NE250 Homework 1 **Mitch Negus**
9/22/2017

Problem 1

The number of molecules, N, found in a sample of a compound with mass M is

$$N(\cdot) = \frac{M(\cdot)N_A}{m(\cdot)}$$

where m is the molar mass of the compound, and N_A is Avogadro's number ($N_A = 6.022 \times 10^{23}$ molecules per mole). Where each actinide isotope is found only once in a molecule of its respective oxide, N also gives the number of atoms of an isotope in the sample.

To find N, we begin by finding the masses of the compounds in the fuel. We can decompose the total mass of the fuel, M_f, into its mixed oxide components:

$$M_f = M(\mathrm{UO_2}) + M(\mathrm{PuO_2}).$$

Given a weight percent for plutonium, w_P, we note that $w_\mathrm{U} = 1 - w_\mathrm{P}$ and so calculate the total masses of both the $\mathrm{UO_2}$ and the $\mathrm{PuO_2}$ to be

$$M(\mathrm{UO_2}) = (1 - w_\mathrm{P})M_f$$
$$M(\mathrm{PuO_2}) = w_\mathrm{P} M_f.$$

We are told that the uranium is all $^{238}\mathrm{U}$, so

$$M(^{238}\mathrm{UO_2}) = M(\mathrm{UO_2}) = (1 - w_\mathrm{P})M_f.$$

¡¡¡¡¡¡¡ HEAD The weight percents of the plutonium isotope oxides are also given (as a fraction of total plutonium oxide). Using $^{239}\mathrm{PuO_2}$ as an example

$$M(^{239}\mathrm{PuO_2}) = w_\mathrm{P9} M(\mathrm{PuO_2}) = w_\mathrm{P9} w_\mathrm{P} M_f.$$

Next, we must determine the molar masses of the various oxides. For uranium,

$$m(^{238}\mathrm{UO_2}) = m(^{238}\mathrm{U}) + 2m(\mathrm{O}),$$

and similarly for plutonium.

When we combine the total and molar masses to determine the total number of atoms for each isotope, we find:
6.69×10^{20} atoms of $^{238}\mathrm{U}$
4.65×10^{20} atoms of $^{239}\mathrm{Pu}$
1.45×10^{20} atoms of $^{240}\mathrm{Pu}$
3.84×10^{19} atoms of $^{241}\mathrm{Pu}$
1.78×10^{19} atoms of $^{242}\mathrm{Pu}$

(for full calculation, see Jupyter notebook, attached)

Problem 2

We use the

a.)

NE250_HW01_mnegus-notebook

September 16, 2017

1 NE 250 – Homework 1

9/22/2017

1.1 Problem 1

The number of molecules, N, found in a sample of a compound with mass M is

$$N(\cdot) = \frac{M(\cdot)N_A}{m(\cdot)}$$

where m is the molar mass of the compound, and N_A is Avogadro's number ($N_A = 6.022 \times 10^{23}$ molecules per mole). Since each actinide isotope is found only once in a molecule of its respective oxide, N also gives the number of atoms of an isotope in the sample.

```
In [1]: def molecule_count(M,m):
            N_A = 6.022e23
            N = M*N_A/m
            return N
```

To find N, we begin by finding the masses of the compounds in the fuel. We can decompose the total mass of the fuel, M_f, into its mixed oxide components:

$$M_f = M(\text{UO}_2) + M(\text{PuO}_2).$$

Given a weight percent for plutonium, w_P, we note that $w_\text{U} = 1 - w_\text{P}$ and so calculate the total masses of both the UO_2 and the PuO_2 to be

$$M(\text{UO}_2) = (1 - w_\text{P})M_f$$

$$M(\text{PuO}_2) = w_\text{P}M_f.$$

```
In [2]: w_p = 0.3
```

```
In [3]: def mass_oxide(w,M_f):
            M_oxide = w*M_f
            return M_oxide
```

The mass of the oxide component for a given isotope is given by

$$M(^i\mathrm{XO}_2) = w_i M(\mathrm{XO}_2)$$

where w_i is the weight percent of the oxide of isotope ^iX out of element X.

```
In [4]: def mass_isotope_oxide(w_i,M_oxide):
            M_i_oxide = w_i*M_oxide
            return M_i_oxide
```

```
In [5]: # Provided weight percents
        w = {'U238': 1, # all U is U238
             'Pu239': 0.697,
             'Pu240': 0.218,
             'Pu241': 0.058,
             'Pu242': 0.027
            }
```

Next, we must determine the molar masses of the various oxides. In general,

$$m(^i\mathrm{XO}_2) = m(^i\mathrm{X}) + 2m(\mathrm{O}),$$

```
In [6]: def molar_mass_isotope_oxide(m_i,m_o):
            m_i_oxide = m_i + 2*m_o
            return m_i_oxide
```

Finally, we use both the total mass of a compound with its molar mass in the original formula, using provided or tabulated values:

```
In [9]: # Tabulated molar masses [g/mol]
        m = {'U238':  238.051,
             'Pu239': 239.052,
             'Pu240': 240.054,
             'Pu241': 241.057,
             'Pu242': 242.059,
             'O16': 15.995
            }
```

```
In [10]: # Assume 1 gram of total fuel
         M_f = 1

         isotopes = ['U238','Pu239','Pu240','Pu241','Pu242']
         for i in isotopes:
             M_i_ox = mass_isotope_oxide(w[i],mass_oxide(w_p,M_f))
             m_i_ox = molar_mass_isotope_oxide(m[i],m['O16'])
             N = molecule_count(M_i_ox,m_i_ox)
             print(i,': ',N)
```

```
U238 :  6.690095207764747e+20
Pu239 :  4.645775193512445e+20
Pu240 :  1.4477025775242242e+20
Pu241 :  3.837537127307754e+19
Pu242 :  1.7799079726618233e+19
```