Today, we will:

- Discuss **Stoichiometric Combustion**, using **Methane** as an example
- Discuss how to generate **Emission Factors** from combustion analysis
- Do some example problems

Stoichiometric Combustion:

Consider **stoichiometric combustion** of a fuel. Let's use **methane** as our example fuel.

Definition: **Stoichiometric Combustion** (or **Ideal Combustion**) means that every kmol of carbon (C) in the (combusted) fuel produces one kmol of CO_2 in the exhaust.

Example: *EF*s from stoichiometric combustion of natural gas

Given: Methane is burned in simple dry air.

To do: Solve for the molar coefficients, assuming stoichiometric combustion.

Solution: Assumptions and Approximations:

- Assume ideal or stoichiometric combustion, meaning that *all* the carbon in the fuel gets converted to carbon dioxide in the combustion gases (exhaust gases).
- Assume **simple air** (also called **simple dry air**): 21% O_2, 79% N_2 by volume or by mol. So we write the chemical equation as follows:

$$\underset{\uparrow}{CH_4} + \underbrace{a(O_2 + \overset{\checkmark}{3.76}\, N_2)}_{air} \rightarrow \underset{\uparrow}{b}CO_2 + cH_2O + dN_2$$

$$\frac{n_{N_2}}{n_{O_2}} = \frac{79}{21} = 3.76$$

Calc coeffs:

$C \rightarrow 1 = b \quad \boxed{b=1}$

$H \rightarrow 4 = 2c \quad \boxed{c=2}$

$O \rightarrow 2a = 2b + c = 2+2 = 4 \rightarrow \boxed{a=2}$

$N \rightarrow 2(3.76\, a) = 2d \rightarrow d = 3.76\, a$

$\boxed{d = 7.52}$

Final chemical equation for stoichiometric combustion of methane and simple dry air:

$$\boxed{CH_4 + 2(O_2 + 3.76\, N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2}$$

Notice that *all* the carbon in the fuel is converted to carbon dioxide in the products.

Estimating Combustion EFs from Basic Chemistry:

Example: *EF*s from combustion of natural gas (assume it is all methane)

Given: Natural gas is burned in a power plant. There is no APCS. Exhaust gases go up the stack at $T = 500$ K and $P = 100$ kPa.

GW gas CO_2

(a) To do: Assuming stoichiometric combustion, estimate the mol fraction, mass fraction, mass concentration, and molar concentration of CO_2 going up the stack.

(b) To do: Estimate (from first principles and chemistry) the *EF* of CO_2 emitted by burning methane, and compare with EPA's published *EF*s for burning natural gas (NG).

Solution (continued from last class): We had,

Chemical equation:

$$CH_4 + 2(O_2 + 3.76\,N_2) \rightarrow \overbrace{\underset{b}{CO_2} + \underset{c}{2H_2O} + \underset{d}{7.52N_2}}^{\text{exh.}} \qquad \text{Stoich.}$$

Notice that *all* the carbon in the fuel is converted to carbon dioxide in the products.

(a) Estimate mol fraction ✓, mass fraction, mass concentration, and molar concentration of CO_2 going up the stack. *Note*: The exhaust going up the stack includes *all* the combustion products on the right side of the chemical equation, i.e., CO_2, H_2O, and N_2.

- $y_{CO_2} = \frac{n_{CO_2}}{n_t} = \frac{b}{b+c+d} = \frac{1}{1+2+7.52} = 0.09506$

(mol fraction)

$$\therefore \boxed{y_{CO_2} = 95{,}100 \text{ PPM}} \quad ☆$$

- Mass fraction of CO_2

recall $$\boxed{f_{CO_2} = \frac{m_{CO_2}}{m_t}} = \frac{n_{CO_2} M_{CO_2}}{n_t M_t} = y_{CO_2} \frac{M_{CO_2}}{M_t}$$

where $$\boxed{M_t = \sum (y_j M_j)}$$

$$\boxed{f_{CO_2} = 0.151 \frac{\text{kg } CO_2}{\text{kg exhaust}}}$$

★ Do the rest of Part (a) on your own for practice

$$\boxed{C_{CO_2} = 0.101 \frac{kg}{m^3}}$$

$$\boxed{C_{molar,CO_2} = 0.00229 \frac{kg}{m^3}}$$

Error in the video. This should be kmol not kg.

(b) Estimate (from first principles and chemistry) the *EF* (emission factor) of CO_2 emitted by burning methane, and compare with EPA's published *EF*s for burning natural gas (NG).

Solution:

- First, we define ***our*** *EF* as the mass of CO_2 emitted per mass of fuel burned.

$$\boxed{EF = \frac{m_{CO_2}}{m_{CH_4}}}$$

- The key is that for **stoichiometric combustion**, **every kmol of methane fuel emits one kmol of CO_2 into the atmosphere**. Thus,

$$EF = \frac{m_{CO_2}}{m_{CH_4}} = \frac{n_{CO_2} M_{CO_2}}{n_{CH_4} M_{CH_4}} = \frac{M_{CO_2}}{M_{CH_4}} = \frac{44.0095 \text{ kg CO}_2/\text{kmol}}{16.04246 \text{ kg CH}_4/\text{kmol}}$$

$$= 2.7433 \frac{\text{kg CO}_2}{\text{kg CH}_4}\left(\frac{1000 \text{ kg CH}_4}{\text{Mg CH}_4}\right) = 27433 \frac{\text{kg CO}_2}{\text{Mg CH}_4}$$

- So, our estimated *EF* is $\boxed{EF = 2740 \frac{\text{kg CO}_2}{\text{Mg CH}_4}}$. Call this $(EF)_{ours}$ $\boxed{(EF)_{ours} = 2740 \frac{\text{kg CO}_2}{\text{Mg CH}_4}}$

- Let's look up and compare EPA's published EFs for burning natural gas. I found 3:

$\boxed{EF = 53 \frac{\text{kg CO}_2}{\text{thousand SCF NG}}}$ and $\boxed{EF = 120{,}000 \frac{\text{lbm CO}_2}{10^6 \text{ SCF NG}}}$ and $\boxed{EF = 1135 \frac{\text{lbm CO}_2}{\text{MW-hr elec}}}$

- Problem: EPA's published *EF*s and our *EF* are in different units. We must convert!

OUR EF is $\dfrac{\text{mass of CO}_2}{\text{mass of fuel}}$

EPA's (First & Second) EF is $\dfrac{\text{mass of CO}_2}{\text{Volume of fuel}}$

To convert, multiply our EF by $\dfrac{\text{mass of fuel}}{\text{volume of fuel}} = \rho_{fuel}$

$$P = \rho R T = \rho \frac{R_u}{M} T \rightarrow \boxed{\rho = \frac{PM}{R_u T}}$$

(P & T of exhaust)

EPA uses SCF of fuel

$$(EF)_{\text{ours in EPA's units}} = (EF)_{\text{ours}} * \rho_{\text{SCF of the fuel}}$$

$$\boxed{(EF)_{\text{ours in EPA's units}} = (EF)_{\text{ours}} * \frac{P\,M_{\text{fuel}}}{R_u T}}$$

$$(EF)_{\substack{\text{ours in}\\ \text{EPA's units}}} = \left(2743.38\,\frac{\boxed{\text{kg CO}_2}}{\cancel{\text{Mg fuel}}}\right)\frac{\left(\overset{P_{SATP}}{101.325}\,\frac{\cancel{\text{kN}}}{\cancel{\text{m}^2}}\right)\left(16.043\,\frac{\cancel{\text{kg}}}{\cancel{\text{kmol}}}\right)}{\left(8.314\,\frac{\cancel{\text{kJ}}}{\cancel{\text{kmol}\cdot\text{K}}}\right)\left(\underset{T_{SATP}}{298.15}\,\cancel{\text{K}}\right)}\cdot\left(\frac{\cancel{\text{kJ}}}{\cancel{\text{kN}\cdot\text{m}}}\right)\cdot\left(\frac{0.3048\,\cancel{\text{m}}}{\cancel{\text{ft}}}\right)^3\left(\frac{1\,\cancel{\text{Mg}}}{1000\,\cancel{\text{kg}}}\right)\left(\frac{1000\,\cancel{\text{ft}^3}}{\boxed{\text{"thousand SCF"}}}\right)$$

$$\boxed{(EF)_{\text{ours in EPA's units}} = 50.9\,\frac{\text{kg CO}_2}{\text{thousand SCF of fuel}}}$$

$$\boxed{(EF)_{\text{EPA (\#1)}} = 53\,\frac{\text{kg CO}_2}{\text{thousand SCF of NG}}}$$

Reasons for diff.

- we use methane, EPA uses NG
- we assumed stoichiometric combustion (but real life is not ideal)

EPA's 2nd EF:

$$\boxed{(EF)_{\text{ours in EPA's units}} = 112{,}000\,\frac{\text{lbm CO}_2}{\text{million SCF fuel}}}$$

EPA's value

~~110,000~~

120,000

Now let's look at the *third* EF from EPA, and $\boxed{EF = 1135 \frac{\text{lbm CO}_2}{\text{MW-hr elec}}}$.

Notice the denominator – this is perhaps a more practical EF for power plants because we typically know how much electrical power is being produced by the power plant, so this *EF* provides a quick estimate of how much CO_2 is emitted for a power plant that burns methane.

First convert to kg instead of lbm: $EF = 1135 \frac{\text{lbm CO}_2}{\text{MW-hr elec}} \left(\frac{1 \text{ kg}}{2.204 \text{ lbm}} \right) = 514.83 \frac{\text{kg CO}_2}{\text{MW-hr elec}}$

Let's call this the third $(EF)_{\text{EPA}}$ → $\boxed{(EF)_{\text{EPA}} = 514.83 \frac{\text{kg CO}_2}{\text{MW-hr elec}}}$

Compare to our previous estimate $(EF)_{\text{ours}}$ from Part (b) → $\boxed{(EF)_{\text{ours}} = 2743.3 \frac{\text{kg CO}_2}{\text{Mg CH}_4}}$.

But how to compare these two *EF*s with such drastically different denominators?

The key here is to take into account the ***overall power plant efficiency***, which is typically less than 40% for a standard power plant producing electricity.

We define the power plant efficiency as

$$\boxed{\eta_{\text{plant}} = \frac{\text{actual power produced}}{\text{maximum possible power produced}} \quad \text{or} \quad \eta_{\text{plant}} = \frac{\text{actual energy produced}}{\text{maximum possible energy produced}}}$$

To do: Estimate the overall power plant efficiency (%) that EPA assumed in order to obtain the above emission factor that we call $(EF)_{\text{EPA}}$.

Solution: HHV = higher heating value of methane

☆ HHV = maximum energy you can get by burning a unit mass of fuel

Look up for methane $\boxed{HHV = 55.5 \frac{\text{MJ}}{\text{kg of fuel}}}$

$$\boxed{\text{Max. possible energy} = (HHV)(m_{\text{fuel}})} \quad (1)$$

Our estimate of EF assumes 100% efficiency

$$\text{Our } (EF)_{\text{ours}} = 2743.3 \frac{\text{kg of CO}_2 \text{ emitted}}{\text{Mg of methane burned}}$$

$$\boxed{m_{CO_2\text{ emitted}} = (EF)_{avg} \cdot m_{fuel} \quad \text{@ max possible efficiency} \quad (2)}$$

$$\downarrow$$

Combine (1) & (2)

$$(2) \rightarrow \quad m_{fuel} = \frac{m_{CO_2\text{ emitted}}}{(EF)_{avg}}$$

$$(1) \rightarrow \quad \text{max possible energy} = (HHV)(m_{fuel})$$

$$\boxed{\text{max possible energy} = HHV \cdot \frac{m_{CO_2\text{ emitted}}}{(EF)_{avg}}} \quad (3)$$

But EPA's EF is

$$(EF)_{EPA} = \frac{m_{CO_2\text{ emitted}}}{\text{MW}\cdot\text{h of elec}}$$

ACTUAL ELEC. ENERGY GENERATED (includes η)

$$\therefore \quad \boxed{\text{actual energy generated} = \frac{m_{CO_2\text{ emitted}}}{(EF)_{EPA}}} \quad (4)$$

Finally combine (3) & (4) and our above definition of η_{plant} to calculate η_{plant}

$$\therefore \quad \eta_{plant} = \frac{\overset{\text{Eq(4)}}{\text{actual energy}}}{\underset{\text{Eq(3)}}{\text{max possible energy}}} = \frac{\cancel{m_{CO_2}}}{(EF)_{EPA}} \cdot \frac{(EF)_{avg}}{(HHV)(\cancel{m_{CO_2}})}$$

$$\boxed{\eta_{plant} = \frac{(EF)_{avg}}{(EF)_{EPA} \cdot HHV}}$$

ANSWER IN VARIABLE FORM

Final answer: The answer (in variable form) is $\boxed{\eta_{\text{plant}} = \frac{(EF)_{\text{ours}}}{(EF)_{\text{EPA}} \cdot HHV}}$.

Now we plug in the numbers to get the final numerical answer, being very careful of units!

Plug in $\boxed{(EF)_{\text{EPA}} = 514.83 \frac{\text{kg CO}_2}{\text{MW-hr elec}}}$ $\boxed{(EF)_{\text{ours}} = 2743.3 \frac{\text{kg CO}_2}{\text{Mg CH}_4}}$ $\boxed{HHV = 55.5 \frac{\text{MJ}}{\text{kg CH}_4}}$:

$$\eta_{plant} = \left(\frac{2743.3 \text{ kg CO}_2}{\text{Mg CH}_4}\right)\left(\frac{\text{MW}\cdot\text{h elec}}{514.83 \text{ kg CO}_2}\right)\left(\frac{\text{kg CH}_4}{55.5 \text{ MJ}}\right)\underbrace{\left(\frac{1 \text{ Mg CH}_4}{1000 \text{ kg CH}_4}\right)\left(\frac{\text{MJ}}{\text{s}\cdot\text{MW}}\right)\left(\frac{3600 \text{ s}}{\text{h}}\right)}_{\text{conv.}}$$

$$= 0.346$$

$$\boxed{\eta_{plant} = 34.6\%}$$