ME 410 Day 7

Topics

- Combustion -- Why? (Other than it's the second word in the course title.)
- Fuels
- Air
- Basic Chemical Equations - Combustion of a Hydrocarbon
- Combustion of a Hydrocarbon in Air
- Examples

1. Combustion -- Why?

- Important in basic understanding of engine processes
- Important in creating models of engine processes, i.e. predictions of fuel conversion efficiency.
- Relates to the emissions issue
- Fun and interesting

In this course we will be very interested in finding the properties of the burned gas at the end of combustion.

As the power stroke begins, the burned gas is in a state of chemical equilibrium. There are techniques which allow us to predict its composition, based fuel and fuel air ratio.

When we know its composition, we can model it thermodynamically.

2. Fuels

These are described in Section 3.3. What's interesting is that gasoline and diesel fuel are very complex mixtures of hydrocarbons. Alternative fuels are also of importance.

3. Air

Also described in the same section. We take it to consist of oxygen and atmospheric nitrogen. I.e. all inert gases have their properties lumped together and are then called atmospheric nitrogen.

Dry air is taken to be 21% O_2 and 79% atmospheric N_2 by VOLUME. This means that the ratio of

$$\frac{\text{moles}\, N_2}{\text{moles}\, O_2} = \frac{79}{21} = 3.773$$

In this course we will keep the thermodynamics simple by working with dry air.

Here are two recipes for air:

$$.21 \text{ moles } O_2 \quad + \quad .79 \text{ moles } N_2 = 1 \text{ mole air}$$

$$1 \text{ mole } O_2 + 3.773 \text{ moles } N_2 = 4.773 \text{ moles air}$$

What's the molecular weight of air? The molecular weight of O2 is 32.00. The molecular weight of atmospheric nitrogen is 28.16.

Use the first of these two equations,

$$M_{air} = .21(32) + .79(28.16) = 28.962 \approx 29$$

Air is a mixture of ideal gases. This course will spend some amount of time studying and characterizing such mixtures.

Basic Chemical Equations

Let's review simple chemistry. We want a balanced equation for the combustion of a hydorcarbon. Let's pick C_8H_{18}, octane as an example.

What happens when we burn one mole of this stuff in pure oxygen?

$$C_8H_{18} + a\,O_2 = b\,CO_2 + c\,H_2O$$

We get

- water
- carbon dioxide

These are basic results of combustion.

Let's balance the species: C,O,H

$$8 = b$$

$$2a = 2b + c$$

$$18 = 2c$$

Solving find that a=12.5, b=8 and c=9. So it's going to take 12.5 moles of O_2 to burn (completely) one mole of C_8H_{18}.

Quick exercise:

How many moles of O_2 are needed in the combustion of propane, C_3H_8?

$$3 = b$$

$$2a = 2b + c$$

$$8 = 2c$$

Solving we find a = 5, also b = 3, c = 4.

What about the general hydrocarbon $C_\alpha H_\beta$?

$$C_\alpha H_\beta + a\,O_2 = b\,CO_2 + c\,H_2O$$

$$\alpha = b$$

$$2a = 2b + c$$

$$\beta = 2c$$

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> eq1 := alpha = b;
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$$eq1 := \alpha = b$$

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> eq2 := 2*a = 2*b+c;
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$$eq2 := 2\,a = 2\,b + c$$

```
> eq3 := beta = 2*c;
```

$$eq3 := \beta = 2\,c$$

```
> solve({eq1,eq2,eq3},{a,b,c});
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$$\{b = \alpha,\ a = \alpha + \frac{1}{4}\beta,\ c = \frac{1}{2}\beta\}$$

The interesting result is that for the general hydrocarbon, $C_\alpha H_\beta$, the number of moles of oxygen per mole of the fuel is

$$a_s = \alpha + \frac{\beta}{4}$$

The subscript “s” used with a stands for stoichiometric. It implies complete combustion with no excess oxygen or fuel left over.

Does burning in air change anything?

Not really.

$$C_{\alpha}H_{\beta} + a\,(O_2 + 3.773\,N_2) = b\,CO_2 + c\,H_2O + d\,N_2$$

$$\alpha = b$$

$$2a = 2b + c$$

$$\beta = 2c$$

$$3.773(2a) = 2d$$

The nitrogen is unaffected by combustion. We balance exactly as before, including

$$a_s = \alpha + \frac{\beta}{4}$$

The simple d=3.773 a_s gives the number of moles nitrogen in the exhaust per mole fuel.

Again, this was stoichiometric combustion, with the proportions of fuel and air (oxygen) mixed so that there will be a complete combustion. No excess of either fuel or oxygen.

Exercise

Some fuels, e.g. alcohol, are not simple hydrocarbons. They have formula $C_{\alpha}H_{\beta}O_{\gamma}$. Repeat the previous analysis for this case.

Calculating the Stoichiometric Fuel Air Ratio

Exercise: use propane. The previous result was a = 5, also b = 3, c = 4.

$$C_3H_8 + 5(O_2 + 3.773\,N_2) = 3CO_2 + 4H_2O + 18.865\,N_2$$

Five moles of air per mole of fuel. Next we need the molecular weights. For now, let air be 29 and propane be 44. The stoichiometric fuel air and air fuel ratios are:

$$(F/A)_s = \frac{1(44)}{5(29)} = 0.305 \quad \text{and} \quad A/F = 3.3$$

Mole Fractions in the Burned Gas

This is often an important thing to know. Continue the propane exercise.

For each mole of propane there will be 25.865 moles of burned products.

Mole fractions are

$$y_{CO_2} = \frac{3}{25.865} = 0.116$$

$$y_{H_2O} = \frac{4}{25.865} = 0.155$$

$$y_{N_2} = \frac{18.865}{25.865} = 0.729$$

Fuel Air Equivalence Ratio

It is possible to burn fuels with more or less air than stoichiometric.

This dimensionless number is used often in engine analysis. It is

$$\phi = \frac{(F/A)_{actual}}{(F/A)_s}$$

So for $\phi > 1$ we say we have a rich mixture. For $\phi < 1$ the mixture is lean.

Sometimes the term "excess air" is used. 100% excess air means that F/A is 1/2 stoichiometric so $\phi = 0.5$. etc.

In the next class we will talk about combustion when ϕ is not 1.

Exercise:

Gasoline might be represented by the chemical formula C_8H_{15}. We burn in dry air.

Questions to be answered

- How many moles of air are needed per mole of fuel?
- How many kg of air are needed per kg of fuel?
- A/F and F/A are...
- How many moles of product gas are produced per mole of fuel?
- How many moles of CO_2 are produced per mole of fuel?
- How many kg of CO_2 are produced per kg of air?
- How many kg of H_2O are produced per kg of fuel?
- What are the molar fractions of the various components of the exhaust gas?
- What is the effective molecular weight of the exhaust gas?