

Today, we will:

- Continue our discussion about emission factors (EFs) and do some example problems
- Discuss how to *calculate*, *estimate*, and *measure* EFs

Example: EFs and APCS (Air Pollution Control System)

Given: A steel plant produces 820 Mg of steel per day using a basic oxygen furnace (BOF). Fumes are cleaned with an electrostatic precipitator before going up the stack. Measurements of the stack exhaust show that 32 kg of particulate matter are emitted per day.

To do: Calculate the overall efficiency of the APCS as a percentage (to 3 digits). E

Solution: First we look up the EF of particle emissions in a BOF: EF = 14.25 kg/Mg.

• With NO APCS, estimate emission = $\frac{14.25 \text{ kg}}{\text{Mg}} \left(820 \frac{\text{Mg}}{\text{day}} \right) = 11,685 \frac{\text{kg}}{\text{day}}$

Actual emission = 32 kg/day

$E = \text{efficiency} = \text{removal efficiency of APCS}$

$$\dot{m}_d = (1 - E) \dot{m}_g \rightarrow E = 1 - \frac{\dot{m}_d}{\dot{m}_g} = 1 - \frac{32}{11,685} = 0.99726$$

99.7%

How to estimate EFs

- VOCs from paint, varnish, etc. → easy

typical oil-based paint has

- pigments
- solvent (VOC) (e.g. toluene)
- other stuff

typ ~ 1/2
by mass

All the solvent goes into the atmosphere

e.g. 1 Mg of paint we emit 0.5 Mg of VOC ≈ 500 kg

product $EF = 500 \frac{\text{kg VOC}}{\text{Mg paint}}$

Compare to EFs published

$EF = 560 \frac{\text{kg}}{\text{Mg}}$ for paint

Estimating EFs from Basic Chemistry

Example: EFs from combustion of natural gas

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 $P = 100\text{ kPa}$.

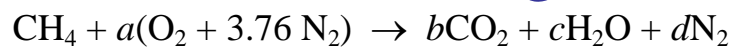
(a) To do: Estimate the mol fraction, mass fraction, mass concentration, and molar concentration of CO_2 going up the stack. Give all answers to 3 significant digits.

(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: Assumptions and Approximations:

- Assume NG is mostly methane CH_4 . For simplicity, let's assume it is 100% methane.
- 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.

(a) Chemical equation:



N_2 goes along for the ride

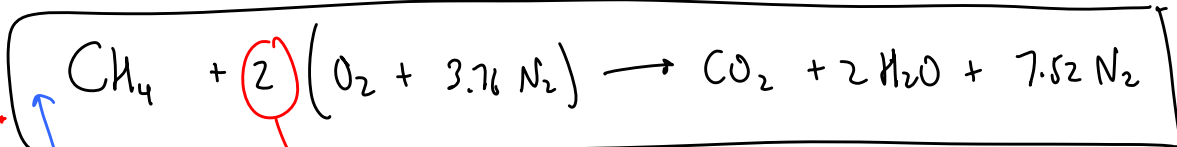
Solve for the molar coefficients:

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

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

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

$$\text{N: } 2(3.76)a = 2d \rightarrow \boxed{d=7.52}$$



★ Ideal combustion

$a_{\text{stich}} = 2$

let a_{stich} = coeff. a in the chem. eq. that leads to stoichiometric balance

In real life, not ideal comb.

$$\text{Define } (F/A)_n = \text{molar fuel-to-air ratio} = \frac{\# \text{ mols fuel}}{\# \text{ mols air}} = \frac{1}{a}$$

molar fuel-air ratio

$$\Phi = \text{Equivalence Ratio} = \frac{(F/A)_n \text{ actual}}{(F/A)_n \text{ stich}} = \frac{\frac{1}{a}}{\frac{1}{a_{\text{stich}}}}$$

3 cases:

a) $a = a_{\text{stoich}} \rightarrow$ IDEAL COMBUSTION

$$\boxed{\Phi = 1} \quad (F/A)_n = (F/A)_{n, \text{stoich}}$$

b) $\overset{\text{actual}}{a} > a_{\text{stoich}} \rightarrow$ excess air
LEAN COMBUSTION

$$\boxed{\Phi < 1} \quad (F/A)_n < (F/A)_{n, \text{stoich}}$$

get additional comb. products eg $\text{CO}, \text{NO}, \text{NO}_2$, soot
alcohol, aldehydes
unburned HC

c) $a < a_{\text{stoich}} \rightarrow$ excess fuel
RICH COMBUSTION

$$\boxed{\Phi > 1} \quad \text{— get additional comb. products}$$

$$y_{\text{CO}_2} = \frac{n_{\text{CO}_2}}{n_t} = \frac{b}{b+c+d} = \frac{\# \text{ mols of CO}_2}{\text{total \# mols}} \quad \text{in exhaust gases}$$

(In comb. products)

$$\frac{1}{1+(2)+7.52} = \frac{y_{\text{CO}_2}}{0.095057}$$

$$\boxed{y_{\text{CO}_2} = 95,100 \text{ ppm}}$$

Calculate RH in % of the exhaust

$P = 100 \text{ kPa}$
 $T = 500 \text{ K} \rightarrow$ look up $P_{v, \text{H}_2\text{O}} = 2669.4 \text{ kPa}$

$$\text{RH} = \frac{P_{\text{H}_2\text{O}}}{P_{v, \text{H}_2\text{O}}} \times 100\%$$

$$\frac{y_{\text{H}_2\text{O}}}{b+c+d} = \frac{P_{\text{H}_2\text{O}}}{P_{\text{atm}}}$$

$$\frac{c}{b+c+d} = \frac{2}{1+2+7.52}$$

$$\text{RH} = \frac{\left(\frac{c}{b+c+d}\right) P_{\text{atm}}}{P_{v, \text{H}_2\text{O}}} \times 100\% \rightarrow \frac{\frac{2}{10.52} (100 \text{ kPa})}{2669.4 \text{ kPa}} \times 100\% = \boxed{0.712\%}$$

• mass fraction of CO_2 $f_j = \frac{m_j}{m_t} = \frac{n_j M_j}{n_t M_t} = y_j \frac{M_j}{M_t}$

Atomic mass

C 12.0107

O 15.9994

H 1.00794

N 14.00674

$$M_t = \sum (y_j M_j)$$

$M_t = \left(\frac{b}{b+c+d} \right) (44.0095) + \left(\frac{c}{b+c+d} \right) (18.0153) + \left(\frac{d}{b+c+d} \right) (28.01348) = 27.6332 \frac{\text{kg}}{\text{kmol}}$

↓
of the exhaust gases

CO_2 H_2O N_2

f_j for $\text{CO}_2 \rightarrow f_{\text{CO}_2} = y_{\text{CO}_2} \frac{M_{\text{CO}_2}}{M_t} = (0.095057) \frac{44.0095}{27.6332} = 0.151391$

$$f_{\text{CO}_2} = 0.151 \frac{\text{kg CO}_2}{\text{kg comb. product}}$$

• mol/ concentration

$$C_j = y_j \frac{M_j}{R_u} \frac{P}{T}$$

$$C_{\text{CO}_2} = (0.095057) \frac{44.0095 \text{ kg/kmol}}{8.314 \text{ kJ/kmol} \cdot \text{K}} \frac{100 \text{ kPa}}{500 \text{ K}} \left(\frac{1 \text{ kN}}{\text{m}^2 \cdot \text{kPa}} \right) \left(\frac{1 \text{ kJ}}{1 \text{ kN} \cdot \text{m}} \right)$$

$$C_{\text{CO}_2} = 0.100635 \frac{\text{kg}}{\text{m}^3}$$

$$\rightarrow C_{\text{CO}_2} = 0.101 \frac{\text{kg}}{\text{m}^3}$$

• Molar concentration of CO_2

$$\rightarrow C_{\text{molar},j} = \frac{C_j}{M_j} = 0.00229 \frac{\text{kmol}}{\text{m}^3}$$

(6) EF

$$m_{\text{CH}_4} = n_{\text{CH}_4} \cdot M_{\text{CH}_4}$$

$$m_{\text{CO}_2} = n_{\text{CO}_2} \cdot M_{\text{CO}_2}$$

$$\text{but } \underline{n_{\text{CH}_4} = n_{\text{CO}_2}}$$

$$EF = \frac{m_{\text{CO}_2}}{m_{\text{CH}_4}} = \frac{M_{\text{CO}_2}}{M_{\text{CH}_4}} = \frac{44.0095}{16.04246} = 2.74 \frac{\text{kg CO}_2}{\text{kg CH}_4} \left(\frac{1000 \text{ kg}}{\text{Mg}} \right)$$

$$\star EF = 2740 \frac{\text{kg CO}_2}{\text{Mg CH}_4}$$

Estimate from first principles
for ideal comb.

Added after class:

To compare with EF published by EPA, we need to do some conversions

need $\frac{\text{kg CO}_2}{1000 \text{ SCF of Natural gas}}$ (NG)

OR

$\frac{1 \text{bm CO}_2}{10^6 \text{ SCF of NG}}$ (Standard cubic ft)

PUBLISHED EFs →

I found
3 different
EFs on the
Internet

$$\frac{53 \text{ kg CO}_2}{\text{thousand SCF NG}}$$

OR

$$\frac{120,000 \text{ lbm CO}_2}{10^6 \text{ SCF}}$$

OR $\frac{1135 \text{ lbm CO}_2}{\text{MWh of electricity produced}}$

We will do the conversions next class & compare our
estimate to the published values