

**Health, Safety and Environment Management in Petroleum and offshore
Engineering**

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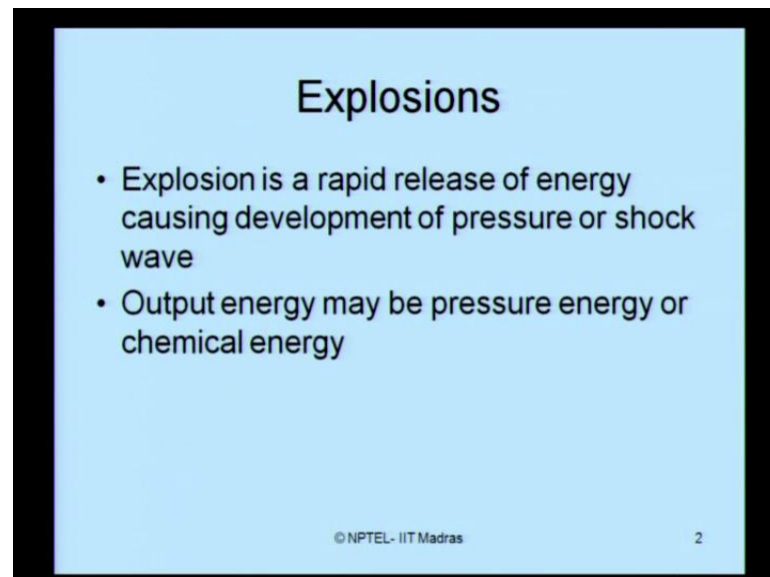
Module No. # 03

Lecture No. # 09

Explosion modeling

Dear friends, in the last lecture, we discussed about the fire and explosion models, we discussed about fire triangle. I hope you have understood, how to draw a flammability diagrams and how to read an existing flammability diagram to understand whether a given mixture is flammable or not. In the present lecture, we will talk about explosion modeling. This is on module-three lecture- nine for HSE under NPTEL, IIT madras.

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Before we discuss about different modeling techniques for explosion, let us try to understand what is explosion? Explosion is a rapid release of energy causing development of pressure or shock wave. The output energy may be pressure energy or a chemical energy.

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Explosion damage estimate

- Explosions result in a blast or a pressure wave moving out from explosion center at the speed of sound
- Shock wave or overpressure is the basic cause for damage
- Missiles or projectiles are other important source of damage
- Damage is function of rate of pressure increase and duration of blast wave
- Blast damage are estimated based on the peak side-on overpressure

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If you want to really estimate the explosion damages, let us try to understand that the explosion actually results in a blast or a pressure wave moving out from an explosion centre at a speed of sound. The shock wave or over pressure is the basic cause for the damage which is resulting from an explosion missiles or projectiles or other important sources of damage; however, damage is expressed as a function of rate of pressure increase and duration of the blast wave. The blast damage is estimated based on the peak side on overpressure. So, if one is interested to estimate the explosion damage, one should understand the rate of pressure increased on the duration of blast wave.

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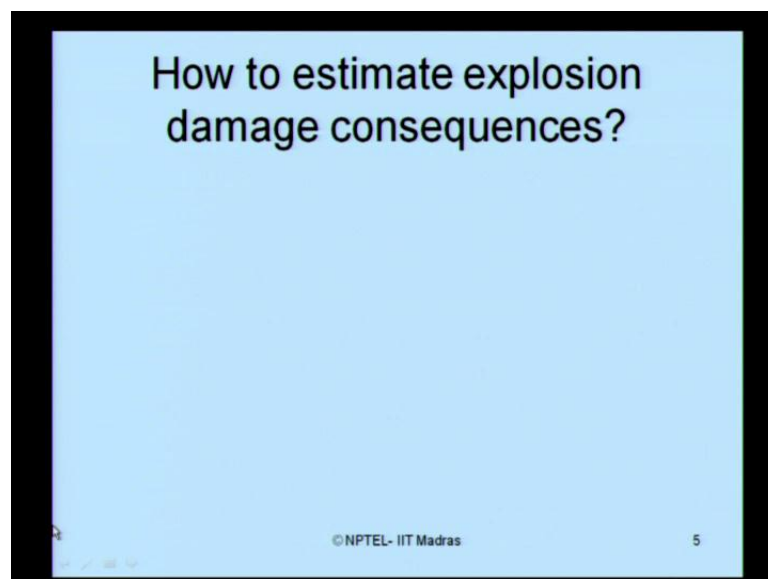
- Explosion generates a rapid rise in pressure
- The propagating wave causes damage to objects located on its path
- It is then followed by negative pressure wave which causes further damage before pressure returns to atmospheric
- Thus damage depends on maximum pressure reached, velocity of propagation and environmental characteristics
- Area under the curve is the measure of severity of explosion

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In this context, let us understand this figure. The explosion actually generates a rapid rise in pressure. Look at this figure, which is plotting the pressure with respect to time before the pressure overshoots to become its peak value; there is always a time delay what we call as arrival time, once the pressure reaches its peak value, which we call as Peak Over Pressure. The explosion actually generates a rapid rise in the pressure, practically within no instant of time the pressure rises from atmospheric to the over pressure. So, that is what we explain here as a result of explosion which generates a very instantaneous rise in pressure. Now, the propagating wave causes damage to the objects located on its path; it is then followed by a pressure drop which goes through even a negative value below the atmospheric. So, the negative pressure wave which will cause a further damage before the pressure returns to atmospheric.

So, the explosion, ladies and gentlemen after an arrival time delay shoots at the pressure to a peak value what we call as peak over pressure. As the wave propagates in the advanced direction, the pressure drops comes to negative causes damage before it returns back to atmospheric. Thus, the damage depends on the maximum pressure reached caused by the explosion; the velocity of course the propagation, because it is the time function; and of course, the environmental characteristics which is present at that sight of explosion. Area under this curve is actually the measure of severity of explosion, if you want to actually calculate the area of positive and the area negative the net area under this curve will actually give you the measure of severity of the explosion.

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Now, the fundamental question comes, how to estimate the explosion damage consequence? For example, I understand that explosion results in instantaneous increase in pressure to a very high value then, the pressure drops down goes to negative before it returns to atmosphere, it causes damage. Now, how to estimate these damage consequences on any object ?

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TNT equivalence method

- What is TNT?
- It is Tri nitro toluene- an important explosive
- $2C_7H_5N_3O_6(s) \rightarrow 3N_2(g) + 7CO(g) + 5H_2O(g) + 7C(s)$

Soot (a black powder)

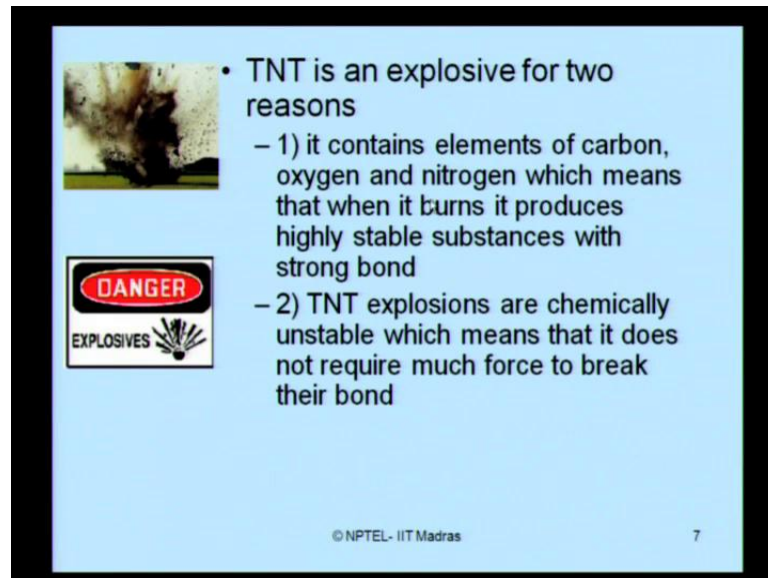
TNT

- TNT can very quickly change from solid to hot expanding gas

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There are many methods available in the literature. One common method which is being used in the literature is what we call as TNT equivalence method. Now, the first question comes in mind is, what do you understand by TNT? TNT is tri nitro toluene- an important explosive. The chemical reaction of this explosive is given by an equation as shown in the screen now. In this equation, the C 7 H 5 N 3 O 6 component is what we call as TNT and this reaction leaves a black powder, which is generally addressed as soot. Now, what is the problem with TNT? TNT can very quickly change from solid to a hot expanding gas.

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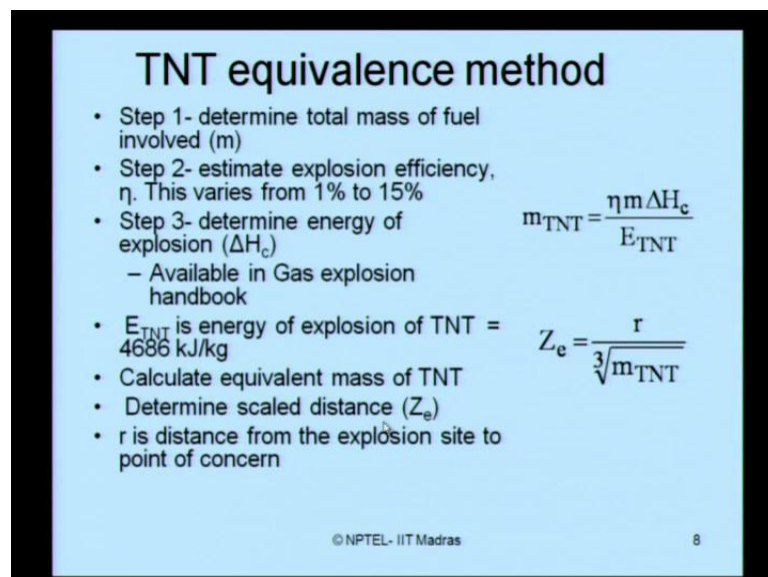
• TNT is an explosive for two reasons

- 1) it contains elements of carbon, oxygen and nitrogen which means that when it burns it produces highly stable substances with strong bond
- 2) TNT explosions are chemically unstable which means that it does not require much force to break their bond

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TNT is an explosive because of two fundamental reasons. It contains elements of carbon, oxygen and nitrogen which mean that when it burns it produces highly stable substances with strong bond between them. TNT explosions are chemically unstable, which means that it does not require much force to break their bond, because of these two fundamental reasons TNT is considered to be very powerful explosive.

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TNT equivalence method

- Step 1- determine total mass of fuel involved (m)
- Step 2- estimate explosion efficiency, η . This varies from 1% to 15%
- Step 3- determine energy of explosion (ΔH_c)
 - Available in Gas explosion handbook
- E_{TNT} is energy of explosion of TNT = 4686 kJ/kg
- Calculate equivalent mass of TNT
- Determine scaled distance (Z_e)
- r is distance from the explosion site to point of concern

$$m_{TNT} = \frac{\eta m \Delta H_c}{E_{TNT}}$$
$$Z_e = \frac{r}{\sqrt[3]{m_{TNT}}}$$

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Then, what is TNT equivalence method? How do you compute that? Step number one - determine the total mass of fuel involved in terms of TNT equivalence; that is given by

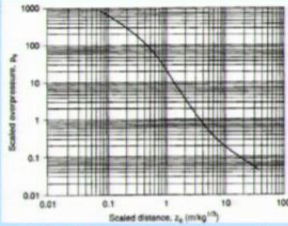
the equation on right side which you see on the screen now. Mass of TNT equivalence is given by $n m \Delta H_c$ by E_{TNT} . What do we understand by this values estimate the explosion efficiency η ? This actually is varied from 1 to 15 percent depending upon how the TNT chemical is packed. So, assume an η value anywhere from 1 to 15 percent. Step number three - determine the energy of explosion that is what we call as ΔH_c in this equation. Generally, for all chemical composition of explosions the energy of explosion is available in what we call as gas explosion handbook.

So, for TNT try to pick up or for any chemical explosion combination you have try to pick up ΔH_c value from the gas explosion handbook. So, on the numerator η is assumed anywhere from 1 to 15 percent. ΔH_c is available from the chemical in the gas explosion handbook; E_{TNT} is what we call as equivalent energy of explosion of TNT, which is generally given in the literature as 4686 kilo joules per kilogram.

So, what you want is an equivalent mass of TNT, if you know the mass of an explosive. So, what is the equivalency of that mass of explosive in terms of TNT is what I get from this equation. Once you obtain the equivalent mass of TNT, then determine what we called as a scaled distance - Z_e ; the scaled distance Z_e is given by this equation in terms of distance in meters by mass of TNT in kilogram which is a cubic root of that value. r is the distance in meters from the explosion site to the point of your concern.

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- Use the figure to determine over pressure P_s
- $P_0 = P_s \times P_a$
- P_s is the scaled over pressure read from the figure and P_a is atmospheric pressure
- Alternatively, P_0 can also be calculated from the equation
- After determining over pressure (P_0), using Table, one can estimate the damage



Source: Crowl D.A., Louvar J.F. 2002. Chemical Process Safety: Fundamentals with applications, 2nd Ed. Upper Saddle River, N.J. Prentice-Hall PTR.

$$P_0 = P_a \left[\frac{1616 \left[1 + \left[\frac{Z_e}{4.5} \right]^2 \right]}{\sqrt{1 + \left[\frac{Z_e}{0.048} \right]^2} \times \sqrt{1 + \left[\frac{Z_e}{0.32} \right]^2} \times \sqrt{1 + \left[\frac{Z_e}{1.35} \right]^2}} \right]$$

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Once you get the scaled distance then let us look at this curve which plots the scale distance in meter per cubic root of the kilogram that is $m \sqrt[3]{TNT}$ over the scaled over pressure P_s . So, once you know Z_e from the previous equation using this curve which is given at the source of Crowl D A and Louvar 2002, try to locate Z_e value on the x axis and equivalently get my scaled over pressure P_s .

So, use the figure to determine the over pressure what we call as P_o . The over pressure P_o is given as, the scaled pressure multiplied by atmospheric pressure. The scaled pressure is what you get from this curve and over pressure is what you compute using a simple relationship like this. P_o is what we call as scaled pressure which is read from here and P_a is the atmospheric pressure. Alternatively, the over pressure can also be computed from a given equation as shown here. If you know the atmospheric pressure value, and if you know the Z_e value which is computed from the previous slide equation use this relationship to compute P_o which is we call as over pressure. After determining the over pressure, how will you estimate the damage our interest is to estimate the damage because of the explosion. So, use a table which is given in the next slide.

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Overpressure (kpa)	Damage	Overpressure (kpa)	Damage
0.28	Loud noise (143 dB) – glass failure	17.2	Destruction of brick houses
0.69	Breakage of small windows	27.6	Cladding of industrial building ruptures, oil tank ruptures, 50% probability of human fatality
2.07	Safe distance (probability of 0.95 of no serious damage below this value)	34.5 to 48.2	Nearly complete destruction of houses
3.4 to 3.6	Windows shatter; occasional damage to window frames	62	Loaded trains completely gets damaged
4.8	Minor damage to house structure	68.9	Probable total destruction of buildings, heavy machinery
6.9 to 13.8	Significant damage to wooden and asbestos	75	90% probability of human fatality; concrete and steel structures completely gets damaged etc
15.8	Lower limit of serious damage		

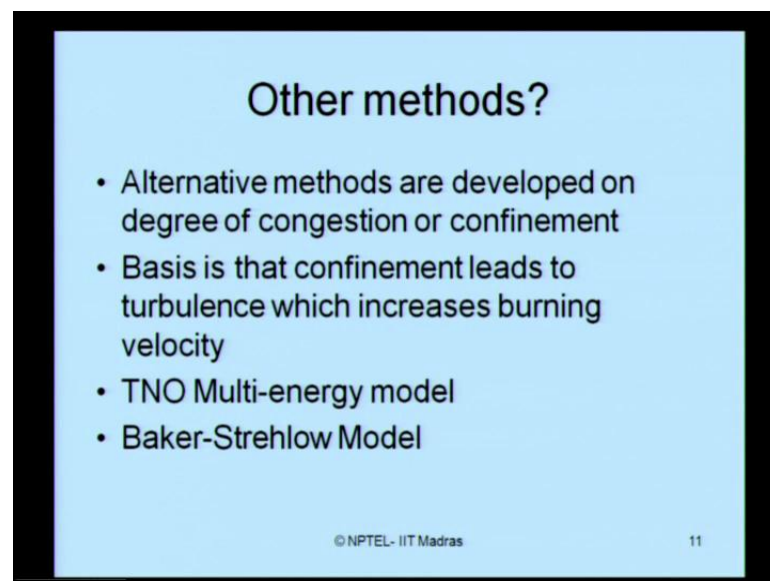
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So, this table gives you a relative index of, if you know the over pressure value in kilopascal, for example, if that arrives to be at 0.28, then the equivalence damage that over pressure can cause is nothing but a loud noise is about 143decibels which can at least break a glass. If that value is about 2.07, then the safe distance that is the

probability of 0.95 of no serious damage below this value can be rewritten. For example, the over pressure is as high as 75, then it can result the damage of ninety percent probability of human fatality. So, the concrete and steel structures can get completely damaged etcetera. That is the energy, what this explosion will have which results in an over pressure of about 75, which you computed from the relationship or from the curve which I showed you in the last slide.

So, ladies and gentlemen, if you know the Z_e value, if you know the mass of your explosive try to convert that mass value into equivalent mass of TNT and from the equivalent mass of TNT find out the Z_e distance; from this Z_e distance use the curve or the equation which I gave you in the last slide to compute what I call as overpressure. The moment estimate the overpressure equivalence amount of damage resulted from that kind of explosion is available in the table which you currently see on your screen. Is that clear?

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Other methods?

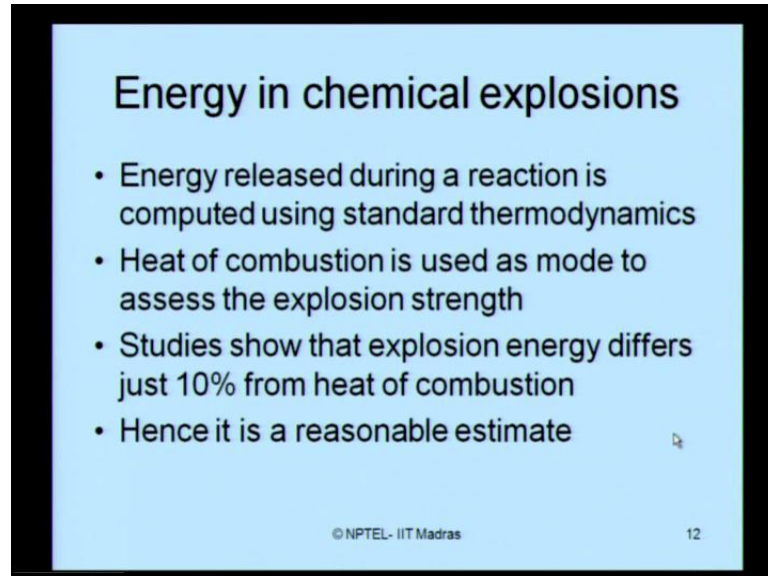
- Alternative methods are developed on degree of congestion or confinement
- Basis is that confinement leads to turbulence which increases burning velocity
- TNO Multi-energy model
- Baker-Strehlow Model

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Once we understand this, let us also see what are the other alternatives methods which are used for measuring the consequences of damage caused from explosion; alternatives methods are developed based on the degree of congestion or confinement. The bases for these methods are that the, confinement leads to turbulence which increases burning velocity. The different methods which are available in literature are TNO multi-energy model or Baker- Strehlow model; however, the equivalence TNT method is one of the

more popular methods being used for estimating the consequences of explosion damages, which I discussed in the previous couple of slides.

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Energy in chemical explosions

- Energy released during a reaction is computed using standard thermodynamics
- Heat of combustion is used as mode to assess the explosion strength
- Studies show that explosion energy differs just 10% from heat of combustion
- Hence it is a reasonable estimate

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Now, lets us ask a question how do I measure the energy in chemical explosions? In chemical explosions, energy released during a reaction is actually computed using standard thermodynamic principles. The heat of combustion is used as mode to assess the explosion strength. Studies show that the explosion energy calculated by this method differs just about 10 percent from the heat of combustion, which is a good agreement for a reasonable estimate at least for gases.

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Explosion energy in physical explosions

- In mechanical or physical explosions, a reaction does not occur
- Energy is obtained from the energy content of the contained substance
- Four approaches are available
 - Brode's method
 - Isentropic expansion method
 - Isothermal expansion method
 - Thermodynamic availability
- E is explosion energy, P_1 is atmospheric pressure, P_2 is bursting pressure, V is volume of vessel, γ is heat capacity ratio

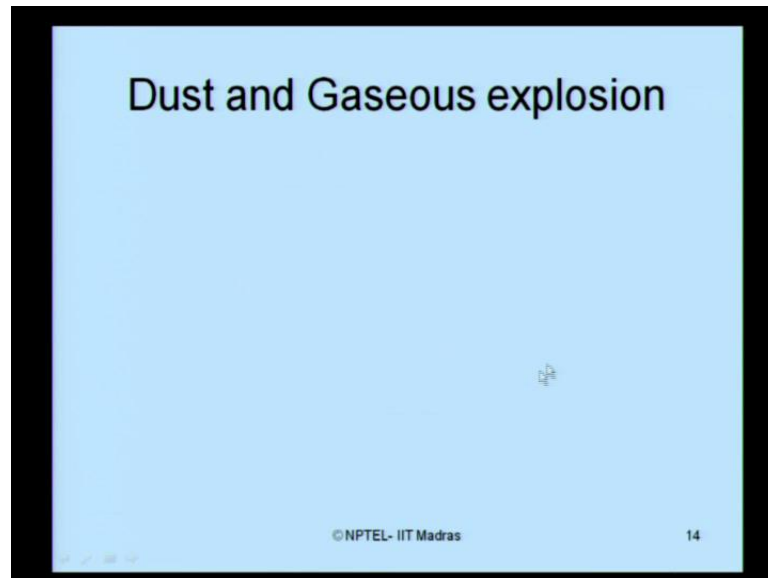
$$E_{\text{Brode}} = \frac{(P_2 - P_1)V}{\gamma - 1}$$
$$E_{\text{isentropic}} = \frac{P_2 V}{\gamma - 1} \left[1 - \left(\frac{P_1}{P_2} \right)^{\frac{\gamma - 1}{\gamma}} \right]$$
$$E_{\text{isothermal}} = P_2 V \ln \left(\frac{P_2}{P_1} \right)$$

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Now, the question comes how do we estimate the explosion energy in physical explosions? In mechanical or physical explosions the reaction does not occur then what do we do? Energy is obtained from the energy content of the contained substance actually. There are four approaches available in the literature to estimate the explosion energy in case of physical explosions namely Brode's method, isentropic expansion method, isothermal expansion method and thermodynamic availability. The brode's method, isentropic expansion method, isothermal expansion method, and thermodynamic availability estimate the explosion energy in case of, physical explosions by the following equations given to you. For example, if you want to estimate the explosion energy in physical explosion using Brode's method, I will pick up this equation and substitute for P_2 and P_1 and v and γ .

Another question comes, what are these values? E, what you see from this equation is the explosion energy resulting from physical explosion. P_1 is the atmospheric pressure, and P_2 is a pressure at which the explosion is occurring what we call as bursting pressure; of course, v is the volume of the vessel or the containment which is getting exploded and γ is the heat capacity ratio. So, once you have these values available for your specific case, you can always estimate the explosion energy either by Brode's method or by isentropic expansion method or by isothermal expansion method or using existing thermodynamic loss.

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Ladies and gentlemen, we have discussed in detail about the fire models. We are now discussing about the explosion models. In explosion models, we discussed about the chemical explosion, physical explosion. Now, you can also have explosion resulting from dust and gas - what we call as dust and gaseous explosions.

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- For a gas, molecules are small and of well-defined size
- For dust particles, size is varying and is of many orders in magnitude larger than molecules
- Gravity also affects dust particle behavior
- K_G and K_{st} are deflagration index for gas and dust respectively

$\left(\frac{dp}{dt}\right)_{\max} \sqrt{V} = K_{st}$

$\left(\frac{dp}{dt}\right)_{\max} \sqrt{V} = K_G$

Pressure in bar (abs)

Time in ms

$P_{\max}=8.5$

dp/dt

Dust injection

Time Delay

Ignition

1 atm

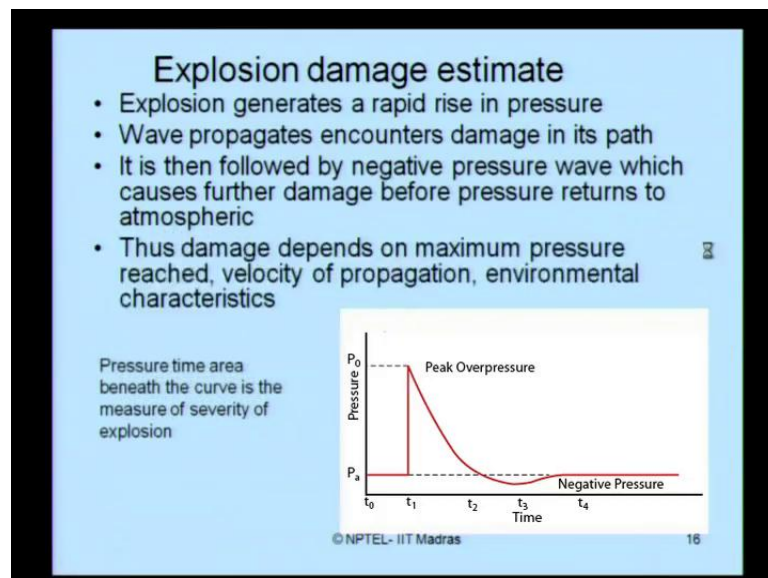
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For a gas, molecules are very small and of well-defined size. For dust particles, size is anyway varying and is of many orders in magnitude larger than the molecules. Now, in case of such explosions, gravity affects the dust particle behavior. If you look at the

explosion rate for gas and dust respectively, for example, in case of a gas, the pressure rise is sudden and then the pressure drops - what we called as a pressure rate dp by dt ; and it reaches the maximum of 8.5 then the pressure drops gradually.

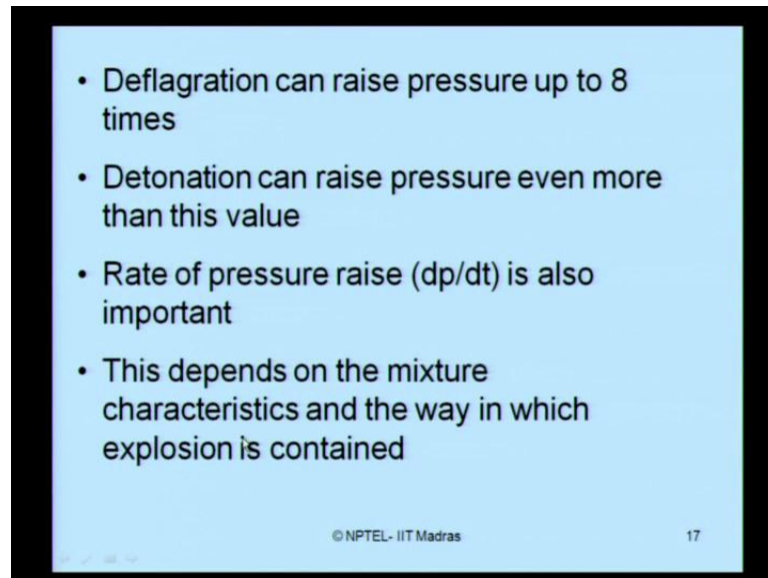
Where in the case of the dust, there is a time delay which is caused for injecting dust in the process. Once a dust is injected, then it happens at a constant atmospheric pressure then the ignition happens and the pressure rises, and of course, the maximum rise in both the cases is about 8.5 then the pressure drops. So, the rate of change of pressure or let say dp by dt in case of gas and dust are given by this equation which is dp by dt max into cube root of V is equal to K_{st} or K_G as the case may be - where K_G and K_{st} are called deflagration index for the gas and for the dust respectively.

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Now, if you look at the explosion damage estimates we have already seen that the explosion damage cause a rapid rise in the pressure. The wave propagates encounters the damage in its path; it is then followed by a negative pressure and area of this curve gives you the measures of severity of explosion

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• Deflagration can raise pressure up to 8 times

• Detonation can raise pressure even more than this value

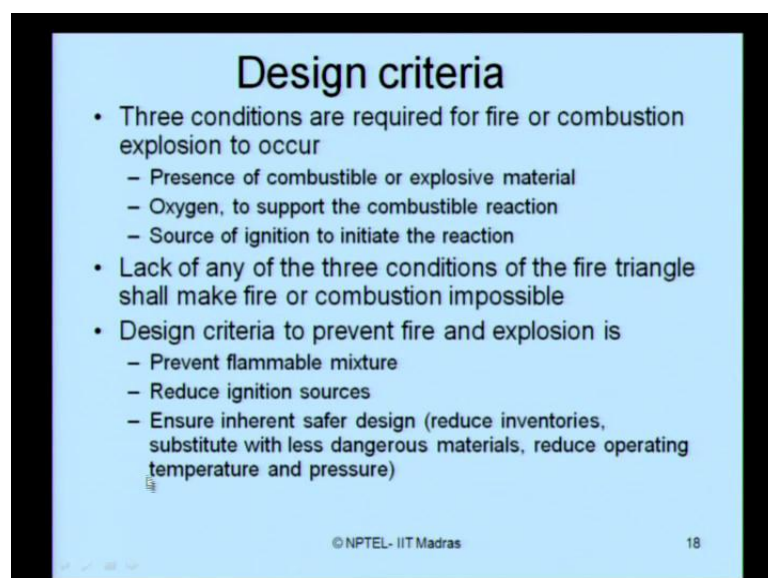
• Rate of pressure raise (dp/dt) is also important

• This depends on the mixture characteristics and the way in which explosion is contained

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Now, the deflagration can raise pressure up to 8 times of its value, whereas, the detonation can raise pressure even more than this value. The rate of pressure rise which we call as dp by dt is also important to estimate the damage caused by dust or by gas. Now, the pressure raise depends on the mixture characteristics on the way in which explosion is contained.

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Design criteria

- Three conditions are required for fire or combustion explosion to occur
 - Presence of combustible or explosive material
 - Oxygen, to support the combustible reaction
 - Source of ignition to initiate the reaction
- Lack of any of the three conditions of the fire triangle shall make fire or combustion impossible
- Design criteria to prevent fire and explosion is
 - Prevent flammable mixture
 - Reduce ignition sources
 - Ensure inherent safer design (reduce inventories, substitute with less dangerous materials, reduce operating temperature and pressure)

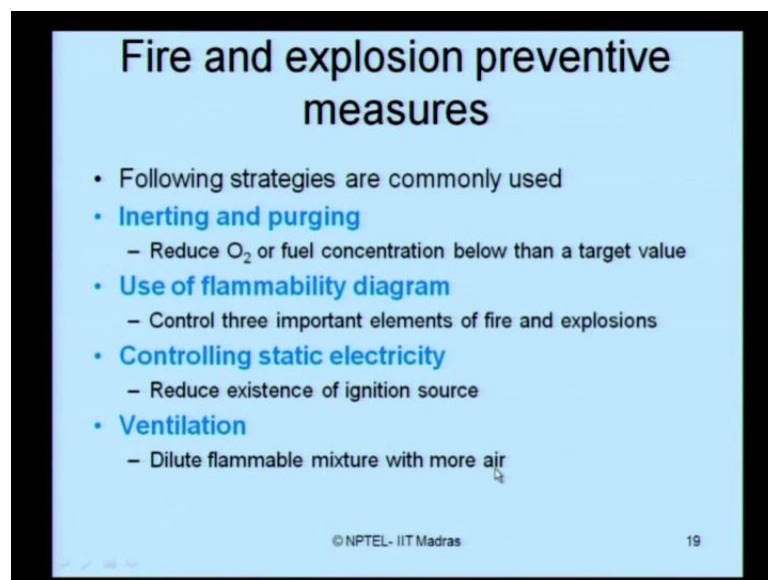
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If we look at the design criteria to control this kind of explosions, then three conditions actually are required for fire or combustion explosion to occur. Presence of combustible

or explosive material is mandatory; oxygen presence is also mandatory to support actually the combustible reaction, and of course, you need the source of ignition to initiate the reaction.

Now, is as simple as that if you really want to control any combustion explosion or fire then absence of any one of them will be helpful. Lack of any one of the three conditions given above in a fire triangle shall make the fire or combustion impossible; however, the design criteria to prevent fire and explosion is to prevent the flammable mixture or and to reduce ignition sources and to ensure inherent safer design; that is reduce the inventories present on board, substitute these inventories with less dangerous materials, reduce the operating temperature and pressure in your process plant.

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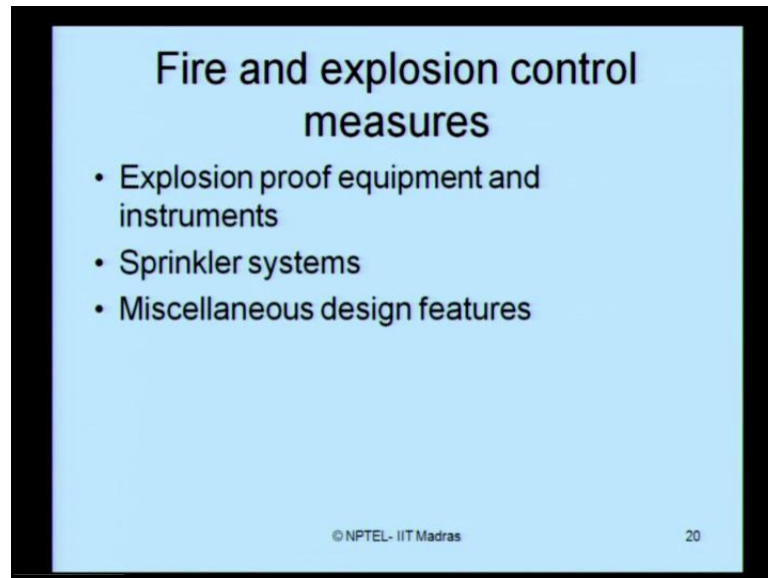
Fire and explosion preventive measures

- Following strategies are commonly used
- **Inerting and purging**
 - Reduce O₂ or fuel concentration below than a target value
- **Use of flammability diagram**
 - Control three important elements of fire and explosions
- **Controlling static electricity**
 - Reduce existence of ignition source
- **Ventilation**
 - Dilute flammable mixture with more air

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There are some preventive measures for fire and explosion. Let us see what are they. Following strategies are commonly used as preventive measures. The top in the list is what we call inerting and purging. Inerting and purging is actually a process where you reduce the oxygen or fuel concentration below than a target value. The next method to prevent fire and explosion is use the flammability diagram; on the other hand control three important elements of fire and explosion of the flammability diagram. The third concept, what we have as a preventive measure is that controlling static electricity in your process plant - reduce the existence of ignitions of source. Dilute the flammable mixture with more air we call this as ventilation method and so on.

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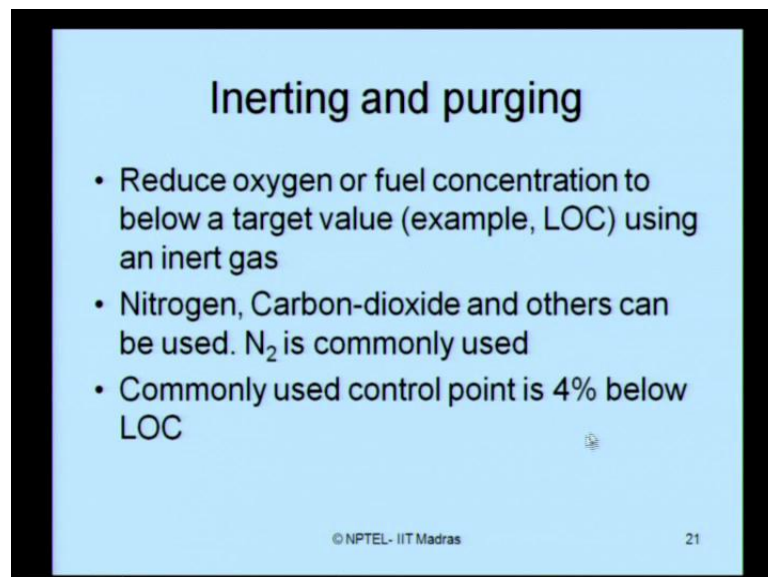
Fire and explosion control measures

- Explosion proof equipment and instruments
- Sprinkler systems
- Miscellaneous design features

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If you look at the fire and explosion control measures, you can also use explosion proof equipment and instruments. You can also use sprinkler systems and you can also use other miscellaneous designed features. Now, we will see these methods one by one in detail.

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Inerting and purging

- Reduce oxygen or fuel concentration to below a target value (example, LOC) using an inert gas
- Nitrogen, Carbon-dioxide and others can be used. N_2 is commonly used
- Commonly used control point is 4% below LOC

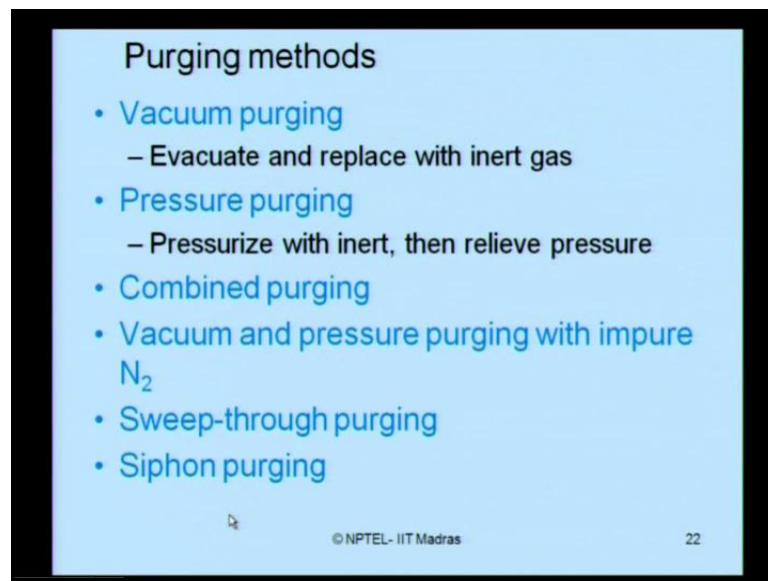
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Let us look at inerting and purging. Basically, our target is to reduce the scenario which can cause explosion or fire. Fire is possible only when the arms of the fire triangle are present in the situation. In this context, inerting or purging is actually a process where

you reduce oxygen or fuel concentration up to what level, to a level below a target value. Another question comes what is a target value? The target value, for example, could be a limiting oxygen concentration. You recollect the definition of limiting oxygen concentration, which we discuss in the previous slides or in the previous modules of this lecture.

We have said that, it is that minimum oxygen content required to cause fire or to cause combustion for a mixture. So, reduce your oxygen concentration or the fuel concentration below that specific target value. How do you do that? You can use an inert gas to reduce the oxygen concentration. What are the common kinds or type of inert gas being used for purging - nitrogen and carbon dioxide or most commonly used amongst this nitrogen is very popularly used for inerting and purging. The commonly used control point to add nitrogen to the system for inerting is about 4 percent below to the limiting oxygen concentration of the fuel.

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There are different purging methods which we can do. One is what we call as vacuum purging. You evacuate and replace it with the inert gas, for example, nitrogen. The other method is what we call as pressure purging pressurize, the vessel with an inert gas then relieve the pressure. The third method is what we call as combined purging So, combination of both vacuum and pressure purging. The fourth method is what we called as vacuum and pressure purging with impure nitrogen. The fifth method is what we call

as sweep-through purging. And the sixth and last method is what we call as siphon purging.

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Purge assumptions

- Purged pure Nitrogen
- Well-mixed conditions inside the vessel
 - It is a good assumption for gases
- Ideal gas law

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Now, we look at them in detail. Before we look at these purging models in detail; let us see what are those purge assumptions to be made before we model them. Purged pure nitrogen is being assumed well mixed condition inside the vessel is prevalent, that is the good assumptions for gases and ideal gas law is valid.

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Vacuum purging

- Most commonly used inerting procedure for vessels
- Procedure
 - Drawing vacuum on the vessel
 - Relieve the vacuum with inert gas
 - Repeat the cycle until desired concentration is reached

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Let us look at the vacuum purging. The figure below shows you the pressure variation with respect to time on a time scale. There are two pressure levels P H and P L. Let us see this process first. Most commonly used inerting procedure for vessels is vacuum purging. The procedure goes like this; you first draw the vacuum on the vessel. So, when you do that the pressure will drop from P H value to P L value. So, that there is a pressure drop, there is the pressure drop in the first cycle then relieve the vacuum with inert gas, once you do that again repeat this cycle for n number of times. Now, while you do this cycle, in all this cycles where you are drawing the vacuum on the vessel oxygen concentration is kept constant, and of course, the moles oxygen is also kept as constant in this process. Now, the concentration of the mixture keeps on varying for every cycle namely y naught for the initial cycle once you do one cycle of purging then becomes y 1. If you do the next cycle of purging the concentration becomes y 2. You keep on repeating the cycle until your concentration becomes to a desired value.

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- Initial oxidant concentration under vacuum (y_0) is the same as the initial concentration
- # of moles at initial high pressure (P_H) and initial low pressure (P_L) are computed using an initial equation of state, for an ideal gas behavior
- n_H and n_L are total moles in the atm and vacuum states, respectively
- # of moles for oxidants are calculated using Dalton's Law
- At the end of 1st cycle, new oxidant (lower) concentration is y_1 , where y_1 is the O_2 concentration after the first purge with N_2
- Similarly at the end of 2nd cycle, oxidant concentration is given by y_2 and so on.
- For i th cycle, $y_i = y_0 (P_L/P_H)^i$
- Total mass added to each cycle is constant. For i cycles, total N_2 gas moles is given by Δn_{N_2}

at A, $n_{\text{oxygen}} = y_0 \left[\frac{P_L V}{R_g T} \right]$
 at B, $n_{\text{total}} = \left[\frac{P_H V}{R_g T} \right]$
 $y_1 = \frac{n_{\text{oxygen}}}{n_{\text{total}}} = \frac{y_0 \left[\frac{P_L V}{R_g T} \right]}{\left[\frac{P_H V}{R_g T} \right]} = y_0 \frac{P_L}{P_H}$
 $y_2 = y_1 \frac{P_L}{P_H} = y_0 \frac{P_L}{P_H} \left[\frac{P_L}{P_H} \right] = y_0 \left[\frac{P_L}{P_H} \right]^2$
 $\Delta n_{N_2} = i(P_H - P_L) \frac{V}{R_g T}$

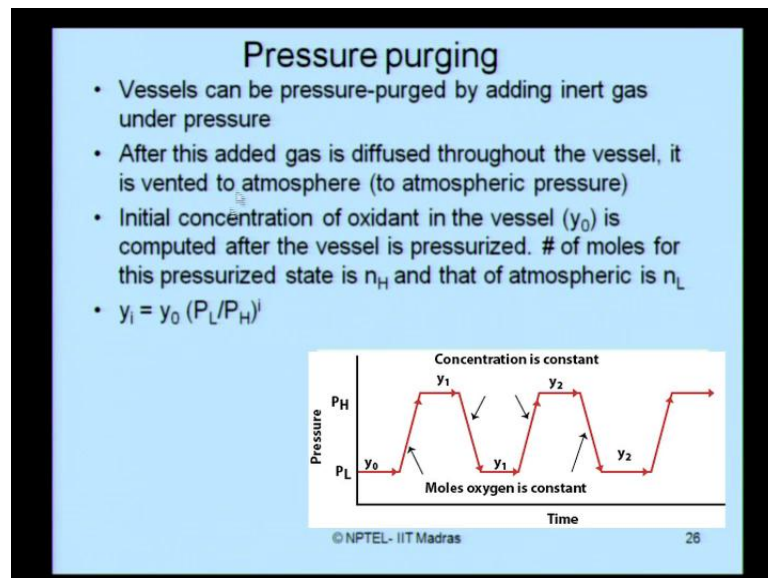
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Now, initial oxidant concentration under vacuum is what we called as y naught is same as the initial concentration which is present. At A arm, the number of moles at initial high pressure P H and the initial low pressure P L are computed using an initial equation of state, for an ideal gas behavior. In the equation, at A and B, n H and n L are the total moles in atmospheric and vacuum states respectively. The numbers of moles for oxidants are calculated using the Dalton's law.

At the end of the first cycle, the new oxidant concentration is y_1 . Then y_1 is given by this equation, which is the oxygen concentration after the first purging with nitrogen. Similarly, y_2 will be the concentration after the second purging with nitrogen. So, if you want to relate y_1 concentration or y_2 concentration with respect to the initial concentration what we say y_0 , then it gives you a simple relationship as you see on the slide now.

Similarly, at the end of second cycle, the oxidant concentration is given as y_2 . Similarly, if you keep on continuing then for an i th cycle then y_i is a concentration i th cycle is given by P_L by P_H raised to the power i multiplied by the initial concentration y_0 . You understand, P_L is actually the initial low pressure what you had in the problem and P_H is the initial i pressure what you are having in the problem. The total added mass to each cycle is constant therefore, for i cycles total nitrogen gas moles is given by a simple expression as you see from here which is P_H minus P_L v by $R g T$ of nitrogen.

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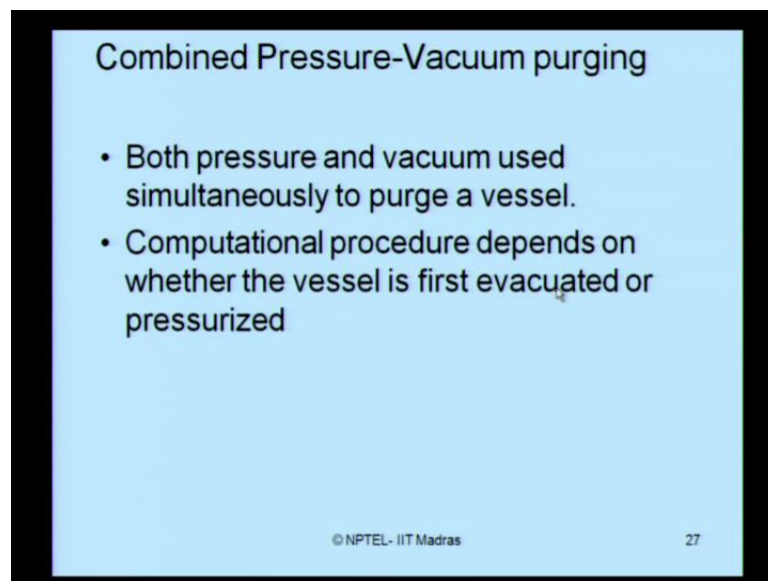


There is another method by which you can do purging - what we call as pressure purging. The first one, what we saw, is what we call as vacuum purging. So, you draw a vacuum from the vessel. So, the pressure is dropped from P_H to P_L ; obviously, in pressure purging it is a reverse process; from the low pressure you pump up the pressure to P_H value that is why the entry level of the pressure is P_L . In this problem, whereas a pressure is raised from P_L to P_H and y_0 is the entry level oxygen concentration; y_1 is the concentration after the first cycle; y_2 after the second cycle and so on. In all

these cycles, moles of oxygen present is taken as constant and the concentration is maintained at constant.

Vessels can also be pressure-purged by adding inert gas under a specific pressure into the vessel. After this is added, gas is diffused throughout the vessel, it is vented to atmospheric therefore the pressure will again drop back from the high pressure initiation to the atmospheric pressure, where again you will pressure-purge the gas into the vessel back to the second cycle of operation. The initial concentration of oxidant in the vessel, which I say as y_{naught} , is computed after the vessel is first pressurized. The number of moles for this pressurized state is n_H and that of atmospheric is n_L . And the concentration at y_i at i th cycle is given by the same expression what we saw in case of the previous case of purging which is inert purging.

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Combined Pressure-Vacuum purging

- Both pressure and vacuum used simultaneously to purge a vessel.
- Computational procedure depends on whether the vessel is first evacuated or pressurized

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We can now also do, what we call as combined pressure and vacuum purging. Both pressure and vacuum used simultaneously to purge a vessel. Now, the computational procedure depends on whether the vessel is first evacuated or pressurized.

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Pressurize first

- Beginning of the cycle is defined as the end of the initial pressurization
- Oxygen mole fraction at this point is the same as the initial mole fraction
- Remaining cycles are identical to the pressure purge operation
- If the initial oxygen mole fraction is 0.21, then the oxygen mole fraction at the end of this initial pressurization is given by:

$$y_0 = 0.21 \left[\frac{P_0}{P_H} \right]$$

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Let us see the first case as the vessel is first pressurized. If the vessel is first pressurized, beginning of the cycle is defined as the end of the initial pressurization. The oxygen mole fraction at this point is same as the initial mole fraction. The remaining cycles are identical to the pressure purge operation. If the initial oxygen mole fraction is 0.21, for example, then the oxygen mole fraction at the end of this initial pressurization is given by this relationship where y_0 is given as 0.21 of product of ratio of P_0 by P_H .

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- Let i be # of cycles after the initial pressurization
- For $(i+1)^{\text{th}}$ cycle,

$$y_i = y_0 \left[\frac{n_L}{n_H} \right]^i = y_0 \left[\frac{P_L}{P_H} \right]^i$$

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So, let i be the number of cycles after the initial pressurization; the p naught is where you are introducing the pressuring-purging operation; y naught becomes the concentration at that level and after the first cycle it becomes y_1 . And after the i th cycle, it becomes y_i , which is given by this equation at i plus one eth cycle y_i will be $y_{naught} n_L$ by n_H , which is given by y_{naught} of ratio of P_L by P_H raise to the power i and P_L and P_H values are known to me for the current operation.

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Evacuate first

- Beginning of the cycle is defined as the end of the initial evacuation
- Oxygen mole fraction at this point is the same as the initial mole fraction
- Remaining cycles are identical to the vacuum purge operation. For $i+1^{\text{th}}$ cycle,

$$y_i = y_0 \left[\frac{n_L}{n_H} \right]^i = y_0 \left[\frac{P_L^i}{P_H} \right]^i$$

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If you are evacuating the vessel first, before you do the pressure purging then in the beginning of the cycle is defined as the end of the initial evacuation. So, from the pressure p naught you evacuate it and bring the pressure to specific low level value then purge it and then bring the concentration to y naught and during this the concentration is kept constant and the moles oxygen is also kept constant in all the cycles. So, keep on doing this as long as your concentration becomes to the accepted value. The oxygen mole fraction at this point is the same as the initial mole fraction. The remaining cycles are identical that the vacuum purge operation, therefore for i plus one eth cycle the concentration is given by y naught ratio of P_L by P_H raised to the power i .

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Pressure and vacuum purging with impure purging

- For a pressure purging, total moles of oxygen at the end of first pressurization is given by the moles initially present plus the moles included with the nitrogen
- This is given by:

$$n_{\text{oxy}} = y_0 \left[\frac{P_L V}{R_g T} \right] + y_{\text{oxy}} (P_H - P_L) \left[\frac{V}{R_g T} \right]$$

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You can also do pressure and vacuum purging with impure purging that is you can use in impure nitrogen for this. For a pressure purging, the total moles of oxygen at the end of the first pressurization is given by the moles initially present plus the moles included with the nitrogen, which is given by this equation as seen in the slide just now. That the moles of oxygen present will be the initial value plus that you have includes along with what you added with nitrogen.

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• Mole fraction of oxygen at the end of the first cycle is given by:

$$y_1 = \frac{n_{oxy}}{n_{total}} = y_0 \left[\frac{P_L}{P_H} \right] + y_{oxy} \left[1 - \frac{P_L}{P_H} \right]$$

• Generalizing the equation, oxygen concentration at the end of i^{th} pressure cycle is given by:

$$y_i = y_{i-1} \left[\frac{P_L}{P_H} \right] + y_{oxy} \left[1 - \frac{P_L}{P_H} \right]$$
$$(y_i - y_{i-1}) = \left[\frac{P_L}{P_H} \right]^i (y_0 - y_{oxy})$$

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The mole fraction of oxygen at the end of the first cycle is given by this equation which has again got two components as you saw in the last slide. Now, when we keep on generalizing this equations for i eth cycle as well the oxygen concentration at the end of the i eth pressure cycle can be given by this equation which has again got two components as you saw in the previous slide.

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Comparison of pressure purging and vacuum purging

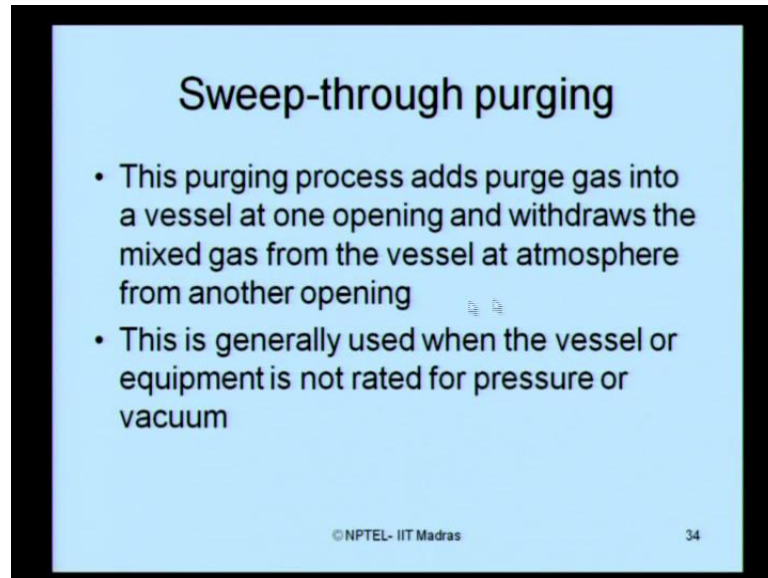
- Pressure purging is faster
 - Because pressure differentials are greater
- Pressure purging uses more inert gas than vacuum purging
- Vacuum purging uses less inert gas because oxygen concentration is reduced primarily by vacuum

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Now, if you want to compare the operation of pressure purging with that of vacuum purging then the pressure purging is faster it is because the pressure differentials are

much greater. Pressure purging uses more inert gas than the vacuum purging vacuum; purging uses less inert gas because the oxygen concentration is actually reduced primarily by vacuum in itself.

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Sweep-through purging

- This purging process adds purge gas into a vessel at one opening and withdraws the mixed gas from the vessel at atmosphere from another opening
- This is generally used when the vessel or equipment is not rated for pressure or vacuum

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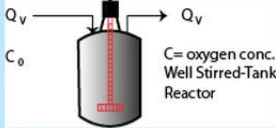
The other method of purging what we see in the literature is sweep-through purging. This purging process adds purge gas into a vessel at one opening and withdraws the mixed gas from the vessel at an atmospheric from another opening. This is generally used when the vessels or equipment is not rated for pressure or vacuum. Ladies and gentlemen, remember that if any vessel has got to be purged the vessel should be rated for that kind of pressure and vacuum purging operation. If you do not have a vessel of that kind, then sweep-through purging is what is being adopted in the industry. Where on one end the pure gas is added into the vessel for purging and on the other end there is a mixed gas is withdrawn to atmosphere from another opening.

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• Mass balance on oxygen is given by:

$$V \frac{dC}{dt} = C_0 Q_v - C Q_v$$

• Hence, volumetric quantity of inert gas required to reduce oxidant concentration from C_1 to C_2 is $Q_v t$ and is given by:

$$Q_v t = V \ln \left[\frac{C_1 - C_0}{C_2 - C_0} \right]$$


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So, I have got a pure gas entry and the withdrawal, the mass balance on oxygen is given by this equation as you see from here. Hence, the volumetric quantity of inert gas required to reduce the oxygen concentration from C_1 to C_2 is $Q_v t$ and is given by a simple relationship as you see here which is V into natural logarithm of $C_1 - C_0$ divided by $C_2 - C_0$ - where C_1 and C_2 are different oxidant concentrations which you want to reduce from C_1 to C_2 .

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Siphon purging

- The sweep-through purging requires large quantities of nitrogen
- This could be expensive when purging is done on a large storage vessel
- In such cases, siphon purging is done (reduces the expenses)
- Purging process starts by filling the vessel with liquid
 - May be water or other liquid

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The sweep-through purging actually requires large quantities of nitrogen; this could be expensive. When the purging is actually done for a large storage vessel, then what do we do in such cases? In large storage vessel, siphon purging is done basically to reduce the expenses, because the sweep through purging can be expensive due to large quantity of nitrogen being involved in that case. Then, the question comes what do you understand by siphon purging? Siphon purging is a process which starts by filling the vessel with liquid; this liquid can be water or any other liquid.

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Siphon purging

- Purged gas is subsequently added to the vapor space as liquid is drained from the vessel
- Volume of purge gas is equal to the volume of the vessel
- Rate of purging is equivalent to volumetric rate of liquid discharge from the vessel

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So, the purged gas is subsequently added to the vapor space as the liquid is drained of from the vessel. The volume of the purge gas is exactly equal to the volume of the vessel. And the rate of purging will be equivalent to the volumetric rate of liquid discharge from the vessel which you are doing siphon purging. So, this explains the different methods of purging as operation available for your problem. In the next class, we discuss about the different methods where we can use flammability diagrams for explosion control models.

Thank you.