

NE250_HW01_mnegus-notebook

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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 $w_U = 1 - w_P$ and so calculate the total masses of both the UO_2 and the PuO_2 to be

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

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

```
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

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

where w_i is the weight percent of the oxide of isotope ${}^i\text{X}$ 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,

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

```
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