

Choose Focus Analyze Exercise
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BT04B004

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ACKNOWLEDGEMENT

I would like to thank Prof GK Suraish for giving me an opportunity to augment my experiences through the CFA exercise.

Doing the CFA exercise second time was an incredible experience. It forced me to think creatively and innovatively. At every step of this exercise I learnt new things.

I am greatly thankful to Prof GK Suraish for inspiring me to do this wonderful exercise.

INSPIRATION FOR THE TOPIC

Prof GK Suraish gave us the CFA exercise on the very first day. The most challenging part of the CFA exercise is to choose an appropriate topic. From the very first week of the semester I was thinking about my CFA topic.

One day I was generally browsing net when I came across the article on Gulf War Syndrome or Gulf War Illness. The disease leads to immune system disorders and birth defects.

During the 1991 Gulf War, Depleted Uranium munitions were used extensively. Depleted uranium (DU) was used in tank kinetic energy penetrator and machine-gun bullets on a large scale during Gulf War. DU munitions often burn when they impact a hard target, producing toxic combustion products. Accidental exposure to toxic DU particles during the war lead to serious health defects in US soldiers and Iraqi civilians. These disorders also lead to birth defects in the US soldiers' babies.

The following pictures depict the severity of the effects of GWS in newly born babies.



Sabo for NEWS



Guardsman Gerard Darren Matthew, sent home from Iraq with mysterious illnesses, holds baby daughter, Victoria, who has deformed hand. He has tested positive for uranium contamination. (Sept 2003)

Moved by the impact of GWS, I kept reading and searching more about properties of DU. The same day when I was lying on bed to sleep I decided to design a DU Mask for my CFA topic.

PROBLEM STATEMENT

- In this project I have proposed a design of a Mask used to remove Depleted Uranium (DU) from air inhaled. DU is extensively used in making arms and ammunition. Recent studies have shown the hazardous effects of inhalation and ingestion of DU. Hence this mask will find application in arms and ammunition industry where the concentration of DU particles is high.
- I have calculated the pressure developed inside the mask as a result of diffusion of contaminated air through the mask.
- Also I have hypothesized when the mask should be replaced by a new mask.

INTRODUCTION

Uranium-

It's a naturally occurring radioactive element with an atomic number of 92. Uranium has two stable oxidation states +4 and +6. Naturally occurring Uranium occurs in three isotopes:-

- U-235
- U-238
- U-234

The relative abundance of each is as depicted in table below:-

Isotope	U-238	U-235	U-234
Relative Abundance (%)	99.27	0.72	0.0055
Half life (years)	4.47 billion	700 million	246,000

Uranium is used in:

- Nuclear reactors
- Nuclear propelled Navy ships and submarines
- Nuclear weapons.

Out of all the isotopes U-235 is radioactive and is primarily used as fuel in nuclear reactors. Naturally U-235 occurs in a small percentage. Hence Enrichment of U is done in order to increase the relative concentration of U-235 in nuclear fuel.

This leads to the production of Depleted Uranium.

Depleted Uranium-

Depleted Uranium (DU) is what is left over when most of the highly radioactive types of uranium are removed used as nuclear fuel. Composition of DU is essentially U-238 with traces of U-235.

Depleted Uranium has wide application due to its high strength and density.

It is used in

- Kinetic energy accelerators
- Armor plating
- Counter Weights in helicopters and airplanes

The radiological dangers of pure DU are relatively lower (60%) than those of naturally-occurring uranium due to the removal of the more radioactive isotopes. The three main pathways exist by which internalization of DU may occur:

- Inhalation
- Ingestion
- Through abrasions

The chemical toxicity of DU is greater than the radiological toxicity. Chemical toxicity effects have been discovered very recently.

It can cause:-

- Respiratory and Kidney problems
- Painful joints
- Gulf War Syndrome
- Harmful Mutations in DNA
- Birth Effects

Concentration of DU particles in atmosphere is very less to cause any significant toxicity. However in arms and ammunition industries, the concentration of DU particle in air is high. This can lead to DU chemical toxicity among the workers. In DU munitions, the predominant chemical forms of uranium present in the atmosphere are likely to be uranium trioxide (UO_3), uranium octoxide (U_3O_8) and uranium dioxide (UO_2), According to WHO, the eight hour time weighted average limitation in worker inhalation of soluble and insoluble DU compounds is $50 \mu\text{g}/\text{m}^3$ DU in air.

In the following report I have proposed a design for mask which can be used to purify inhaled air from DU particles.

MODEL OF THE MASK

The mask has a hemi spherical structure consisting of three layers through which air along with dust particles, organic impurities, and DU particles can diffuse.

The three layers are packed one after one other such that it limits the course of air. The inhaled air flows through filter layers which removes harmful dusts, toxic gases ,carbon impurities and DU particles ,letting only purified air inside the body.

The three layers are:-

- **First Layer**
Aerosol Filters:-

This is the outer most layer, exposed to the atmosphere. This thin layer traps tiny suspended solid or liquid particles and often referred to as particulate. Dust particles have size of the order of 0.3 microns. Also size of DU is of the order of 1 Angstrom. Hence the pore size of the mesh equal to 1 nano meter will trap all particulate and let air and DU particles diffuse in.

- **Second Layer**
Activated Charcoal:-

This is next to aerosol filter. It is used to adsorb carbon based impurities (organic chemicals) from air .Activated charcoal is charcoal that has been treated with oxygen to open up millions of tiny pores between the carbon atoms. The use of special manufacturing techniques results in highly porous charcoals that have surface areas of 300-2,000 square meters per gram. The huge surface area of activated charcoal gives it countless bonding sites. When certain chemicals pass next to the carbon surface, they attach to the surface and are trapped. Activated, charcoals are widely used to adsorb odorous or colored substances from gases or liquids. The substance is highly porous with a porosity factor (65%-75%).

- **Third Layer**

EDTA (Ethylenediaminetetraacetate)-

This is the final and the inner most layer. EDTA is a very good chelating agent, and forms coordination compounds with most monovalent, divalent, trivalent and tetravalent metal ions. EDTA contains 4 carboxylic acid and 2 tertiary amine groups that can participate in acid-base reactions. Thus DU uranium particles when in their stable oxidation state of +4 and +6 can bind to the EDTA . Thus trapping DU and letting only purified air in side.

PRINCIPLE OF THE DU MASK

In short the mask works as follow. Air in the atmosphere contains many impurities like dust,pollen,DU particles, Organic chemicals etc. The mask is designed such that all the impurities are trapped one by one in one of the three layer depending upon the nature of the impurity. As air enters inside mask and diffuses through first layer-the aerosol layer all particulate impurities(dust and pollen) are trapped. As the air enters the second layer –the activated charcoal carbon based impurities are adsorbed to it . In the final layer that is the EDTA layer DU particles are trapped by forming a coordination complex. Hence finally we get purified air.

For calculation purpose I have taken mask to be a hemi sphere with outer diameter 10.2 cm where as inner diameter 8cm

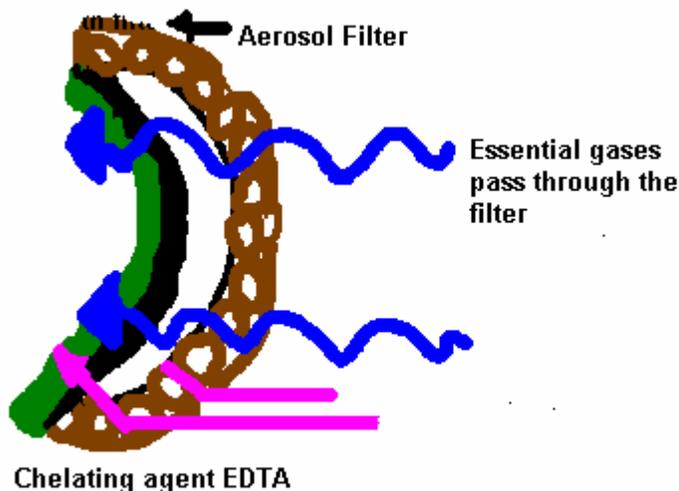
Also the thickness of each layer is taken as in the table below

Layer Number	Layer Name	Thickness (cm)
First Layer	Aerosol Filter	0.2
Second Layer	Activated Charcoal	1.0
Third Layer	EDTA	1.0

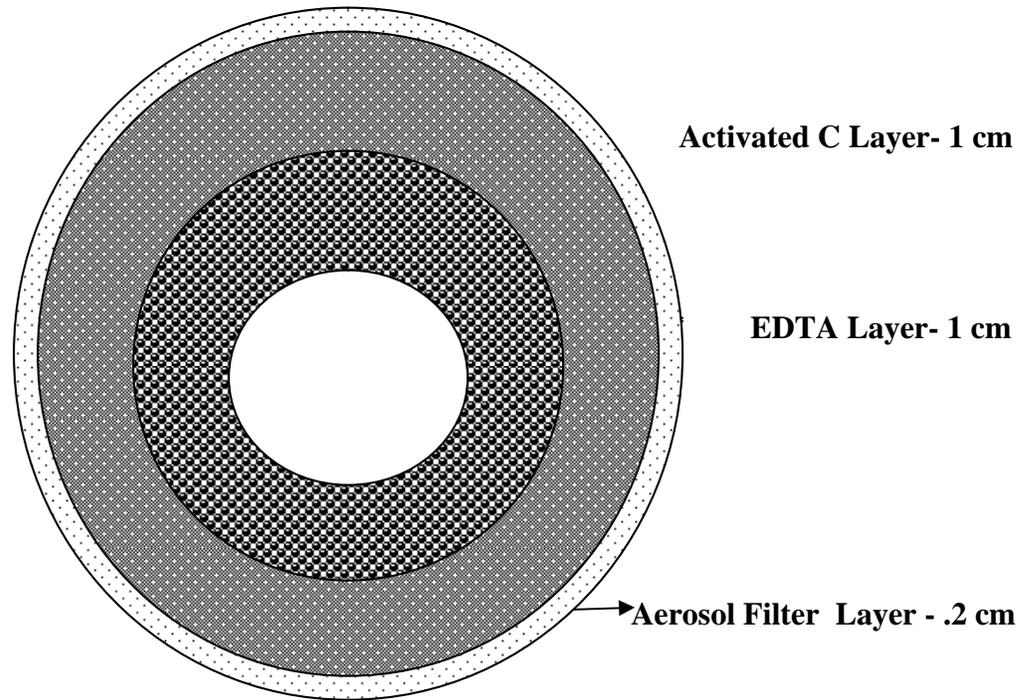
SCHEMATIC OF THE DEPLETED URANIUM MASK



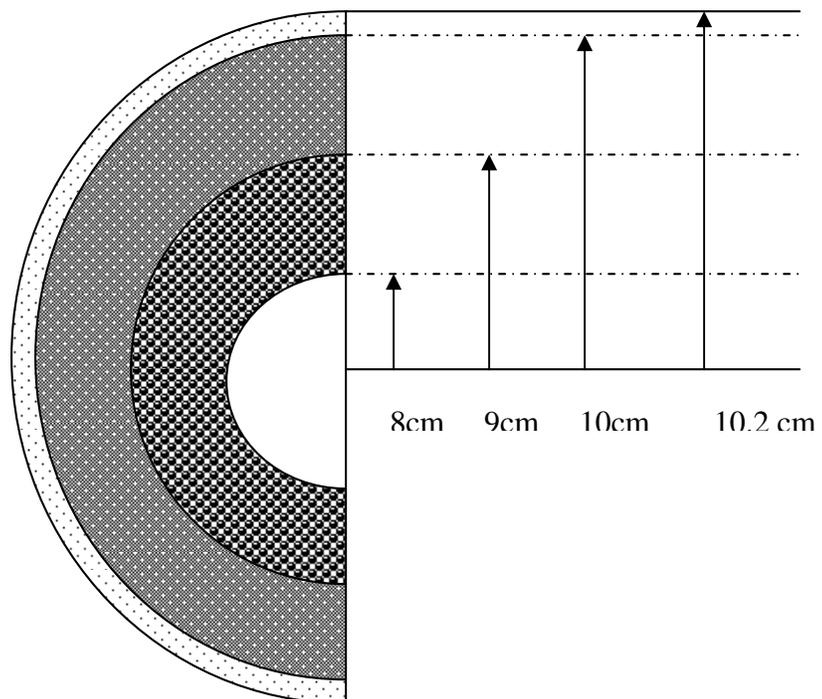
www.affiliateshellmills.com



TOP VIEW OF THE DU MASK



SIDE VIEW CROSS SECTION OF THE DU MASK



CALCULATION OF AIR PRESSURE DEVELOPED INSIDE THE MASK THROUGH DIFFUSION OF AIR.

ASSUMPTIONS

- Air to be an ideal gas for all purposes at a temperature of 30°C.
- Flux of air through mask is constant
- I am doing an analysis for only one breath inhaled.
- In order to keep my system simple and solvable I have not considered the diffusion of the exhaled air.
- Initially there was no air inside the mask that is pressure inside the mask zero initially.
- Outside the mask the pressure of air is atmospheric that is 1 Pascal or 760mm of Hg.
- For calculation of pressure inside the mask I have neglected DU concentration in air.
- Also since the first layer the aerosol layer is thin as compared to other two layers the pressure drop across this layer is negligible, hence I have assumed the pressure across this layer is essentially atmospheric.

EQUATIONS USED

According to Ficks law [7]

$$N_A = - D_p dP_A / dZ$$

When the material is porous Ficks law is modified to

$$N_A = - D_{eff} dP_A / dZ$$

Where $D_{eff} = (e / t) D_{AK}$

Also according to Knudsen Formula [2] for transport of gases at ideal conditions [7]

$$N_A = - 8a / 3 * (1 / (2 \Pi M_A RT)^{1/2}) (dP_A / dZ)$$

N_A = Flux of species A that is number of moles diffusing per unit area per unit time

P_A = Partial pressure of species A

D_p = Diffusion constant

e = Porosity factor i.e. fractional void space in the porous material

t = Tortuosity factor i.e. total mean path traveled by gas / thickness of porous material

M_A = Molecular mass of the gas diffused

a = Effective radius of the pores

R = Universal Gas constant

T = Temperature in Kelvin

DATA USED

- For activated charcoal layer $e/t = .7/2.0$
- For EDTA layer $e/t = .4/2.4$
- $a = 1 \text{ cm}$
- $M_A = 28.94 \text{ g/mol}$
- $R = 8.314 \text{ m}^3 \cdot \text{Pa} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
- $T = 298 \text{ K}$

CALCULATIONS

Now consider a hemispherical shell of thickness dr inside the second layer. Now applying the above equations to the hemispherical shell we get.

$$W_A = -8a/3 * (1/(2 \pi M_A RT))^{1/2} (dP_A/dr) (-2 \pi r^2)(e/t)$$

W_A = molar rate of air

For calculation purposes W_A is assumed to be constant.

Integrating the above equation for **Activated Charcoal** layer we get

$$(W_A/D_{\text{eff}}) [1/r_i - 1/r_1] = [P_{A1} - P_{Ai}] \quad \text{I}$$

r_1 = Outer most radius

r_i = Radius at the interface of activated charcoal and EDTA layer

P_{A1} = Pressure outside

P_{Ai} = Pressure at interface of activated charcoal and EDTA layer

$$D_{\text{eff}} = (16 \pi a/3) * (1/(2 \pi M_A RT))^{1/2} * (e/t)$$

Similarly solving for **EDTA layer** we get

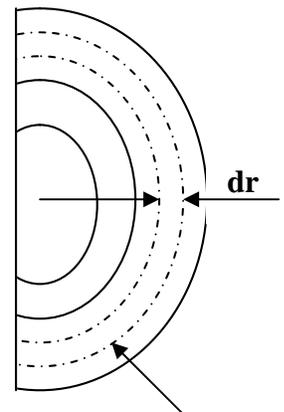
$$(W_A/D'_{\text{eff}}) [1/r_2 - 1/r_i] = [P_{Ai} - P_{A2}] \quad \text{II}$$

P_{A2} = Pressure inside the mask

r_2 = inner radius of mask

Adding **I** and **II** we get

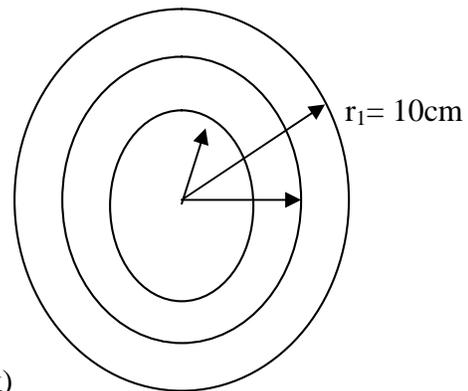
$$P_{A2} = P_{A1} - [(W_A/D_{\text{eff}}) [1/r_i - 1/r_1] + (W_A/D'_{\text{eff}}) [1/r_2 - 1/r_i]] \quad \text{III}$$



Flux of air going inside differential ring

Plugging in value from the figure

- $r_1 = 10 \text{ cm}$
- $r_i = 9 \text{ cm}$
- $r_2 = 8 \text{ cm}$
- $W_A = 1 \text{ mol/breath}$
- $P_{A1} = 1 \text{ atm}$



Solving we get

$P_{A2} = .999 \text{ atm}$ (Pressure developed inside the mask)

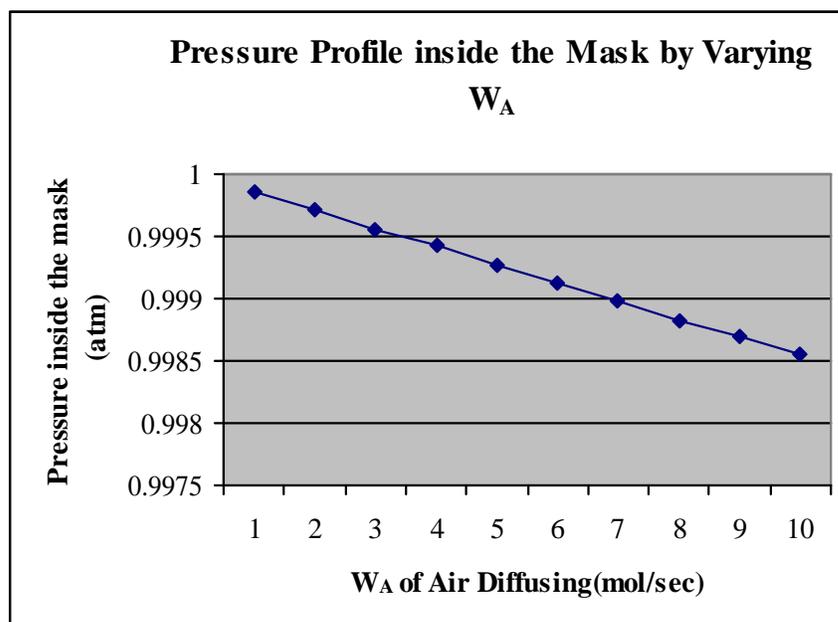
ANALYSIS

Analyzing the equation **III** further we can see that Final Pressure i.e. P_{A2} depends upon many factors i.e.

- Flux of the air ' W_A '
- Effective Size of The pores ' a '
- Dimensions of the mask
- Thickness of each layer

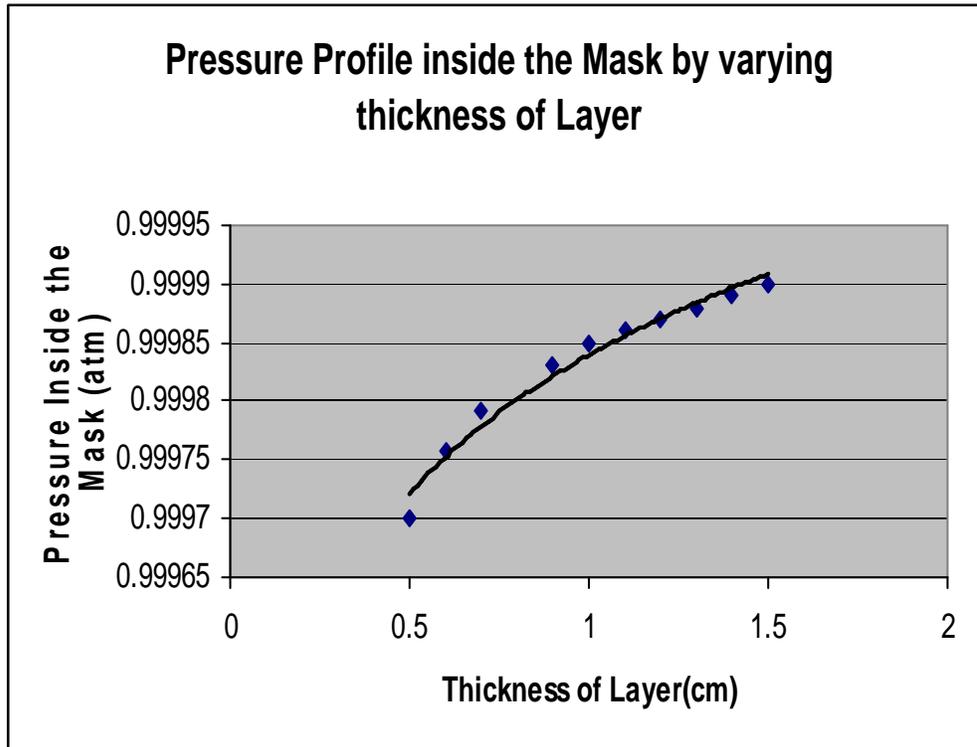
Now we shall look at P_{A2} profile by varying one of the factors and keeping others constant

1) Variation of P_{A2} by varying W_A



As you can see from the graph above ; P_{A2} varies ;linearly with W_A . As we increase W_A P_{A2} decreases.

2) Variation Of P_{A2} by varying thickness of the layer



As we can see from the graph above P_{A2} and Thickness of the layer vary non linearly. Since thickness of the layers is directly proportional to the radii of the mask. By analyzing the thickness of the layer we have also taken into account the factor when the radii of the Mask are varied.

REPLACEMENT TIME OF THE EDTA LAYER - SATURATED WITH DU

APPROACH USED

Consider the situation of DU binding to the EDTA hemi spherical shell analogous to the situation where an enzyme that is EDTA is immobilized in a hemispherical shell and DU that is substrate is binding to EDTA inside the shell with constant flux.

Stoichiometric Analysis tells that U binds to EDTA in one is to one ratio i.e. for one mole of DU particles entering 1 mole of EDTA is required.

ASSUMPTIONS

- Assume steady state i.e. rate of flux of DU particle is constant
- Input of DU is
- Output of DU is zero
- DU diffuses in the shell with a constant velocity V_{el}
- Binding of DU to EDTA follows Michael Menton Equation
- Concentration of DU is very small
- Concentration of EDTA is constant

EQUATIONS USED

Balance equation

$$I - O + G - C = dA/dt$$

I = Input

O = Output

G = Generation

C = Consumption

dA/dt = Accumulation

Michael Menton Equation [7]

$$V = V_m S / (K + S)$$

V = Rate at which one EDTA binds to DU per unit time

V_m = Maximum rate

S = Concentration of DU

K = Constant

Ficks Law [6]

$$N_A = -D_c \frac{dC_A}{dZ}$$

N_A = Flux of species A that is number of moles diffusing per unit area per unit time

C_A = Concentration of species A

D_c = Diffusion constant

CALCULATIONS AND ANALYSIS

Considering a differential hemi spherical element in the EDTA layer of thickness dr .

Applying DU balance on this differential element

Acc to mass balance equation

$$I - O = C \quad \text{I}$$

$dA/dt = 0$ (steady state)

$G = 0$ (no generation of DU)

Ficks law gives

$$\text{Input : } 2 \Pi r^2 [- D_{\text{eff}} * dS/dr]_{r+dr} \quad (-)$$

$$\text{Output : } 2 \Pi r^2 [- D_{\text{eff}} * dS/dr]_r \quad (-)$$

$$\text{Consumption : } [V_m * S / (K + S)] [2 \Pi r^2 dr]$$

Substituting in I

$$r^2 [(D_{\text{eff}} * dS/dr)]_{r+dr} - r^2 [(D_{\text{eff}} * dS/dr)]_r = [V_m * S / (K+S)] [r^2 dr]$$

Dividing by dr and taking limit $dr \rightarrow 0$

$$D_{\text{eff}} [d^2S/dr^2 + dS/dr (2/r)] = V_m * S / (K+S) \quad \text{II}$$

Boundary conditions

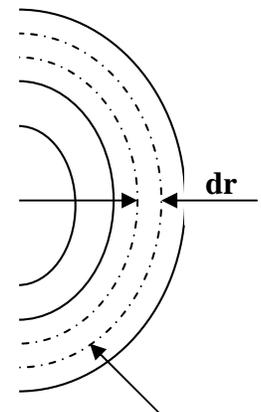
$$\text{At } r = 0, dS/dr = 0 \quad (1)$$

$$\text{At } r = r_i, S = S_o \quad (2)$$

r_i = radius from the centre of the mass to the EDTA and activated Charcoal interface

Also

$$dS/dr = dS/dt * dt/dr \quad \text{IV}$$



Flux of air going inside differential ring

where $dt/dr = (1/Vel)$ [as stated in assumption]

Substituting **IV** in **II**

$$D_{eff} [d^2S/dt^2 + dS/dt (2/t)] = V_m * Vel^2 * S / (K+S) \quad \mathbf{V}$$

Above equation is a second order differential equation in 'S' and 't'
To solve this equation requires complex program .

However equation **V** be solved in a special case when $S \gg \gg K$

Equation **V** can be modified to

$$D_{eff} [d^2S/dt^2 + dS/dt (2/t)] = V_m * Vel^2$$

Integrating the above equation we get

$$S = S_0 - (V_m * Vel^2 / 6 * D_{eff}) t^2$$

The above equation can calculate time t, when EDTA will be saturated if the value of V_m is found out through experiments.

RESULTS

- The design of the DU mask is modeled. It can purify the contaminated air from dust, pollen, DU particles and organic impurities.
- The pressure inside the mask is calculated to be .999 atm. This implies there is not much decrease in pressure of inhaled air by diffusion through the various mask layers. This is good because a large decrease in atmospheric pressure leads to difficulty in breathing. This is analogous to the situation at higher altitudes where there is difficulty in breathing due to decrease in pressure of Oxygen.
- The pressure inside the mask depends on many factors like flux of contaminated air, dimension of the mask, effective radius of the pores etc. As the flux of air increases pressure inside the mask decreases.
- Analysis of the Replacement time for the EDTA layer is done. Though a numeric figure for the model couldn't be calculated due to unavailability of experimental data.

POINTS TO PONDER

- In the above analysis I have not considered the replacement time for aerosol filter layer and Activated Charcoal layer. This can be achieved by similar analysis as done for Depleted Uranium.
- In the EDTA layer I have considered only complex formation with DU. However with EDTA multiple complexing can occur. Ions of Fe, Ca, and Mg present in air can also bind.
- I have done the analysis for one breath inhaled assuming there was no air inside the mask initially. Practically this is incorrect as some amount of air will be present inside the mask. In order to keep my system simple and solvable I have not considered the diffusion of the exhaled air.
- Disposal of the EDTA mesh with DU – Disposal of radioactive waste is a big environment concern. Under oxic conditions the stable form of uranium is U~VI, which is highly soluble. [6]Reduction of soluble U~VI to relatively insoluble U~IV can serve as one potential method. Uranium IV is sparingly soluble, and will tend to precipitate forming amorphous $UO_2(s)$. Very recently bacterial dissimilatory U~VI reduction, leading to U~IV! Precipitation as $UO_2(am)$, has been proposed as an alternative means of promoting U mineralization under industrial conditions. Bacteria like *Shewanella putrefaciens* are capable of dissimilatory U~VI reduction, in many cases obtaining energy for growth by coupling U~VI Reduction to the oxidation of organic carbon or H
- Some implementation problems like cost factor of designing the mask has not been calculated.

REFERENCES

- 1) www.wikipedia.org
- 2) <http://www.fuelcellknowledge.org/>
- 3) www.howthingswork.com
- 4) Elizabeth J.P. Phillips, Edward R. Landa and Derek R. Lovley, **Remediation of uranium contaminated soils with bicarbonate extraction and microbial U (VI) reduction**, Journal of Microbiology (1995), 14,203-207.
- 5) Johnson R. Haasa and Abraham Northup, **Effects of aqueous complexation on reductive precipitation of uranium by Shewanella putrefaciens**, 2004 American Institute of Physics
- 6) Transport Phenomena by Edwin N.Lightfoot
- 7) Bioprocess Engineering by Michael L. Shuler