Chemical Process Safety
Professor Shishir Sinha
Department of Chemical Engineering, IIT Roorkee
Fundamental Principles
Lecture 04
Scale-up & Runaway Reaction

Welcome to this module of runaway reaction or reaction runaway problems because this runaway problems are more critical in chemical process safety, so we thought that we must give you an overview about those reaction runaways and scale-up aspect, so in this particular module we are going to discuss certain fundamental principles those who are related to the reaction runaway.

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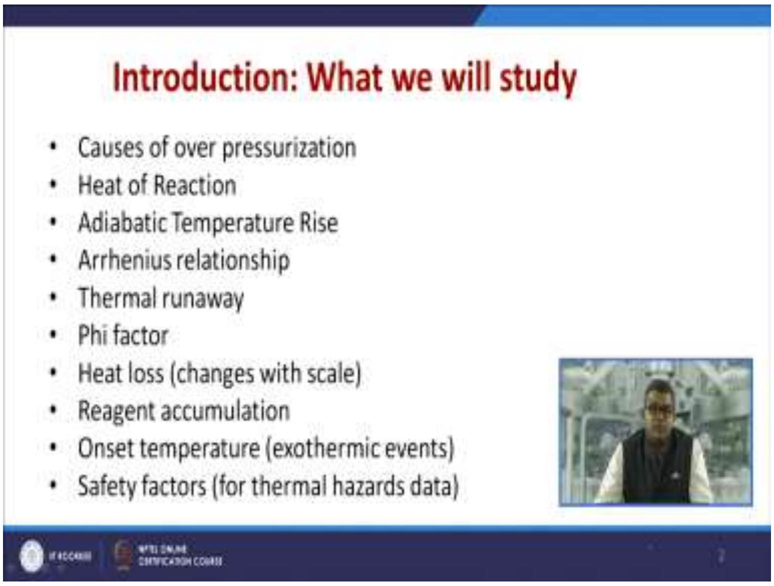
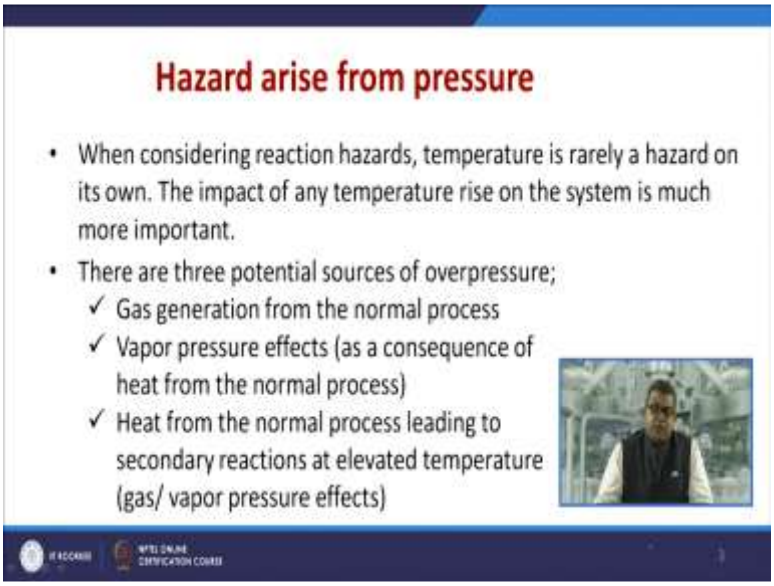


Introduction: What we will study

- Causes of over pressurization
- Heat of Reaction
- Adiabatic Temperature Rise
- Arrhenius relationship
- Thermal runaway
- Phi factor
- Heat loss (changes with scale)
- Reagent accumulation
- Onset temperature (exothermic events)
- Safety factors (for thermal hazards data)



Hazard arise from pressure

- When considering reaction hazards, temperature is rarely a hazard on its own. The impact of any temperature rise on the system is much more important.
- There are three potential sources of overpressure;
  - ✓ Gas generation from the normal process
  - ✓ Vapor pressure effects (as a consequence of heat from the normal process)
  - ✓ Heat from the normal process leading to secondary reactions at elevated temperature (gas/ vapor pressure effects)

We will discuss about the causes of various kind of over pressurization will discuss about the basic concept of heat of reaction, Adiabatic temperature rise, Arrhenius relationship and will discuss about the thermal runaway aspects, then Phi factor, heat losses changes with time of scales, then we will discuss about reagent accumulation and onset temperature related to the exothermic aspects and will discuss about certain safety factors for thermal hazard data.

So let us have a look about the hazards, those who are arising from the pressure, so while we consider the reaction hazard the temperature is rarely a hazard on its own, although sometimes when it is within the domain, within the controllable domain then temperature never put forward any kind of hazard, so the impact of any temperature rise, sometimes this temperature rise may take place because of certain conditions like exothermicity or cooling temperature failures etc.

So the impact of any kind of temperature rise on the system is much more important, because this may lead to the other catastrophic problems, so there are three potential sources of overpressure. One is the gas generation from the normal processes and this took place in the Bhopal gas tragedy, when because of the high temperature the CO_2 built up inside the MIC tank while reacted with the water and it create a lot of problem and all the safety processes were failed, the second aspect is the vapour pressure effect as a consequence of heat from the normal processes, the third one is the heat from the normal process leading to the secondary reaction at elevated temperature that is gas or a vapour pressure effects in other words, you can say.

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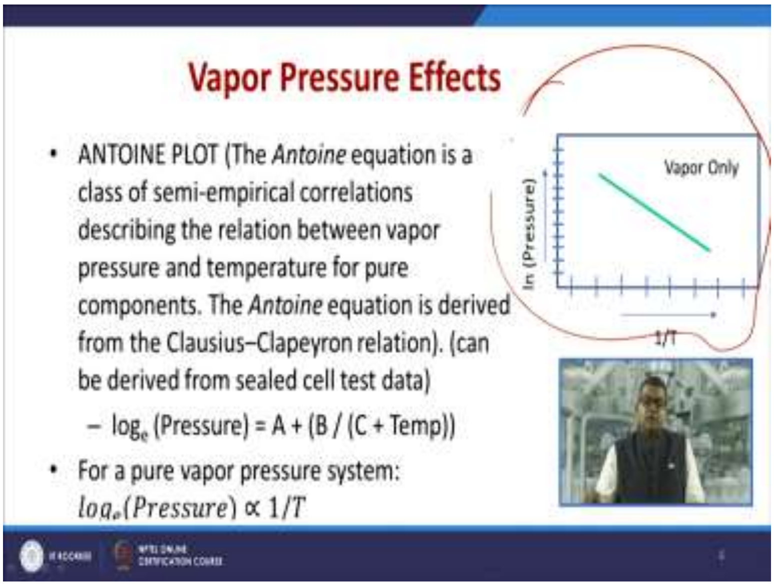

Vapor Pressure Effects

- ANTOINE PLOT (The *Antoine* equation is a class of semi-empirical correlations describing the relation between vapor pressure and temperature for pure components. The *Antoine* equation is derived from the Clausius–Clapeyron relation). (can be derived from sealed cell test data)
  - $\log_e(\text{Pressure}) = A + (B / (C + \text{Temp}))$
- For a pure vapor pressure system: $log_e(Pressure) \propto 1/T$

Now let us have a look about a vapour pressure effect, now this vapour pressure effect is attributed to the Antoine theory and this theory you can look in the chemical engineering thermodynamics aspects, so this vapour pressure effect is attributed to the Antoine plot, now this plot is attributed to the Antoine equation, so the Antoine equation is a class of semi-empirical correlation describing the relation between the vapour pressure and a temperature for pure components.

Now why there is a need of this plot or this relationship because in the previous slide we have discussed that sometimes the temperature may lead to because temperature sometimes is in a safer limit, but this temperature may create the problem of overpressure, so whenever you talking about the relationship between the temperature and pressure, then we must have a certain correlations, so Antoine equation provide the solution for this particular aspects.

Now this Antoine equation is derived from the Clausis-Clapeyron relations and it can be derived by from the sealed cell data, so this is the Antoine plot log of

– $\log_e(\text{Pressure}) = A + (B / (C + \text{Temp}))$

that is the T is the temperature, so for a vapour pressure system, the log pressure, the

$$log_e(Pressure) \propto 1/T$$

so by this way you can plot this logarithmic plot with the pressure versus 1 by T.

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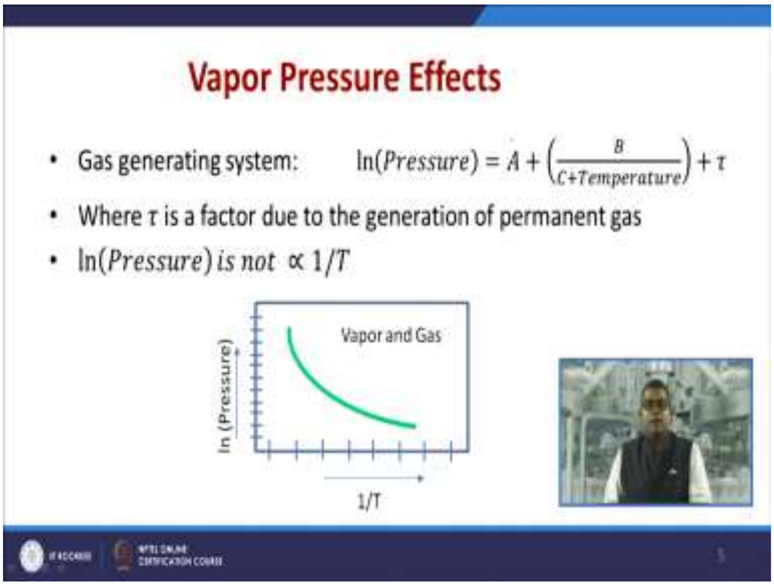

Vapor Pressure Effects

- Gas generating system: $\ln(Pressure) = A + \left(\frac{B}{C+Temperature}\right) + \tau$
- Where τ is a factor due to the generation of permanent gas
- $\ln(Pressure)$ is not $\propto 1/T$

Now if you recall, if we have a gas generating system, then

$$\ln(Pressure) = A + \left(\frac{B}{C+Temperature}\right) + \tau$$

now a τ is a factor that is due to the generation of permanent gas and in that particular case this log LN pressure is not directly proportion to 1/ T and you may see that the nature of the plot would be like this.

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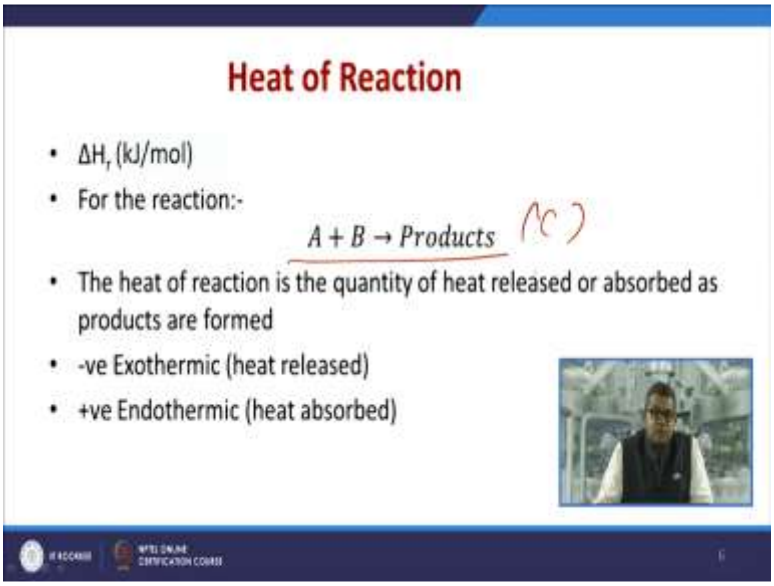

Heat of Reaction

- ΔH_r (kJ/mol)
- For the reaction:-

$$\underline{A + B \rightarrow Products} \quad (C)$$

- The heat of reaction is the quantity of heat released or absorbed as products are formed
- -ve Exothermic (heat released)
- +ve Endothermic (heat absorbed)

Let us have a look about the heat of a reaction, this is a very common phenomena, so we will not devote much time towards this particular aspects because in chemical thermodynamic or engineering thermodynamics we have gone through this heat of reaction aspects, usually represented by ΔH_r and it is having the unit of kilojoule per mole, so let us see that for a reaction A plus B this gives the product say may be C, so the heat of a reaction is the quantity of a heat released or absorbed as a products are formed, so there are two type of heat of reaction one is exothermic when the heat is released and second is the endothermic when heat is absorbed by the system.

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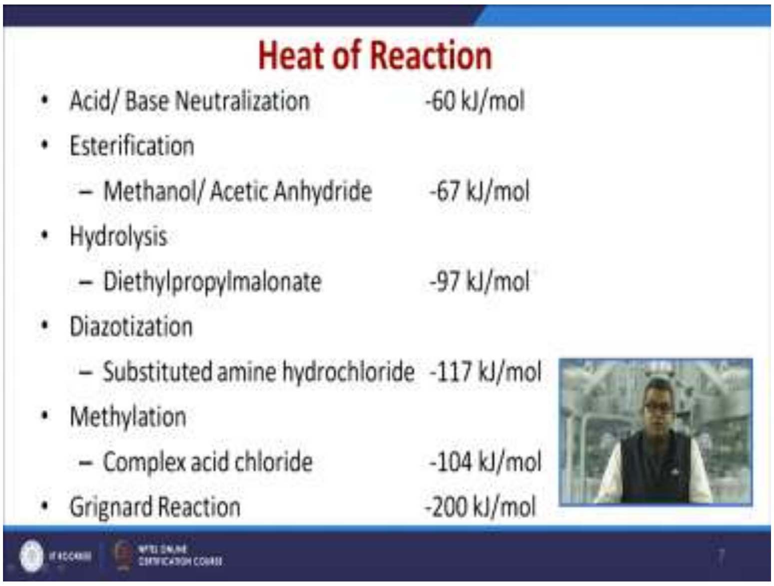

Heat of Reaction

- Acid/ Base Neutralization -60 kJ/mol
- Esterification
  - Methanol/ Acetic Anhydride -67 kJ/mol
- Hydrolysis
  - Diethylpropylmalonate -97 kJ/mol
- Diazotization
  - Substituted amine hydrochloride -117 kJ/mol
- Methylation
  - Complex acid chloride -104 kJ/mol
- Grignard Reaction -200 kJ/mol

Now you can see in this particular slide will have listed some reference heat of reaction like Acid or Base neutralization may have an exothermicity of 60 KJ/mole, then Esterification of a methanol or acetic anhydride is having the exothermic heat of reaction 67 KJ/mole, then hydrolysis may have a heat of a reaction of minus 97 KJ/mole, Diazotization that is the substituted amine hydrochloride having the heat of reaction. In the range of say minus 117 KJ/mole, then Methylation that is, this may have heat of reaction of minus 104 KJ/mole and Grignard reaction may have a heat of a reaction minus 200 KJ/mole.

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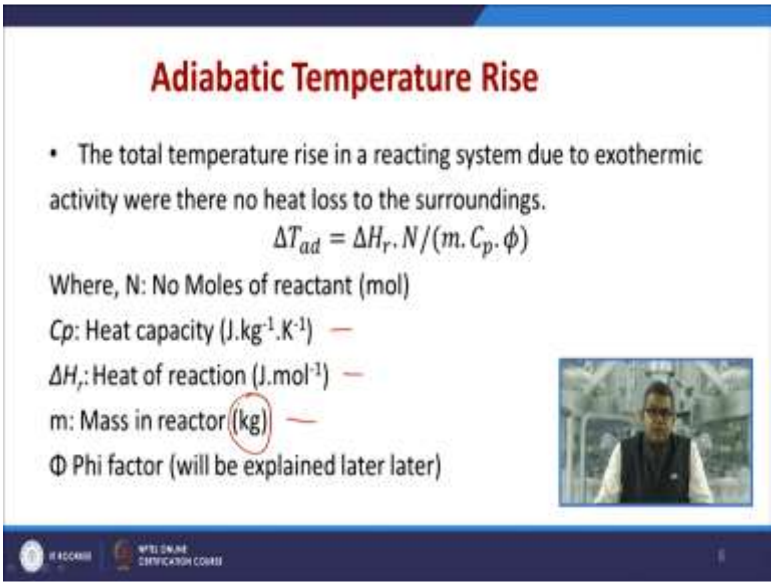

Adiabatic Temperature Rise

- The total temperature rise in a reacting system due to exothermic activity were there no heat loss to the surroundings.

$$\Delta T_{ad} = \Delta H_r . N/(m.C_p.\phi)$$

Where, N: No Moles of reactant (mol)

Cp: Heat capacity ($J.kg^{-1}.K^{-1}$)

ΔH_r: Heat of reaction ($J.mol^{-1}$)

m: Mass in reactor (kg)

Φ Phi factor (will be explained later later)

Now the standard heat of reaction you can have from various handbooks. Now let us have a look about the adiabatic temperature rise, so the total temperature rise in the reacting system due to exothermic activities were there no heat loss to the surrounding and it is given by

$$\Delta T_{ad} = \Delta H_r . N/(m.C_p.\phi)$$

Now here N is the number of moles of reactant, C_p is the heat capacity having the units of Joule kilogram inverse and Calvin versus, delta Hr is having the heat of reaction, m is the mass in the reactor, which is having the unit of kilogram and Phi factor, we will explain this in the subsequent slides later on.

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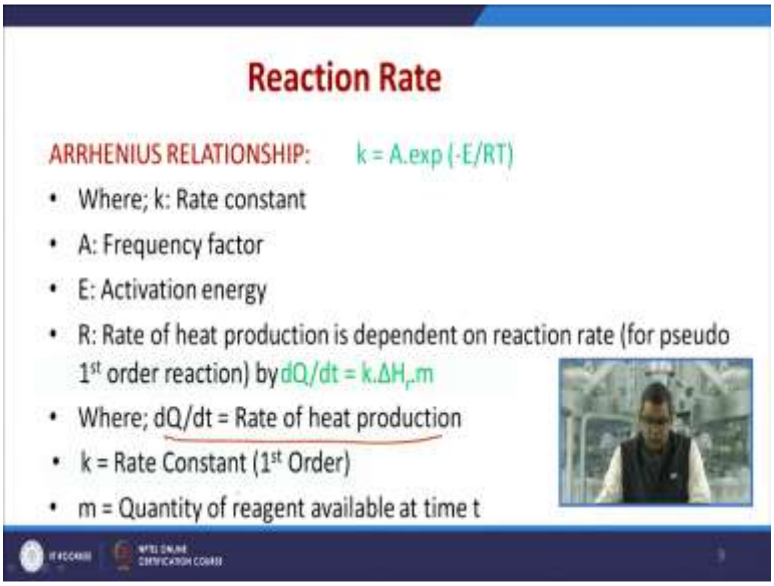

Reaction Rate

ARRHENIUS RELATIONSHIP: $k = A.\exp(-E/RT)$

- Where; k: Rate constant
- A: Frequency factor
- E: Activation energy
- R: Rate of heat production is dependent on reaction rate (for pseudo 1^{st} order reaction) by $dQ/dt = k.\Delta H_r.m$
- Where; dQ/dt = Rate of heat production
- k = Rate Constant (1^{st} Order)
- m = Quantity of reagent available at time t

Another aspect is the reaction rate, this is attributed to the Arrhenius relationship and which is represented as

$$k = A.\exp(-E/RT)$$

Where K is the rate constant, A is the frequency factor, E is the activation energy, R is the rate of heat production is dependent on reaction rate for the pseudo 1^{st} order by

$$dQ/dt = k.\Delta H_r.m$$

now this dQ, dt is the rate of heat production, now this K is the rate constant having the 1^{st} order and m is the quantity of reagent available at time t.

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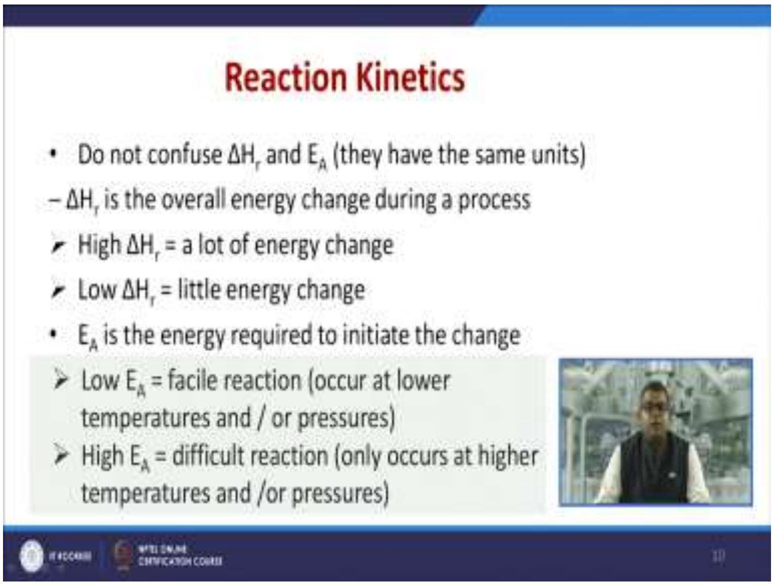

Reaction Kinetics

- Do not confuse ΔH_r and E_A (they have the same units)

– ΔH_r is the overall energy change during a process

- High ΔH_r = a lot of energy change
- Low ΔH_r = little energy change
- E_A is the energy required to initiate the change
  - Low E_A = facile reaction (occur at lower temperatures and / or pressures)
  - High E_A = difficult reaction (only occurs at higher temperatures and /or pressures)

Now let us have a brief look about the reaction kinetics and you must not confuse about the ΔH_r and E_A, they have the same units, so ΔH_r that is heat of the reaction is the overall energy change during a process, so high ΔH_r that is the heat of reaction, a lot of energy change and a low heat of a reaction, then a small amount of energy change takes place, so low E_A, E_A is the energy required to initiate a change, so if you are having the low E_A that is facile reaction occur at a lower temperatures or pressures and if you are having the high E_A that is the difficult reaction only occurs at high temperature or a pressure, so these are the certain suggestive measures for the reaction kinetics.

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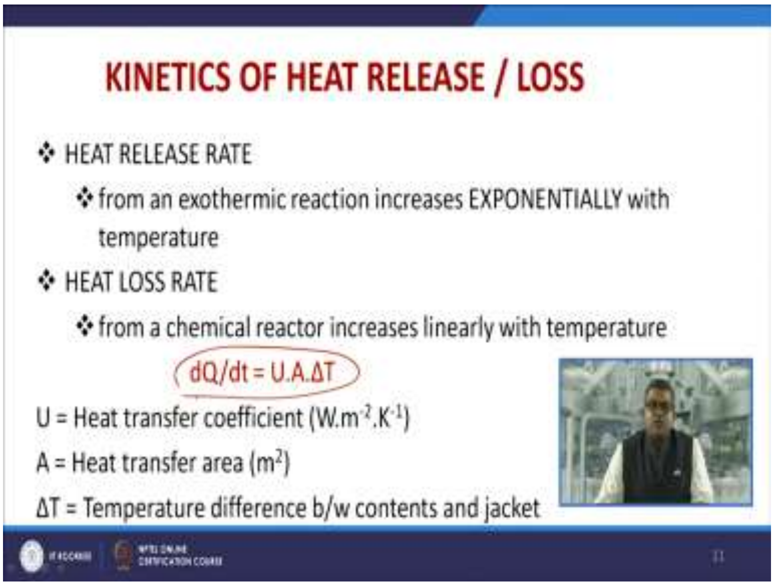

KINETICS OF HEAT RELEASE / LOSS

- HEAT RELEASE RATE
  - from an exothermic reaction increases EXPONENTIALLY with temperature
- HEAT LOSS RATE
  - from a chemical reactor increases linearly with temperature

$$dQ/dt = U.A.\Delta T$$

U = Heat transfer coefficient ($W.m^{-2}.K^{-1}$)

A = Heat transfer area (m^2)

ΔT = Temperature difference b/w contents and jacket

Let us have a discussion about the kinetics of heat release or sometimes loss, the heat release rate that is from an exothermic reaction increases exponentially with the temperature, so this is a very, you can say the catchy line, so that you can analyse that if any kind of catastrophe may take place then how we can analyse that how much quantum of the heat release from the kinetics studies.

Now heat loss rate, now from a chemical reactor increases linearly with the temperature with this formula

$dQ/dt = U.A.\Delta T$

Where, U is the heat transfer coefficient having the unit of Watt/m^2K and A is the heat transfer area, usually represented in a m^2 and ΔT the temperature difference between contents and a jacket, so ΔT is important.

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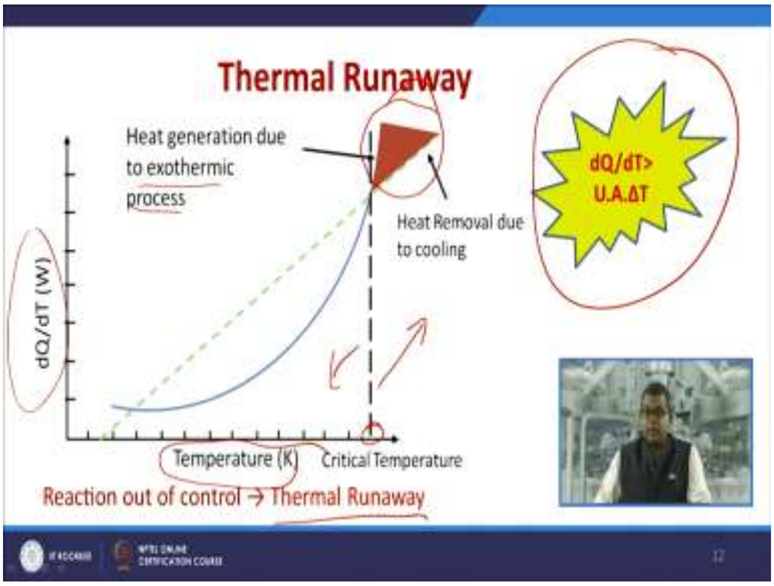

Thermal Runaway

$dQ/dT > U.A.\Delta T$

Reaction out of control → Thermal Runaway

Sometimes you may experience a thermal runaway problems, and as we have discussed the governing equation is this one, now here the dQ by dt is on the y-axis and the temperature on the x-axis, so you need to find out that what is the critical temperature over which there may be a chances of thermal runaway reaction, so in case if by any means if there is any exothermic process and access heat been liberated then you need to find out that how much quantity of heat removal is required for cooling so that it may work below this critical temperature radiation.

Now since if by any means it goes beyond this critical temperature range, then there may be a chance of thermal runaway and you need to take the appropriate safety measures to overcome such kind of scenario, in past there may have several reaction that took place because of this thermal runaway aspect, now remember a thermal runaway is the progressive production of heat from a chemical process and occurs when the rate of heat production exceeds the rate of heat removal. So, that means certain imbalance took place between the cooling aspects and the heat production of aspect because the exothermicity is known.

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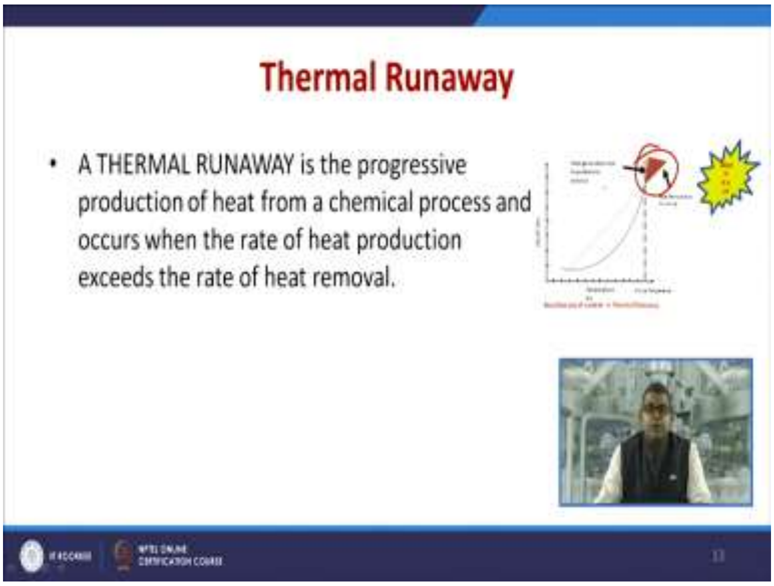

Thermal Runaway

- A THERMAL RUNAWAY is the progressive production of heat from a chemical process and occurs when the rate of heat production exceeds the rate of heat removal.

So you can analyse this scenario and you can take the appropriate measures to control this particular catastrophic approach.

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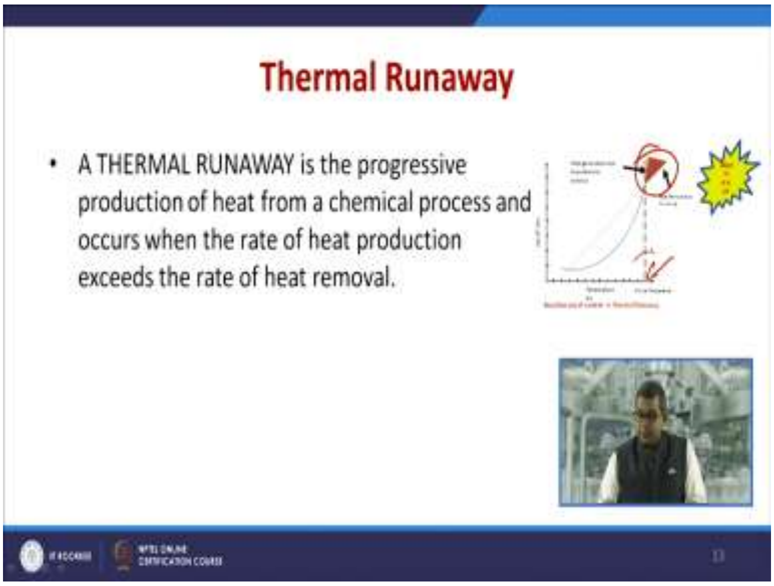
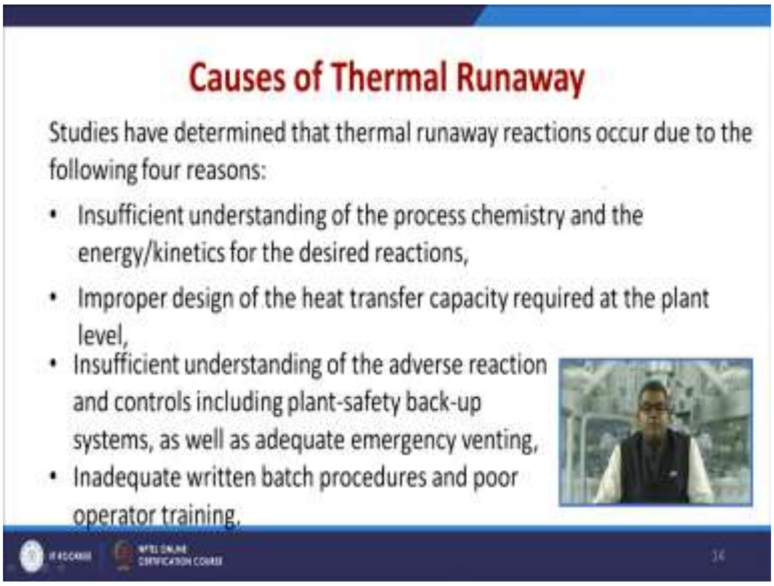


Thermal Runaway

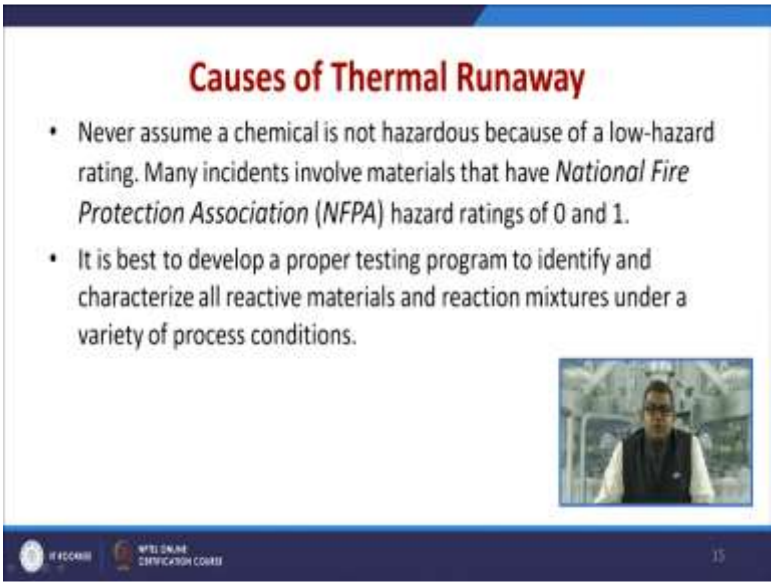
- A THERMAL RUNAWAY is the progressive production of heat from a chemical process and occurs when the rate of heat production exceeds the rate of heat removal.



Causes of Thermal Runaway

Studies have determined that thermal runaway reactions occur due to the following four reasons:

- Insufficient understanding of the process chemistry and the energy/kinetics for the desired reactions,
- Improper design of the heat transfer capacity required at the plant level,
- Insufficient understanding of the adverse reaction and controls including plant-safety back-up systems, as well as adequate emergency venting,
- Inadequate written batch procedures and poor operator training.



Causes of Thermal Runaway

- Never assume a chemical is not hazardous because of a low-hazard rating. Many incidents involve materials that have *National Fire Protection Association* (*NFPA*) hazard ratings of 0 and 1.
- It is best to develop a proper testing program to identify and characterize all reactive materials and reaction mixtures under a variety of process conditions.

Now there may be several causes for the thermal runaway, so studies have determine that thermal runaway reactions occur due to the various reasons and we have enlisted four reasons for this one, sometimes insufficient understanding of the process chemistry and the energy kinetics of the desired reaction, that means sometimes you may negate the effect of exothermicity.

Sometimes it may lead to the improper design of heat transfer capacity required for the plant, now this is again very important because you know theoretically that how much quantum of heat been generated in that particular process, so if your design is below the particular heat capacity, then definitely you are approaching towards the thermal runaway aspect, sometimes insufficient understanding of the adverse reaction and control including plant safety backup system as well as adequate emergency venting.

Again, it is very crucial aspect and attributed to the design of the reactor, sometimes inadequate return batch procedures and a poor operator training because sometimes it may approach to this particular reason and the process conditions surpasses this particular critical temperature zone and if the operator they are not trained to handle the scenario, then definitely the plant may land in trouble because of that thermal runaway aspect, so never assume a chemical is non-hazardous because of a low hazard rating and many incident involve material having the National Fire Protection Association hazard rating between 0 to 1, but they became the catastrophic in due course of time

so it is best to develop proper testing program to identify and characterize all reactive materials and reaction mixtures under a variety of process condition, so that is very much needed because like in Bhopal, there was I mean it was unlikely that water will meet MIC and these are the very much reactive and created and the reaction is exothermic in nature and the system was not designed at all for to cater this type of scenario, so if you are having the hazard rating in between 0 to 1, do not say that, dont think that this particular system is safe, you to take the proper measures to safeguard the system.

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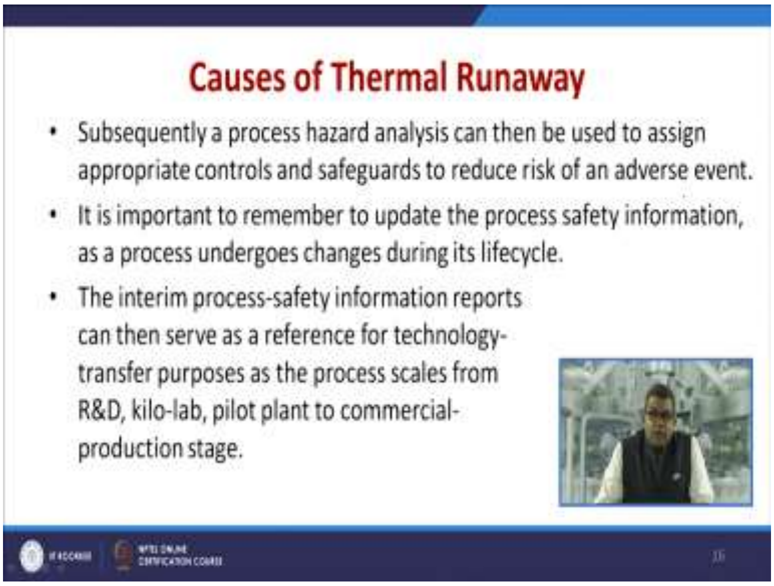

Causes of Thermal Runaway

- Subsequently a process hazard analysis can then be used to assign appropriate controls and safeguards to reduce risk of an adverse event.
- It is important to remember to update the process safety information, as a process undergoes changes during its lifecycle.
- The interim process-safety information reports can then serve as a reference for technology-transfer purposes as the process scales from R&D, kilo-lab, pilot plant to commercial-production stage.

Subsequently a process hazard analysis that can be used to assign the appropriate control and a safeguard to reduce risk of an adverse event, that is again very important aspect because no chemical is non-hazardous. Now, it is important to remember to update the process safety information as the process undergoes changes during the life cycle. Now, the interim process safety information reports can then serve as a reference for the technology transfer purpose, as a process scales from research and development aspect, labs, pilot plants to the commercial production stages.

Now, once the process has been set the final process safety report then can be used by the variety of end users, maybe in-house or by outsourced facilities. So, when developing the safety documentation, it is important to keep in mind that it must comply with the company or industry policy and procedures as well as the country and a local regulation because sometimes based on the gravity of the system, the local authorities or national authorities may impose certain regulation to the thing.

So while designing or while developing all kinds of safety-related issues we must know (because certain areas may be designated as a green area, certain maybe as an industrial area), so we must know that what are those regulations those who are governing and which we need to comply while designing the safety documentation.

There are certain things they are related to the kinetic complications. Now, beware of assuming simple kinetics for autocatalytic reactions, sometimes heterogeneous reaction, mass transfer may be the rate determining step, sometimes face transfer agents may dictate the rate, so you must know the complexity of the reactions, maybe the multiple steps or in a single step, what are the different routes of those complex reactions? These are the various complications they are associated with the kinetics or chemical kinetics of the process in question.

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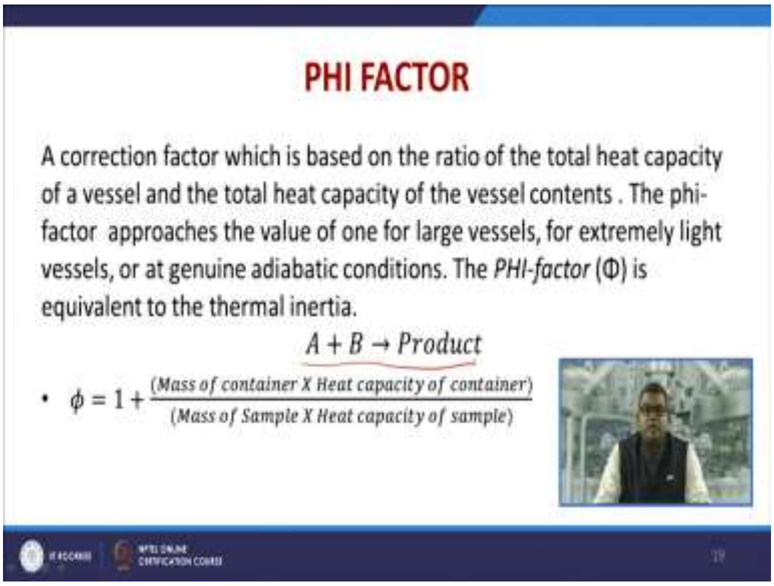

PHI FACTOR

A correction factor which is based on the ratio of the total heat capacity of a vessel and the total heat capacity of the vessel contents . The phi-factor approaches the value of one for large vessels, for extremely light vessels, or at genuine adiabatic conditions. The *PHI-factor* (Φ) is equivalent to the thermal inertia.

$$\underline{A + B \rightarrow Product}$$

- $\phi = 1 + \frac{(Mass\ of\ container\ X\ Heat\ capacity\ of\ container)}{(Mass\ of\ Sample\ X\ Heat\ capacity\ of\ sample)}$

Now let us have a look about the phi factor, this is a correction factor which is based on the ratio of the total heat capacity of the vessel and the total heat capacity of the vessel contents, so the phi factor approaches the value of one for a large vessels and for extremely light vessels or at a genuine adiabatic conditions. Now, Phi factor is usually equivalent to the thermal inertia.

Let us have a look about this again the basic equation A plus B, they are converting into the product, so phi factor is designated as

$$\phi = 1 + \frac{(Mass\ of\ container\ X\ Heat\ capacity\ of\ container)}{(Mass\ of\ Sample\ X\ Heat\ capacity\ of\ sample)}$$

so it is quite simple.

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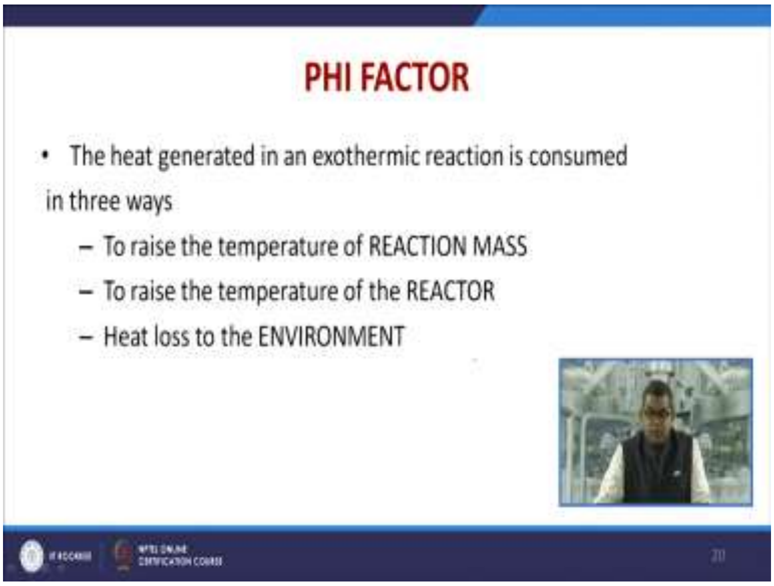

PHI FACTOR

- The heat generated in an exothermic reaction is consumed in three ways
  - To raise the temperature of REACTION MASS
  - To raise the temperature of the REACTOR
  - Heat loss to the ENVIRONMENT

Now the heat generated in an exothermic reaction is consumed in three ways.

Usual way is to raise a temperature of the reaction mass, so whatever inside the reactor. Sometimes it is used to raise the temperature of the reactor and sometimes it may attributed to the heat loss to the environment, so you may experience that reactor is having the heat.

Now if phi is greater than 1 then it is considered in a thermodynamic and a kinetic calculation, so we have enlisted several cases when 1 cubic meter glass lined reactor, then jacket is empty, the phi factor is 1.41. 10 metre cube glass lined reactor when jacket is empty, 1.13. 10 gram of carious tube screening test that is 2.50. Accelerating rate calorimeter 1.50. Then adiabatic pressure Dewar calorimeter are 1.05.

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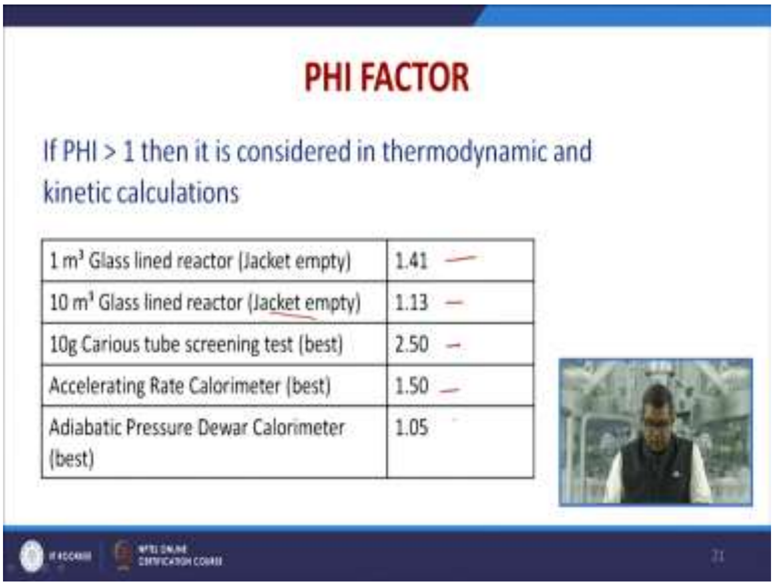

PHI FACTOR

If PHI > 1 then it is considered in thermodynamic and kinetic calculations

1 m^3 Glass lined reactor (Jacket empty)	1.41
10 m^3 Glass lined reactor (Jacket empty)	1.13
10g Carious tube screening test (best)	2.50
Accelerating Rate Calorimeter (best)	1.50
Adiabatic Pressure Dewar Calorimeter (best)	1.05

So let us think about the testing. The testing should consider the consequences of all conceivable process deviation, this should be conducted under the plant scale heat loss condition or have an appropriate safety factor applied, they should replicate the plant condition in all ways possible, including the use of plant material consideration of material of plant construction etc.

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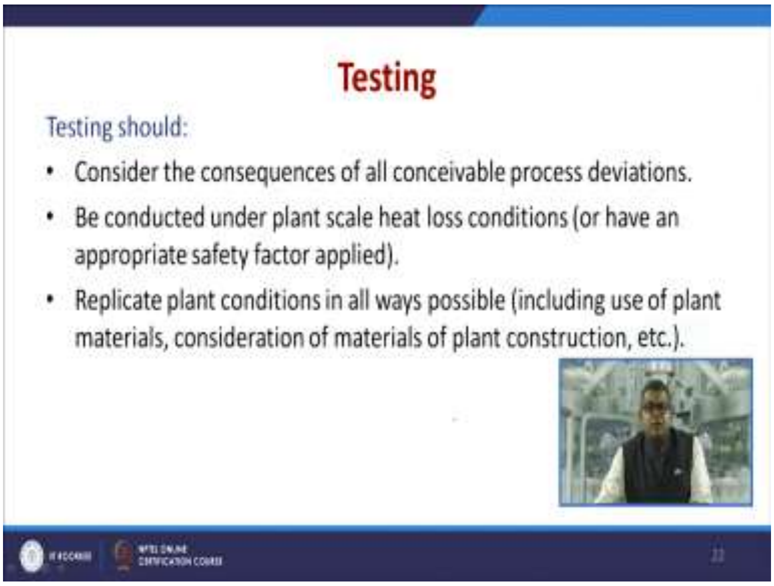
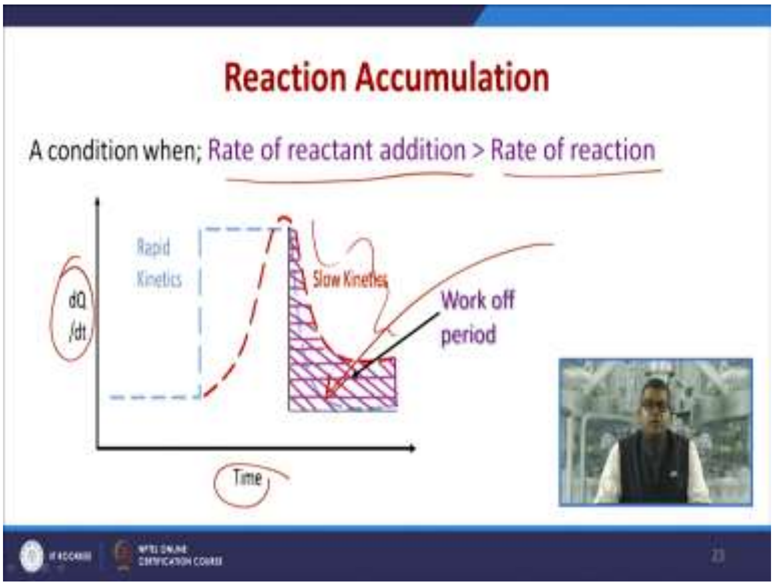


Testing

Testing should:

- Consider the consequences of all conceivable process deviations.
- Be conducted under plant scale heat loss conditions (or have an appropriate safety factor applied).
- Replicate plant conditions in all ways possible (including use of plant materials, consideration of materials of plant construction, etc.).



Reaction Accumulation

A condition when; Rate of reactant addition > Rate of reaction

Now let us have a look about the rate reaction accumulation, we are not going to devote much time because we are all aware about the accumulation, so this is a condition when a rate of reactor in addition is more than the rate of reaction, so you need to plot this dQ/ dt versus time, so initially you may experience the rapid reaction growth and then there is a scenario when there may be chances of slow kinetics, so this is, the zone where you can think about the work of a period.

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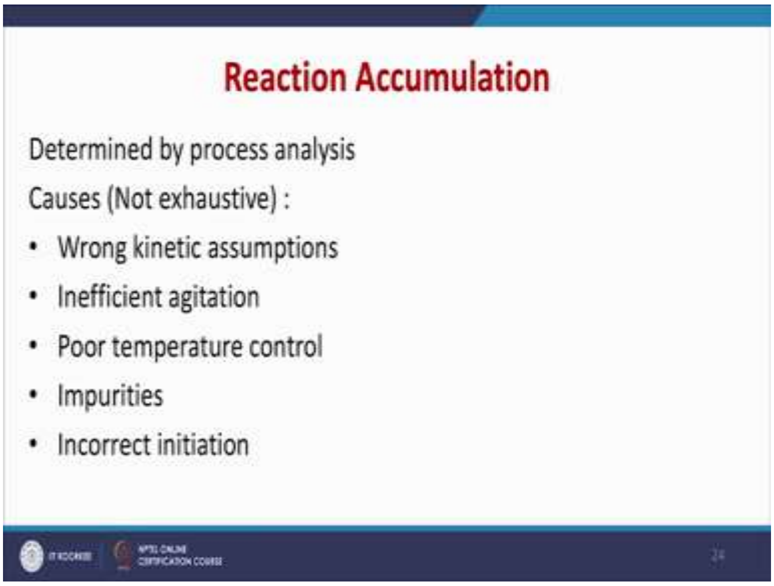

Reaction Accumulation

Determined by process analysis

Causes (Not exhaustive) :

- Wrong kinetic assumptions
- Inefficient agitation
- Poor temperature control
- Impurities
- Incorrect initiation

Now this is usually determined by the process analysis, discuss about the causes not in a very exhaustive manner, now sometimes you may take the wrong kinetic assumptions and this may be a very extremely catastrophic, but fortunately in chemical engineering aspect, whatever wrong kinetics we take it is only just at the design level, so when it is scale up, when it is under the pilot plant study, then we can remove all kind of deficiencies which we have taken the list stages.

Sometimes it may attributed to the inefficient agitation because in agitations, sometimes the particle may get deposited to the impellers et cetera, if you are using those impellers, then the rate of agitation may go on decreasing and that particular things, maybe the problematic and attributed to the reaction accumulation, sometimes the poor temperature control may lead to the reaction accumulation, sometimes the impurities is attributed to either to the reactant and sometimes the non-intermediate remover of those impurities from the reaction mass may create the problem of reaction accumulation and sometimes the incorrect initiation, maybe because of the contaminated raw material, sometimes may be attributed to the poor temperature and a pressure control at start-up, this may attributed to the (())(21:43) reaction accumulation.

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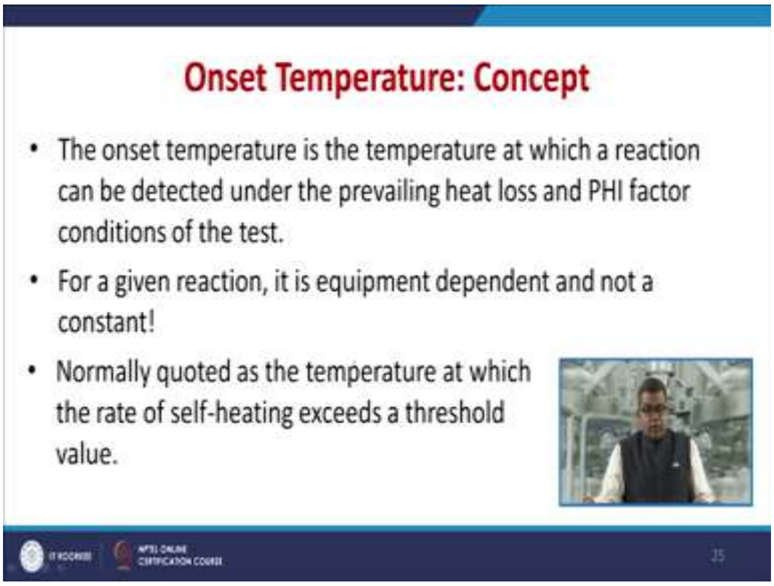

Onset Temperature: Concept

- The onset temperature is the temperature at which a reaction can be detected under the prevailing heat loss and PHI factor conditions of the test.
- For a given reaction, it is equipment dependent and not a constant!
- Normally quoted as the temperature at which the rate of self-heating exceeds a threshold value.

Now let us have a look about the onset temperature, that is the basic concept, the onset temperature is a temperature at which a reaction can be detected under the prevailing heat loss and a phi factor condition of the test, so for a given reaction, it is equipment dependent and they are not a constant and normally quoted as a temperature at which the rate of self-heating exceeds a threshold value, so sometimes the knowledge about this particular aspect is essential while designing the safety aspect.

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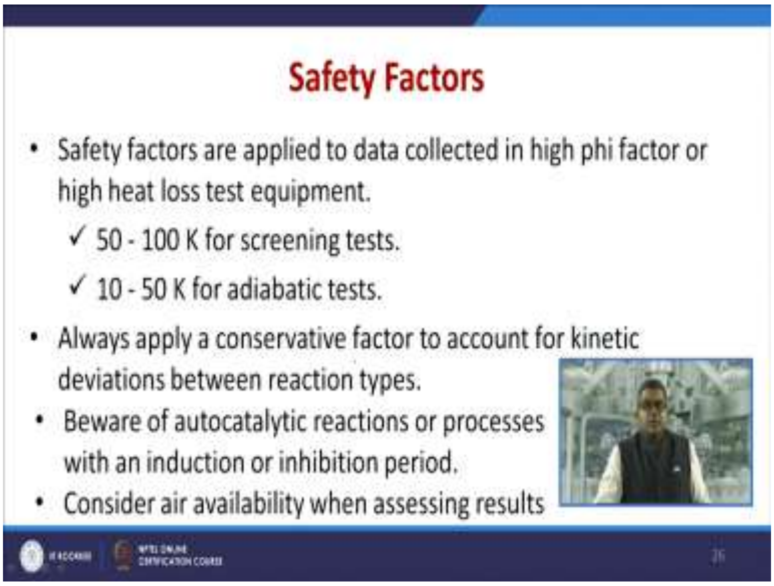

Safety Factors

- Safety factors are applied to data collected in high phi factor or high heat loss test equipment.
  - ✓ 50 - 100 K for screening tests.
  - ✓ 10 - 50 K for adiabatic tests.
- Always apply a conservative factor to account for kinetic deviations between reaction types.
- Beware of autocatalytic reactions or processes with an induction or inhibition period.
- Consider air availability when assessing results

Now let us have a look about there is safety factors, so safety factors are applied for this runaway reactions to collect data in high phi factor or high heat loss test equipment, now 5200 Kelvin for screen test, 10 to 15 K for the adiabatic test, now this is always apply for a conservative factor to account for kinetic deviation between the reaction types, now one must beware of autocatalytic reaction or process within induction or inhibition period, you may also consider the availability of air, while accessing the results.

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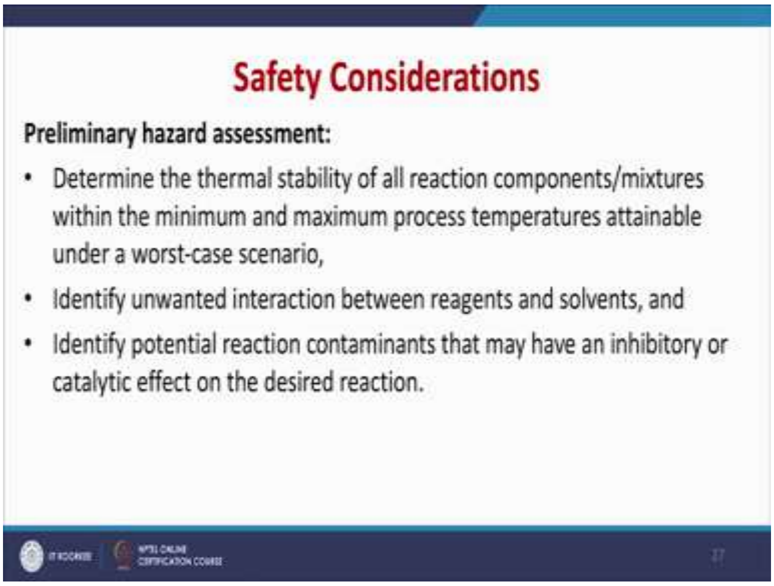

Safety Considerations

Preliminary hazard assessment:

- Determine the thermal stability of all reaction components/mixtures within the minimum and maximum process temperatures attainable under a worst-case scenario,
- Identify unwanted interaction between reagents and solvents, and
- Identify potential reaction contaminants that may have an inhibitory or catalytic effect on the desired reaction.

So let us have a preliminary hazard assessment in safety consideration, you need to determine the thermal stability of all reaction components or mixtures within the minimum and maximum process temperature which you can attend under the worst-case scenario because worst-case scenario, they are sometimes the designing factors, you need to identify the unwanted interactions between the reagents and a solvent, sometimes you need to identify the potential reaction contaminants that may have an inhibitory or catalytic effect on the desired reactions.

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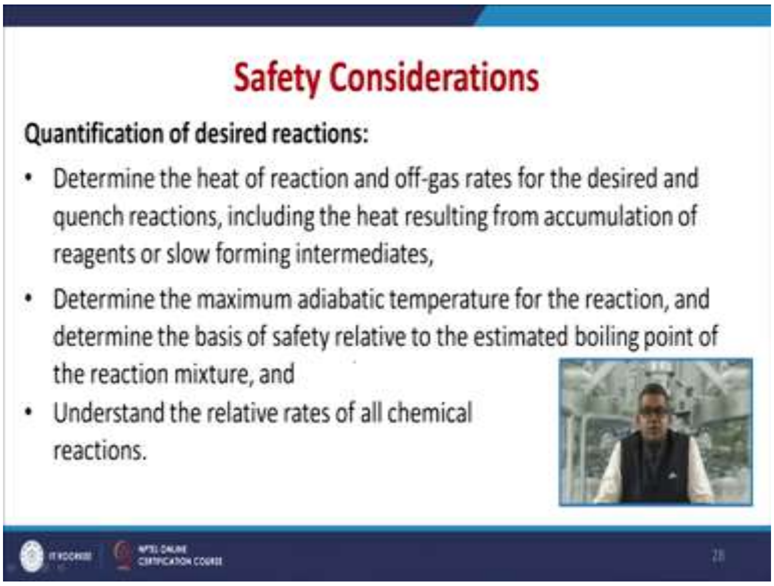

Safety Considerations

Quantification of desired reactions:

- Determine the heat of reaction and off-gas rates for the desired and quench reactions, including the heat resulting from accumulation of reagents or slow forming intermediates,
- Determine the maximum adiabatic temperature for the reaction, and determine the basis of safety relative to the estimated boiling point of the reaction mixture, and
- Understand the relative rates of all chemical reactions.

Now another is the quantification of the desired reactions, so you need to determine the heat of reaction and off-gas rates for the desired and quench reaction including the heat resulting from accumulation of reagent or slow forming intermediates, sometimes you need to determine the maximum adiabatic temperature for the reaction and determine the basis of safety relative to estimate boiling point of the reaction mixture and understand the relative rate of all chemical reaction and sometimes this inclusive of all kind of side, unwanted reactions and a major reactions, et cetera.

Then you need to go for the quantification of the adverse reaction, now by this way you need to assess the thermal stability of a reaction mixture over a wide temperature range.

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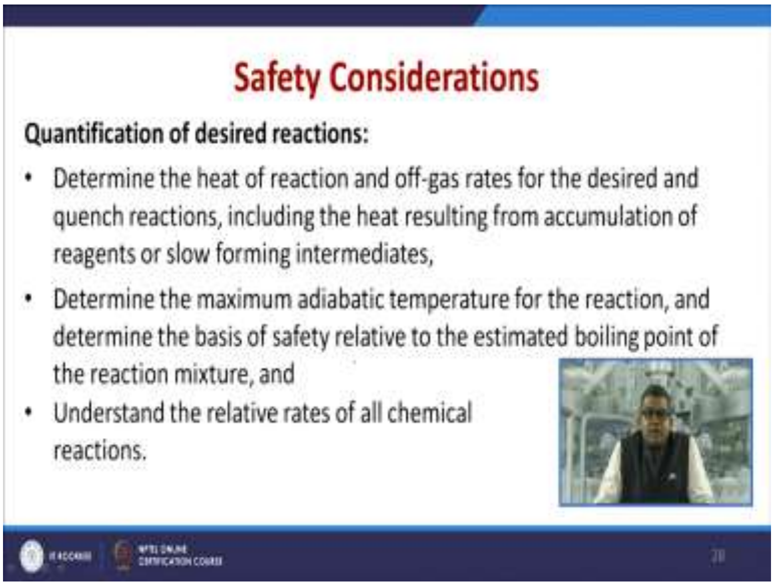

Safety Considerations

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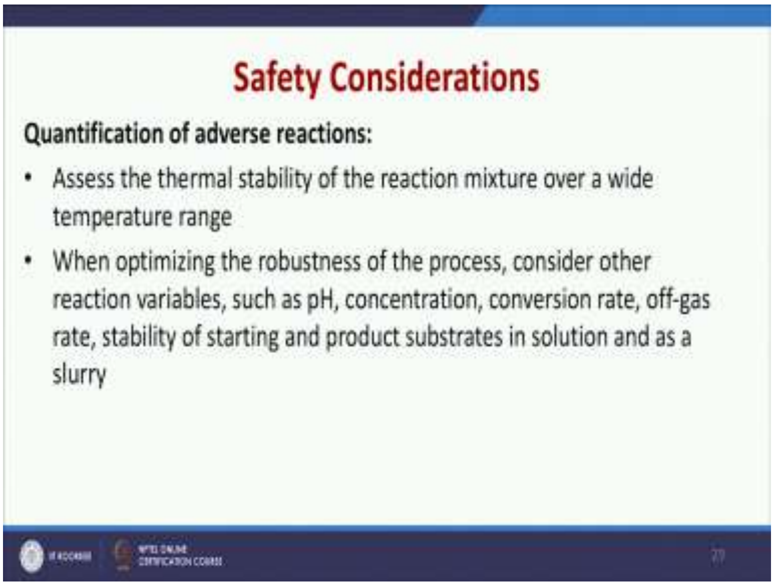

Safety Considerations

Quantification of adverse reactions:

- Assess the thermal stability of the reaction mixture over a wide temperature range
- When optimizing the robustness of the process, consider other reaction variables, such as pH, concentration, conversion rate, off-gas rate, stability of starting and product substrates in solution and as a slurry

So while optimising the robustness of the process, consider other reaction variables such as pH, concentration, conversion rate, off-gas rate, stability of starting and product substrate et cetera in solution or as a slurry et cetera, so you may consider all the probabilities, all the prospects of this particular thing, then consider the potential and impact of unwanted vapour-phase reactions and develop a chemical interaction matrix for material present in the reaction mixture, when you need to classify the reactivity and communicate this information to the operational personnel, so it has a various step involve for whenever the quantification of these adverse reactions are in questions.

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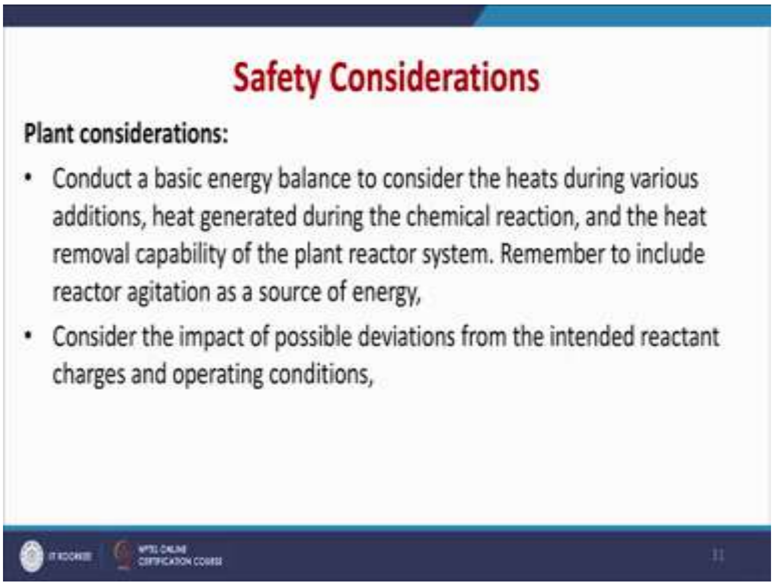

Safety Considerations

Plant considerations:

- Conduct a basic energy balance to consider the heats during various additions, heat generated during the chemical reaction, and the heat removal capability of the plant reactor system. Remember to include reactor agitation as a source of energy,
- Consider the impact of possible deviations from the intended reactant charges and operating conditions,

Then next phases the plant consideration, now you need to conduct a basic energy balance to consider the heat during the various editions, heat generation, during the chemical reaction and the heating removal capacity or capability of the plant reactor system, now remember to include the reactor agitation as a source of energy because sometimes we may skip this important aspects while considering this plant consideration, now consider the impact of possible deviation from the intended reactant charges and operating conditions.

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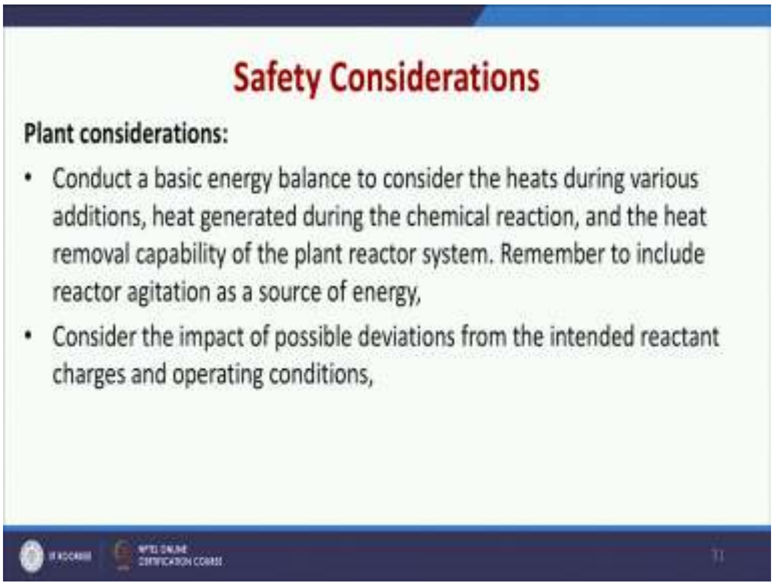
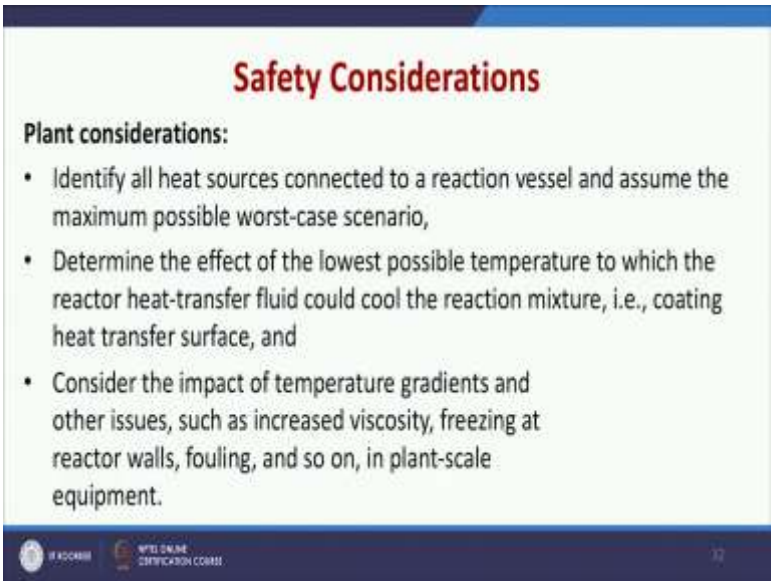


Safety Considerations

Plant considerations:

- Conduct a basic energy balance to consider the heats during various additions, heat generated during the chemical reaction, and the heat removal capability of the plant reactor system. Remember to include reactor agitation as a source of energy,
- Consider the impact of possible deviations from the intended reactant charges and operating conditions,



Safety Considerations

Plant considerations:

- Identify all heat sources connected to a reaction vessel and assume the maximum possible worst-case scenario,
- Determine the effect of the lowest possible temperature to which the reactor heat-transfer fluid could cool the reaction mixture, i.e., coating heat transfer surface, and
- Consider the impact of temperature gradients and other issues, such as increased viscosity, freezing at reactor walls, fouling, and so on, in plant-scale equipment.

References

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- Fauske & Associates, blog, How to Scale-up Chemical Reactions/ Runaway Reactions in a Safer Way, link: https://www.fauske.com/blog/bid/401398/how-to-scale-up-chemical-reactions-runaway-reactions-in-a-safer-way
- Safety Issues In The Scale-up Of Chemical Reactions, RSC Publication, URL: http://www.rsc.org/globalassets/04-campaigning-outreach/realising-potential-of-scientists/regulations-health-safety/safety-issues-in-the-scaleup-of-chemical-reactions.pdf

Then you need to identify all heat sources connected to a reaction vessel and assume the maximum possible worst-case scenario. Then you determine the effect of lowest possible temperature to which the reactor heat transfer fluid could cool the reaction mixture, maybe that is the coating of heat transfer surfaces et cetera and then consider the impact of temperature gradient and other issues such as increased viscosity, freezing at reactor walls, falling and so on and plant scale equipment.

So in this particular module we have consider the various aspects of runaway reactions, what is the importance we discuss about the safety consideration issues et cetera, so if you wish, you can have a look for all this references in this particular slides those are given. Thank you very much.