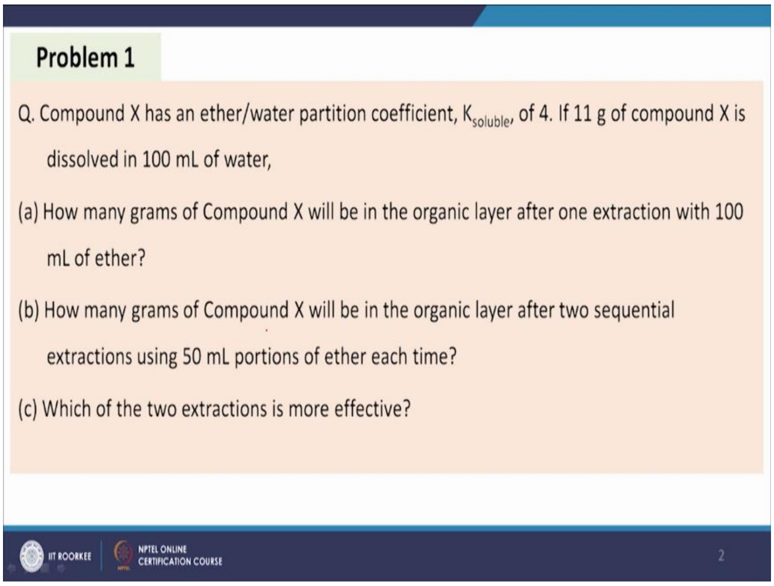
Basic Environmental Engineering and Pollution Abatement
Professor Prasenjit Mondal
Department of Chemical Engineering
Indian Institute of Technology, Roorkee
Lecture 05
Tutorial 1

Hello everyone, today, we will solve some numerical problems based on the discussion we have made in the last 4 classes.

(Refer Slide Time: 00:37)



Problem 1

Q. Compound X has an ether/water partition coefficient, $K_{soluble}$, of 4. If 11 g of compound X is dissolved in 100 mL of water,

(a) How many grams of Compound X will be in the organic layer after one extraction with 100 mL of ether?

(b) How many grams of Compound X will be in the organic layer after two sequential extractions using 50 mL portions of ether each time?

(c) Which of the two extractions is more effective?

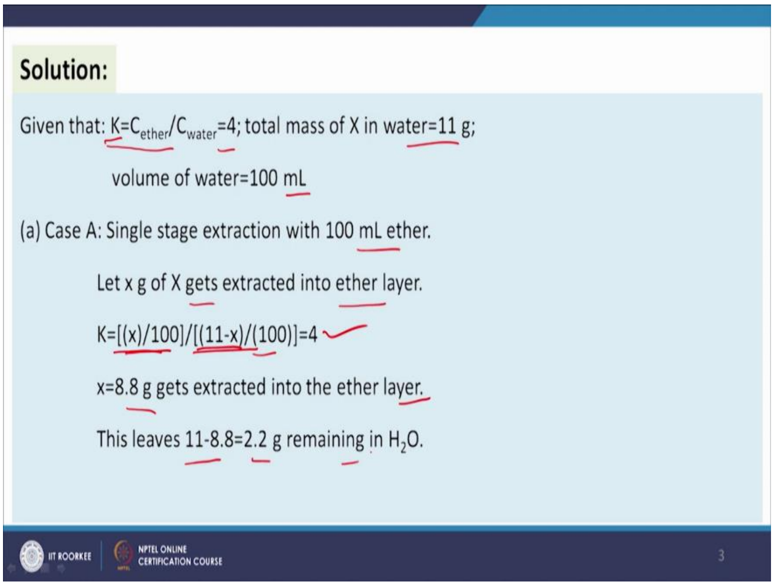
So, problem number 1. So, compound X has an ether/water partition coefficient, $K_{soluble}$ of 4. If 11 g of compound X is dissolved in 100 mL of water, then how many grams of compound X will be in the organic layer after one extraction with 100 mL of ether. So, this is problem number 1(a).

And then (b) how many grams of compound X will be in the organic layer after two sequential extractions using 50 mL portions of ether each time and (c) which of the two extractions is more effective. So, we have to solve this problem. We will solve it and as you see, this is a problem based on the distribution of organic compounds in aqueous and organic phase when some pollutants are present in water, so that becomes in equilibrium with the biomass of the living organisms.

So, there is some partition coefficient and the concentration of organic phase is more than the concentration of the pollutants in the water phase, we have discussed in the previous class and we have also seen that every time it is not possible to measure it.

So, there are some standard process with specific organic solvent and water to the pollutants which are used in the laboratory and it is separated into two different phase that is organic and aqueous phase and then the from that partition coefficient, there is some relationship we find out the BCF (Bio-Concentration Factor). So, similar concept we will be using here. So, what we will do?

(Refer Slide Time: 02:38)



Solution:

Given that: $K=C_{ether}/C_{water}=4$; total mass of X in water=11 g;

volume of water=100 mL

(a) Case A: Single stage extraction with 100 mL ether.

Let x g of X gets extracted into ether layer.

K=[(x)/100]/[(11-x)/(100)]=4

x=8.8 g gets extracted into the ether layer.

This leaves 11-8.8=2.2 g remaining in H_2O.

We have K that is equal to concentration of the pollutant X, Cether/Cwater that is equal to K it is given 4 and total mass is also given. That is equal to 11 g. So, volume of the water is given that is equal to 100 mL. So, for the case 1, say single stage extraction with 100 mL ether what do we get?

Let x g of X get extracted into ether layer

K= x/100 , this is the concentration, x g/100 mL, we have taken so, gram/mL (x/100) (11- x), that is the amount of x present in the aqueous phase.

(11- X)/100 that is the volume

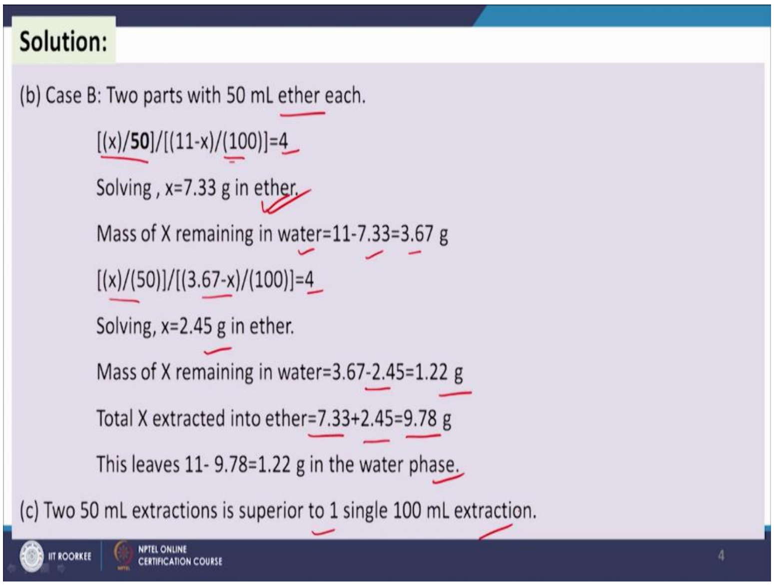
So, concentration is equal to (11- X)/100

So, K= [(x/100)]/[(11- x)/100]=4

X =8.8 g.

So, 8.8 g x gets extracted into the ether layer, so how many is present in the aqueous phase, that is 11-8.8 = 2.2 g-remaining in the water. So, first case a, we are able to solve now then case b.

(Refer Slide Time: 04:14)



Solution:

(b) Case B: Two parts with 50 mL ether each.

$[(x)/\mathbf{50}]/[(11-x)/(100)]=4$

Solving , x=7.33 g in ether.

Mass of X remaining in water=11-7.33=3.67 g

$[(x)/(50)]/[(3.67-x)/(100)]=4$

Solving, x=2.45 g in ether.

Mass of X remaining in water=3.67-2.45=1.22 g

Total X extracted into ether=7.33+2.45=9.78 g

This leaves 11- 9.78=1.22 g in the water phase.

(c) Two 50 mL extractions is superior to 1 single 100 mL extraction.

Two parts with 50 mL ether each, so, we will be taking 50 mL of ether and we will mix these one with the pollutants and water we will also get that is equal to 100 mL,

x/50 that is the concentration of x in the organic phase that is ether and 100 mL water we have taken and (11- x) is going into the water then

$[(x)/50]/[(11-x)/(100)]=4$

x = 7.33g in ether.

So, mass of X is remaining in the water equal to 11-7.33 = 3.67 g

Again, for next 50 mL

$[(x)/50]/[(3.67-x)/(100)]=4$

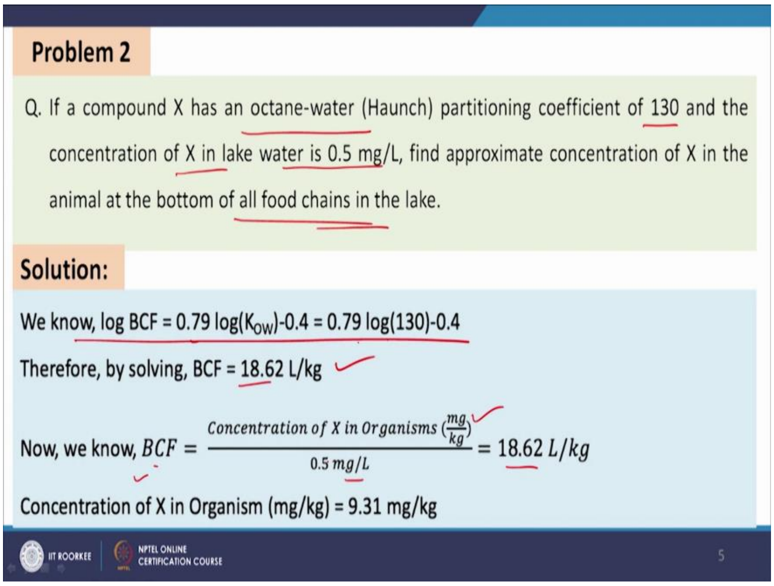
x = 2.45 g in ether.

So, mass of X remaining in water = 3.67 – 2.45 = 1.22 g So, total X extracted into this case into 2 ether steps to separation steps using 50 mL ether in each step, that is equal to 7.33 + 2.45= 9.78 g.

So, total 9.78 gram is separated into the organic phase. So, it lives 1.22 g in the water phase. So, that second part is also done.

Now, third part. So, two 50 mL extractions is superior to one single stage, because we see here in the second case using two steps consecutively, only 1.22 gram X is remaining in the water, whereas in the previous case, it was 2.22 gram X remaining in the water. So, now the problem is solved.

(Refer Slide Time: 06:38)



Problem 2

Q. If a compound X has an octane-water (Haunch) partitioning coefficient of 130 and the concentration of X in lake water is 0.5 mg/L, find approximate concentration of X in the animal at the bottom of all food chains in the lake.

Solution:

We know, $\log BCF = 0.79 \log(K_{OW}) - 0.4 = 0.79 \log(130) - 0.4$

Therefore, by solving, BCF = 18.62 L/kg

Now, we know, $BCF = \dfrac{Concentration\ of\ X\ in\ Organisms\ (\frac{mg}{kg})}{0.5\ mg/L} = 18.62\ L/kg$

Concentration of X in Organism (mg/kg) = 9.31 mg/kg

See the next problem. So, problem number 2, here, if your compound X has an octane-water partitioning coefficient of 130 and the concentration of X in lake water is 0.5 mg/litre, find approximate concentration of X in the animal at the bottom of all food chains in the lake. So, that we have to calculate. That means, in this case, in this aquatic environment, so, pollutant is present in this water.

So, in that case, the pollutant will be in equilibrium with zooplankton, and phytoplankton. So, phytoplankton will be taken up by the living organism show we have to find out the X in the animal at the bottom of all food chains. So, that means if we know the bio concentration factor, then you can calculate it. So, that way here octane-water system, has been given. So, here we are seeing how we calculate the BCF. BCF, we know the formula

$\log BFC = 0.79 \log(Kow) – 0.4 = 0.79 \log(130) – 0.4$

130 that is the partition coefficient K_{OW}.

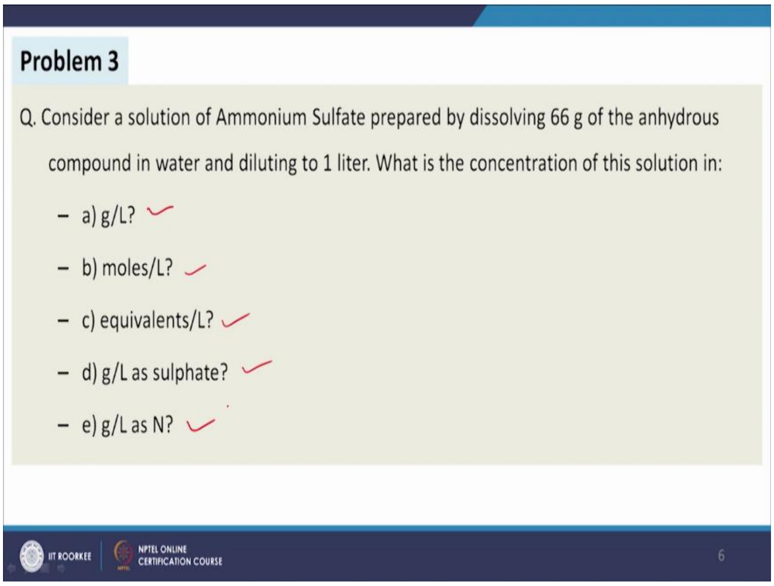
BCF= 18.62 L/kg.

By the concept or by the definition of bioconcentration factor we can get concentration of X in organic organisms mg/kg divided by concentration of the pollutants in the lake water that is 0.5 mg/litre.

BCF= concentration of X in organic organisms (mg/kg)/0.5mg/l = 18.62 L/kg*0.5mg/L= 9.31mg/kg

Concentration of X in organism = 9.31mg/kg. So, this is the concentration of X in the organism that we are asked to calculate and now we are able to find out the value of it. So, now we will see problem number 3. So, here the statement is like this.

(Refer Slide Time: 09:32)



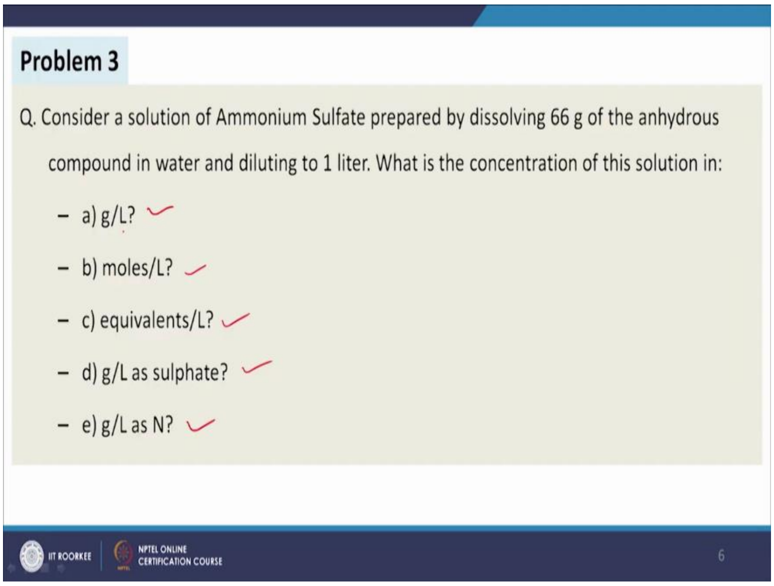
Problem 3

Q. Consider a solution of Ammonium Sulfate prepared by dissolving 66 g of the anhydrous compound in water and diluting to 1 liter. What is the concentration of this solution in:

- a) g/L?
- b) moles/L?
- c) equivalents/L?
- d) g/L as sulphate?
- e) g/L as N?

Consider a solution of ammonium sulphate prepared by dissolving 66 g of the nitrous compound in water and diluting to 1 litre. Then what is the concentration of the solution in gram per litre, moles per litre, equivalents per litre, gram per litre as sulphate, and gram per litre as nitrogen? So, we have to calculate this as per the statement. Now let us see.

(Refer Slide Time: 10:01)



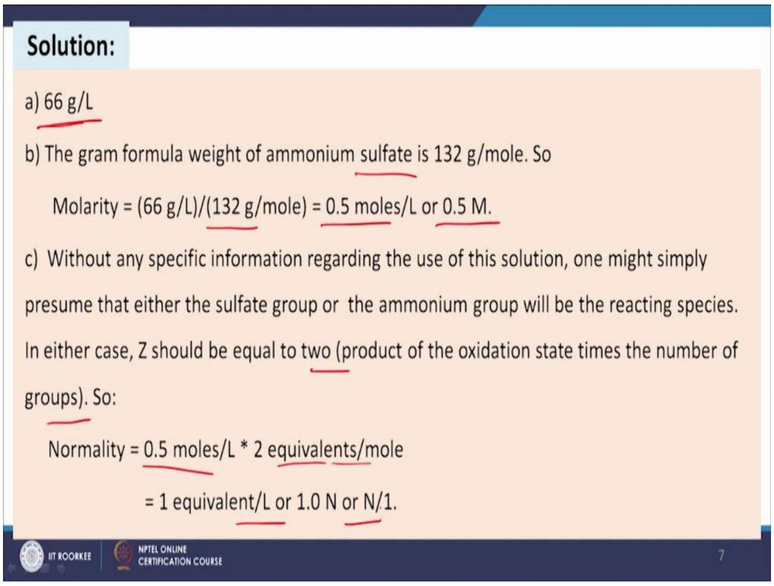
Problem 3

Q. Consider a solution of Ammonium Sulfate prepared by dissolving 66 g of the anhydrous compound in water and diluting to 1 liter. What is the concentration of this solution in:

- a) g/L?
- b) moles/L?
- c) equivalents/L?
- d) g/L as sulphate?
- e) g/L as N?

IIT ROORKEE
NPTEL ONLINE CERTIFICATION COURSE

6



Solution:

a) 66 g/L

b) The gram formula weight of ammonium sulfate is 132 g/mole. So

Molarity = (66 g/L)/(132 g/mole) = 0.5 moles/L or 0.5 M.

c) Without any specific information regarding the use of this solution, one might simply presume that either the sulfate group or the ammonium group will be the reacting species. In either case, Z should be equal to two (product of the oxidation state times the number of groups). So:

Normality = 0.5 moles/L * 2 equivalents/mole

= 1 equivalent/L or 1.0 N or N/1.

So, what we will see here we have 66 g/L ammonium sulphate.

Then the gram formula weight of ammonium sulphate $(NH_4)_2SO_4$ is 132 g/mole,

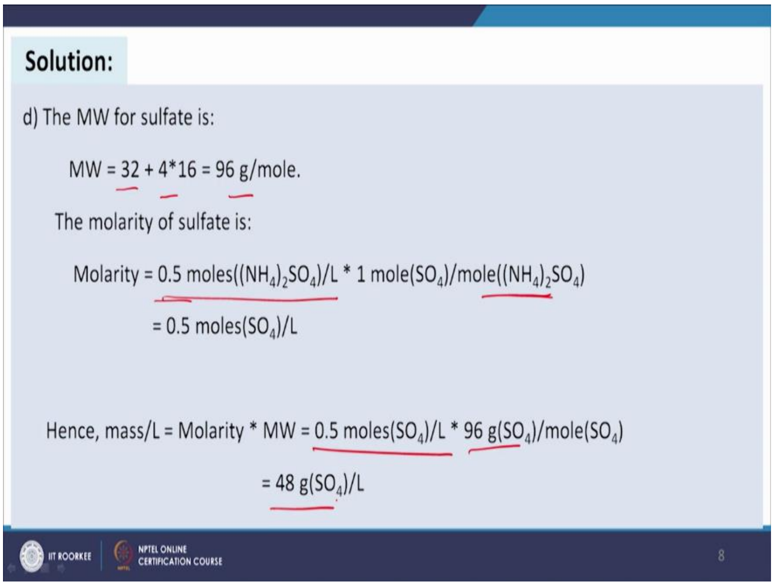
molarity = (66 g/ l)/ (132 g/mole) = 0.5 moles/L or 0.5 M.

without any specific information regarding the use of the solution. One might simply presume that either the sulphate group or the ammonium group will be the reacting species and in either case, Z would be equal to 2 product of the oxidation state times the number of groups

Normality = 0.5 moles/L*2 equivalents/mole

We are getting 1 equivalent/litre or 1.0 normal, N/1

(Refer Slide Time: 12:00)



Solution:

d) The MW for sulfate is:

MW = 32 + 4*16 = 96 g/mole.

The molarity of sulfate is:

Molarity = 0.5 moles($(NH_4)_2SO_4$)/L * 1 mole(SO_4)/mole($(NH_4)_2SO_4$)

= 0.5 moles(SO_4)/L

Hence, mass/L = Molarity * MW = 0.5 moles(SO_4)/L * 96 g(SO_4)/mole(SO_4)

= 48 g(SO_4)/L

Then, for question part d, let us see the molecular weight of sulphate.

SO_4 = 32 + 4*16 = 96 gram/mole, and the molarity of sulphate is 0.5 moles, this is the molar strength we have ammonium sulphate. Now, I have to convert in terms of sulphate.

Molarity = 0.5 moles $[(NH_4)_2SO_4]$/L* 1mole(SO_4)/mole($(NH_4)_2SO_4$),

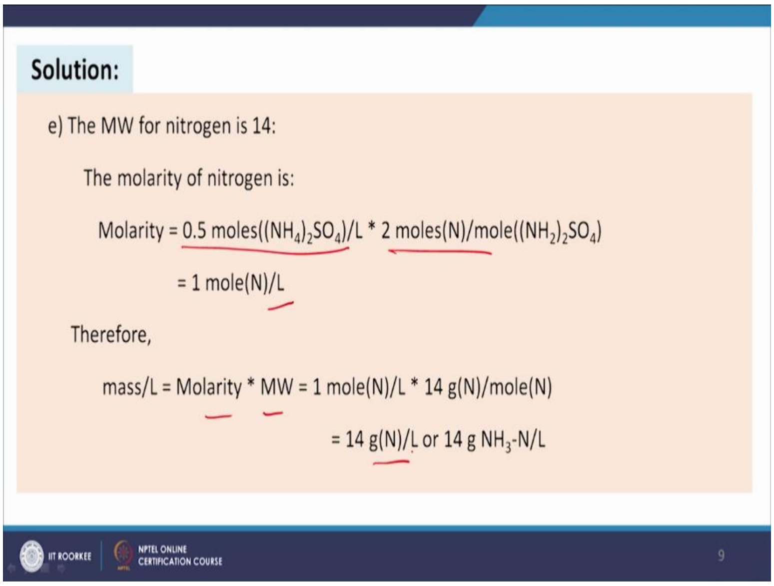
=0.5 moles (SO_4)/litre,

Hence, mass/L = Molarity* MW (molecular weight)

= 0.5 moles(SO_4)/L* 96 g (SO_4) /mole(SO_4)

= 48 g(SO_4)/L

(Refer Slide Time: 13:02)



Solution:

e) The MW for nitrogen is 14:

The molarity of nitrogen is:

Molarity = 0.5 moles($(NH_4)_2SO_4$)/L * 2 moles(N)/mole($(NH_2)_2SO_4$)

= 1 mole(N)/L

Therefore,

mass/L = Molarity * MW = 1 mole(N)/L * 14 g(N)/mole(N)

= 14 g(N)/L or 14 g NH_3-N/L

For part e,

The molecular weight of nitrogen is 14

so, molarity of nitrogen is = 0.5 moles$[(NH_4)_2SO_4)]$/L* 2 moles(N)/mole$[(NH_4)_2SO_4)$

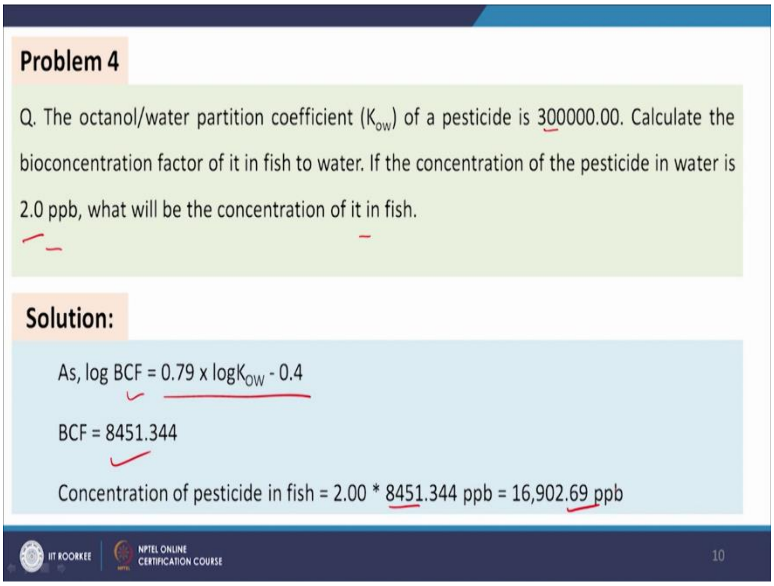
= 1 mole N/L.

Therefore, mass/litre = molarity * molecular weight

= 1 mole N/L*14g(N)/mole(N)

= 14g (N)/L, or 14 g NH_3-N (ammoniacal nitrogen)/litre, we can say. So, that way we can solve the problem. Now, we see the problem number 4.

(Refer Slide Time: 13:50)



Problem 4

Q. The octanol/water partition coefficient (K_{ow}) of a pesticide is 300000.00. Calculate the bioconcentration factor of it in fish to water. If the concentration of the pesticide in water is 2.0 ppb, what will be the concentration of it in fish.

Solution:

As, log BCF = 0.79 x logK_{OW} - 0.4

BCF = 8451.344

Concentration of pesticide in fish = 2.00 * 8451.344 ppb = 16,902.69 ppb

The statement is, the octanol/water partition coefficient K_{OW} of a pesticide is these 300000 calculate the bioconcentration factor of it in fish to water. If the concentration of the pesticide in water is 2 ppb, what will be the concentration of it in fish?

So, again, similar to that problem we have discussed just before few minutes.

So, then here log bioconcentration factor equal to the empirical formula we will be using

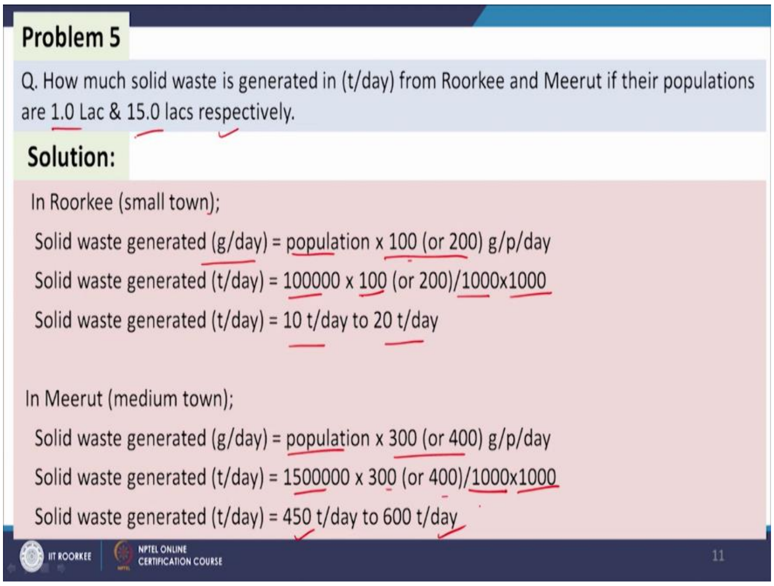
Log BFC = 0.79 log(Kow) – 0.4

BCF= 0.79 log(300000) – 0.4 = 8451.344

So, concentration of pesticide in fish = 2ppb*8451.344= 16,902.69 ppb.

So, now, we will come to the next problem.

(Refer Slide Time: 14:57)



Problem 5

Q. How much solid waste is generated in (t/day) from Roorkee and Meerut if their populations are 1.0 Lac & 15.0 lacs respectively.

Solution:

In Roorkee (small town);

Solid waste generated (g/day) = population x 100 (or 200) g/p/day

Solid waste generated (t/day) = 100000 x 100 (or 200)/1000x1000

Solid waste generated (t/day) = 10 t/day to 20 t/day

In Meerut (medium town);

Solid waste generated (g/day) = population x 300 (or 400) g/p/day

Solid waste generated (t/day) = 1500000 x 300 (or 400)/1000x1000

Solid waste generated (t/day) = 450 t/day to 600 t/day

So, problem number 5. The statement is how much solid waste is generated in tonne per day from Roorkee and Meerut, if their populations are 1 lakh and 15 lakhs, respectively. So, this problem is based on the pollution generation capacity per capita waste, solid waste generation capacity. So, Roorkee 1 lakhs and this is 15 lakhs, Meerut. So, if we compare one is small city and other is your medium town.

So, as you have discussed in the previous class, so, here we are getting the small town Roorkee, solid waste generation gram/day, we know that 100 to 200 g/day per capita, so,

Solid waste generation (g/day) = population*100(or 200) g/day

Solid waste generation (t/day) = 100000*100(or 200)/(1000*1000)

Solid waste generation (t/day) = 10 t/day to 20 t/day

So, this is a waste to generation in Roorkee per day and for Meerut that value will change, because we know that for medium city per capita waste generation is different from that of the small city and it is 300 to 400 gram per person per day.

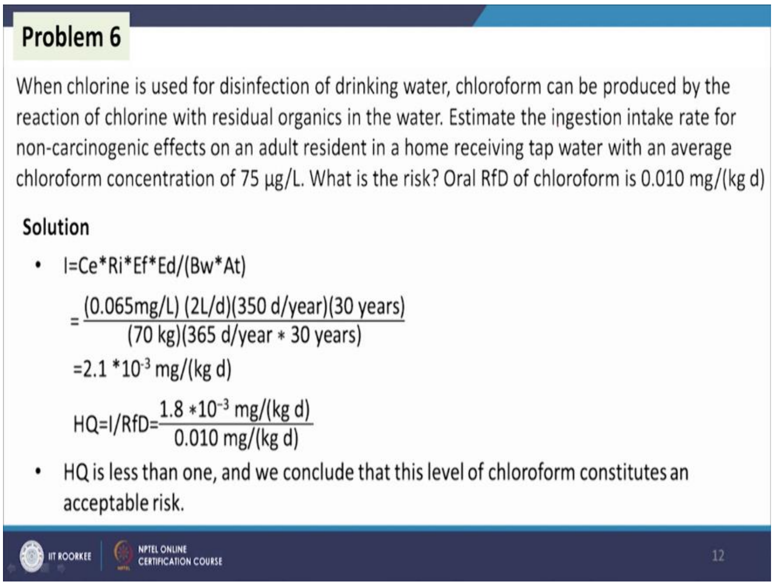
Solid waste generation (g/day) = population*300(or 400) g/day

Solid waste generation (t/day) = 1500000*300(or 400)/(1000*1000)

Solid waste generation (t/day) = 450 t/day to 600 t/day

So, we will be getting our 450 t/day to 600 t/day. So, now, we are able to find out the waste generated in this two city per day.

(Refer Slide Time: 17:06)



Problem 6

When chlorine is used for disinfection of drinking water, chloroform can be produced by the reaction of chlorine with residual organics in the water. Estimate the ingestion intake rate for non-carcinogenic effects on an adult resident in a home receiving tap water with an average chloroform concentration of 75 μg/L. What is the risk? Oral RfD of chloroform is 0.010 mg/(kg d)

Solution

- I=Ce*Ri*Ef*Ed/(Bw*At)

  $$= \frac{(0.065 mg/L)\,(2L/d)(350\ d/year)(30\ years)}{(70\ kg)(365\ d/year * 30\ years)}$$

  $$= 2.1 * 10^{-3}\ mg/(kg\ d)$$

  $$HQ = I/RfD = \frac{1.8 * 10^{-3}\ mg/(kg\ d)}{0.010\ mg/(kg\ d)}$$

- HQ is less than one, and we conclude that this level of chloroform constitutes an acceptable risk.

So, the statement of the next problem is when chlorine is used for disinfection of drinking water chloroform can be produced by the reaction of chlorine with residual organics in the water, estimate the ingestion integrate for non-carcinogenic effects on an adult resident in a home receiving tap water with an average chloroform concentration of 65 microgram per litre. What is the risk? Oral RfD of chloroform is 0.010 mg/kg day. So, now we have to solve it. So, this is a problem related to the risk assessment which we have discussed in the previous class and we had one expression as given here,

$I = C_e * R_i * E_f * E_d / (B_w * A_t)$

$I = (0.065 mg/l)(2L/d)(350\ d/year)(30\ year)/(70\ kg)(365\ d/year*30\ year)$

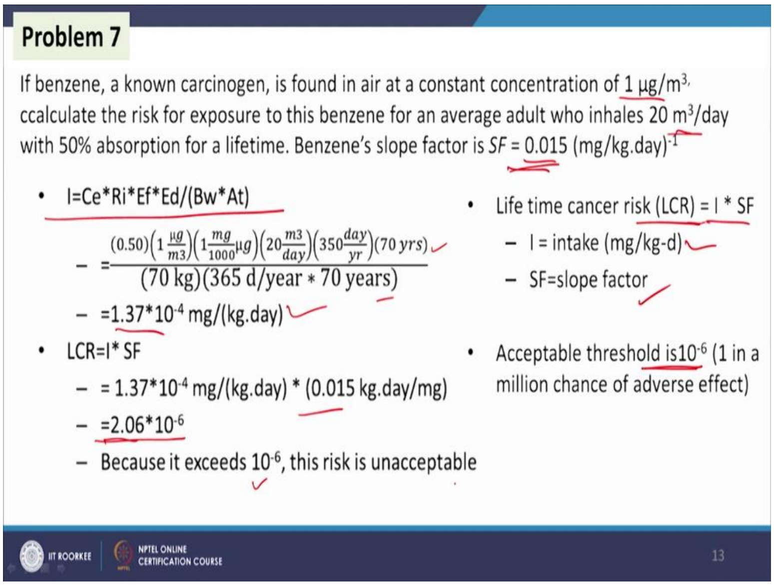
$I = 1.8*10^{-3}\ mg/(kg\ d)$

So, this part is now over we are able to find out ingestion integrate, but we have to find out the risk as well. So, how can you find out the risk? So, risk is equal to we know that relationship hazardous quotient. Risk can be calculated on the basis of hazardous quotient. So, then HQ =I/RfD

$$= 1.8*10^{-3}\ mg/(kg\ d) / 0.010\ mg/(kg\ d)$$

So, this equal to we are getting that HQ is less than 1 in this case it is less than 1 and we conclude that this level of chloroform concentration constitutes an acceptable risk. So, this risk is not much it is acceptable risk because it is less than 1. So, when the HQ is less than 1, then the concentration is acceptable. So, another question that is problem number 6.

(Refer Slide Time: 20:06)



Problem 7

If benzene, a known carcinogen, is found in air at a constant concentration of 1 μg/m^{3,} ccalculate the risk for exposure to this benzene for an average adult who inhales 20 m^3/day with 50% absorption for a lifetime. Benzene's slope factor is *SF* = 0.015 (mg/kg.day)$^{-1}$

- I=Ce*Ri*Ef*Ed/(Bw*At)
  - $= \frac{(0.50)\left(1\frac{\mu g}{m3}\right)\left(1\frac{mg}{1000}\mu g\right)\left(20\frac{m3}{day}\right)\left(350\frac{day}{yr}\right)(70\,yrs)}{(70\text{ kg})(365\text{ d/year} * 70\text{ years})}$
  - =1.37*10^{-4} mg/(kg.day)
- LCR=I* SF
  - = 1.37*10^{-4} mg/(kg.day) * (0.015 kg.day/mg)
  - =2.06*10^{-6}
  - Because it exceeds 10^{-6}, this risk is unacceptable
- Life time cancer risk (LCR) = I * SF
  - I = intake (mg/kg-d)
  - SF=slope factor
- Acceptable threshold is10^{-6} (1 in a million chance of adverse effect)

The statement is if benzene a known carcinogen is found in air at a constant concentration of 1 microgram per metre cube, calculate the risk for exposure to this benzene for an average adult who inhales 20 metre cube per day with 50% absorption for a lifetime. Benzene's slope factor is SF 0.015mg per kg per day.

So, this is again another problem related to the risk analysis and we have this expression

$I = C_e*R_i*E_f*E_d/(B_w*A_t)$ and this is a carcinogenic effect. This may have carcinogenic effect. So, risk we can calculate with the help of SF that is your slope factor and what is that? That is lifetime cancer risk, LCR =I*SF.

And if the value is 10^{-6} then it is acceptable or less than this then it is acceptable threshold. If it is more than that it is not acceptable. So, then now, let us see the value of I.

I= (0.50) (1μg/m^3) (1mg μg/1000) (20 m^3/day)/(350day/yr) (70 yrs.)/(70kg) (365 d/year*70 year)

I = 1.37*10^{-4} mg/(kg day)

LCR =I*SF=1.37*10^{-4} mg/(kg day) *(0.015 kg day/mg)

=2.06*10^{-6}

Acceptable threshold value is 10^{-6}, but here the value is more 2.06*10^{-6}.

So, this exceeds the 10^{-6} limit. So, this risk is unacceptable, so, that will be hazardous for the health. So, after this in this class, now we are able to solve 6 numerical problems based on our previous 4 classes. Thank you for your patience.