NE250_HW01_mnegus-prob1-ntbk

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1 NE 250 – Homework 1

1.1 Problem 1

9/22/2017

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:

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

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 UO_2 and the PuO_2 to be

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

```
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 [7]: # 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 [8]: # 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
```