Today, we will:

• Continue example problem from last time – EFs from combustion chemistry
• Do some example problems
• If time, discuss *equivalence ratio* for combustion

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

*Given:* Natural gas is burned in a power plant. There is no APCS. Exhaust gases go up the stack at \(T = 500\, \text{K}\) and \(P = 100\, \text{kPa}\).

(a) **To do:** Estimate the mol fraction, mass fraction, mass concentration, and molar concentration of CO\(_2\) going up the stack. Give all answers to 3 significant digits.

(b) **To do:** Estimate (from first principles and chemistry) the EF of CO\(_2\) 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:

\[
\text{CH}_4 + a(\text{O}_2 + 3.76\, \text{N}_2) \rightarrow b\text{CO}_2 + c\text{H}_2\text{O} + d\text{N}_2
\]

Solve for the molar coefficients: \(a = 2, b = 1, c = 2, d = 3.76a = 7.52\). So, the equation is

\[
\text{CH}_4 + 2(\text{O}_2 + 3.76\, \text{N}_2) \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 7.52\text{N}_2
\]

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

(a) Now calculate *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\(_2\)O, and N\(_2\).
(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.

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

- The key is that for **stoichiometric combustion**, every kmol of methane fuel emits one kmol of CO$_2$ into the atmosphere. Thus,

$$EF = \frac{m_{\text{CO}_2}}{m_{\text{CH}_4}} = \frac{n_{\text{CO}_2} M_{\text{CO}_2}}{n_{\text{CH}_4} M_{\text{CH}_4}} = 44.0095 \frac{1000 \text{ kg CH}_4}{16.04246 \text{ Mg CH}_4}$$

$$= 2.740 \frac{\text{kg CO}_2}{\text{kg CH}_4} \left( \frac{1000 \text{ kg CH}_4}{\text{Mg CH}_4} \right) = 2740 \frac{\text{kg CO}_2}{\text{Mg CH}_4}$$

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

- 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:
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\(_2\) 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 \((EF)_{EPA}\) → \((EF)_{EPA} = 514.83 \frac{\text{kg CO}_2}{\text{MW-hr elec}}\).

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

**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 \((EF)_{EPA}\).

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

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

Plug in $\begin{align*}
(EF)_{\text{EPA}} &= 514.83 \frac{\text{kg CO}_2}{\text{MW-hr elec}} \\
(EF)_{\text{ours}} &= 2743.3 \frac{\text{kg CO}_2}{\text{Mg CH}_4} \\
\text{HHV} &= 55.5 \frac{\text{MJ}}{\text{kg CH}_4}
\end{align*}$.
Equivalence ratio:
Consider the chemical equation above for burning a fuel, like methane,
\[ \text{CH}_4 + a(\text{O}_2 + 3.76 \text{ N}_2) \rightarrow b\text{CO}_2 + c\text{H}_2\text{O} + d\text{N}_2 \]

Notation:
- \( a = \text{actual} \) molar coefficient: molar coefficient \( a \) in the combustion chemical equation \((a\) is not necessarily the \textit{stoichiometric} value – can be smaller or larger than \( a_{\text{stoich}} \)).
- \( a_{\text{stoich}} = \text{stoichiometric} \) molar coefficient: molar coefficient \( a \) in the combustion chemical equation that leads to exact stoichiometric balance, or \textit{ideal combustion}. Again, this means that \textit{all} the carbon in the fuel gets converted to carbon dioxide in the combustion gases (exhaust gases).
- \((F/A)_n = \text{molar fuel-to-air ratio} = \frac{\text{(# mols of fuel)}}{\text{( # mols of air)}} = 1/a.\)
  - \((F/A)_n = \text{actual molar fuel-to-air ratio} = 1/a.
  - \((F/A)_{n, \text{stoich}} = \text{stoichiometric molar fuel-to-air ratio} = 1/ a_{\text{stoich}}.\)

Equivalence ratio \( \Phi \) is defined as the ratio of the \textit{actual} fuel/air ratio to the \textit{stoichiometric} fuel/air ratio.

\[
\text{Equivalence ratio} = \Phi = \frac{(F/A)_{n}}{(F/A)_{n, \text{stoich}}} = \frac{1/a}{1/a_{\text{stoich}}} = \frac{a_{\text{stoich}}}{a}
\]

- If \( \Phi = 1 \), the combustion is \textit{stoichiometric}.
- If \( \Phi < 1 \), the combustion is \textit{lean} (there is excess air).
- If \( \Phi > 1 \), the combustion is \textit{rich} (there is too much air, and incomplete combustion).