ENGR-3000:
Renewable Energy, Technology, and Resource Economics

Energy in Fuels

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World Learning SIT Study Abroad

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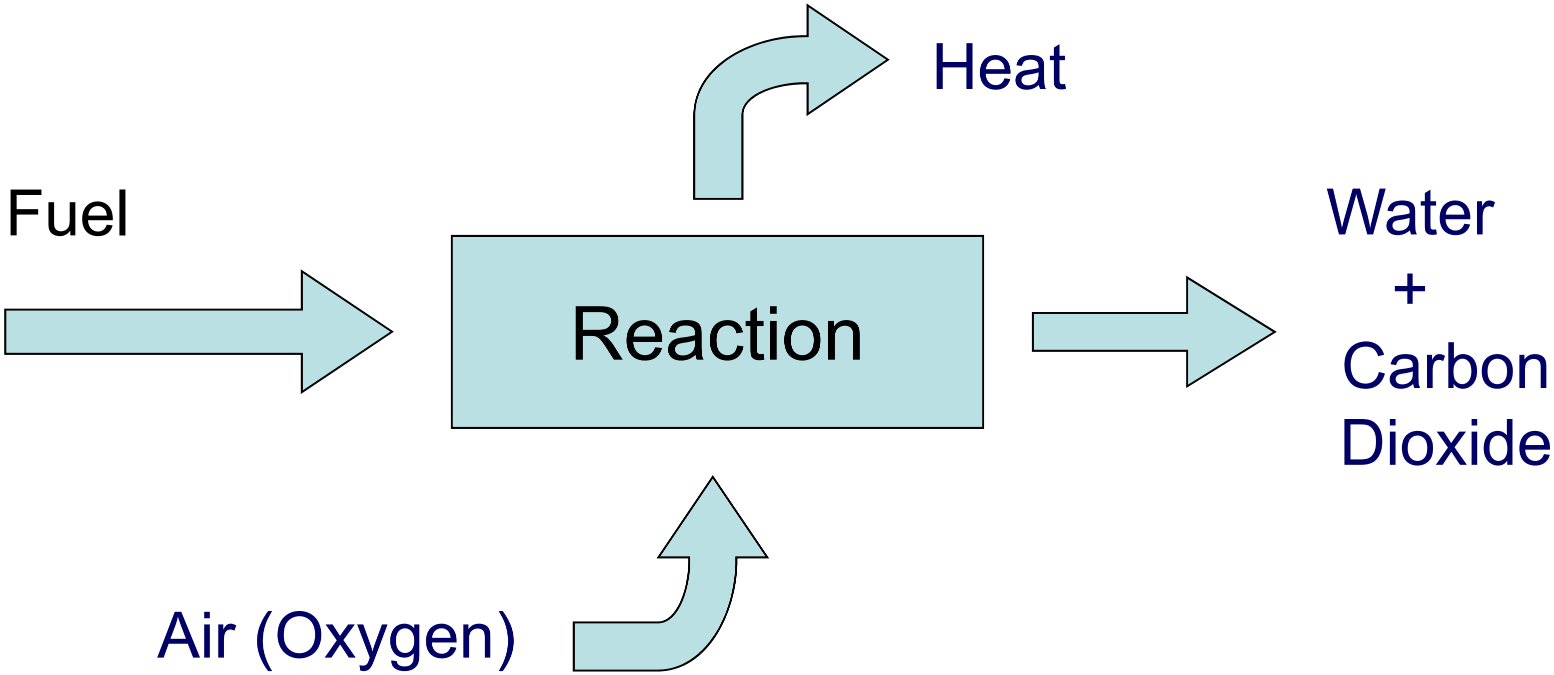
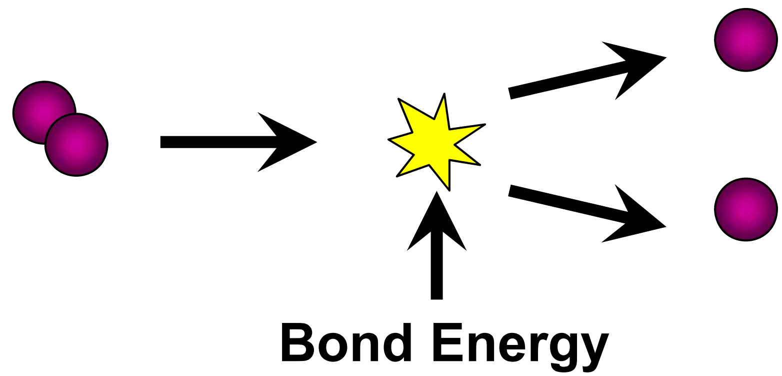
Combustion Reactions, General Form



$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + Heat$$

Energy Stored in Chemical Bonds

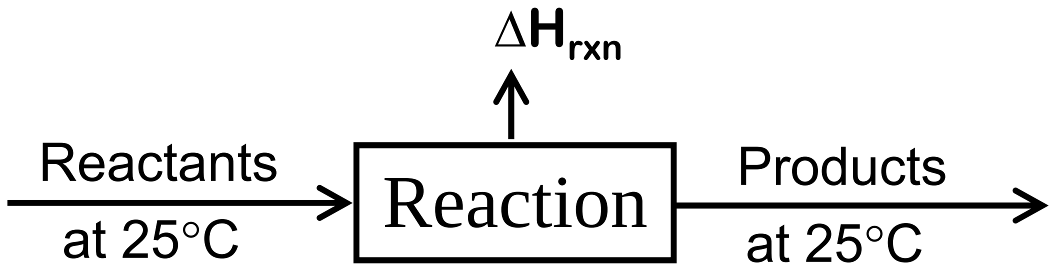


- Breaking a bond is an endothermic process: you must put energy into the system to break a bond
- Forming a bond is an exothermic process: energy is released into the surroundings when a bond is formed
- <u>Estimate</u> the change in enthalpy (ΔH) for a chemical reaction as follows:

$$\Delta H = (\text{Energy of bonds broken}) - (\text{energy of bonds formed})$$

The “Heating Value” of Combustion Reactions

- Start with reactants at standard state (25°C, 1 Bar)
- Allow reaction to occur (at constant pressure)
- Allow products to return to standard state (25°C, 1 Bar)
- Track change in enthalpy from initial state (at standard conditions) to final state (at standard conditions):

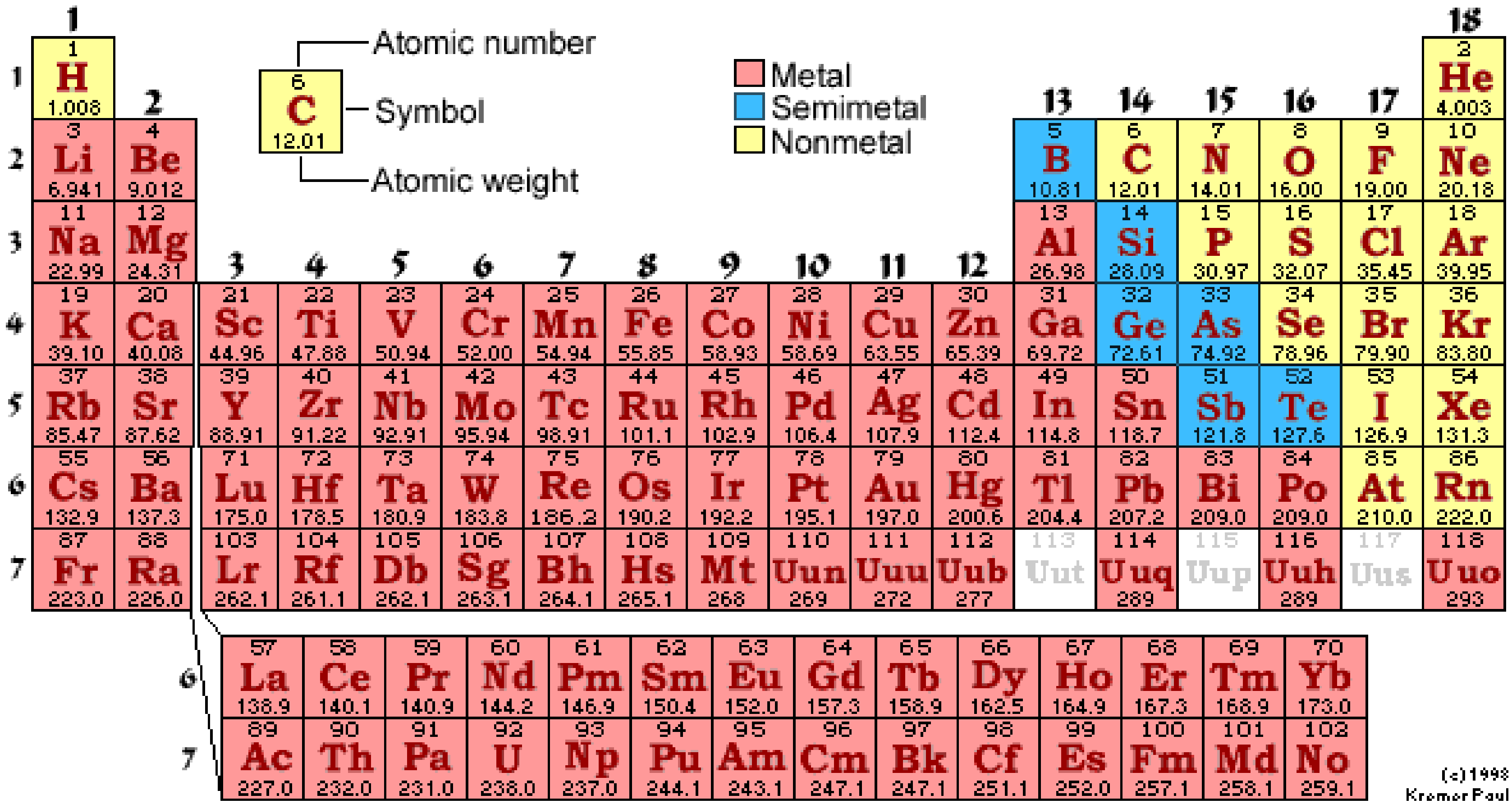


Higher and Lower Heating Values

- When fuel is burned one product is water.
  - If water vapor exits stack then its energy is lost, about 2440 kJ per kg of water vapor (1060 BTU/lb)

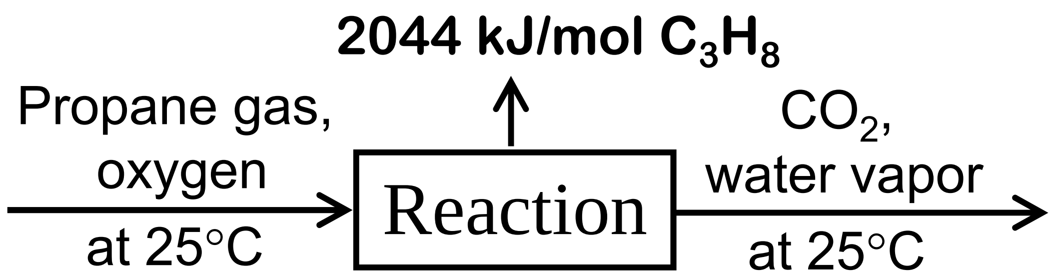
- Heat of Combustion for fuels
  - Higher Heating Value (HHV) – gross heat, accounts for latent heat in water vapor
  - Lower Heating Value (LHV) – net heat, assumes latent heat in water vapor is not recovered

Atomic Weights



Hydrogen: 1g/mole; Carbon: 12g/mole; Oxygen 16g/mole

Calculating Lower Heating Value

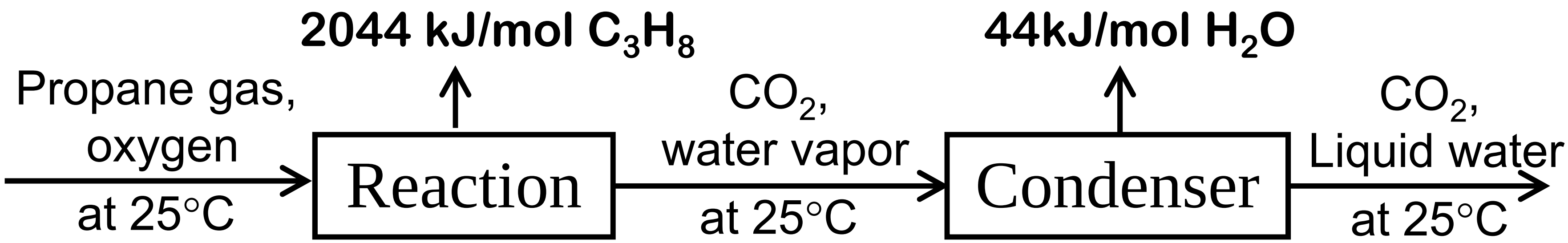


$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O(g) + 2044\ \text{kJ/mol}$$

$$MW_{Propane} = (3)\left(\frac{12\text{g}}{\text{mol}}\right) + (8)\left(\frac{1\text{g}}{\text{mol}}\right) = 44\,\frac{\text{grams}}{\text{mole}}$$

$$LHV = \left(2044\,\frac{\text{kJ}}{\text{mol}}\right)\left(\frac{\text{mol}}{44\text{g}}\right)\left(\frac{1000\text{g}}{\text{kg}}\right) = 46450\,\frac{\text{kJ}}{\text{kg}}$$

Calculating Higher Heating Value



$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O(g) + 2044\ \text{kJ/mol}$$

$$H_2O(g) \rightarrow H_2O(L) + 44\ \text{kJ/mol}$$

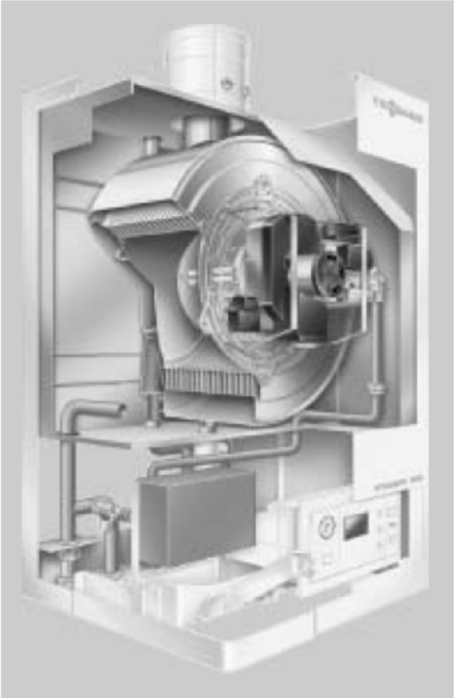
$$\Delta H = 2044\ \text{kJ/mol} + 4(44\ \text{kJ/mol}) = 2220\ \text{kJ/mol}$$

$$\text{HHV} = \left(2220\frac{\text{kJ}}{\text{mol}}\right)\left(\frac{\text{mol}}{44\text{g}}\right)\left(\frac{1000\text{g}}{\text{kg}}\right) = 50450\frac{\text{kJ}}{\text{kg}}$$

Higher and Lower Heating Values

- Conventional Multifuel Boiler: Smith Series 19 HE
  - fuel = natural gas or #2 oil
  - stack temp = 370°F
  - Efficiency = 83%

- Condensing Boiler: Vitodens 200 WB2
  - fuel = natural gas
  - stack temp = 104°F
  - Efficiency = 95%



Combustion Reactions (HHV)

- Hydrogen

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O(L) + 285.8 \text{ kJ/mol}$$

- Methane

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O(L) + 891 \text{ kJ/mol}$$

- Ethanol

$$C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O(L) + 1366 \text{ kJ/mol}$$

- Gasolene (Trimethylpentane)

$$C_8H_{18} + 12\tfrac{1}{2}O_2 \rightarrow 8CO_2 + 9H_2O(L) + 5463 \text{ kJ/mol}$$

- Diesel (hexadacane, or cetane)

$$C_{16}H_{34} + 24\tfrac{1}{2}O_2 \rightarrow 16CO_2 + 17H_2O(L) + 10698 \text{ kJ/mol}$$

Comparison of Fuels

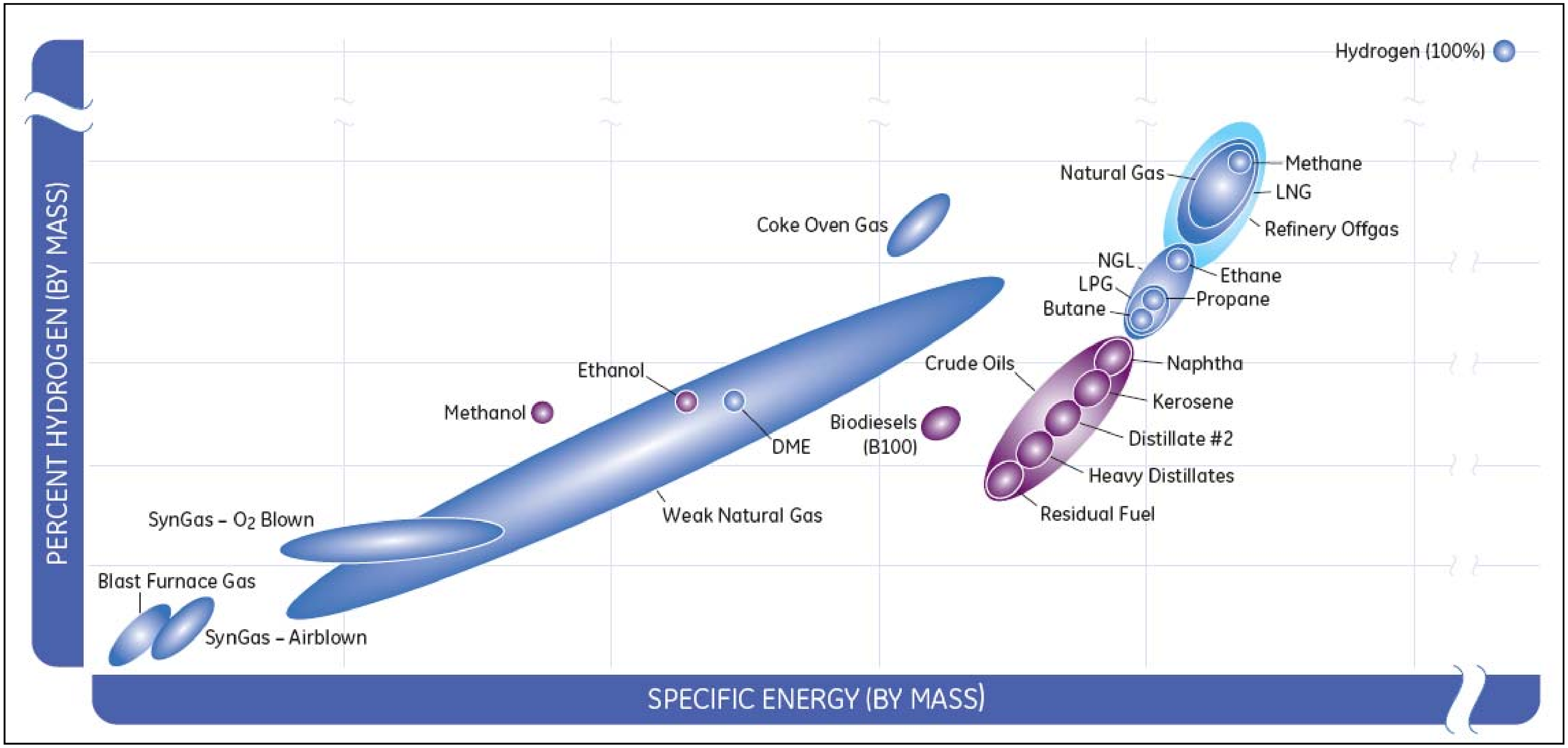
Specific Energy, Energy Density & CO_2

Fuel	Specific Energy kj/g	Density KWH/gal	Chemical Formula	lbs CO2/gal
Propane	50.4	26.8	C_3H_8	13
Ethanol	29.7	24.7	C_2H_5OH	13
Gasoline	46.5	36.6	C_7H_{16}	20
Diesel	45.8	40.6	$C_{12}H_{26}$	22
Biodiesel	39.6	35.0	$C_{18}H_{32}O_2$	19
Methane	55.8	27.0	CH_4	3
Oil	47.9	40.5	$C_{14}H_{30}$	20
Wood	14.9	11.3	approx weight	9
Coal	30.2	22.9	approx weight	19
Hydrogen	141.9	10.1	H_2	0

Source: DOE, Stanford University, College of the Desert, & Green Econometrics research

- Energies based on higher heating values

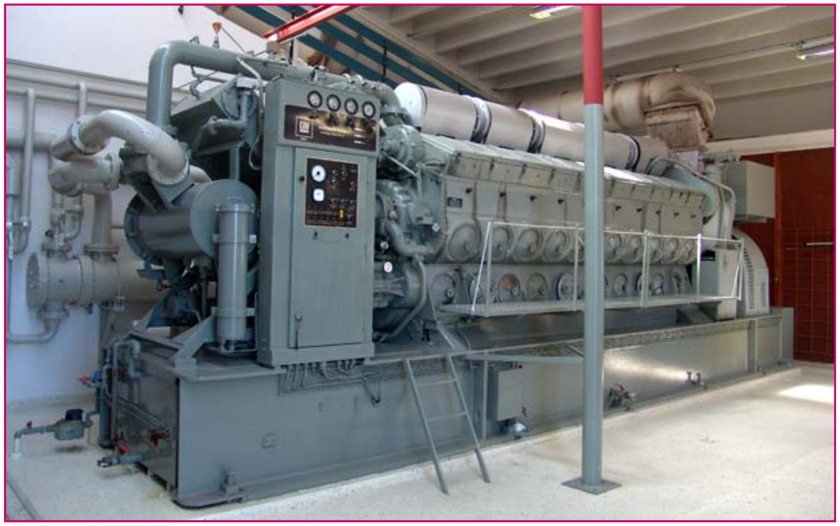
Percent Hydrogen vs. Specific Energy

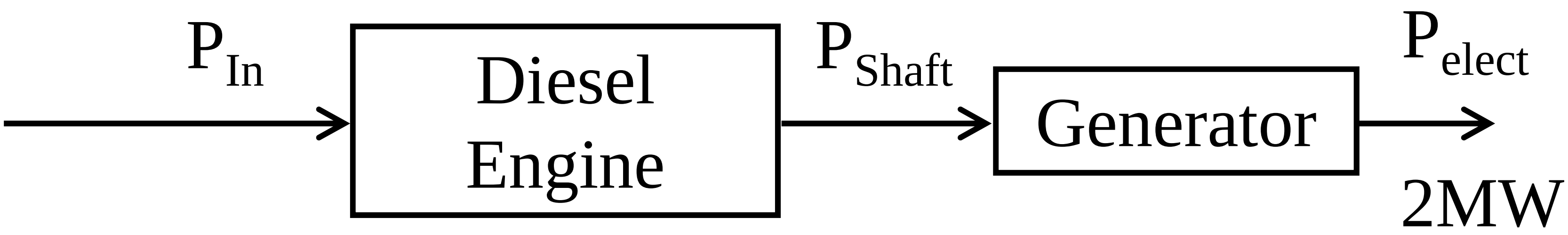


www.gepower.com

Example: Diesel and Gas Engine

- Estimate the fuel consumption (in liter/hr) and overall efficiency of a 2MW diesel generator operating at its rated power.
  - Specific fuel consumption = 200g/kWh$_m$.
  - Generator efficiency = 96%
  - Energy content of #2 diesel (HHV) = 44.8 MJ/kg
  - density of #2 diesel = 0.85kg/liter





$$P_{In} = \left(\dot{m}_{Fuel}\right)(HHV) \qquad \eta_{Diesel} = \frac{P_{Shaft}}{P_{In}} \qquad \eta_{Gen} = \frac{P_{Elec}}{P_{Shaft}} = 0.96$$

- Mechanical Output

$$\eta_{Gen} = \frac{P_{Elec}}{P_{Shaft}} \Rightarrow \quad P_{Shaft} = \frac{P_{Elec}}{\eta_{Gen}} = \frac{2MW_e}{0.96} = 2.083MW_m$$

- Fuel Flow Rate

$$\dot{m}_{Fuel} = (SFC)(P_{Shaft}) = \left(\frac{200g/h}{kW}\right)(2083kW)$$

$$\dot{m}_{Fuel} = 416.6\times10^3\frac{g}{h}\left(\frac{kg}{10^3 g}\right) = 417\frac{kg}{h}$$

- Fuel Consumption

$$Q_{Fuel} = 417\frac{kg}{hr}\left(\frac{liter}{0.85kg}\right) = 490\frac{liter}{hr}$$

- Rate of Heat Addition

$$P_{In} = \left(\dot{m}_{Fuel}\right)(HHV) = \left(417\frac{kg}{hr}\right)\left(\frac{44.8MJ}{kg}\right) = 18612\frac{MJ}{hr}$$

$$P_{In} = \left(18612\frac{MJ}{hr}\right)\left(\frac{hr}{3600s}\right) = 5.19\frac{MJ}{hr} = 5.19MW_{th}$$

- Diesel Engine Efficiency

$$\eta_{Diesel} = \frac{P_{Shaft}}{P_{In}} = \frac{2.08MW_m}{5.19MW_{th}} = 0.40$$

CO_2 Emission from Diesel Fuel

- Estimate the production of CO_2 (in g CO_2/kWh).
  - Use Cetane ($C_{16}H_{34}$) as a model reaction for diesel combustion. ΔH = 10,700kJ/mol

$$C_{16}H_{34} + 24\tfrac{1}{2}O_2 \rightarrow 16CO_2 + 17H_2O$$

  - Atomic weights,
    - Carbon = 12g/mol,
    - Hydrogen = 1 g/mol
    - Oxygen = 16g/mol

- Reference: CO_2 emission from coal $\simeq$ 325 gCO_2/kWh

- Molecular weight of CO_2

$$\frac{12\text{g}}{\text{mole}} + 2\left(\frac{16\text{g}}{\text{mole}}\right) = \frac{44\text{g}}{\text{mole}}$$

- There are 16 moles of CO_2 produced per mole of Cetane:

$$\frac{16\left(\frac{44\text{g}}{\text{mole}}\right)}{10700\,\frac{\text{kJ}}{\text{mole}}} = \frac{65.8\times10^{-3}\,\text{gCO}_2}{\text{kJ}}\left(\frac{3600\text{kJ}}{\text{kWh}}\right) = 237\,\frac{\text{gCO}_2}{\text{kWh}}$$

➢ Determine the Carbon intensity of the electricity generation

$$237\,\frac{\text{gCO}_2}{\text{kWh}} \longrightarrow \boxed{\begin{array}{c}\text{Diesel}\\ \text{Power Plant}\\ \eta = 38.4\%\end{array}} \longrightarrow$$

$$237\,\frac{\text{gCO}_2}{\text{kWh}}\left(\frac{1}{0.384}\right) = 617\,\frac{\text{gCO}_2}{\text{kWh}}$$

Exercise, Gas Engine

- If we replaced the diesel generator in the previous example with a natural gas generator with the same efficiency, would the CO_2 emissions change?
  - Use methane (CH_4) as the model reaction for natural gas combustion. ΔH = 891 kJ/mol

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

Carbon Intensity of Electricity

- Generated from Coal:

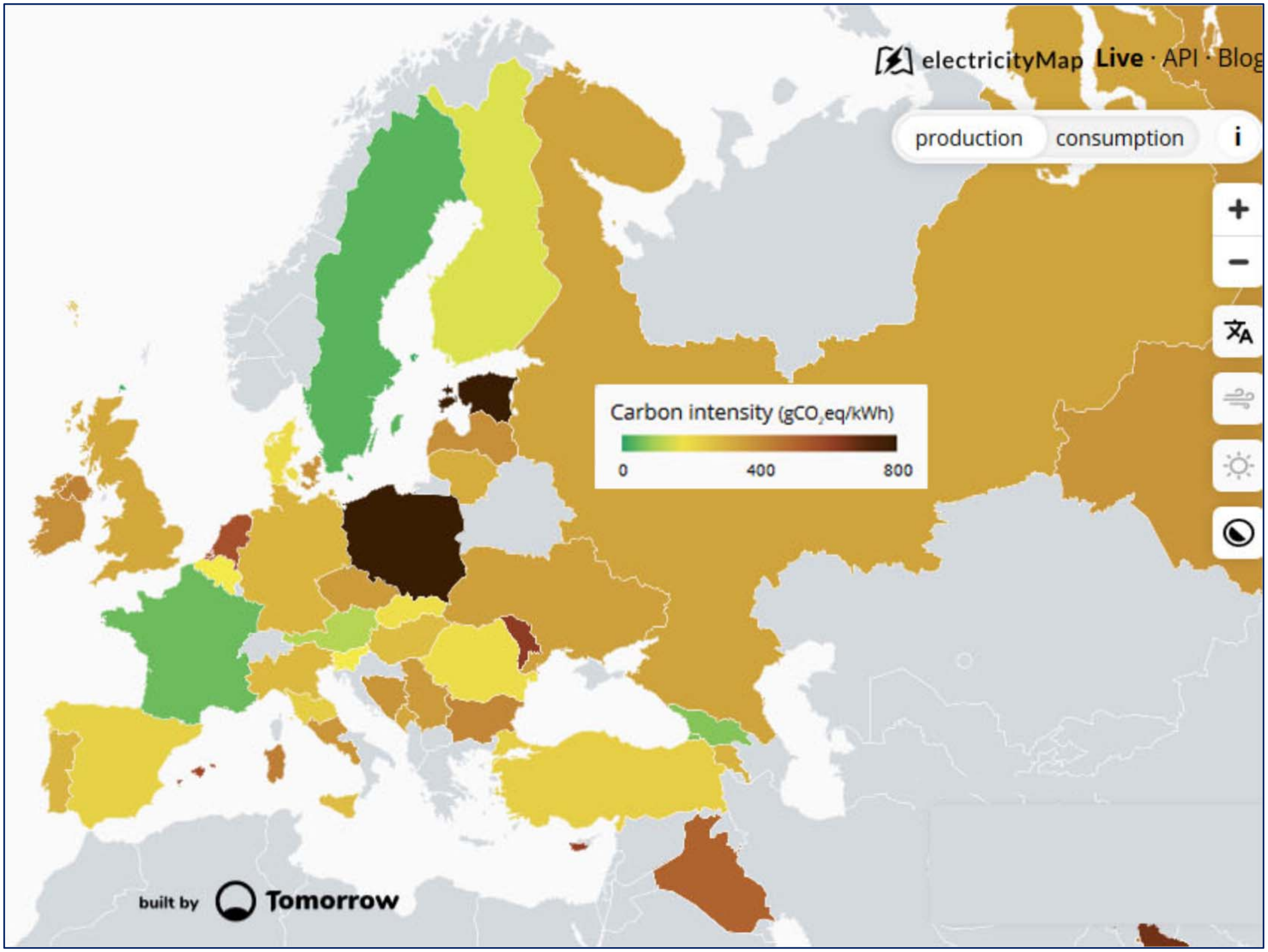
$$325\,\frac{\mathrm{gCO_2}}{\mathrm{kWh}} \longrightarrow \boxed{\begin{array}{c}\text{Coal}\\ \text{Power Plant}\\ \eta = 37.5\%\end{array}} \longrightarrow 325\,\frac{\mathrm{gCO_2}}{\mathrm{kWh}}\left(\frac{1}{0.375}\right) = 867\,\frac{\mathrm{gCO_2}}{\mathrm{kWh}}$$

- Generated from Natural Gas

$$178\,\frac{\mathrm{gCO_2}}{\mathrm{kWh}} \longrightarrow \boxed{\begin{array}{c}\text{Natural Gas}\\ \text{Power Plant}\\ \eta = 44.4\%\end{array}} \longrightarrow 178\,\frac{\mathrm{gCO_2}}{\mathrm{kWh}}\left(\frac{1}{0.444}\right) = 401\,\frac{\mathrm{gCO_2}}{\mathrm{kWh}}$$

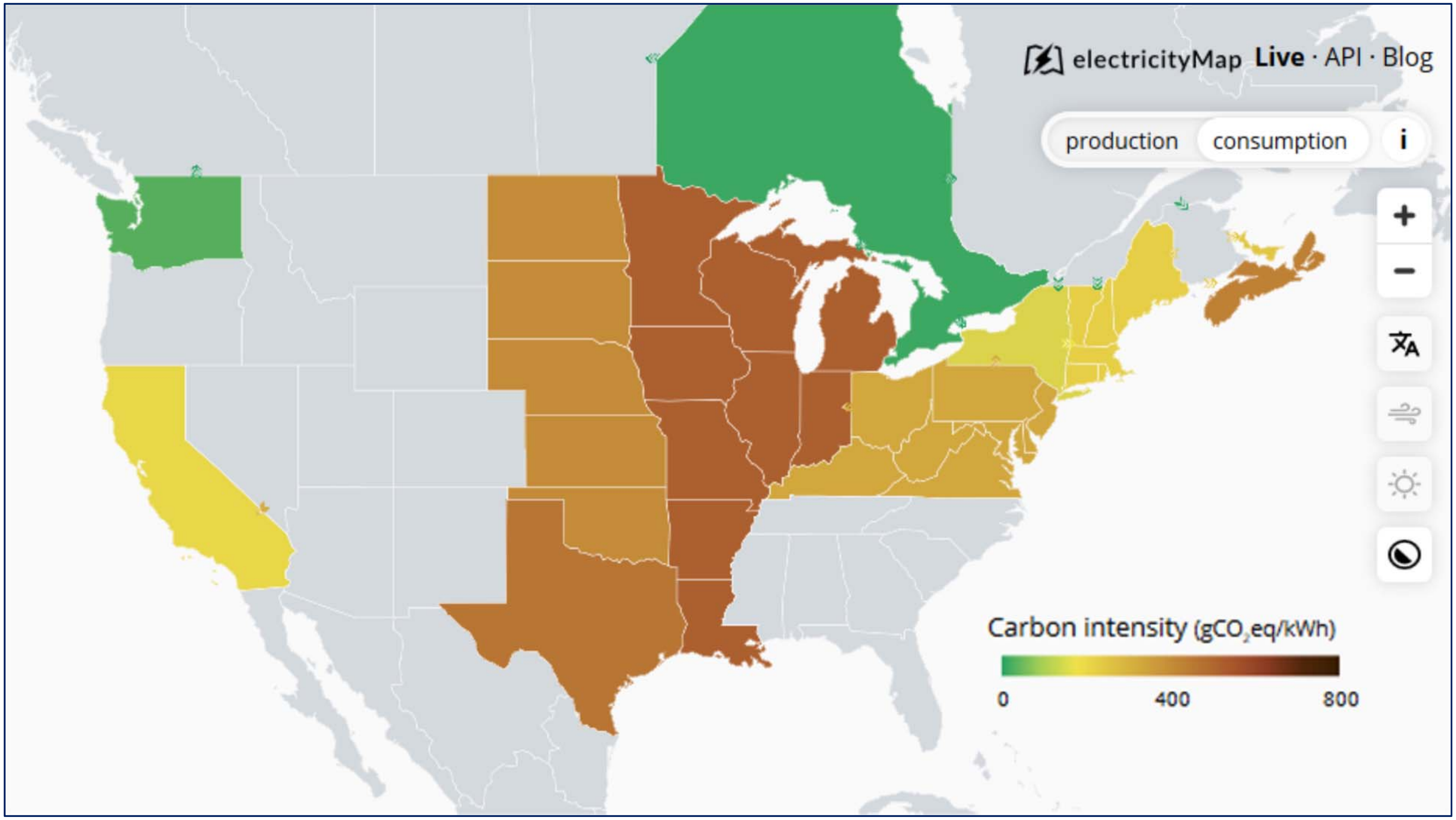
➢ Average Electrical Grid Carbon Intensity = 430 $\mathrm{gCO_2/kWh_e}$

Carbon Intensity of Electricity: Europe



https://www.electricitymap.org

Carbon Intensity of Electricity: USA



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