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 = $\frac{14.25 \text{ kg}}{\text{Mg}}\left(820 \frac{\text{Mg}}{\text{day}}\right) = 11685 \frac{\text{kg}}{\text{day}}$

Actual emission = 32 kg/day

E = efficiency = removal efficiency of APCS

$\dot{m}_d = (1-E)\,\dot{m}_g \rightarrow E = 1 - \frac{\dot{m}_d}{\dot{m}_g} = 1 - \frac{32}{11685} = 0.99726$

$\boxed{99.7\%}$

How to estimate EFs

• VOCs from paint, varnish, etc. → easy

typical oil-based paint has
- pigments
- $\boxed{\text{solvent (VOC) (e.g. toluene)}}$
- 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

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

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 $T = 500$ K and $P = 100$ 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:

$$\boxed{CH_4 + a(O_2 + 3.76\ N_2) \rightarrow bCO_2 + cH_2O + dN_2}$$

N_2 goes along for the ride

Solve for the molar coefficients:

C: $1 = b \rightarrow \boxed{b=1}$ O: $2a = 2b + c \rightarrow \boxed{a=2}$

H: $4 = 2c \rightarrow \boxed{c=2}$ N: $2(3.76)a = 2d \rightarrow \boxed{d=7.52}$

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

ideal combustion

$a_{stoich} = 2$

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

In real life, not ideal comb,

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

molar fuel-air ratio

$$\boxed{\Phi = \text{Equivalence Ratio} = \frac{(F/A)_{n,\ actual}}{(F/A)_{n,\ stoich}}} = \frac{\frac{1}{a}}{\frac{1}{a_{stoich}}}$$

3 cases:

a) $a = a_{stoich}$ → IDEAL COMBUSTION $\boxed{\Phi = 1}$ $(F/A)_n = (F/A)_{n,stoich}$

b) actual → $a > a_{stoich}$ → excess air

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

get additional comb. products eg CO, NO, NO_2, soot

alcohols, aldehydes

unburned HC

c) $a < a_{stoich}$ → excess fuel

RICH COMBUSTION $\boxed{\Phi > 1}$ — get additional comb. products

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$$y_{CO_2} = \frac{n_{CO_2}}{n_t} = \frac{b}{b+c+d} = \frac{\#\text{ mols of } CO_2}{\text{total } \#\text{ mols}}$$ in exhaust gases

(In comb. products)

$$\frac{1}{1+2+7.52} = 0.095057 \quad y_{CO_2}$$

$$\boxed{y_{CO_2} = 95{,}100 \text{ ppm}}$$

Calculate RH in % of the exhaust

P = 100 kPa

T = 500 K → look up P_{v,H_2O} = 2669.4 kPa

$$RH = \frac{P_{H_2O}}{P_{v,H_2O}} \times 100\%$$

$$y_{H_2O} = \frac{P_{H_2O}}{P_{atm}}$$

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

$$RH = \frac{\left(\frac{c}{b+c+d}\right) P_{atm}}{P_{v,H_2O}} \times 100\% \rightarrow \frac{\frac{2}{10.52}(100\text{ kPa})}{2669.4\text{ kPa}} \times 100\% = \boxed{0.712\%}$$

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

Atomic mass

C 12.0107

O 15.9994

H 1.00794

N 14.00674

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

$$M_t = \underbrace{\left(\frac{b}{b+c+d}\right)(44.0095)}_{CO_2} + \underbrace{\left(\frac{c}{b+c+d}\right)(18.0153)}_{H_2O} + \underbrace{\left(\frac{d}{b+c+d}\right)(28.01348)}_{N_2} = 27.6332 \frac{kg}{kmol}$$

M_t of the exhaust gases

f_j for CO_2 → $f_{CO_2} = y_{CO_2} \dfrac{M_{CO_2}}{M_t} = (0.095057) \dfrac{44.0095}{27.6332} = 0.151391$

$$\boxed{f_{CO_2} = 0.151 \frac{kg\ CO_2}{kg\ comb.\ products}}$$

• mass concentration $\quad \boxed{c_j = y_j \dfrac{M_j}{R_u} \dfrac{P}{T}}$

$$c_{CO_2} = (0.095057) \frac{44.0095\ kg/kmol}{8.314\ kJ/kmol \cdot K} \frac{100\ kPa}{500\ K} \left(\frac{1\ kN}{m^2 \cdot kPa}\right)\left(\frac{1\ kJ}{1\ kN \cdot m}\right)$$

$c_{CO_2} = 0.100635 \dfrac{kg}{m^3}$ → $\boxed{c_{CO_2} = 0.101 \dfrac{kg}{m^3}}$

• Molar concentration of CO_2 → $\boxed{C_{molar,j} = \dfrac{c_j}{M_j} = 0.00229 \dfrac{kmol}{m^3}}$

(b) EF

$$m_{CH_4} = n_{CH_4} \cdot M_{CH_4}$$

$$m_{CO_2} = n_{CO_2} \cdot M_{CO_2}$$

but $n_{CH_4} = n_{CO_2}$

$$EF = \frac{m_{CO_2}}{m_{CH_4}} = \frac{M_{CO_2}}{M_{CH_4}} = \frac{44.0095}{16.04246} = 2.74 \frac{\text{kg } CO_2}{\text{kg } CH_4}\left(\frac{1000 \text{ kg}}{\text{Mg}}\right)$$

$$\boxed{EF = 2740 \frac{\text{kg } CO_2}{\text{Mg } CH_4}}$$

Estimate from first principles for ideal comb.

Added after class:

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

need $\frac{\text{kg } CO_2}{\text{1000 SCF of Natural gas}}$ (NG) OR $\frac{\text{lbm } CO_2}{10^6 \text{ SCF of NG}}$

SCF: Standard cubic ft

PUBLISHED EFs → $\boxed{\frac{53 \text{ kg } CO_2}{\text{thousand SCF NG}}}$ OR $\boxed{\frac{120{,}000 \text{ lbm } CO_2}{10^6 \text{ SCF}}}$

I found 3 different EFs on the Internet

or $\boxed{\frac{1135 \text{ lbm } CO_2}{\text{MWh of electricity produced}}}$

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