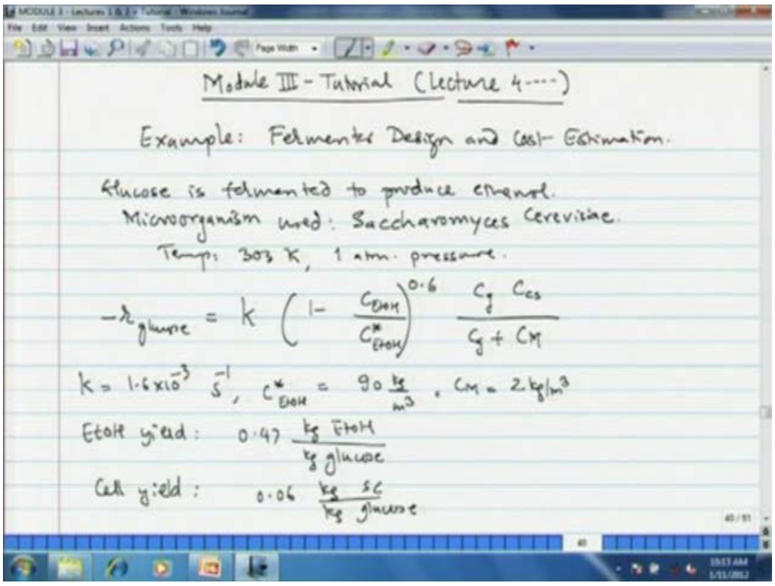
Process Design Decisions and Project Economics
Dr. V. S. Moholkar
Department of Chemical Engineering
Indian Institute of Technology, Gawahati

Module - 3
Reactor Design and Cost Estimation
Lecture - 16
Tutorial on Reactor Design and Cost Estimation

Welcome, we are now in module 3, the Reactor Design and Cost Estimation, and in the previous 3 lectures, we saw the various aspects of reactor design, the qualitative and quantitative treatments of various aspects. And in attend of last lecture, I had given you a problem of fermented design, that we have to solve in this lecture. And we shall also see another problem on a design of a fix bed reactor for methanol manufacture, for your convenience, now I repeat the problem statement briefly.

(Refer Slide Time: 00:57)



Module III - Tutorial (Lecture 4----)

Example: Fermenter Design and Cost Estimation.

Glucose is fermented to produce ethanol.
Microorganism used: Saccharomyces Cerevisiae.
Temp: 303 K, 1 atm. pressure.

$$-r_{glucose} = k\left(1-\frac{C_{EtOH}}{C^*_{EtOH}}\right)^{0.6}\frac{C_g\,C_{cs}}{C_g + C_M}$$

$k = 1.6\times10^{-3}\ s^{-1}$, $C^*_{EtOH} = 90\ \frac{kg}{m^3}$, $C_M = 2\ kg/m^3$

EtOH yield: $0.47\ \frac{kg\ EtOH}{kg\ glucose}$

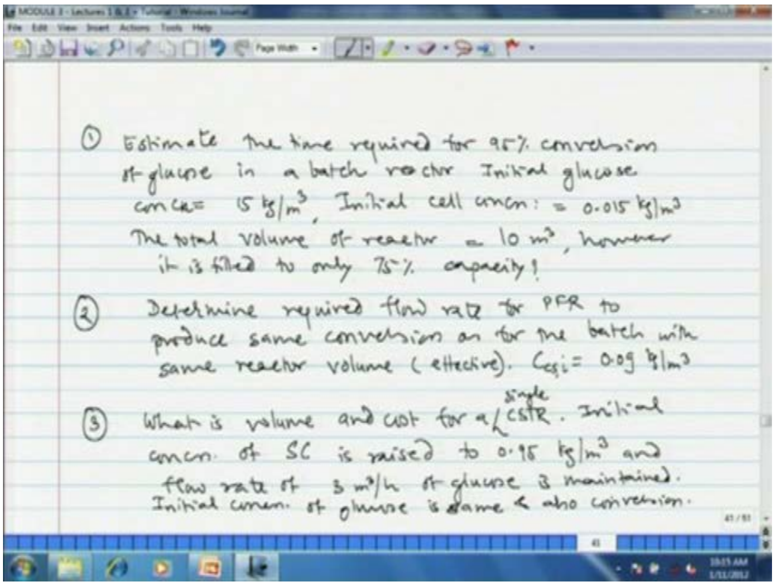
Cell yield: $0.06\ \frac{kg\ SC}{kg\ glucose}$

We have been given the reactor of fermentation, glucose fermentation to produce ethanol, the microorganism used is Saccharomyces cerevisiae, the temperature of the fermenter is 303 Kelvin at atmospheric pressure. The rate of glucose consumption has been given as K into 1 minus C ethanol by C star ethanol raise to 0.6. Now, this process is self inhibitory which means the ethanol that is formed in the process kills the bacteria.

And therefore, at certain concentration of ethanol, all the bacteria are killed and the ethanol, the glucose fermentation stops, that particular concentration, inhibitory concentration of ethanol C star has been given as 90 kg per meter cube. And then we have a simple monod kinetics K into 1 minus C ethanol by C star ethanol raise to 0.6 into C g, the concentration of glucose into C c s, the concentration of bacteria divided by C g plus C M, C M is the Michaelis menten constant.

Various values are given as K is equal to 1.6 into 10 to minus 3 second inverse, the inhibitory concentration, as I just said is 90 kg per meter cube, the Michaelis menten constant is 2 kg per meter cube. Ethanol yield has been given as 0.47 kg ethanol per kg glucose consumed and the cell yield is 0.06 kg Saccharomyces cerevisiae per kg glucose consumed. Cell yield means, basically the amount of cell that gets deactivated, work yield.

(Refer Slide Time: 02:47)



① Estimate the time required for 95% conversion of glucose in a batch reactor Initial glucose concn= 15 kg/m^3, Initial cell concn: = 0.015 kg/m^3 The total volume of reactor = 10 m^3, however it is filled to only 75% capacity!

② Determine required flow rate for PFR to produce same conversion as for the batch with same reactor volume (effective). C_{csi} = 0.09 kg/m^3

③ What is volume and cost for a single CSTR. Initial concn. of SC is raised to 0.95 kg/m^3 and flow rate of 3 m^3/h of glucose is maintained. Initial concn. of glucose is same & also conversion.

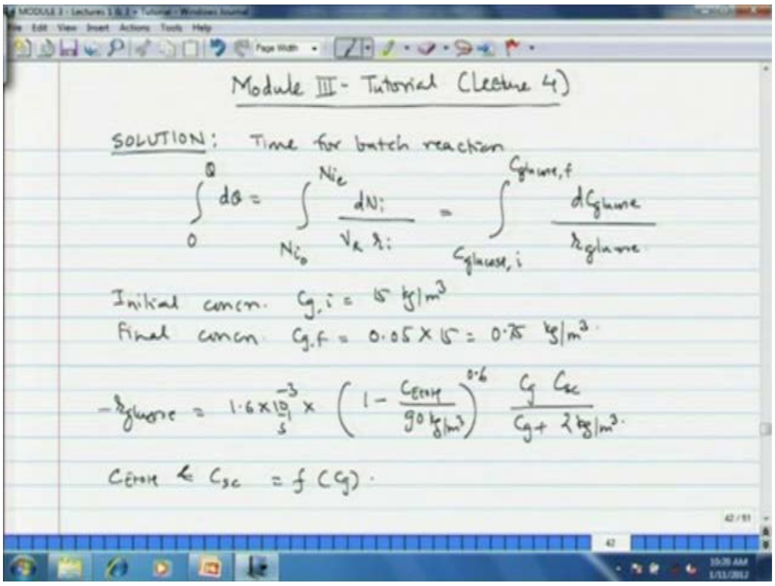
We have to answer 3 questions in this, first of all we have to estimate the time required for 95 percent conversion of glucose in a batch reactor, initial glucose concentration has been given as 15 kg per meter cube, initial cell concentration has been given as 0.015 kg per meter cube. The total volume of the reactor is 10 meter cube however, it is filled only to 75 percent of the capacity, so the total working volume is 7.5 meter cube.

In the second question, we have to determine the flow rate required for a PFR suppose, the batch reactor is converted into a PFR, then we have to estimate the flow rate in this

PFR to produce the same conversion, as for the batch reactor, and the same reactor volume effective. And then the concentration of the bacteria here however is larger, it is 0.09 kg per meter cube, the initial concentration.

And the third question is about converting the same PFR into a single CSTR, initial concentration is of bacteria, is further raised almost 10 times to 0.95 kg per meter cube. And the flow rate is maintained at 3 meter cube per hour of glucose and then initial concentration of glucose is same and also the conversion. So, we have to estimate here the volume and cost of this particular CSTR.

(Refer Slide Time: 04:12)



Module III - Tutorial (Lecture 4)

SOLUTION: Time for batch reaction

$$\int_0^{\theta} d\theta = \int_{N_{i_0}}^{N_{i_e}} \frac{dN_i}{V_R\, r_i} = \int_{C_{glucose,i}}^{C_{glucose,f}} \frac{dC_{glucose}}{r_{glucose}}$$

Initial concn. $C_{g,i} = 15\ kg/m^3$

Final concn. $C_{g,f} = 0.05 \times 15 = 0.75\ kg/m^3$

$$-r_{glucose} = 1.6 \times 10^{-3}\ s^{-1} \times \left(1 - \frac{C_{EtOH}}{90\ kg/m^3}\right)^{0.6} \frac{C_g\, C_{sc}}{C_g + 2\ kg/m^3}$$

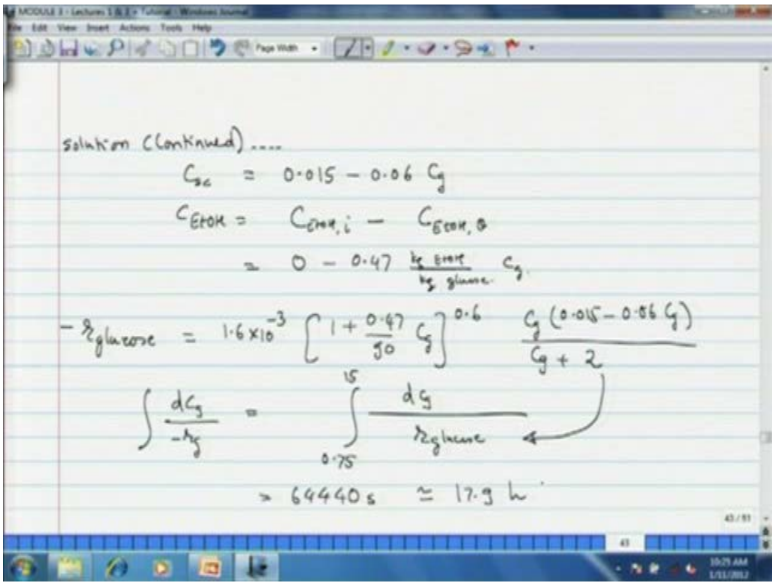
C_{EtOH} & C_{sc} $= f(C_g)$

Now, let us deal with each of this problem one by one, the first one batch reactor now, we have to estimate the time. The time for batch reaction is given as integral 0 to theta d theta where, theta is a time is equal to integral Ni naught to N i e, d N i divided by V R into r i. This is a rate expression, general rate expression for batch reactors that we had seen in the previous lecture, N i are the number of moles of the reacting species, 0 indicates the initial moles, e indicates at equilibrium, V R is the volume of the reactor.

Now, in the present situation, the volume of reactor is going to stay constant so we can convert the number of moles into concentration. Now here, the main reacting species is glucose so N i i is glucose so C glucose initial to C glucose final, d C glucose divided by r glucose, this is the rate expression. Now, we here onwards, we will indicate glucose concentration by C g and not glucose as a full word for gravity. We have been given that, the initial concentration C g i is equal to 15 kg per meter cube and we have to go for 95 percent.

So, the final concentration is 0.05 into 15 that is, 0.75 kg per meter cube, we have to evaluate this integral and we have a complicated expression. You have 2 options, either integrate in the form of a summation or integrate directly using some basic software like polymath or math cad, however we have to first write the integrant, the r glucose. If we substitute all values, k 1.6 into 10 to the power minus 3 into 1 minus C ethanol divided by 90 kg per meter cube. This unit, K unit is second inverse, this point kg has 90 kg per meter cube raise to 0.6 C g into C s c divided by C g plus the Michaelis menten constant 2 kg per meter cube. Now, we have to integrate this, we have to convert C ethanol and C saccharomyces cerevisiae, as a function of glucose concentration.

(Refer Slide Time: 07:31)



solution (Continued) ....

$$C_{sc} = 0.015 - 0.06\, C_g$$

$$C_{EtOH} = C_{EtOH,i} - C_{EtOH,0}$$

$$= 0 - 0.47\, \frac{\text{kg EtOH}}{\text{kg glucose}}\, C_g$$

$$-r_{glucose} = 1.6\times10^{-3}\left[1 + \frac{0.47}{90}\, C_g\right]^{0.6} \frac{C_g\,(0.015 - 0.06\, C_g)}{C_g + 2}$$

$$\int \frac{dC_g}{-r_g} = \int_{0.75}^{15} \frac{dg}{r_{glucose}}$$

$$= 64440\,s \simeq 17.9\,h$$

And for this purpose, we use the yield that has been given to us, the concentration of the cells reduces as ethanol forms and the reduction yields in terms of glucose. Initial concentration is 0.015 kg per meter cube minus the yield 0.06 C g into the concentration of glucose. Then similarly, C ethanol is initial C ethanol by ethanol per glucose yield into C g and this turns out to be 0.047 this is plus, initial plus the ethanol that forms into C g. And now, we substitute all these values in the expression, please make a correction here.

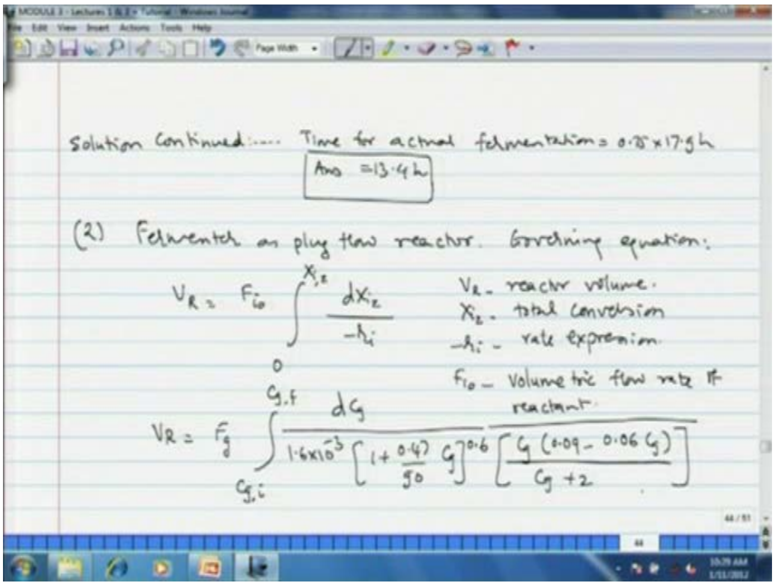
The concentration of ethanol, instantaneous concentration of ethanol C ETOH is the initial concentration minus the final concentration, all are instantaneous concentration at time theta. And then initial concentration is 0, the yield of ethanol per glucose fermented is 0.47 kg so 0.47 kg ethanol, per kg glucose now, volume is going to remain constant so we multiplied by C g, concentration of glucose.

And now, we substitute everything into the expression, r glucose is equal to or minus r glucose is equal to 1.6 into 10 to the power minus 3 into 1 plus 0.47 by 90 C glucose plus 2.6 into C glucose into 0.015 minus 0.06 C glucose divided by C glucose plus 2. And then putting this into the previous integral, integral d C g by r glucose with limits as, initial concentration 15 and final concentration 0.75.

Now, if we absorb this minus sign then the limits get exchanged so that we do here, we absorb the minus sign and exchanged limits d C g divided by r g, r glucose, which is this expression, substitute here. And then we can carry out this integral using any basic software like a math cad or math lab, and then we get the total time as 64440 seconds, which is equivalent to 17.9 hours this is how, we find out the time for fermentation.

However, this time is for the process, if the entire reactor was filled with glucose remember that, we are signed we absorbed in, if you see the previous integral, we had this V R and V R was absorbed as it is into for making out the concentration. However, we have been given that, only 75 percent of the volume of the reactor has been filled therefore, now that variation is linear. Therefore obviously, the time for fermentation is reduced by that much quantity.

(Refer Slide Time: 12:07)



Solution Continued:.... Time for actual fermentation = 0.75 × 17.9 h

$$\boxed{\text{Ans } = 13.4 \text{ h}}$$

(2) Fermenter as plug flow reactor. Governing equation:

$$V_R = F_{i0} \int_0^{X_{i,t}} \frac{dX_{it}}{-r_i}$$

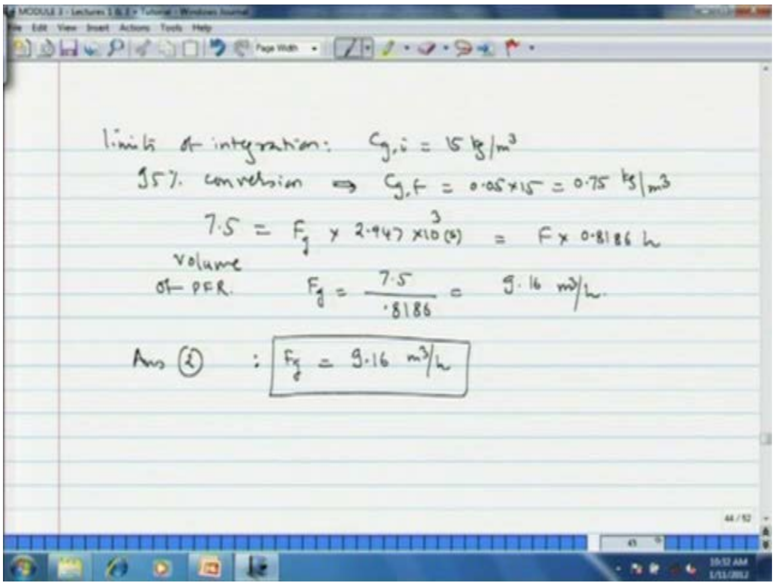
V_R - reactor volume.
X_{it} - total conversion
$-r_i$ - rate expression.
F_{i0} - Volumetric flow rate of reactant.

$$V_R = F_g \int_{C_{g,i}}^{C_{g,f}} \frac{dC_g}{1.6\times10^{-3}\left[1+\frac{0.47}{90}C_g\right]^{0.6}\left[\frac{C_g\,(0.09-0.06\,C_g)}{C_g+2}\right]}$$

So, the time for actual fermentation is 0.75 into 17.9 hours that is equal to 13.4 hours so this is the answer to the first question, the time required for 95 percent of conversion of the glucose for those conditions, that we stated earlier so this is the answer to the first question. Now, second question is about the PFR, fermenter as plug flow reactor now, here again we do the same thing, the governing equation for plug flow reactor is V R, is equal to F i naught integral 0 to X i z d X i z divided by minus r i.

Now, notations are V R, the reactor volume then X i z, the conversion total conversion obtained, minus r i is the rate expression and F i naught is the volumetric flow rate of the reactant. Now, again volume is going to remain constant so what we do is that, we convert this conversion in terms of concentration V R is equal to F g. Because, here the flow rate is that of glucose C g i to C g F, initial concentration of glucose to final concentration d C g divided by 1.6 into 10 to the power of minus 3. Exactly same thing, but with slight modification of the concentration of the microorganism. So, this is the volume, that we get in the form of integral, now the limits remain the same.

(Refer Slide Time: 15:16)



limits of integration: $C_{g,i} = 15\ \text{kg/m}^3$

95% conversion $\Rightarrow$ $C_{g,f} = 0.05 \times 15 = 0.75\ \text{kg/m}^3$

$7.5 = F_g \times 2.947 \times 10^{3}$ (s) $= F \times 0.8186\ \text{h}$

volume of PFR.

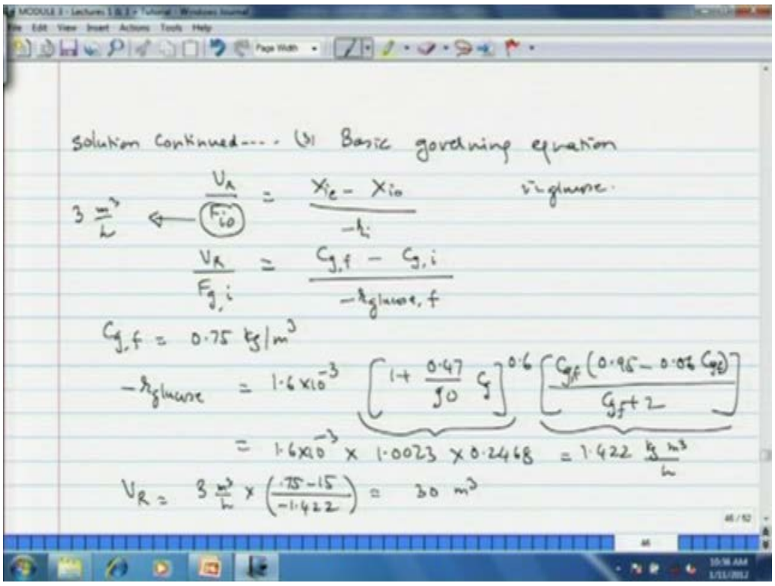
$F_g = \dfrac{7.5}{.8186} = 9.16\ \text{m}^3/\text{h}$.

Ans ② : $\boxed{F_g = 9.16\ \text{m}^3/\text{h}}$

We have been given that, the concentration of glucose is same as, that for the batch reactor 15 kg per meter cube and conversion is also same 95 percent conversion. So, the final concentration is 0.05 into 15 that is, 0.75 kg per meter cube so again you can perform the integral integration using any basic software. This particular integral, you can performing any basic software and then you can find the answer as 7.5, the volume of PFR.

Remember, that we have been given the volume of PFR in this case, we have to find out the flow rate now, 10 meter cube was the volume of the batch reactor but the reactor was filled only to 75 percent of the volume. So, the working volume was 7.5, we have to find flow rate for PFR, which has same volume as that in case of batch. So, we do not take the 10 meter cube total volume of the batch reactor but the 7.5 meter cube working volume, that becomes the left hand side of the integral. That, F glucose and the integral is 2.947 into 10 to power 3, this is what you get and then this seconds and you convert it into hours. So, F into 0.8186 hours and F g then become 7.5 divided by 0.8186 or 9.16 meter cube per hour. So, the answer to second question, the flow rate of glucose in a PFR is 9.16 meter cube per hour.

(Refer Slide Time: 17:51)



solution Continued.... (3) Basic governing equation

$$3\,\frac{m^3}{h} \longleftarrow \boxed{F_{i0}} \qquad \frac{V_R}{F_{i0}} = \frac{X_{ie} - X_{i0}}{-r_i} \qquad i = \text{glucose}$$

$$\frac{V_R}{F_{g,i}} = \frac{C_{g,f} - C_{g,i}}{-r_{glucose,f}}$$

$$C_{g,f} = 0.75\ kg/m^3$$

$$-r_{glucose} = 1.6\times10^{-3}\ \underbrace{\left[1 + \frac{0.47}{50}C_g\right]^{0.6}}\ \underbrace{\left[\frac{C_{gf}(0.95 - 0.06\,C_{gf})}{C_{gf}+2}\right]}$$

$$= 1.6\times10^{-3} \times 1.0023 \times 0.2468 = 1.422\ \frac{kg\ m^3}{h}$$

$$V_R = 3\,\frac{m^3}{h} \times \left(\frac{.75 - 15}{-1.422}\right) = 30\ m^3$$

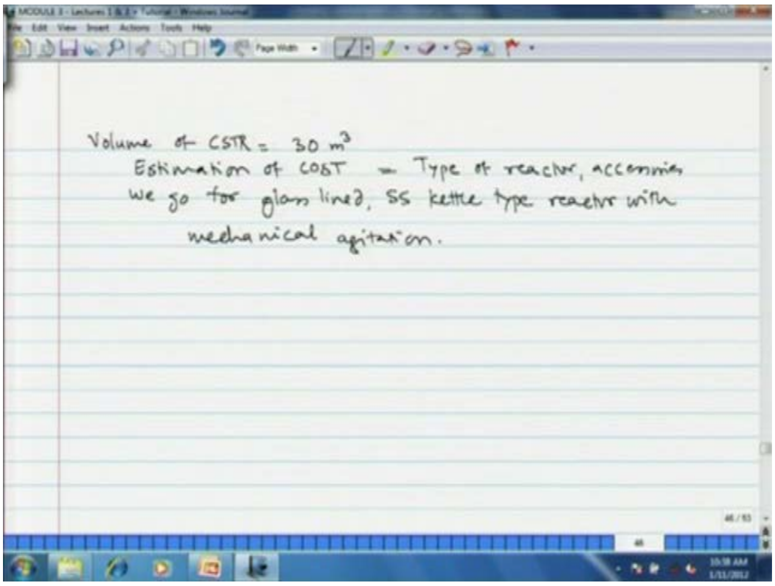
Now the third question, in third question we have 2 problems, first is to find out the volume of the CSTR and then we have to find out the cost. So, we first go for the volume now here, again we take the basic governing equation V R by F i naught is equal to X i e, the equilibrium conversion minus X i naught, the conversion at time 0 divided by rate of constant.

And now, i is essentially glucose so replacing i by g, V R volume of the reactor divided by F g initial into C g here, equilibrium is the final concentration, initial is C g i divided by minus r glucose. Now here, we have to estimate the rate of glucose conversion on the basis of final concentration remember, in CSTR everything is mixed. So, we can estimate the rate of reaction inside the reactor based on the outlet concentration of the glucose because everything is mixed, so concentration is uniform.

So here, we estimate the rate of glucose conversion on the basis of final concentration of glucose, now we know that C g f final concentration of glucose is 0.75 kg per meter cube and then we substitute all the values. Remember here that, the concentration of the microbes, the saccharomyces cerevisiae has been raised 10 times 0.95 kg per meter cube so minus r glucose is 1.6 into 10 to the power minus 3, 1 plus 0.47 divided by 90 into C g raise to 0.6 again, C g into 0.95 minus 0.06 C g divided by C g plus 2.

And then here we do not have to perform any integration, we have to simply substitute C g F at here and then calculate. So, this particular bracket is evaluated as 1.0023, this particular is integrated as 0.2468 and then we get the rate of glucose conversion as 1.422 kg meter cube per hour. Now, we have to calculate V R, now to calculate V R, we have to know F i naught, the flow rate of glucose into the reactor, that has been given to us as 3 meter cube per hour. So, 3 meter cube per hour into the final minus initial, so 0.75 minus 15 divided by now, minus r i because minus r i, so we absorb the sign here, minus 1.422. And then the V R transferred to be 30 meter cube, so we have answered the first bit of this particular.

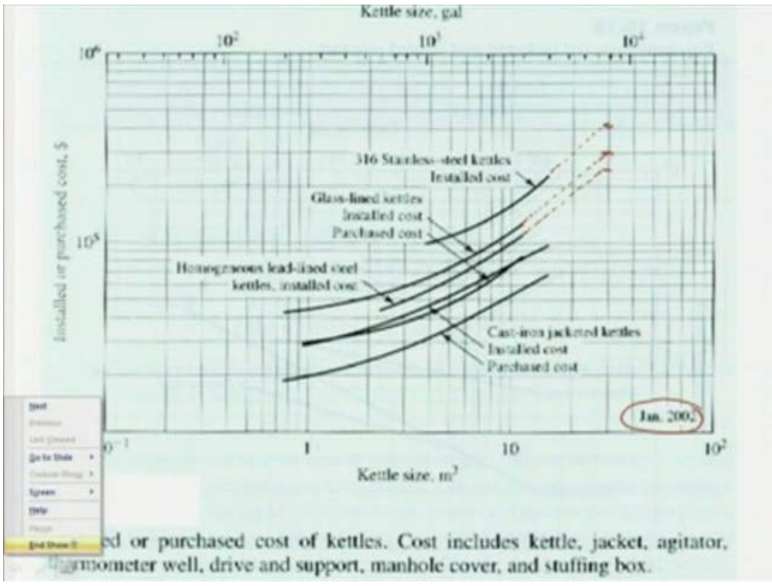
(Refer Slide Time: 22:29)



Volume of CSTR = $30\ m^3$
Estimation of COST — Type of reactor, accessories
we go for glass lined, SS kettle type reactor with
mechanical agitation.

Now, the next task is to estimate the cost now, before we do that, we have to select the type of reactor and accessories. Now, since we are carrying out fermentation, we have to go either for a stainless steel reactor or a carbon steel reactor with some lining for prevention of the erosion let us say, like glass lined. Then it has to be a jacketed reactor to control the temperature and it should have sufficient mechanical agitation. So, that point we note here, we go for glass lined SS kettle type reactor with mechanical agitation now, we have been given the cost correlations.

(Refer Slide Time: 23:55)

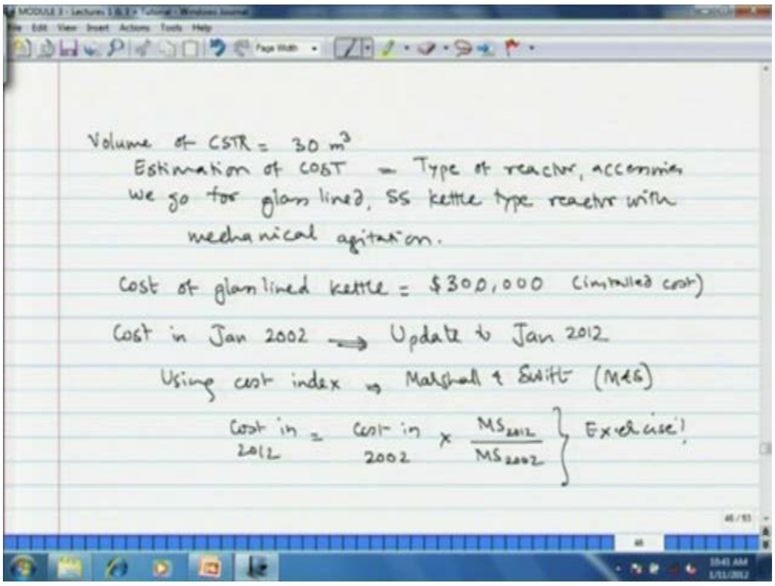


ed or purchased cost of kettles. Cost includes kettle, jacket, agitator, rmometer well, drive and support, manhole cover, and stuffing box.

To estimate the cost, we have to see the cost correlation, several sources of this correlations are available, what you see on the screen now, is the cost correlation for kettles. The cost includes the jacket, the agitator, thermometer well, drive, support and also the manhole cover and stuffing box. Now, various types of reactors are available, we go for the glass lined reactor and then 30 meter cube of volume, so we have to extend this particular line to 30 meter cube 10, 20, 30, so typically this.

So here, we get the cost as approximately 200 thousand dollars, this is the installed cost now, if this cost is not available, is not affordable then we can choose different metal for construction. And then let us say, the 316 stainless steel kettles, here is the cost of the glass lined reactor 200 thousand dollars or 300 thousand dollars, that I just mentioned or if you find this as not suitable then you can go for 316 stainless steel or even the regular stainless steel, lead lined stainless steel. Cost will be little be less but anyway you are not going to get below 200 to 250 thousand dollars. So, that point you note, remember again, this is the cost correlation made in January 2002, we have to update the cost information.

(Refer Slide Time: 25:52)



Volume of CSTR = 30 m^3

Estimation of COST → Type of reactor, accessories

we go for glass lined, SS kettle type reactor with mechanical agitation.

Cost of glass lined kettle = $300,000 (installed cost)

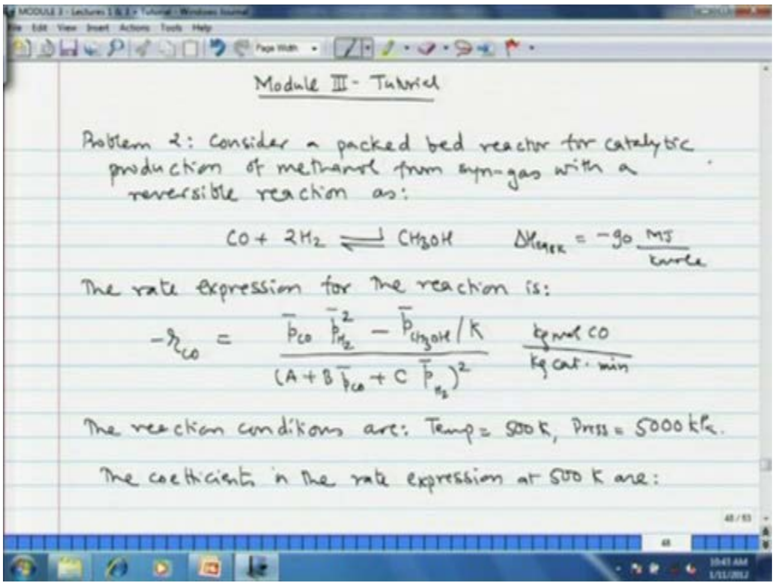
Cost in Jan 2002 $\Longrightarrow$ Update to Jan 2012

Using cost index ⇒ Marshall & Swift (M&S)

$$\text{Cost in } 2012 = \text{Cost in } 2002 \times \frac{MS_{2012}}{MS_{2002}} \Bigg\} \text{ Exercise!}$$

Cost of glass lined kettle is dollar 300 thousand, installed cost in January 2002 is this, we have to update to January 2012 or this we can do using cost indexes such as, Marshall and Swift index, that we denote as M and S. So, the cost in 2012 is essentially cost in 2002 into Marshall and Swift index at 2012 divided by Marshall and Swift index at 2002. Now, this particular thing is rather easy, I will leave it as an exercise for you, you look into the various sources websites as well as a regular journals like journal chemical engineering published by institution of chemical engineers. Now, Marshall and Swift indices are published regularly in these journals, find out the Marshall and Swift index at 2002, 2012, take a ratio and update this cost, this is left as an exercise for you. So, this completes our problem on fermentation now, we have to go for the next problem.

(Refer Slide Time: 27:49)



Module III - Tutorial

Problem 2: Consider a packed bed reactor for catalytic production of methanol from syn-gas with a reversible reaction as:

$$CO + 2H_2 \rightleftharpoons CH_3OH \qquad \Delta H_{498K} = -90 \frac{MJ}{kmole}$$

The rate expression for the reaction is:

$$-r_{CO} = \frac{\bar{p}_{CO}\,\bar{p}_{H_2}^2 - \bar{p}_{CH_3OH}/K}{(A + B\,\bar{p}_{CO} + C\,\bar{p}_{H_2})^2} \quad \frac{kmol\ CO}{kg\ cat \cdot min}$$

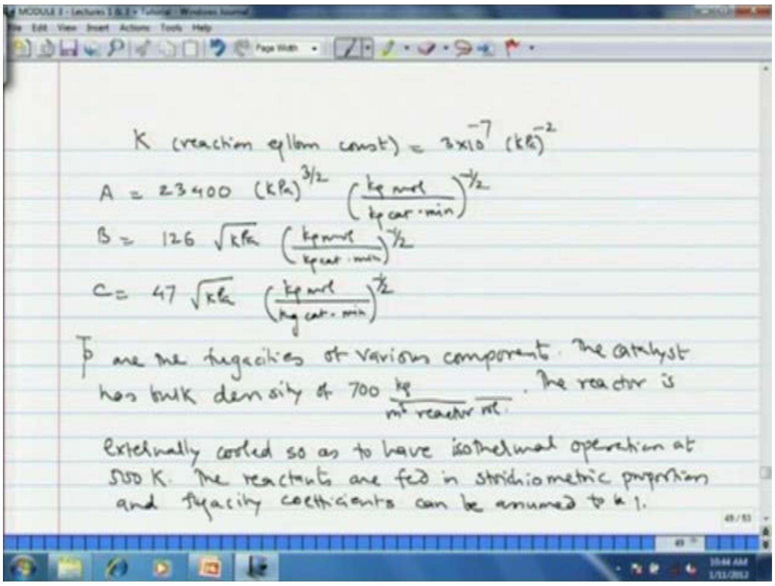
The reaction conditions are: Temp = 500 K, Press = 5000 kPa.

The coefficients in the rate expression at 500 K are:

That is, problem on methanol synthesis in a fixed bed reactor, what you see on screen now is the problem definition. Consider a packed bed reactor for catalytic production of methanol from synthesis gas with a reversible reaction as Co plus 2 H 2 gives CH 3 OH. The reaction is highly exothermic, 90 kilo joules or 90 mega joules per kilo mole heat released, the rate expression is in the form of a Lumber Mitchell Wood kinetics.

Partial pressure of Co, p bar Co into partial pressure of H 2 square minus partial pressure of CH 3 OH divided by K, divided by this particular thing, A plus B partial pressure Co, C partial pressure H 2. Now, partial pressure is applicable only in the case of ideal gas now, the behavior may deviate from ideal gas so we can say fugacities here so or p, p bar are the fugacities of different components. The rate expression is kg moles Co per kg catalyst per minute, the reaction conditions are quite harsh, temperature of 500 Kelvin, pressure of 5000 kilo Pascal or 5 mega Pascal, the coefficient in the rate expression at 500 Kelvin are this A, B, C.

(Refer Slide Time: 29:18)



K (reaction eqllbm const) = $3\times10^{-7}\ (\text{kPa})^{-2}$

$A = 23400\ (\text{kPa})^{3/2}\left(\frac{\text{kg mol}}{\text{kg cat}\cdot\text{min}}\right)^{-1/2}$

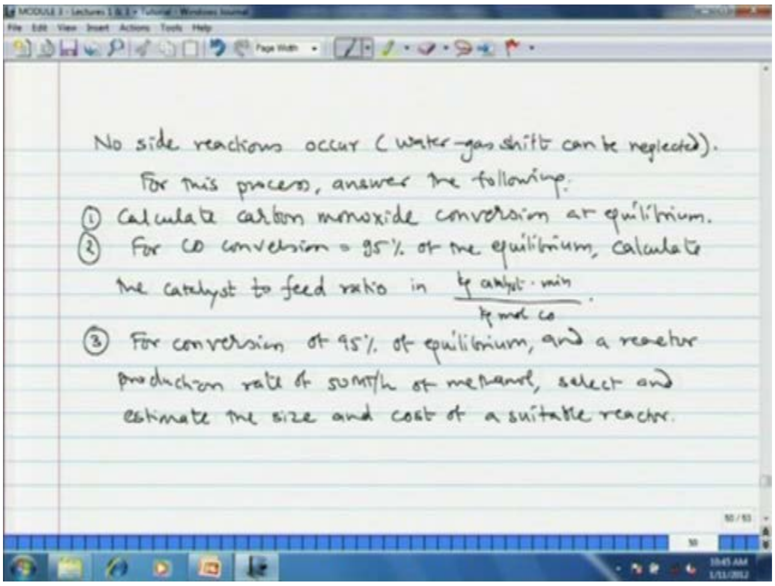
$B = 126\ \sqrt{\text{kPa}}\left(\frac{\text{kg mol}}{\text{kg cat}\cdot\text{min}}\right)^{-1/2}$

$C = 47\ \sqrt{\text{kPa}}\left(\frac{\text{kg mol}}{\text{kg cat}\cdot\text{min}}\right)^{-1/2}$

$\bar{p}$ are the fugacities of various component. The catalyst has bulk density of 700 $\frac{\text{kg}}{\text{m}^3\ \text{reactor vol}}$. The reactor is externally cooled so as to have isothermal operation at 500 K. The reactants are fed in stoichiometric proportion and fugacity coefficients can be assumed to be 1.

K is the equilibrium constant, 3 into 10 to power minus 7 kilo Pascal raise to minus 2, A is 23400 kilo Pascal raise to 3 by 2, into kg mole per kg catalyst per minute raise to minus half, the unit remains the same for other three. For B, the value is 126 unit is root K P a into kg mole divided by K g catalyst per minute raise to minus half, C is 47 root K P a kg mole per kg catalyst per minute raise to minus half. The catalyst has bulk density of 700 kg per meter cube of reactor volume, the reactor is externally cooled so as to, have the isothermal operation at 500 Kelvin. And the reactants are fed in stoichiometric proportion, the fugacity coefficients can be assumed to be 1.

(Refer Slide Time: 30:16)



No side reactions occur (water-gas shift can be neglected).

For this process, answer the following.

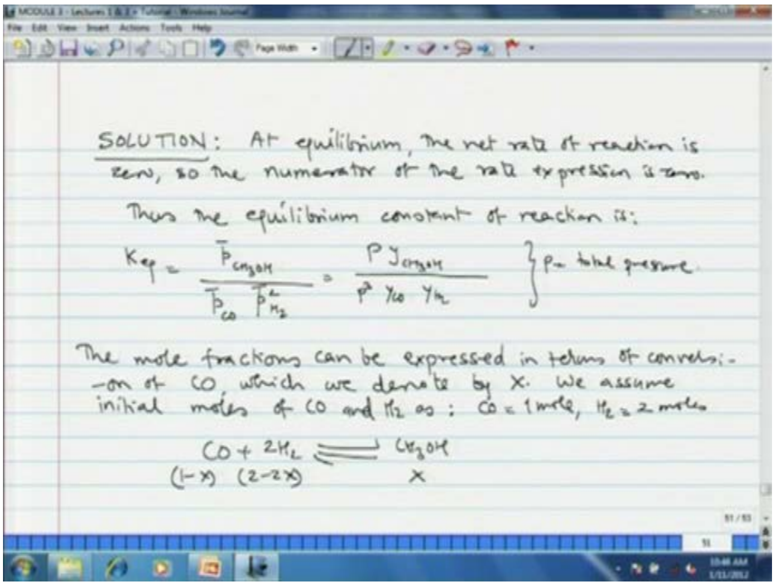
① Calculate carbon monoxide conversion at equilibrium.

② For CO conversion = 95% of the equilibrium, calculate the catalyst to feed ratio in $\frac{\text{kg catalyst}\cdot\text{min}}{\text{kg mol CO}}$.

③ For conversion of 95% of equilibrium, and a reactor production rate of 50 MT/h of methanol, select and estimate the size and cost of a suitable reactor.

Now, we ignore the side reactions in this case, we assume no side reaction occur whatever shift reaction is the possible side reaction but we assume it to be negligible. And then again we have to answer 3 bits here, 3 questions, first calculate the carbon monoxide conversion at equilibrium, second for carbon monoxide conversion equal to 95 percent of the equilibrium. Calculate kettles to feed ratio in kg catalyst per minute per kg moles Co or kg catalyst per kg mole Co per minute. And then third for conversion of 95 percent of the equilibrium and a reactor production rate of 50 metric tons per hour of methanol, select and estimate the size and cost of a suitable reactor.

(Refer Slide Time: 31:08)



SOLUTION: At equilibrium, the net rate of reaction is zero, so the numerator of the rate expression is zero.

Thus the equilibrium constant of reaction is:

$$K_{eq} = \frac{\bar{p}_{CH_3OH}}{\bar{p}_{CO}\,\bar{p}^2_{H_2}} = \frac{P\,y_{CH_3OH}}{P^3\,y_{CO}\,y_{H_2}} \Big\}\ P = \text{total pressure.}$$

The mole fractions can be expressed in terms of conversi--on of CO, which we denote by X. We assume initial moles of CO and H_2 as : CO = 1 mole, H_2 = 2 moles

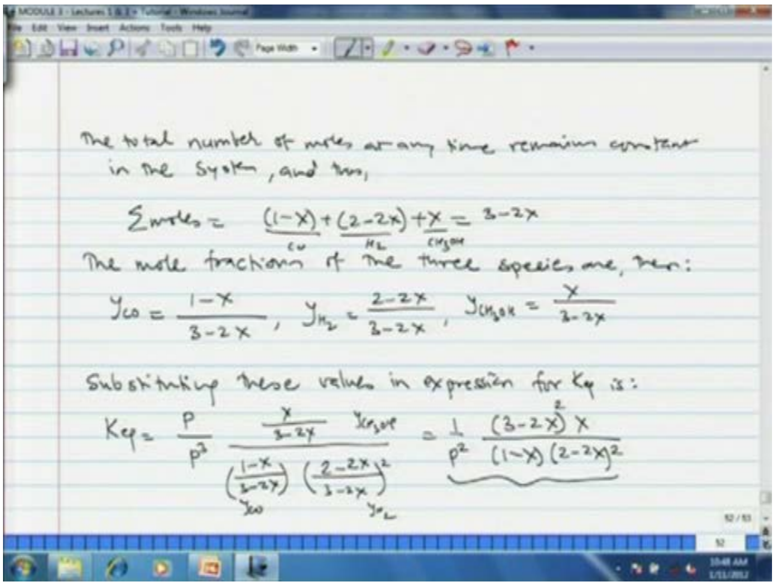
$$\begin{array}{cccc} CO & + & 2H_2 & \rightleftharpoons & CH_3OH \\ (1-X) & & (2-2X) & & X \end{array}$$

So, 3 questions, we take the first one that is the calculating the equilibrium conversion of methanol now at equilibrium, the net rate of reaction is 0. Therefore, the numerator of the rate expression, that we saw should be 0 and if you do that. Then, we can immediately calculate the K equilibrium, equilibrium constant of the reaction, as fugacity of methanol divided by fugacity of carbon monoxide into fugacity of hydrogen that is, 2.

We have been given fugacity coefficient equal to 1 so we can directly convert the fugacity in terms of mole fractions, the fugacity is equal to the total pressure P of the reactor into Y CH 3 OH, the mole fraction of methanol, then for the denominator p cube into Y mole fraction of carbon monoxide, Y mole fraction of hydrogen. The mole fraction now, we have to estimate, these can be expressed in terms of conversion of Co, which is the mean or the reference reactant, which we denote by X.

Now, the conversion of carbon monoxide is X so if we assume, that the initial moles of carbon monoxide and hydrogen are 1 is to 2. Because, we have been given that, the synthesis gas mixture is fed in stoichiometric proportion, there is nothing excess of any component. Co H 2 is 1 is to 2 so Co after conversion of X moles, the moles of Co that remain is 1 minus X then similarly, for H 2, 2 minus X and CH 3 OH, X. Now, since this is a equilibrium limited reaction, the total moles remain constant at any time.

(Refer Slide Time: 32:58)



The total number of moles at any time remains constant in the system, and thus,

$$\Sigma \text{moles} = \underbrace{(1-X)}_{CO} + \underbrace{(2-2X)}_{H_2} + \underbrace{X}_{CH_3OH} = 3-2X$$

The mole fractions of the three species are, then:

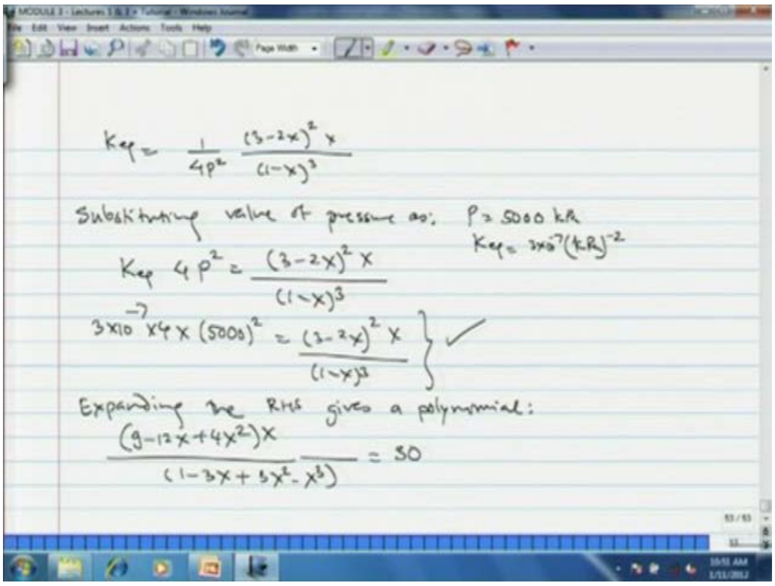
$$y_{CO} = \frac{1-X}{3-2X}, \quad y_{H_2} = \frac{2-2X}{3-2X}, \quad y_{CH_3OH} = \frac{X}{3-2X}$$

Substituting these values in expression for Keq is:

$$K_{eq} = \frac{P}{P^3} \frac{\overset{y_{CH_3OH}}{\frac{X}{3-2X}}}{\underset{y_{CO}}{\left(\frac{1-X}{3-2X}\right)} \underset{y_{H_2}}{\left(\frac{2-2X}{3-2X}\right)^2}} = \underbrace{\frac{1}{P^2} \frac{(3-2X)^2 X}{(1-X)(2-2X)^2}}$$

So, the total moles in the system are 1 minus X plus 2 minus 2 X plus X, carbon monoxide, hydrogen, methanol that is, 3 minus 2 X. And then the mole fraction of the 3 species is Y Co, 1 minus X divided by total moles Y H 2, 2 minus 2 X divided by total moles Y CH 3 OH, X divided by total moles. And now, we substitute these mole fractions into the expression for equilibrium K eq, equilibrium is equal to P divided by P cube into mole fraction of a methanol, X divided by 3 minus 2 X into mole fraction of a carbon monoxide and mole fraction of hydrogen. And then we get this particular expression, K equilibrium equal to 1 divided by P square into 3 minus 2 X into X divided by 1 minus X into 2 minus 2 X square and now, we substitute various values.

(Refer Slide Time: 34:36)



$$K_{eq} = \frac{1}{4P^2}\frac{(3-2x)^2 x}{(1-x)^3}$$

Substituting value of pressure as: $P = 5000\ kPa$

$K_{eq} = 3\times10^{-7}(kPa)^{-2}$

$$K_{eq}\, 4P^2 = \frac{(3-2x)^2 x}{(1-x)^3}$$

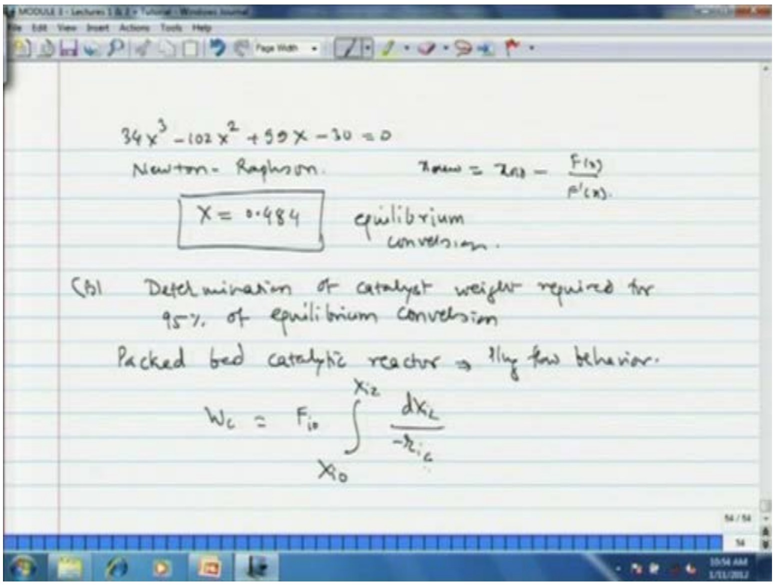
$$3\times10^{-7}\times 4\times(5000)^2 = \frac{(3-2x)^2 x}{(1-x)^3}\Bigg\} \checkmark$$

Expanding the RHS gives a polynomial:

$$\frac{(9-12x+4x^2)x}{(1-3x+3x^2-x^3)} = 30$$

Here, we have been given the total pressure as 5000 kilo Pascal, 5 mega pascal, K equilibrium as 3 into 10 to the power of minus 7 Pascal raise to minus 2. After substituting everything and simplifying, we find that, we get actually a polynomial K after expansion so that polynomial I will give you.

(Refer Slide Time: 35:09)



$$34x^3 - 102x^2 + 99x - 30 = 0$$

Newton-Raphson. $x_{new} = x_{old} - \frac{F(x)}{F'(x)}$

$$\boxed{X = 0.484}$$ equilibrium conversion.

(b) Determination of catalyst weight required for 95% of equilibrium conversion

Packed bed catalytic reactor ⇒ Plug flow behavior.

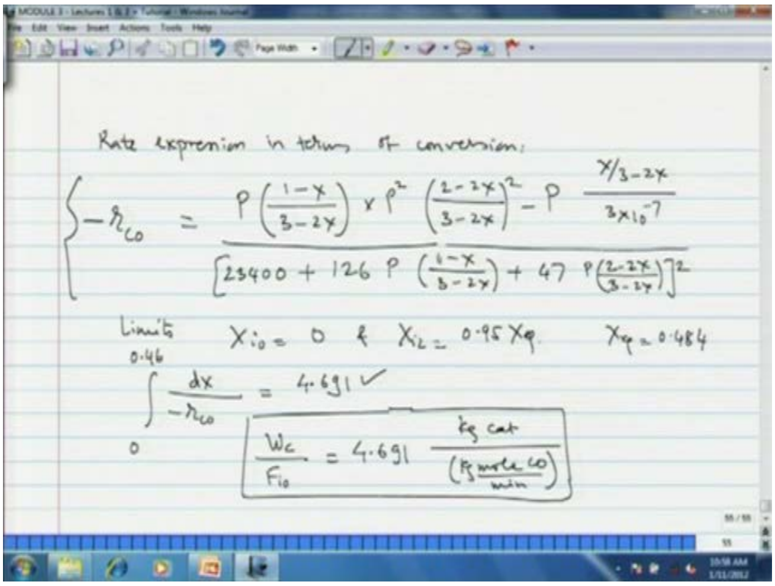
$$W_c = F_{i0}\int_{X_0}^{X_i} \frac{dX_i}{-r_{i_c}}$$

The polynomial that you get after expansion of this particular quantity is, I am going to give you now, 34 X cube minus 102 X square plus 99 X minus 30 is equal to 0. Now, this we have to solve to get the answer of X now, this we can solve using simple

Newton- Raphson technique. And then X new is equal to X old minus F x divided by F dash x, this is the simple formula, you put in any sub routine of math cad or math lab.

And then you can find out X is equal to 0.484, so that is the equilibrium conversion of methanol for given condition. So, that is answer to the first question but the second question is about the determination of the catalyst rate required for 90 percent of this conversion or 95 percent of conversion. Now, the general formula for a catalytic reactor, we have been given a pack bed reactor, the rate expression is in terms of kg catalyst. So, we can assume a plug flow reactor, plug flow behavior however, since the rate expression is in terms of weight of catalyst, we write instead of volume, the weight of catalyst is equal to F i naught to X i naught into X i z divided by d X i z divided by minus r i C, the rate expression with respect to catalyst.

(Refer Slide Time: 37:42)



Rate expression in terms of conversion:

$$-r_{CO} = \frac{P\left(\frac{1-X}{3-2X}\right) \times P^2 \left(\frac{2-2X}{3-2X}\right)^2 - P\,\frac{X/3-2X}{3\times10^{-7}}}{\left[23400 + 126\,P\left(\frac{1-X}{3-2X}\right) + 47\,P\left(\frac{2-2X}{3-2X}\right)\right]^2}$$

Limits $X_{i0} = 0$ & $X_{i} = 0.95\,X_{eq}$ $\quad X_{eq} = 0.484$

$$\int_0^{0.46} \frac{dx}{-r_{CO}} = 4.691 \checkmark$$

$$\boxed{\frac{W_c}{F_{i0}} = 4.691\ \frac{\text{kg cat}}{\left(\text{kg}\frac{\text{mole CO}}{\text{min}}\right)}}$$

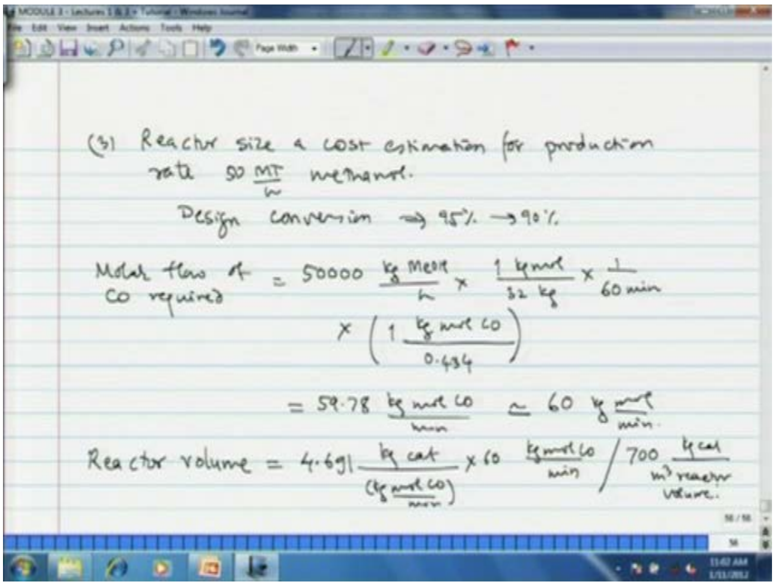
We have to calculate the rate expression in terms of conversion, while we use the same values as before of mole fraction. We have been given fugacity coefficient to be 1 so the fugacity can be converted into total pressure into mole fraction. Now, I am going to directly give that answer using the same mole fraction as before, carbon monoxide 1 minus X divided by 3 minus 2 X into hydrogen fugacity P square, total pressure square 3 minus 2 X square minus the equilibrium X divided by 3 minus 2 X divided by the equilibrium constant 3 into 10 to the power minus 7.

And the whole expression divided by the constant A plus B into P Co, fugacity of a Co that we write, plus 47 into fugacity of hydrogen and whole thing squared. And now, the limits of integration are X i naught equal to 0 and X i z equal to 0.95 of X equilibrium, x equilibrium we have just estimated as 0.484, This is a complicated expression of rate, again I suggest you to use simple softwares.

You go for numerical integration, I will directly give you the value of the integral now depending on the sub routine that you use or the software that you use, your own integral may differ slightly numerically but that depends on the tolerance values that you have used. So, my answer is 4.691, the integral here, we approximate as 0.46, it comes 0.4598 and then what I got is 4.691, the value of the integral.

And then what we have is W c divided by F i naught is equal to 4.691, the catalyst weight required per molar flow rate of carbon monoxide, this is kg catalyst divided by kg mole Co divided per minute. This is the answer to the second question remember, we still have not calculated the value of the molar flow rate of the carbon monoxide, that depends on the total production rate of methanol.

(Refer Slide Time: 41:26)



(3) Reactor size & cost estimation for production rate 50 $\frac{MT}{h}$ methanol.

Design conversion $\Rightarrow$ 95% $\rightarrow$ 90%

Molar flow of CO required $= 50000 \frac{\text{kg MeOH}}{h} \times \frac{1 \text{ kgmol}}{32 \text{ kg}} \times \frac{1}{60 \text{ min}}$

$\times \left(1 \frac{\text{kg mol CO}}{0.434} \right)$

$= 59.78 \frac{\text{kg mol CO}}{\text{min}} \simeq 60 \text{ kg} \frac{\text{mol}}{\text{min}}$.

Reactor volume $= 4.691 \frac{\text{kg cat}}{\left(\text{kg} \frac{\text{mol CO}}{\text{min}}\right)} \times 60 \frac{\text{kgmol CO}}{\text{min}} \Big/ 700 \frac{\text{kg cat}}{\text{m}^3 \text{ reactor volume}}$.

We will move to the third bit of the problem that is, reactor size and cost estimation for production rate of 50 metric ton per hour of methanol. Now, the stoichiometry is 1, 1 mole of methanol is produced per mole of Co converted however, all of the Co is not converted. So, we have to take into account, the equilibrium conversion or let us say, the

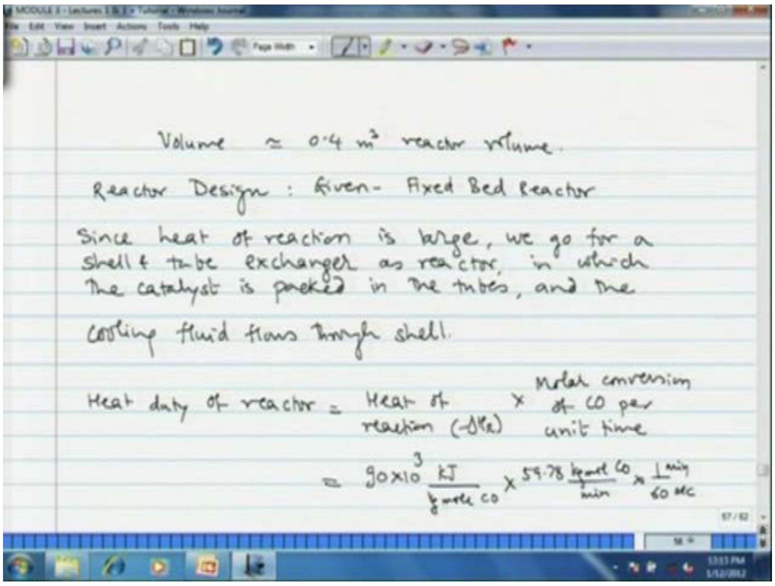
95 percent equilibrium conversion, maybe we can assume a little bit less let us say, 90 percent to make sure that, our reactor operates.

So, we design that point, we note here design conversion, we shift from 95 percent to 90 percent just to make sure, that our reactor operates, 95 percent is very close to equilibrium. The molar flow rate of Co required would be 50000 kg methanol per hour into or we convert this kg into molar production by dividing the molecular weight 32 kg of methanol.

And then we have been given the rate in terms of minute, so we convert hour into minute, the hourly production to minute production and then as I said, that not all of the Co gets converted. So, we take this 90 percent conversion 0.434, 90 percent of 0.484 or 485, that we estimated as equilibrium conversion. This turns out to be something like 59.78 kg mole Co per minute, which you can further approximate as 60 kg mole per minute.

You have to estimated reactor volume, we have just estimated the catalyst weight, that we need per mole of Co reacted. So, the reactor volume can be estimated on the basis of, catalyst weight that we need, divided by the packing density of the catalyst, that has been given to us as 700 meter cube kg per meter cube. 4.691 kg catalyst per kg mole Co per minute into 60 kg mole Co per minute, divided by 700 kg catalyst per meter cube reactor volume remember, this is not the actual density of the catalyst, this is the packing density of catalyst.

(Refer Slide Time: 44:14)



Volume $\simeq$ 0.4 m^3 reactor volume.

Reactor Design : Given - Fixed Bed Reactor

Since heat of reaction is large, we go for a shell & tube exchanger as reactor, in which the catalyst is packed in the tubes, and the cooling fluid flows through shell.

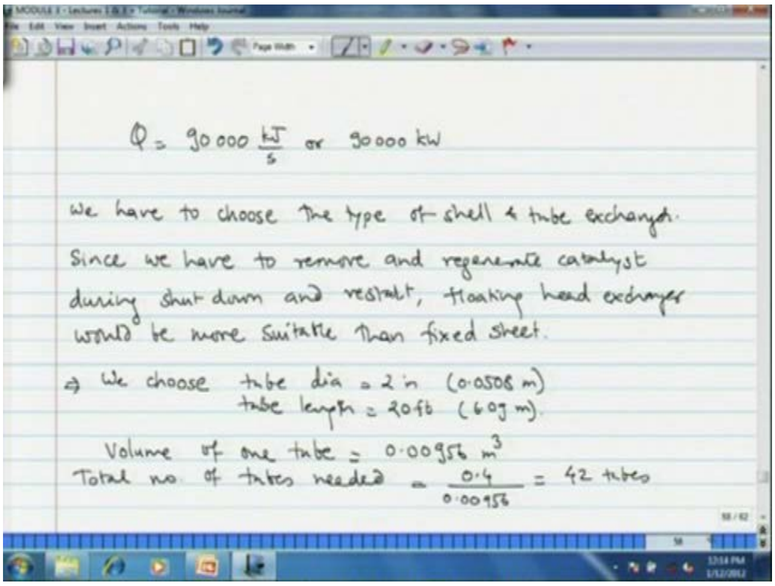
Heat duty of reactor = Heat of reaction ($-\Delta H_R$) × Molar conversion of CO per unit time

$$= 90 \times 10^3 \frac{kJ}{kmole\ CO} \times 59.78 \frac{kmol\ CO}{min} \times \frac{1\ min}{60\ sec}$$

So, this turns out to be, the volume is equal to approximately 0.4 meter cube reactor volume. After calculating the reaction volume, we have to design the reactor, we are given that the reactor is a fixed bed reactor. Since the heat of reaction is quite high, something like 90 kilo joules per mole of Co have to go for a salient tube heat exchanger as a reactor, in which the catalyst will be packed in the tubes and the cooling fluid will flow through the shell.

The heat duty of the reactor we have to first calculate, the heat of reaction into the molar conversion of Co per unit time. We have rate constant in minute but the heat transfer coefficient will be in kilo watt so we convert that flow rate into per second flow rate. So, 59.78 kg mole Co per minute divided by 60 second into 90 into 10 to the power 3 kilo joules per kg mole Co.

(Refer Slide Time: 45:15)



$Q = 90000 \frac{kJ}{s}$ or 90000 kW

We have to choose the type of shell & tube exchanger.

Since we have to remove and regenerate catalyst during shut down and restart, floating head exchanger would be more suitable than fixed sheet.

⇒ We choose tube dia = 2 in (0.0508 m)
tube length = 20 ft (6.09 m).

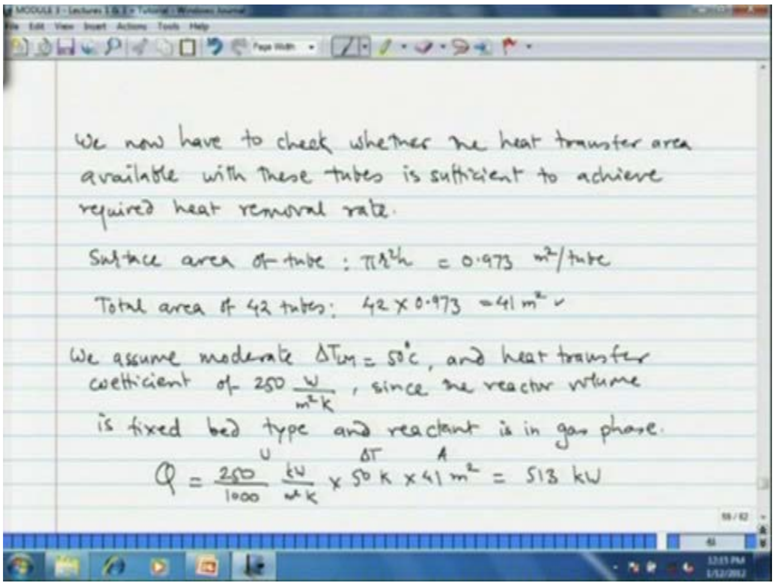
Volume of one tube = $0.00956 \ m^3$

Total no. of tubes needed $= \frac{0.4}{0.00956} = 42$ tubes

So, that gives us the total heat of reaction as 90000 kilo joules per second or 90 megawatt, we have to choose the type of salient tube heat exchanger. We have 2 options, first floating head and fixed tube sheet type of reactor. We have to remove and regenerate a catalyst during shut down and restart, so floating head heat exchanger would be more suitable than the fixed sheet. Therefore, we go for that particular design floating head exchanger now, we have to choose the tube diameter and the tube length.

We choose 2 inch diameter of the tubes so as to, have sufficient flow velocity as well as heat transfer rate and the tube length we choose as 20 feet, depending on the typical sizes of the reactor, that are available. The volume of 1 tube will be 0.00956 meter cube so the total number of tubes, that will be needed for making up the 0.4 meter cube reaction volume will be 0.4 divided by 0.00956 that is equal to 42 tubes.

(Refer Slide Time: 46:25)



We now have to check whether the heat transfer area available with these tubes is sufficient to achieve required heat removal rate.

Surface area of tube : $\pi r^2 h = 0.973\ m^2/\text{tube}$

Total area of 42 tubes: $42 \times 0.973 = 41\ m^2$ ✓

We assume moderate $\Delta T_{lm} = 50^\circ C$, and heat transfer coefficient of $250\ \frac{W}{m^2 K}$, since the reactor volume is fixed bed type and reactant is in gas phase.

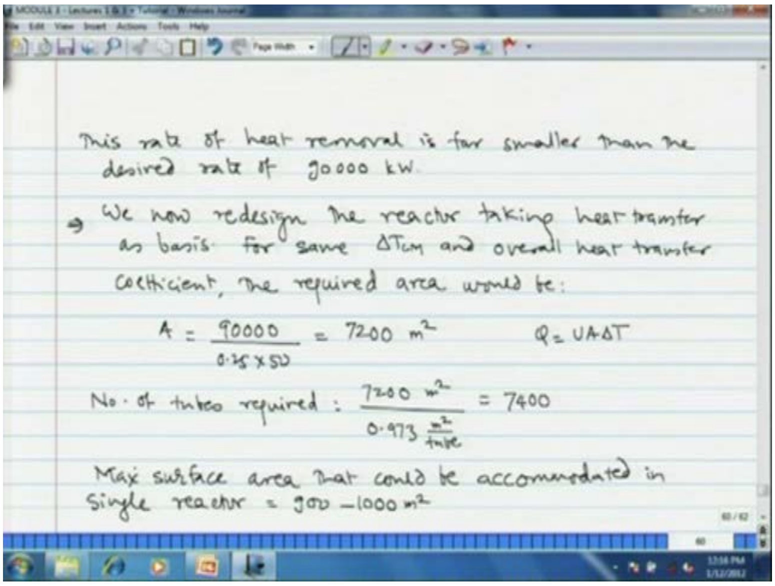
$$Q = \overset{U}{\frac{250}{1000}\ \frac{kW}{m^2 K}} \times \overset{\Delta T}{50\ K} \times \overset{A}{41\ m^2} = 513\ kW$$

Now we have to see, whether the area that is available in these 42 tubes is sufficient to achieve the required heat removal rate of 90000 kilo watt or 90 megawatt. The surface area of the tube can be estimated by standard pi r square h formula and it turns out to be 0.97 meter square per tube. So, the total area of 42 tubes is 42 into 0.973 that is, 41 meter square, we have to assume delta T, delta t log mean in the reactor, that we take typical value as 50 degree centigrade.

And we take the heat transfer coefficient, order of magnitude as 250 watt per meter square per Kelvin this is, because the reactor volume is fixed by time and the reactant is in gas phase. So, we are not likely to achieve very high heat transfer rates there so we have taken a moderate overall heat transfer coefficient of 250 watt per meter square Kelvin.

So, the heat removal rate, that will be achieved Q will be 250 into 50 into 41 U A delta T, Q is equal to U A delta T and then the heat removal rate that can maximum heat removal rate, that could be achieved is 513 kilo watt. Now, this is far smaller than 90000 kilo watt that we want, therefore this design is not feasible now what we do is that, we take heat transfer as basis.

(Refer Slide Time: 47:53)



This rate of heat removal is far smaller than the desired rate of 90000 kW.

⇒ We now redesign the reactor taking heat transfer as basis. For same ΔT_{lm} and overall heat transfer coefficient, the required area would be:

$$A = \frac{90000}{0.25 \times 50} = 7200 \text{ m}^2 \qquad Q = UA\Delta T$$

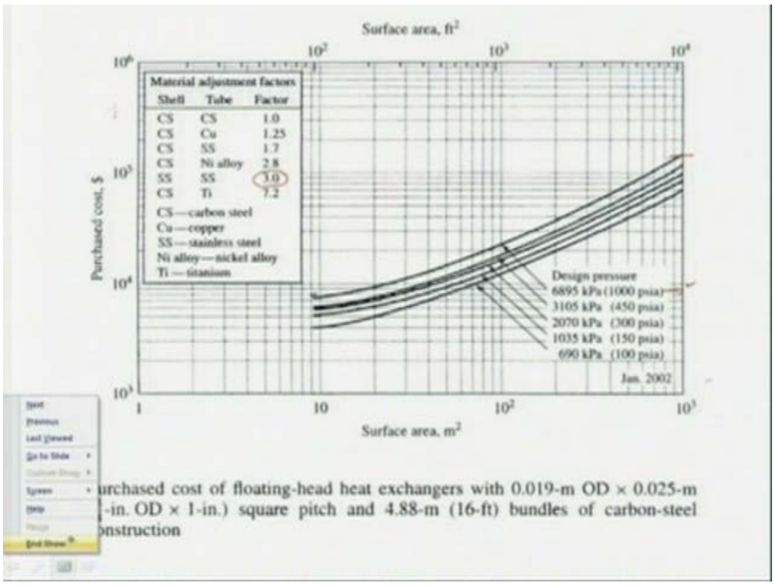
$$\text{No. of tubes required} : \frac{7200 \text{ m}^2}{0.973 \frac{\text{m}^2}{\text{tube}}} = 7400$$

Max surface area that could be accommodated in single reactor = 900 – 1000 m^2

And then redesign the reactor with the same delta T log mean and over all heat transfer coefficient. To achieve 90000 kilo watt heat removal rate, the heat exchanger area that will be required, again using the same formula Q is equal to U A delta T will be area equal to 90000 divided by 0.25 kilowatt, the heat transfer coefficient into 50 so 7200 meter square.

Now, with area of 1 tube as 0.97 meter square per tube now, we keep the dimensions of the tube constant. Because, those have been chosen on the basis of hydro dynamics so the number of total tubes will be required will be 7400. Now, we have a limitation, that maximum surface area that can be accommodated in a single salient heat exchanger with certain dimension like reasonable dimension, is about 900 to 1000 meter square. We take the lower limit 900 meter square therefore to have 7200 meter square total area, we need 8 reactors in parallel, so that is about the design. So, we have floating head and the tube of 2 inch, tube length 20 feet and 8 reactors. Now, we have to go for cost estimation, we have been given cost correlations of floating head heat exchanger.

(Refer Slide Time: 49:16)



Material adjustment factors

Shell	Tube	Factor
CS	CS	1.0
CS	Cu	1.25
CS	SS	1.7
CS	Ni alloy	2.8
SS	SS	3.0
CS	Ti	7.2

CS—carbon steel
Cu—copper
SS—stainless steel
Ni alloy—nickel alloy
Ti—titanium

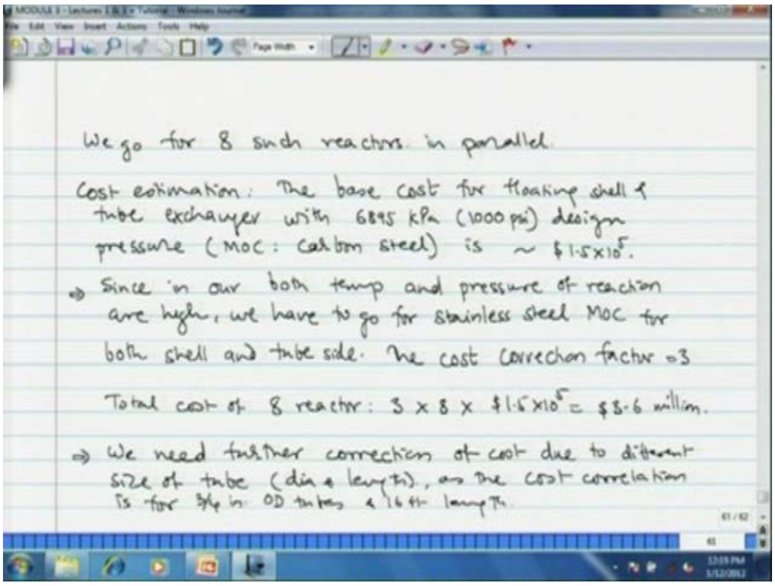
urchased cost of floating-head heat exchangers with 0.019-m OD × 0.025-m -in. OD × 1-in.) square pitch and 4.88-m (16-ft) bundles of carbon-steel onstruction

Now here, the diameter of the tube is 0.025 meter, 1 inch diameter, a square pitch and 16 feet bundle of carbon steel construction. And now, you can see here that, if you take 900 meter square as area then the typical cost, that can be achieved or that is possible is about let us say, 1.5 into 10 to power 5 dollars so this is the purchase cost. Now, another factor is the design pressure, our reaction occurs at 5000 kilo Pascal so we have to choose the design pressure, higher than that 6895 kilo Pascal, we choose the design pressure.

And then for that particular design pressure and 900 meter square area, we get the purchase cost as approximately 1.5 or 105 thousand dollars. But remember, these are for 1 inch diameter and 16 feet bundle of tubes of carbon steel construction. Now, we have quite harsh reaction conditions, we have the temperature of about 500 Kelvin and pressure of 5000 kilo Pascal so carbon steel may not be a suitable material.

So, we have to go for stainless steel, both stainless steel shell and stainless steel tubes therefore, we have to apply correction factor of 3 here. The cost has to be increased by factor of 3, that is a correction factor for the material of construction. Further more, we have to apply correction factor for the diameter as well as length but that, we shall see later.

(Refer Slide Time: 51:02)



We go for 8 such reactors in parallel.

Cost estimation: The base cost for floating shell & tube exchanger with 6895 kPa (1000 psi) design pressure (MOC: carbon steel) is ~ $1.5×10^5.

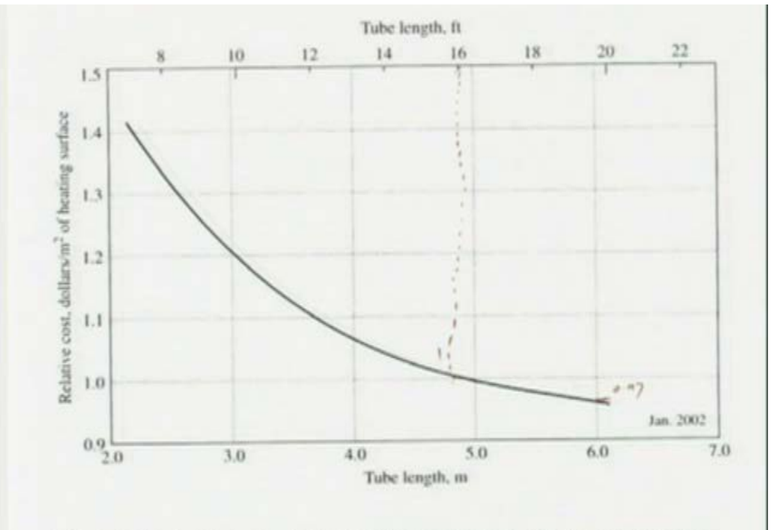
⇒ Since in our both temp and pressure of reaction are high, we have to go for stainless steel MOC for both shell and tube side. The cost correction factor = 3

Total cost of 8 reactor: 3 × 8 × $1.5×10^5 = $3.6 million.

⇒ We need further correction of cost due to different size of tube (dia & length), as the cost correlation is for 3/4 in. OD tubes & 16 ft length.

So, the total cost of 8 reactors after correction for material of construction will be 3 into 8 into 150 thousand dollars so something like 3.6 million dollars.

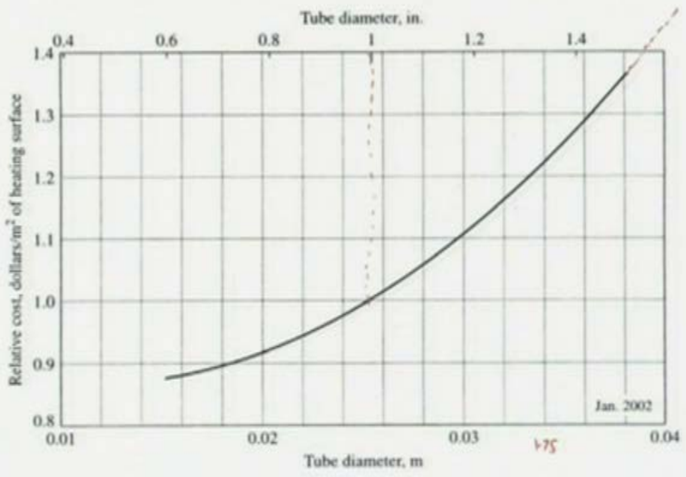
(Refer Slide Time: 51:19)



Effect of tube length on cost of conventional shell-and-tube heat exchangers

Now, we go for the additional correction factors, correction factor for the tube length and correction factor for the diameter. Now, that tube length, which was there in the correlation was 16 feet, our is 20 feet, so we have to choose that particular correction values 16 feet. These are the correction factors and then we have to take a ratio here, we get approximately 1 and here 0.97 for 20 feet, here 0.9 and 1, in between we can say 0.97, this is 1 so that is the ratio of correction factors for the tube length.

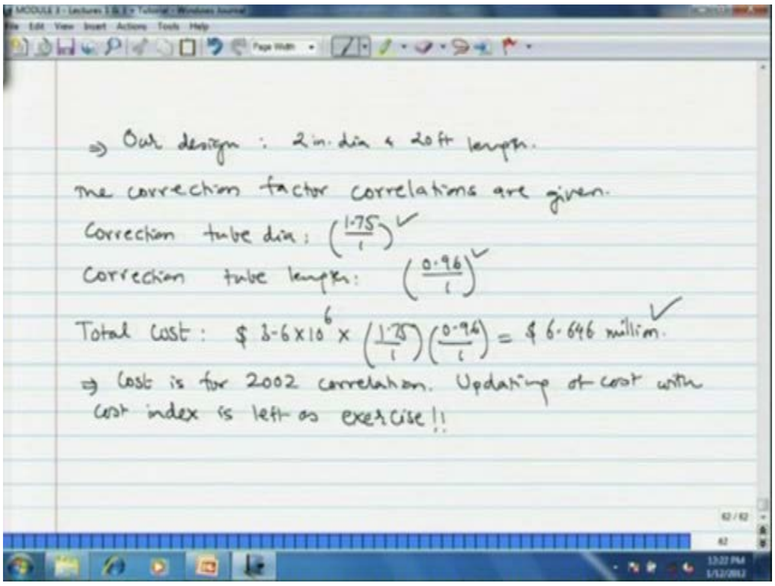
(Refer Slide Time: 52:04)



Effect of tube diameter on cost of conventional shell-and-tube heat exchangers

Thereafter, we have to also go for the ratio of diameters now, our diameter is 2 inch so this particular correlation is only up to 1.4 inch, we have to extrapolate this. So, I have done this and then I have found out that the correction, the relative cost for a 2 inch diameter is something like 1.7, the correction factor 1.75. And now, for 1 inch, you can see here the correction factor is 3.4 inch outer diameter and 1 inch square pitch. So, we have to take the correction factor for 3.4 or 0.75, which is a right here and then this turns out to be something like 0.91. So, the correction factor for the tube diameter is 1.75 divided by 0.91, 0.91 corresponding to 3.3 by 4 inch tube correlation that we just saw, 1 inch was the square pitch of the tubes and that diameter was 3.4 inch, not 1 inch as I said earlier. So, we have to go for correction factor because our diameter is higher of 2 inch.

(Refer Slide Time: 53:45)



⇒ Our design : 2 in. dia & 20 ft length.

The correction factor correlations are given.

Correction tube dia : $\left(\frac{1.75}{1}\right)$ ✓

Correction tube length : $\left(\frac{0.96}{1}\right)$ ✓

Total cost : $\$ 3.6 \times 10^6 \times \left(\frac{1.75}{1}\right)\left(\frac{0.96}{1}\right) = \$ 6.646$ million. ✓

⇒ Cost is for 2002 correlation. Updating of cost with cost index is left as exercise!!

And then after the correction factors, you have to recalculate the cost, correction for tube diameter 1.75 divided by 1, correction for tube length 0.96 divided by 1. So, the total cost of 3.6 million dollars is adjusted for the correction factors and we get the new total cost as 6.646 million dollars. Now, remember that, these correlations were formulated in 2002 so you have to update them. This correlation was given for January 2002, so you have to update it for the 2012 cost.

Now, that I leave as an exercise, updating of the cost is left as an exercise, you can do it by taking the ratio of cost indices like Marshall and Swift index is a standard index used for cost corrections or cost inflation. So, you take the cost index, Marshall and Swift cost index for 2002 then you also take the Martial and Swift cost index for 2012. The ratio of these two indices will be, that ratio you multiply by the total cost in 2002 that will give you the total cost in 2012.

But, I will leave this as an exercise, the cost indices are available in standard journals and these journals are chemical engineering, publication of i chemi, institute of chemical engineers, chemical engineering progress or chemical weekly. So, look into these techno commercial journals to get the cost indices, so that completes module 3 of this course that is, reactor design and cost estimation.