress. Initially for an exothermic reaction, if we consider exothermic reaction and then ΔH is negative and so this will give an optimum temperature that is negative not a physically meaningful or significant results that means C_B at the beginning is 0 and so this term is negative, \ln term in the denominator.

So at the beginning the upper term is positive because ΔH is negative, so the numerator over here at the start of the reaction this is T optimum is negative. So which is not physically meaningful. So the optimum temperature becomes infinite when the quantity inside the logarithm in the denominator is equal to 1. So as a reaction progress the conversion changes the term. The term over here in the denominator under \ln term this becomes 1 then it indicates the optimum temperature is infinite.

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Batch Reactor

Exothermic First-Order Reversible Reaction

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

- 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 batch reactor 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 can be obtained from the equation given above.

That means here

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

So this is a limit where the temperature becomes infinite. That means for convergence smaller than the critical values that means

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

convergence smaller than this critical value the optimal temperature is as high as possible. So if we can initially if we would like to get a higher reaction rate up to this critical conversion

when the $\frac{C_B}{C_A}$ would be equal to this term where the \ln term would be infinite.

So then we can keep the temperature as high as possible to reach the higher conversion with a minimum time. Then as the reaction proceeds past this point, the optimum temperature will decrease. So we have to because it is exothermic reaction and we have to lower down the temperature. So the optimum temperature trajectories for a batch reactor with a single reversible reaction to run the reactor at highest possible temperature that is T_{\max} until the conversion reaches a point where the optimum temperature obtained from the equation above is T_{\max} .

So here till it reaches the critical conversion values we have to keep the temperature as high as possible and that is determined by the no reactor operational limits and the boiling of the reactants. Those parameters will decide at the beginning what temperature we should maintain at this case till the smaller than the critical value and after that point the optimum temperature can be obtained from the equation given above. So then we can obtain the T_{opt} relations from there. What is the optimum temperature we need to maintain, that we can obtain from the relation. Now one can predict how the temperature should vary in time by integrating the equation of concentration with respect to, with rate evaluated at optimum temperature.

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Batch Reactor

Exothermic First-Order Reversible Reaction

$$\frac{dC_A}{dt} = f(C_A)$$

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

- This can be integrated to give the concentration as a function of time, and
- The equation used to obtain the optimal temperature then gives the temperature as a function of time.
- Finally, these temperatures and concentrations can be used in the enthalpy balance equation to obtain the heat removal rate required (as a function of time) to maintain the optimal temperature.

That means we know

$$\frac{dC_A}{dt} = A \exp\left(-\frac{E_a}{RT}\right) \left(1 + \frac{1}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)}\right) C_A - \frac{A \exp\left(-\frac{E_a}{RT}\right)}{k_0 \exp\left(-\frac{\Delta H}{RT}\right)} C_{A0}$$

If we set with

$T = T_{opt}$, so after critical conversion we can write $\frac{dC_A}{dt}$,

$$\frac{dC_A}{dt} = A \left[\frac{(E_a - \Delta H) C_{A0} - C_A}{k_0 E_a C_A} \right]^{\frac{E_a}{\Delta H}} \left[1 + \frac{E_a C}{(E_a - \Delta H)(C_{A0} - C_A)} \right] C_A - \frac{A}{k_0} \left[\frac{(E_a - \Delta H) C_{A0} - C_A}{k_0 E_a C_A} \right]^{\frac{E_a - \Delta H}{\Delta H}} C_{A0}$$

So this is the relation if we consider T is the optimum temperature and then we can substitute T optimum over here in this relation. So dC_A/dt we would obtain like this. So this can be, know integrated to give the concentration as a function of time and the equation used to obtain the optimum temperature then gives the temperature as a function of time. So the earlier equations which we obtained that is dC_A/dt which is a function of conversion or concentration.

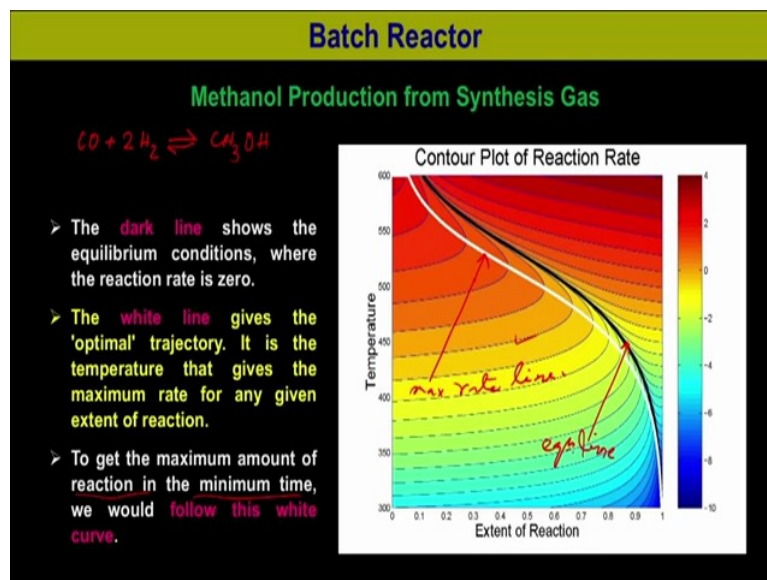
So this we can integrate, the earlier equations which we have developed can be integrated to give the concentration profile that is concentration versus time and then equation used to

obtain the optimum temperature then gives the temperature as a function of time. So that means this concentration versus time we need to incorporate into the relation that is

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

So the concentration profile if we substitute over here in this optimum temperature then we will get the temperature, optimum temperature versus the time. Now finally this temperature and concentration can be used in the enthalpy balance equation to obtain the heat removal rate require as a function of time to maintain the optimum temperature. So we have temperature as a function of time and concentration as a function of time. So both we can use in case of the energy balance equation which will give the heat removal rate required as a function of time. So that we will tell about the, how to maintain the optimum temperature. So this is how, we can do it but since the calculation is know analytical calculation is really lengthy, so we can use the know software like mathematical or maple to solve these equations.

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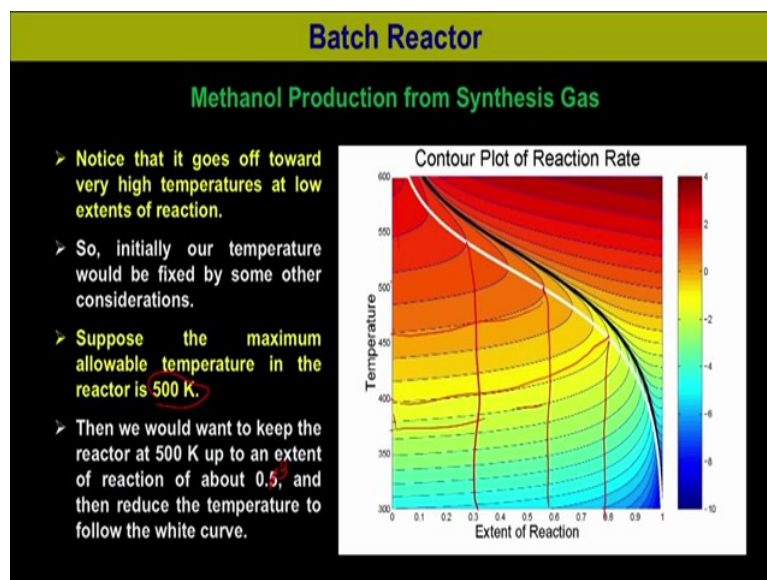


Now let us take an example of methanol production from synthesis gas, so basically the reaction is exothermic in nature. So, like $CO + 2H_2 \rightleftharpoons CH_3OH$ you could see here in this plot the reaction rate is plotted versus temperature and extent of reactions. So we call it Contour Plot. And in this case you could see that there are 2 different, 3 different lines over here. The dark line over here, the thicker dark line at the middle this one, this is basically the

equilibrium line. So the dark line shows the equilibrium conditions where the reaction rate is 0. So at this point the reaction rate is 0. This line, the dark line which is thinner and outline represents how the rate of reaction progress with the extent of reaction and the temperature.

The white line over here you could see, the white line this is the maximum rate trajectories. So it represents maximum rate line. The white line gives the optimal trajectory it is the temperature that gives the maximum rate for any given extent of reactions. So at a particular extent of reactions over here this gives the maximum rate at that temperature. To get the maximum amount of reaction in a minimum time we would follow this white curve. So if we wanted to have maximum amount of reactions to be happen with a minimum time we need to follow this white line.

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So we could notice that it goes off towards very high temperature at low extent of reactions. If we consider low extent of reactions, so very less here say close to that. The maximum rate you could see it is going off. At low conversion the, know maximum goes off at very high temperature. So what is our target, say initially our temperature would be fixed by some other considerations and that would be the maximum temperature we need to fix. Suppose the maximum allowable temperature for this reaction is 500 degree centigrade. So say 500 Kelvin, so maximum allowable temperature for this reaction if we consider say 500 Kelvin. Now at 500 Kelvin say over here, so we should, know run the reactions start with that high temperature and reaction will proceed to this and it will reach like this. So the conversion we would obtained here is about this.

Now if we keep on you know doing the experiment, running the experiments further at this temperature the equally conversion will decrease, the rate will decrease as well as the conversion will decrease because it will reach to the equilibrium. So then we want to keep the reactor at 500 Kelvin up to an extent of reactions say about 0.5 or so. So this is basically, this means that this is the temperature close to you know we cannot keep up to 500.

So we may keep the temperature up to this, so the conversion is about 0.3 and then reduce the temperature to follow the white line. So we need to reduce the temperature say about 450 and then we can you know run for a certain period of time to reach the conversion over here and again we know reduce the temperature say around 400 or so it will reach this conversion. So we have to optimize the temperature step-by-step or reduce the temperature so that we can achieve the maximum conversion possible with a minimum time.

So this is how the batch reactor operation we can do with a minimum time and how the temperature would progress. So thank you very much for attending this lecture and we will continue our discussion on the energy balance and optimum temperature progression for other 2 idealize reactors that is plugged flow reactor and the continuous stir tank reactor in our subsequent lectures, thank you.