ME 410 Day 10

Topics

- Generalized method for computing low temperature combustion reaction - Lean
- Generalized method for computing low temperature combustion reaction - Rich
- Software implementation

1. Mixture of Fuel and Air - Hydrocarbon.

Start with one mole of fuel and the air used to burn it.

$$C_\alpha H_\beta + \frac{1}{\phi}\left(\alpha + \frac{\beta}{4}\right)(O_2 + \psi N_2)$$

where $\psi = 3.773$. Now divide by $\alpha$, let $y = \beta / \alpha$.

$$CH_y + \frac{1}{\phi}\left(1 + \frac{y}{4}\right)(O_2 + \psi N_2)$$

and let

$$\varepsilon = 1 \Big/ \left(1 + \frac{y}{4}\right) = \frac{4}{4+y} \quad \text{so} \quad y = \frac{4(1-\varepsilon)}{\varepsilon}$$

$$CH_y + \frac{1}{\phi\varepsilon}(O_2 + \psi N_2)$$

Now shift over to dealing with a reaction based on one mole of $O_2$. How? Simple, just divide by the coefficient of $O_2$.

$$\phi\varepsilon C + \phi\varepsilon H_y + (O_2 + \psi N_2)$$

or

$$\phi\varepsilon C + 2(1-\varepsilon)\phi H_2 + (O_2 + \psi N_2)$$

This is what we start with and use in balancing the molar equations.

2. Chemical Balance

The reaction of interest is

$$\phi\varepsilon C + 2(1-\varepsilon)\phi H_2 + (O_2 + \psi N_2) = n_{CO_2} CO_2 + n_{CO} CO$$

$$+ n_{H_2O} H_2O + n_{H_2} H_2$$

$$+ n_{O_2} O_2 + n_{N_2} N_2$$

We distinguish the two cases lean $(\phi < 1)$ (which we studied earlier) and rich $(\phi > 1)$.

3. Review of Lean

- $n_{CO} = 0$
- $n_{H_2} = 0$

By balancing C, H, O, and N the remaining molar unknowns are found. The text, in Table 4.3 “Burned gas composition under 1700K” has the answers in the first column.

$$n_{CO_2} = \varepsilon\phi \qquad n_{H_2O} = 2(1-\varepsilon)\phi$$

$$n_{O_2} = 1-\phi \qquad n_{N_2} = \psi$$

Total number of burned gas moles: $n_b = (1-\varepsilon)\phi + 1 + \psi$

4. Rich Mixture Burned Gas Composition

This is a bit more complex. We can assume

- $n_{O_2} = 0$

leaving 5 molar unknowns to be found. The 4 molar equations balancing C, H, O and N must be augmented with an additional relationship.

This relationship involves a subsidiary reaction which takes place between 4 of the products.

$$CO_2 + H_2 = CO + H_2O$$

A condition known as chemical equilibrium is assumed to exist. We will learn more about this later in our combustion studies. For now let me state the implication here.

$$K = \frac{n_{CO} n_{H_2O}}{n_{CO_2} n_{H_2}}$$

The equilibrium constant K is actually a function of temperature.

$$\ln(K) = 2.743 - \frac{1.761 \times 10^3}{T} - \frac{1.611 \times 10^6}{T^2} + \frac{0.2803 \times 10^9}{T^3}$$

(This is Equation 4.5 on page 104. We evaluate it at an appropriate burned gas temperature. Such as 1740 K where its value is 3.5)

What follows next is a bit of algebra. Let “c” stand for $n_{CO}$.

Here’s some Maple which shows the solution for the molar unknowns.

Carbon Balance Equation

```
> eq1 := epsilon*phi = n_CO2 + c;
```

$$eq1 := \varepsilon\,\phi = n\_CO2 + c$$

Hydrogen Balance Equation

```
> eq2 := 2*(1-epsilon)*phi = n_H2O + n_H2;
```

$$eq2 := 2\,(1-\varepsilon)\,\phi = n\_H2O + n\_H2$$

Oxygen Balance Equation

```
> eq3 := 1 = n_CO2 + 1/2*c + 1/2*n_H2O;
```

$$eq3 := 1 = n\_CO2 + \frac{1}{2}\,c + \frac{1}{2}\,n\_H2O$$

Nitrogen balance not needed. We solve these equations for the unknown molar quantities.

```
> s1 := solve({eq1,eq2,eq3},{n_CO2,n_H2,n_H2O});
```

$$s1 := \{n\_CO2 = \varepsilon\,\phi - c,\ n\_H2 = 2\,\phi - 2 - c,\ n\_H2O = 2 - 2\,\varepsilon\,\phi + c\}$$

Now to see how to get c we use the equilibrium equation. Find an expression which must be zero.

```
> ex := K*(n_CO2*n_H2)-(n_H2O * c);
```

$$ex := K\,n\_CO2\,n\_H2 - n\_H2O\,c$$

```
> ex1 := subs(s1,ex);
```

$$ex1 := K\,(\varepsilon\,\phi - c)\,(2\,\phi - 2 - c) - (2 - 2\,\varepsilon\,\phi + c)\,c$$

```
> ex2:=expand(ex1);
```

$$ex2 := 2\,K\,\varepsilon\,\phi^2 - 2\,K\,\varepsilon\,\phi - K\,\varepsilon\,\phi\,c - 2\,K\,c\,\phi + 2\,K\,c + K\,c^2 - 2\,c + 2\,\varepsilon\,\phi\,c - c^2$$

The following show the set up of equation 4.6 on page 104. It is a quadratic equation for c.

```
> quad := coeff(ex2,c,2);
```

$$quad := K - 1$$

```
> lin := coeff(ex2,c,1);
```

$$lin := -K\,\varepsilon\,\phi - 2\,K\,\phi + 2\,K - 2 + 2\,\varepsilon\,\phi$$

```
> const :=coeff(ex2,c,0);
```

$$const := 2\,K\,\varepsilon\,\phi^2 - 2\,K\,\varepsilon\,\phi$$

```
>
```

I.e. we get c by solving

$$(K-1)c^2 - \{K[2(\phi-1)+\varepsilon\phi] + 2(1-\varepsilon\phi)\}c + 2K\varepsilon\phi(\phi-1) = 0$$

If we are using EES the software handles the problem without having to write down this equation explicitly. The basic equation with K is enough.

5. Calculation of the Number of Moles of Fuel

To make it easier to see the balance equations, we have written the fuel as

$$\phi\varepsilon C + 2(1-\varepsilon)\phi H_2$$

(Again, this is per mole of $O_2$.) The actual fuel formula is $(CH_y)_\alpha$.

Now

$$M_f = \alpha(12 + y)$$

After some tedious algebra, which I don't give here we find an equivalent expression for the fuel term.

$$\left[\frac{4}{M_f}(1+2\varepsilon)\phi\right](CH_y)_\alpha$$

The term in square brackets is the number of moles of fuel per mole of oxygen, call it $n_f$.

6. What are we trying to do?

What's going on here is an effort to accurately model the gas in the cylinder just prior to the combustion process. We need to understand what this complicated mixture is composed of. Then we can progress towards calculation of thermodynamic properties.

To complicate things more, the mixture contains not only fresh air and fuel, but also burned gas left over from the previous combustion cycle.

Additionally, with EGR (Exhaust gas recycling) a percentage of the exhaust gas is mixed back in with the intake air to improve the emissions situation.

Let $x_b$ be the fraction of burned gas present in the charge. The formula for this charge is

$$\left\{\left[\frac{4}{M_f}(1+2\varepsilon)\phi\right](CH_y)_\alpha + O_2 + \psi N_2\right\}(1-x_b) +$$

$$x_b\left\{n_{CO_2}CO_2 + n_{CO}CO + n_{H_2O}H_2O + n_{H_2}H_2 + n_{O_2}O_2 + n_{N_2}N_2\right\}$$

If we substitute in the results obtained previously and organize them something like Table 4.4 will come out.

| Species | Lean Mixture | Rich Mixture |
|---|---|---|
| Fuel | $4(1-x_b)(1+2\varepsilon)\phi/M_f$ | $4(1-x_b)(1+2\varepsilon)\phi/M_f$ |
| $O_2$ | $1-x_b\ \phi$ | $1-x_b$ |
| $N_2$ | $\psi$ | $\psi$ |
| $CO_2$ | $x_b\varepsilon\phi$ | $x_b(\varepsilon\phi - c)$ |
| $H_2O$ | $2x_b\ (1-\varepsilon)\phi$ | $x_b\ [2(1-\varepsilon\phi)+c]$ |
| CO | 0 | $x_b\ c$ |
| $H_2$ | 0 | $x_b\ [2(\phi-1)+c]$ |

Finally

$$n_u = (1-x_b)\left\{\left[\frac{4}{M_f}(1+2\varepsilon)\phi\right] + 1 + \psi\right\} + x_b n_b$$

is the total number of moles in the unburned mixture with residual fraction $x_b$.

7. Molecular weights of these mixtures

Notice that the mass (not the number of moles) of the burned and unburned gas must be the same. Following the text notation, this mass is

$$m_{RP} = 4\phi(1+2\varepsilon)(1.00) + 1(32.0) + 28.16\psi$$

Then the molecular weight of the burned mixture is

$$M_b = \frac{m_{RP}}{n_b}$$

and the molecular weight of the unburned mixture is

$$M_u = \frac{m_{RP}}{n_u}$$

Software Implementation

- Combustion Stoichiometry at CSU website. This is just concerned with the products of combustion.
- EES - please see courseware section on website. There are two text files which can be pasted into EES. One is for the lean case and one for the rich case. These not only have the products of combustion, but a chemical analysis of the unburned gas as well taking into account the residual fraction.