JQ.2.5.soln

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(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 (ϕ) 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 stocihiometric 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 ν_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 6.02×10^{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:

$$CH_2O + a(O_2 + 3.76N_2) \rightarrow bCO_2 + dH_2O + 3.76aN_2$$

Find the stoichiometric coefficients a, b,& d.

C: $1 = b$

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

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

$$CH_2O + 1(O_2 + 3.76N_2) \rightarrow 1CO_2 + 1H_2O + 3.76N_2$$

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

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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
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b) The equivalence ratio (ϕ) 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.

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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
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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.

$$2CH_2O + 1(O_2 + 3.76N_2) \rightarrow 1CO_2 + 1H_2O + 3.76N_2 + CH_2O$$

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

In [55]: X_F_PROD

Out[55]: 0.14792899408284024

In [55]:
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