

**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<sub>2</sub> in the exhaust.

**Example: EFs from stoichiometric combustion of natural gas**

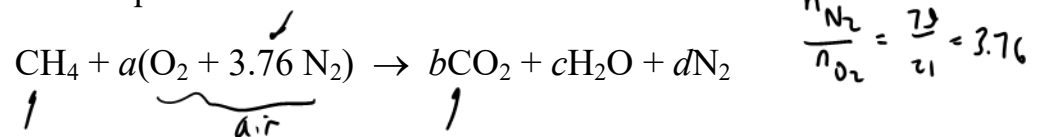
**Given:** Methane is burned in simple dry air.

**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<sub>2</sub>, 79% N<sub>2</sub> by volume or by mol.

So we write the chemical equation as follows:



Calc. coeffs:

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

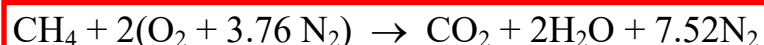
$$\text{H} \rightarrow 4 = 2c \quad \boxed{c=2}$$

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

$$\text{N} \rightarrow 2(3.76 a) = 2d \rightarrow d = 3.76 a$$

$$\boxed{d=7.52}$$

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



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

## Estimating Combustion EFs from Basic Chemistry:

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

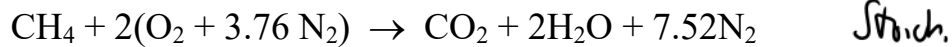
**Given:** Natural gas is burned in a power plant. There is no APCS. Exhaust gases go up the stack at  $T = 500$  K and  $P = 100$  kPa.

**(a) To do:** Assuming stoichiometric combustion, estimate the <sup>GW g<sub>W</sub> CO<sub>2</sub></sup> mol fraction, mass fraction, mass concentration, and molar concentration of CO<sub>2</sub> going up the stack.

**(b) To do:** Estimate (from first principles and chemistry) the EF of CO<sub>2</sub> emitted by burning methane, and compare with EPA's published EFs for burning natural gas (NG).

**Solution** (continued from last class): We had,

Chemical equation:



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<sub>2</sub> 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<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub>.

$$y_{\text{CO}_2} = \frac{n_{\text{CO}_2}}{n_t} = \frac{b}{b+c+d} = \frac{1}{1+2+7.52} = 0.09506$$

(mol fraction)

$$\therefore y_{\text{CO}_2} = 95,100 \text{ ppm} \quad \star$$

• Mass fraction of CO<sub>2</sub>

$$\text{result} \quad f_{\text{CO}_2} = \frac{m_{\text{CO}_2}}{m_t} = \frac{n_{\text{CO}_2} M_{\text{CO}_2}}{n_t M_t} = y_{\text{CO}_2} \frac{M_{\text{CO}_2}}{M_t}$$

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

$$f_{\text{CO}_2} = 0.151 \frac{\text{kg CO}_2}{\text{kg exhaust}}$$

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



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

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

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

(b) Estimate (from first principles and chemistry) the *EF* (emission factor) of CO<sub>2</sub> 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<sub>2</sub> emitted per mass of fuel burned.

$$EF = \frac{m_{\text{CO}_2}}{m_{\text{CH}_4}}$$

- The key is that for **stoichiometric combustion**, **every kmol of methane fuel emits one kmol of CO<sub>2</sub> into the atmosphere**. Thus,

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

$$= 2.7433 \frac{\text{kg CO}_2}{\text{kg CH}_4} \left( \frac{1000 \text{ kg CH}_4}{\text{Mg CH}_4} \right) = 2743.3 \frac{\text{kg CO}_2}{\text{Mg CH}_4}$$

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

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

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

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

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

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

To convert,

multiply our EF by  $\frac{\text{mass of fuel}}{\text{Volume of fuel}}$

$$P = \rho R T = \rho \frac{R_u}{M} T \rightarrow \boxed{\rho = \frac{P \cdot M}{R_u T}} \quad (P, T \text{ of exhaust})$$

EPA uses SCF of fuel

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

$$(EF)_{\text{our in EPA's units}} = (EF)_{\text{our}} * \frac{PM_{\text{fuel}}}{R_u T}$$

$$(EF)_{\text{our in EPA's units}} = \left( 2743.38 \frac{\text{kg CO}_2}{\text{Mg fuel}} \right) \frac{\left( 101.325 \frac{\text{kPa}}{\text{m}^2} \right) \left( 16.043 \frac{\text{kg}}{\text{kmol}} \right)}{\left( 8.314 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}} \right) \left( 298.15 \text{ K} \right)} \cdot \left( \frac{\text{kJ}}{\text{kmol}} \right)$$

$P_{\text{SAT}}$   $T_{\text{SAT}}$

$$\left( \frac{0.3048 \text{ m}}{\text{ft}} \right)^3 \left( \frac{1 \text{ Mg}}{1000 \text{ kg}} \right) \left( \frac{1000 \text{ ft}^3}{\text{"thousand SCF"}} \right)$$

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

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

Reasons for diff.

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

EPA's 2<sup>nd</sup> EF:

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

EPA's value

~~110,000~~

120,000

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

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<sub>2</sub> 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)<sub>EPA</sub> →  $(EF)_{\text{EPA}} = 514.83 \frac{\text{kg CO}_2}{\text{MW-hr elec}}$

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

**But how to compare these two EFs 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

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

**To do:** Estimate the overall power plant efficiency (%) that EPA assumed in order to obtain the above emission factor that we call (EF)<sub>EPA</sub>.

**Solution:**

HHV = higher heating value of methane

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

Look up for methane

$$\boxed{\text{HHV} = 55.5 \frac{\text{MJ}}{\text{kg of fuel}}}$$

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

(1)

Our estimate of EF at 100% efficiency

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

$$m_{\text{CO}_2 \text{ emitted}} = (EF)_{\text{avg}} \cdot m_{\text{fuel}} \quad \text{@ max possible efficiency} \quad (2)$$

Combine (1) & (2)

$$(2) \rightarrow m_{\text{fuel}} = \frac{m_{\text{CO}_2 \text{ emitted}}}{(EF)_{\text{avg}}}$$

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

$$\text{max possible energy} = \text{HHV} \cdot \frac{m_{\text{CO}_2 \text{ emitted}}}{(EF)_{\text{avg}}} \quad (3)$$

But EPA's EF is  $(EF)_{\text{EPA}} = \frac{m_{\text{CO}_2 \text{ emitted}}}{\text{MW} \cdot \text{h of elec}}$

ACTUAL ELEC. ENERGY GENERATED (includes  $\eta$ )

$$\therefore \text{actual energy generated} = \frac{m_{\text{CO}_2 \text{ emitted}}}{(EF)_{\text{EPA}}} \quad (4)$$

Finally combine (3) & (4) and our above definition of  $\eta_{\text{plant}}$  to calculate  $\eta_{\text{plant}}$

$$\therefore \eta_{\text{plant}} = \frac{\text{actual energy} \quad \text{Eq (4)}}{\text{max possible energy} \quad \text{Eq (3)}} = \frac{\cancel{m_{\text{CO}_2}} \cdot (EF)_{\text{avg}}}{(EF)_{\text{EPA}} \cdot (\text{HHV})(\cancel{m_{\text{CO}_2}})}$$

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

ANSWER IN VARIABLE FORM

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

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

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

$$\eta_{\text{plant}} = \left( \frac{2743.3 \text{ kg CO}_2}{\text{Mg CH}_4} \right) \left( \frac{\text{MW-hr elec}}{514.83 \text{ kg CO}_2} \right) \left( \frac{\text{kg CH}_4}{55.5 \text{ MJ}} \right) \underbrace{\left( \frac{1 \text{ Mg CH}_4}{1000 \text{ kg CH}_4} \right) \left( \frac{\text{MJ}}{5 \text{ MW}} \right) \left( \frac{3600 \text{ s}}{\text{h}} \right)}_{\text{conv.}}$$

$$= 0.346$$

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