

## JQ.2.5.soln

September 19, 2014

(2.5) Formaldehyde ( $CH_2O$ ) burns to completeness in air. Compute:

- (a) stoichiometric air to fuel mass ratio
- (b) mole fraction of fuel in the reactant mixture for an equivalence ratio ( $\phi$ ) of 2
- (c) mole fraction of fuel in the product mixture for  $\phi = 2$

In section 2.2, the text describes a complete reaction as one in which “the products are in their most stable state”. For hydrocarbon (i.e.,  $C_mH_n$ ) and alcohol (i.e.,  $C_mH_nOH$ ) fuels, the stable species are considered to be carbon dioxide ( $CO_2$ ) and water vapor ( $H_2O$ ). A stoichiometric reaction is one in which there is no fuel or oxygen on the product side.

Chemical reactions are typically written in a chemical notation that shows the reactants (often shown as the chemical species on the left hand side of the equation) and the products (chemical species on the right hand side). One very simple representation of a chemical reaction is the reaction:  $R \rightarrow P$  where  $R$  is the reactant chemical species and  $P$  is the product chemical species.

We can generalize this as  $\nu_f F + \nu_o Ox + \nu_d D \rightarrow \nu_p P + \nu_d D$

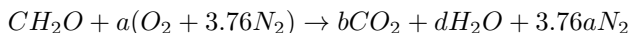
The  $\nu_i$  are called the stoichiometric coefficients or molar coefficients. F represents fuel, Ox represents oxygen, D represents diluent, and P represents products. A diluent is a chemical species that dilutes the chemical reaction process, but that does not play a significant part in the reaction chemical process. Note that equal moles of the diluent exist on the reactant and product sides of the equation. In most combustion and fire problems, the nitrogen in air is considered a diluent.

Before we can answer the questions in this problem, we need to define what we mean by air. Air is generally modeled in combustion and fire problems as a mixture of nitrogen and oxygen. We say that air is 79%  $N_2$  and 21%  $O_2$  by volume. We can describe this in terms of moles. One mole of anything represents a particular number of that thing. There are  $6.02 \times 10^{23}$  components in a mole. This is called Avogadro’s number. At standard temperature and pressure, a mole of gas occupies 22.3 liters. For one mole of oxygen ( $n_O = 1$ ) in air there are 3.76 moles ( $n_N = 3.76$ ) of nitrogen. Said differently 4.76 moles of air contain 1 mole of  $O_2$  and 3.76 moles of  $N_2$ .

Aside: we use the symbol  $X_i$  to denote the mole fraction of chemical species i. The mole fraction of oxygen in air is given by  $X_O = \frac{n_O}{n_O + n_N}$ . Confirm that  $1/4.76 = 0.21$ . The mole fraction is also the same as the volume fraction.

For the formaldehyde combustion we first need to balance the chemical reaction: example 2.1 in the text shows how to balance a chemical reaction by recognizing that elements are conserved between the reactant and product sides of the chemical reaction.

- a) Balance the chemical reaction using elemental balances:

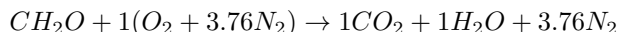


Find the stoichiometric coefficients a, b, & d.

C:  $1 = b$

H:  $2 = 2d$  or  $d = 1$

O:  $1 + 2a = 2b + d = 3$  or  $a = 1$



```
In [48]: b=1.; d=1.; a=1.;
```

the stoichiometric air to fuel ratio is  $A/F$  in which  $A$  is the mass of air and  $F$  is the mass of fuel.  $A = aM_O + 3.76aM_N$  in which  $M_i$  is the molecular weight of chemical species  $i$ . The fuel mass  $F = M_F$  since there is only one mole of fuel.

```
In [49]: M_O=32.0; M_N=28.; M_F_ST=12.+2.+16.; M_A=a*28.8*4.76; AFR_ST=M_A/M_F_ST;
```

```
In [50]: AFR_ST
```

```
Out[50]: 4.569599999999999
```

b) The equivalence ratio ( $\phi$ ) is the actual fuel to air ratio divided by the stoichiometric fuel to air ratio.

$$\phi = \frac{F/A}{F/A|_{ST}}$$

You calculated the stoichiometric air to fuel ratio in part (a). This is the reciprocal of the stoichiometric fuel to air ratio. To find the mole fraction, you will need to know the moles of fuel, oxygen, and nitrogen. It is easiest to assume that the moles of air are fixed and to compute the amount of fuel that would need to be added to the known amount of air.

```
In [51]: phi=2.; FAR=phi*AFR_ST; M_F=M_A*phi*AFR_ST**(-1.); nu_F=M_F/M_F_ST; X_F_RCT=nu_F/(nu_F+4.76*a
```

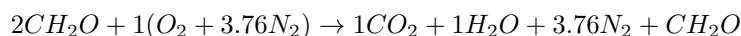
```
In [52]: X_F_RCT
```

```
Out[52]: 0.29585798816568054
```

```
In [53]: nu_F
```

```
Out[53]: 2.0000000000000004
```

c) To find the mole fraction of fuel in the product mixture, you can think about the amount of fuel in excess of the amount of fuel needed to consume the oxygen as diluent. Then you can carry this excess fuel to the product side.



```
In [54]: X_F_PROD=1/(1.+1.+3.76+1.);
```

```
In [55]: X_F_PROD
```

```
Out[55]: 0.14792899408284024
```

```
In [55]:
```