

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

Energy in Fuels

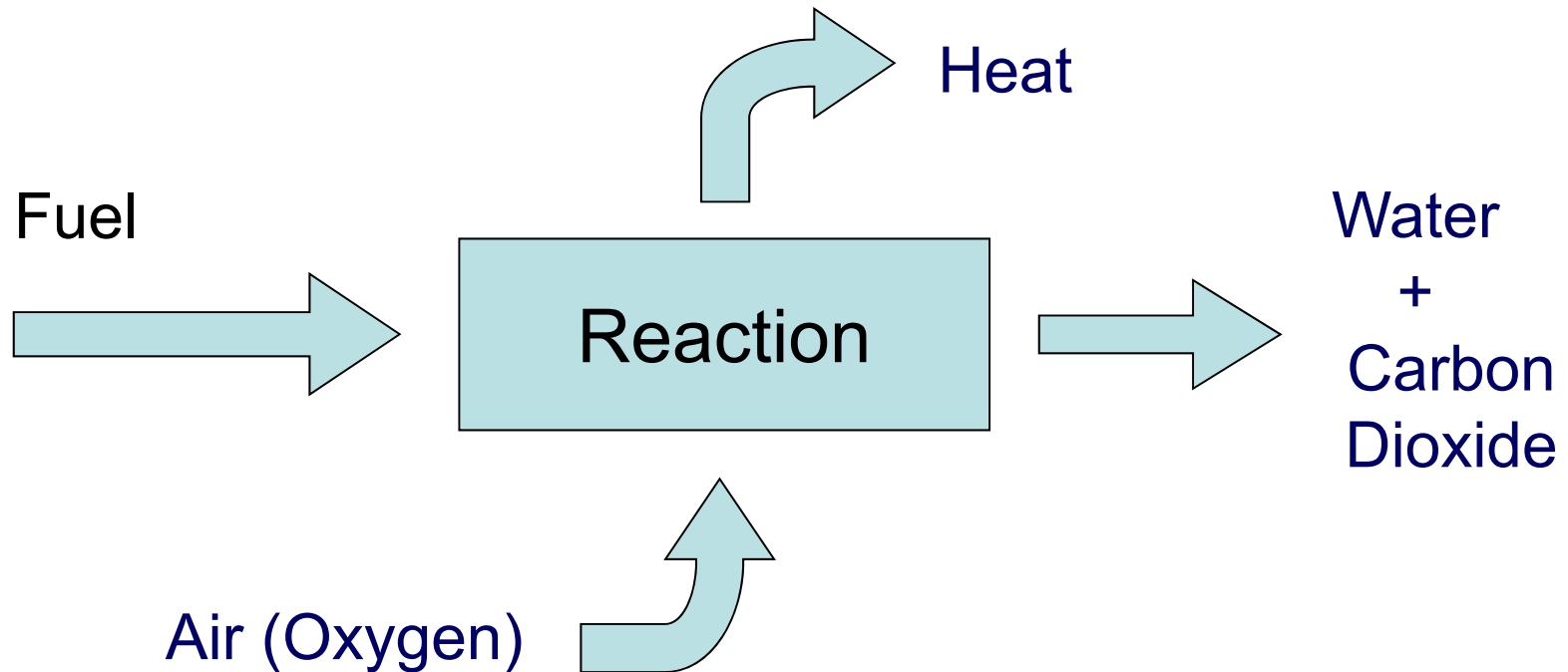
S. David Dvorak. Ph.D, P.E.



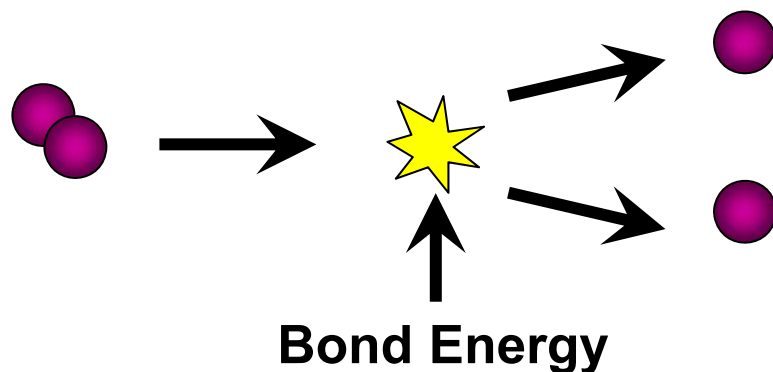
5 June 2019
Ísafjörður, Iceland



Combustion Reactions, General Form



Energy Stored in Chemical Bonds

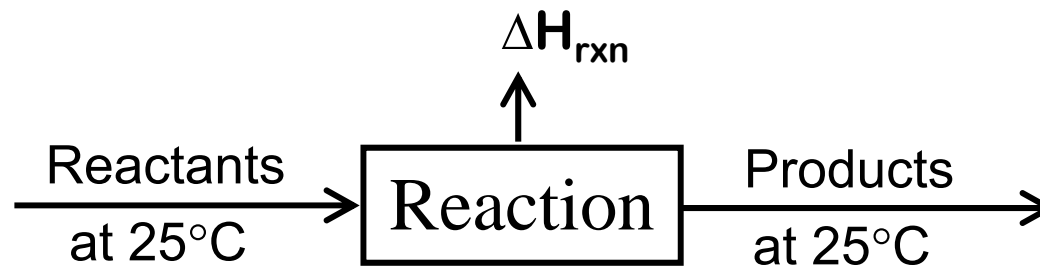


- Breaking a bond is an endothermic process: you must put energy into the system to break a bond
- Forming a bond is an exothermic process: energy is released into the surroundings when a bond is formed
- Estimate the change in enthalpy (ΔH) for a chemical reaction as follows:

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

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

1

1

1

1.008

H

2

4

2

9.012

Be

3

3

3

6.941

Li

6

6

6

12.01

C

11

11

11

22.99

Na

12

12

12

24.31

Mg

13

13

13

26.98

Al

14

14

14

28.09

Si

15

15

15

30.97

P

16

16

16

32.07

S

17

17

17

35.45

Cl

18

18

18

39.95

Ar

19

19

19

39.10

K

20

20

20

40.08

Ca

21

21

21

44.96

Sc

22

22

22

47.88

Ti

23

23

23

50.94

V

24

24

24

52.00

Cr

25

25

25

54.94

Mn

26

26

26

55.85

Fe

27

27

27

58.93

Co

28

28

28

58.69

Ni

29

29

29

63.55

Cu

30

30

30

65.39

Zn

31

31

31

69.72

Ga

32

32

32

72.61

Ge

33

33

33

74.92

As

34

34

34

78.96

Se

35

35

35

79.90

Br

36

36

36

83.80

Kr

37

37

37

85.47

Rb

38

38

38

87.62

Sr

39

39

39

88.91

Y

40

40

40

91.22

Zr

41

41

41

92.91

Nb

42

42

42

95.94

Mo

43

43

43

98.91

Tc

44

44

44

101.1

Ru

45

45

45

102.9

Rh

46

46

46

106.4

Pd

47

47

47

107.9

Ag

48

48

48

112.4

Cd

49

49

49

114.8

In

50

50

50

118.7

Sn

51

51

51

121.8

Sb

52

52

52

127.6

Te

53

53

53

126.9

I

54

54

54

131.3

Xe

55

55

55

132.9

Cs

56

56

56

137.3

Ba

71

71

71

175.0

Lu

72

72

72

178.5

Hf

73

73

73

180.9

Ta

74

74

74

183.8

W

75

75

75

186.2

Re

76

76

76

190.2

Os

77

77

77

192.2

Ir

78

78

78

195.1

Pt

79

79

79

197.0

Au

80

80

80

200.6

Hg

81

81

81

204.4

Tl

82

82

82

207.2

Pb

83

83

83

209.0

Bi

84

84

84

209.0

Po

85

85

85

210.0

At

86

86

86

222.0

Rn

87

87

87

223.0

Fr

88

88

88

226.0

Ra

103

103

103

262.1

Lr

104

104

104

261.1

Rf

105

105

105

262.1

Db

106

106

106

263.1

Sg

107

107

107

264.1

Bh

108

108

108

265.1

Hs

109

109

109

268

Mt

110

110

110

269

Uun

111

111

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272

Uuu

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112

112

277

Uub

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113

Uut

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Uuq

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Uup

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116

Uuh

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117

117

Uus

118

118

118

Uuo

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57

57

138.9

La

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58

58

140.1

Ce

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140.9

Pr

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60

60

144.2

Nd

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61

61

146.9

Pm

62

62

62

150.4

Sm

63

63

63

152.0

Eu

64

64

64

157.3

Gd

65

65

65

158.9

Tb

66

66

66

162.5

Dy

67

67

67

164.9

Ho

68

68

68

167.3

Er

69

69

69

168.9

Tm

70

70

70

173.0

Yb

89

89

89

227.0

Ac

90

90

90

232.0

Th

91

91

91

231.0

Pa

92

92

92

238.0

U

93

93

93

237.0

Np

94

94

94

244.1

Pu

95

95

95

243.1

Am

96

96

96

247.1

Cm

97

97

97

247.1

Bk

98

98

98

251.1

Cf

99

99

99

252.0

Es

100

100

100

257.1

Fm

101

101

101

258.1

Md

102

102

102

259.1

No

Atomic number

Symbol

Atomic weight

Metal

Semimetal

Nonmetal

1

2

3

4

5

6

7

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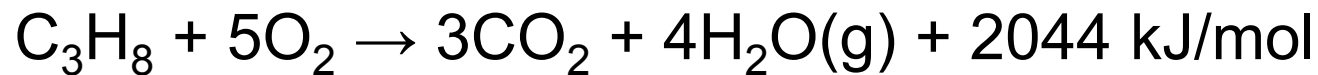
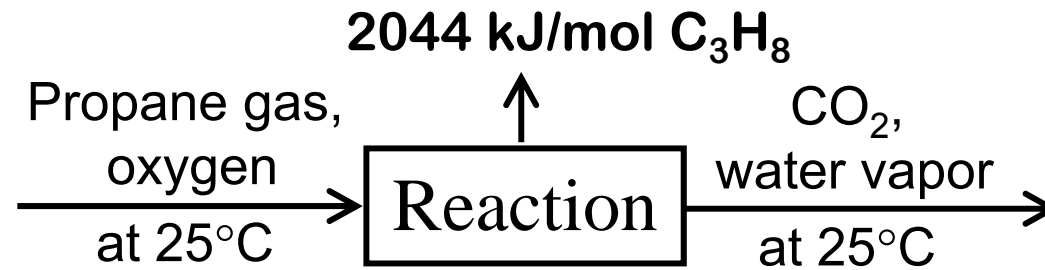
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Hydrogen: 1g/mole; Carbon: 12g/mole; Oxygen 16g/mole

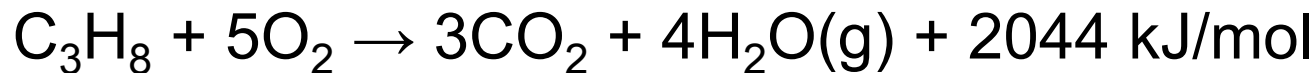
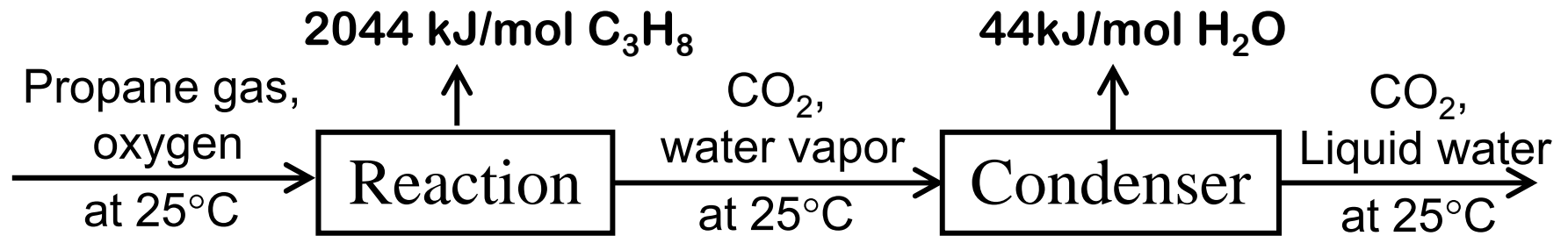
Calculating Lower Heating Value



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

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

Calculating Higher Heating Value



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

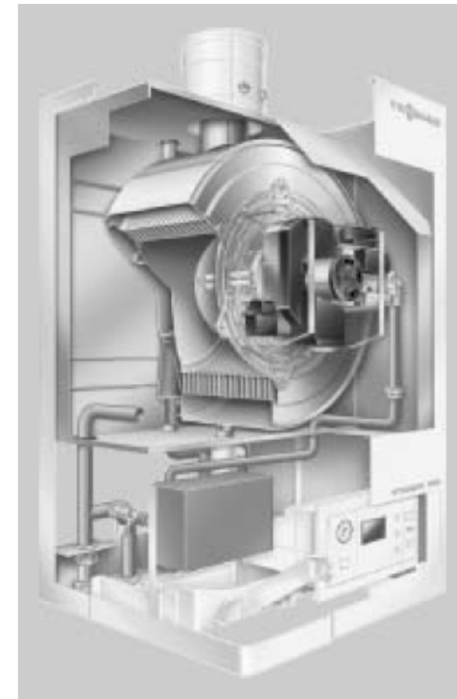
$$\text{HHV} = \left(2220 \frac{\text{kJ}}{\text{mol}} \right) \left(\frac{\text{mol}}{44 \text{ g}} \right) \left(\frac{1000 \text{ g}}{\text{kg}} \right) = 50450 \frac{\text{kJ}}{\text{kg}}$$

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%

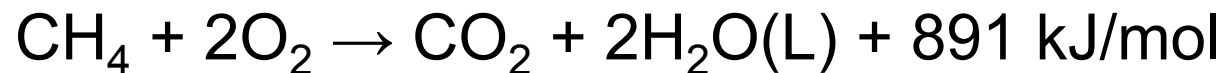


Combustion Reactions (HHV)

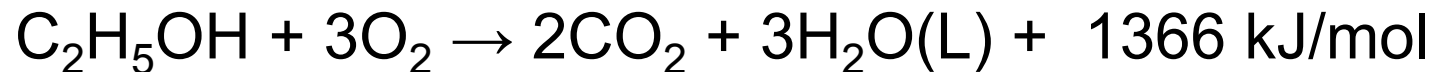
- Hydrogen



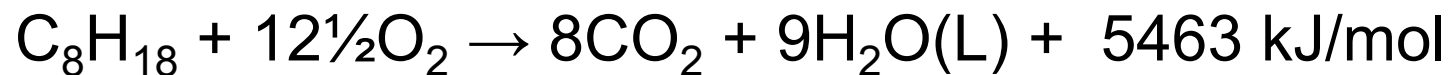
- Methane



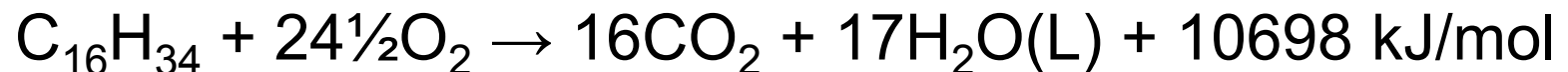
- Ethanol



- Gasolene (Trimethylpentane)



- Diesel (hexadecane, or cetane)



Comparison of Fuels

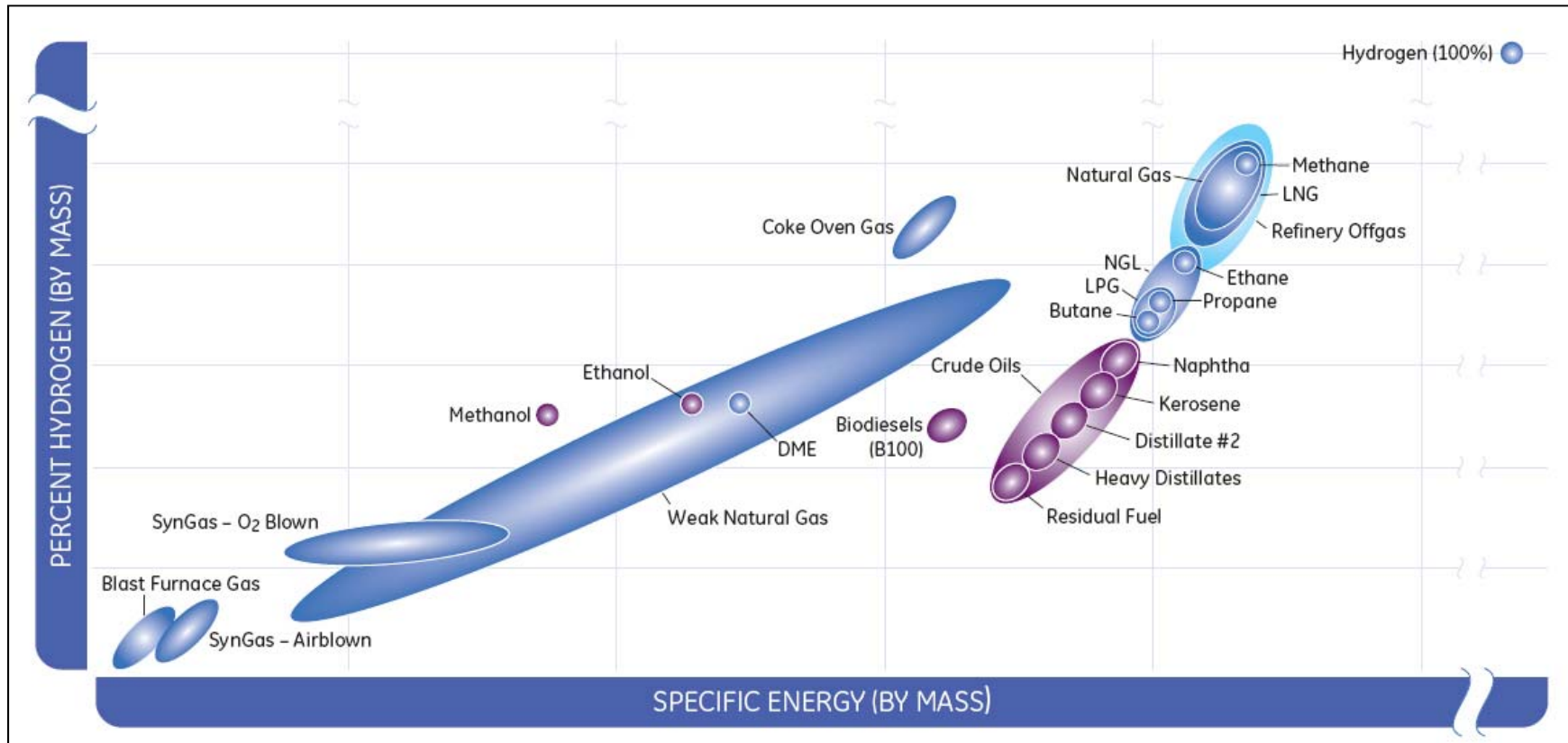
Specific Energy, Energy Density & CO2

Fuel	Specific Energy kj/g	Density KWH/gal	Chemical Formula	lbs CO2/gal
Propane	50.4	26.8	C3H8	13
Ethanol	29.7	24.7	C2H5OH	13
Gasoline	46.5	36.6	C7H16	20
Diesel	45.8	40.6	C12H26	22
Biodiesel	39.6	35.0	C18H32O2	19
Methane	55.8	27.0	CH4	3
Oil	47.9	40.5	C14H30	20
Wood	14.9	11.3	approx weight	9
Coal	30.2	22.9	approx weight	19
Hydrogen	141.9	10.1	H2	0

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

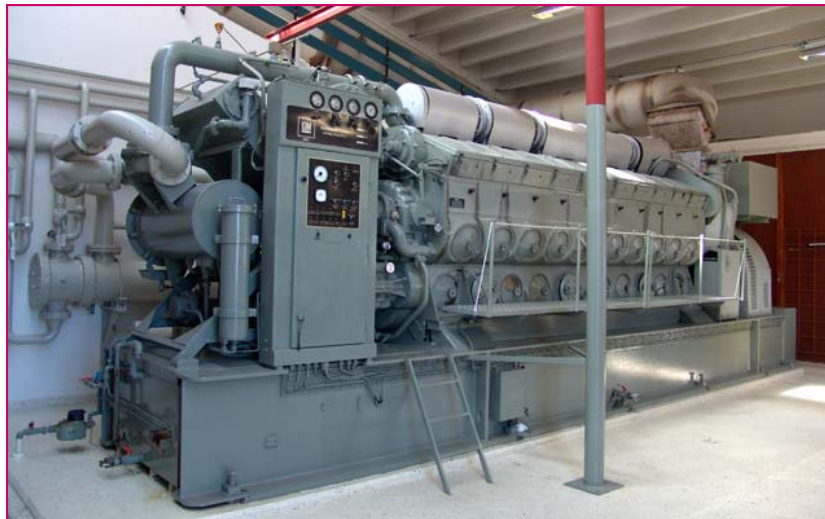
- Energies based on higher heating values

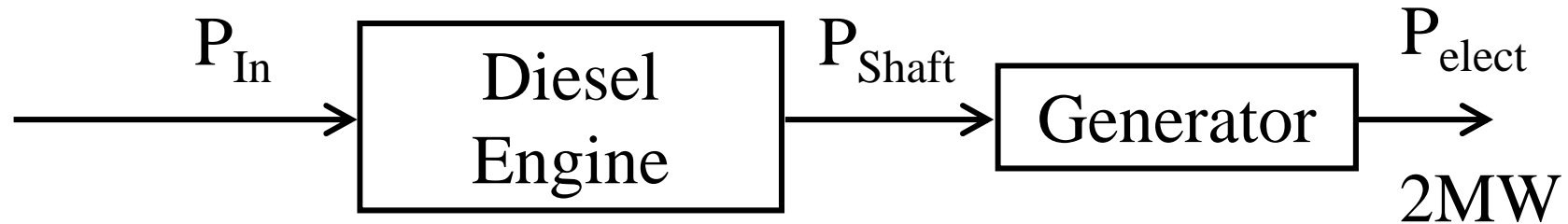
Percent Hydrogen vs. Specific Energy



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





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

- Mechanical Output

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

- Fuel Flow Rate

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

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

- Fuel Consumption

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

- Rate of Heat Addition

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

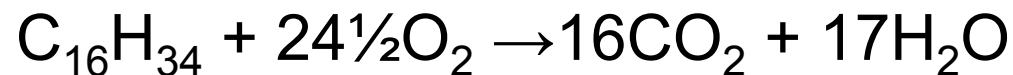
$$P_{\text{In}} = \left(18612 \frac{\text{MJ}}{\text{hr}} \right) \left(\frac{\text{hr}}{3600 \text{s}} \right) = 5.19 \frac{\text{MJ}}{\text{hr}} = 5.19 \text{MW}_{\text{th}}$$

- Diesel Engine Efficiency

$$\eta_{\text{Diesel}} = \frac{P_{\text{Shaft}}}{P_{\text{In}}} = \frac{2.08 \text{MW}_{\text{m}}}{5.19 \text{MW}_{\text{th}}} = 0.40$$

CO₂ Emission from Diesel Fuel

- Estimate the production of CO₂ (in g CO₂/kWh).
 - Use Cetane (C₁₆H₃₄) as a model reaction for diesel combustion. $\Delta H = 10,700\text{kJ/mol}$



- Atomic weights,
 - Carbon = 12g/mol,
 - Hydrogen = 1 g/mol
 - Oxygen = 16g/mol
- Reference: CO₂ emission from coal $\cong 325 \text{ gCO}_2/\text{kWh}$

- Molecular weight of CO₂

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

- There are 16 moles of CO₂ produced per mole of Cetane:

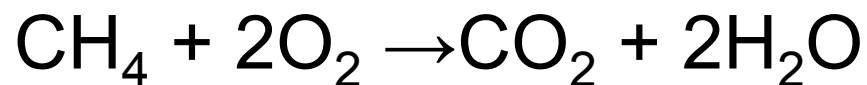
$$\frac{16\left(\frac{44\text{g}}{\text{mole}}\right)}{10700\frac{\text{kJ}}{\text{mole}}} = \frac{65.8 \times 10^{-3} \text{gCO}_2}{\text{kJ}} \left(\frac{3600\text{kJ}}{\text{kWh}}\right) = 237 \frac{\text{gCO}_2}{\text{kWh}}$$

- Determine the Carbon intensity of the electricity generation

$$237 \frac{\text{gCO}_2}{\text{kWh}} \xrightarrow{\text{Diesel Power Plant } \eta = 38.4\%} 237 \frac{\text{gCO}_2}{\text{kWh}} \left(\frac{1}{0.384}\right) = 617 \frac{\text{gCO}_2}{\text{kWh}}$$

Exercise, Gas Engine

- If we replaced the diesel generator in the previous example with a natural gas generator with the same efficiency, would the CO₂ emissions change?
 - Use methane (CH₄) as the model reaction for natural gas combustion. $\Delta H = 891 \text{ kJ/mol}$



Carbon Intensity of Electricity

- Generated from Coal:

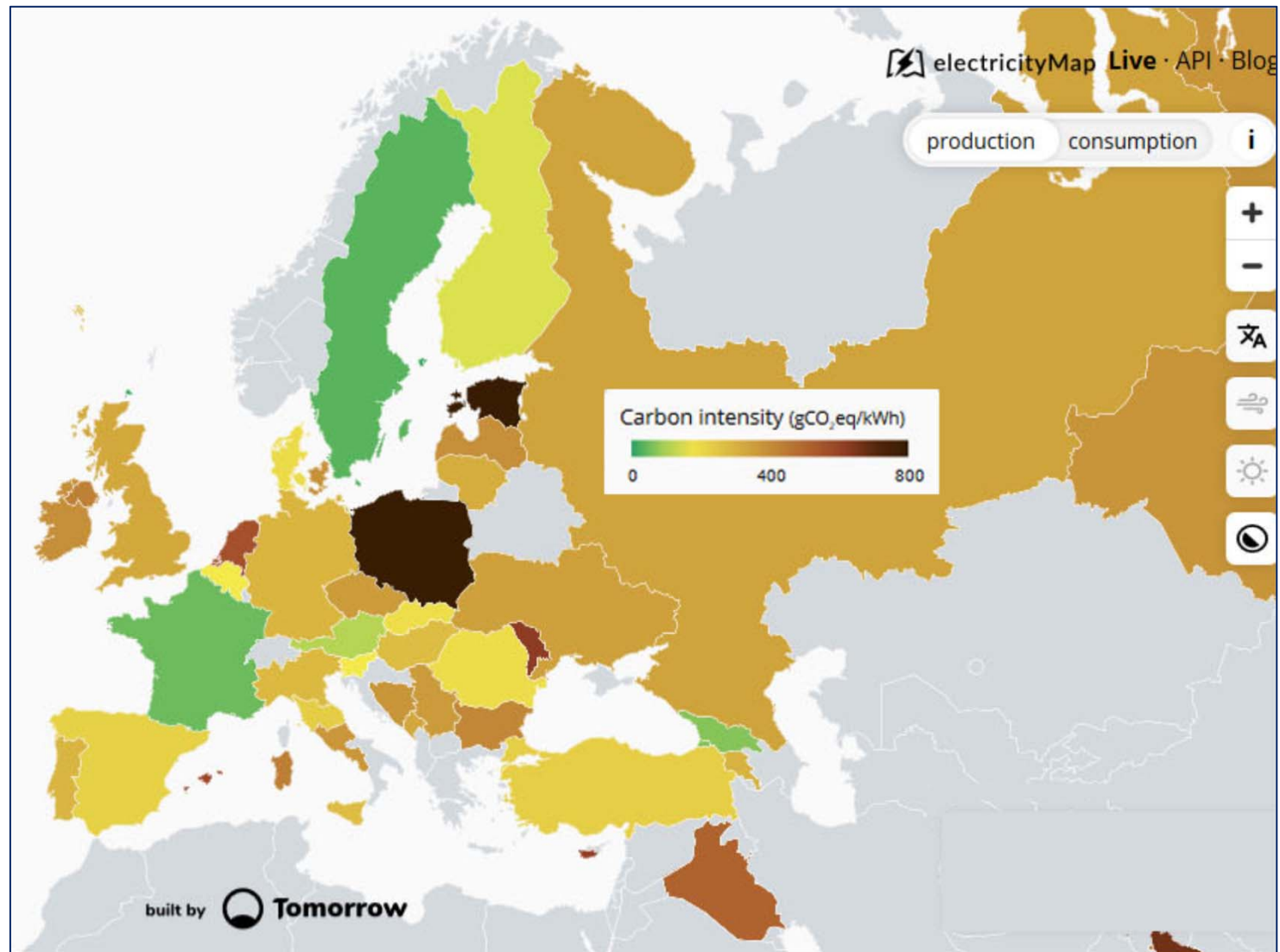
$$325 \frac{\text{gCO}_2}{\text{kWh}} \xrightarrow{\text{Coal Power Plant } \eta = 37.5\%} 325 \frac{\text{gCO}_2}{\text{kWh}} \left(\frac{1}{0.375} \right) = 867 \frac{\text{gCO}_2}{\text{kWh}}$$

- Generated from Natural Gas

$$178 \frac{\text{gCO}_2}{\text{kWh}} \xrightarrow{\text{Natural Gas Power Plant } \eta = 44.4\%} 178 \frac{\text{gCO}_2}{\text{kWh}} \left(\frac{1}{0.444} \right) = 401 \frac{\text{gCO}_2}{\text{kWh}}$$

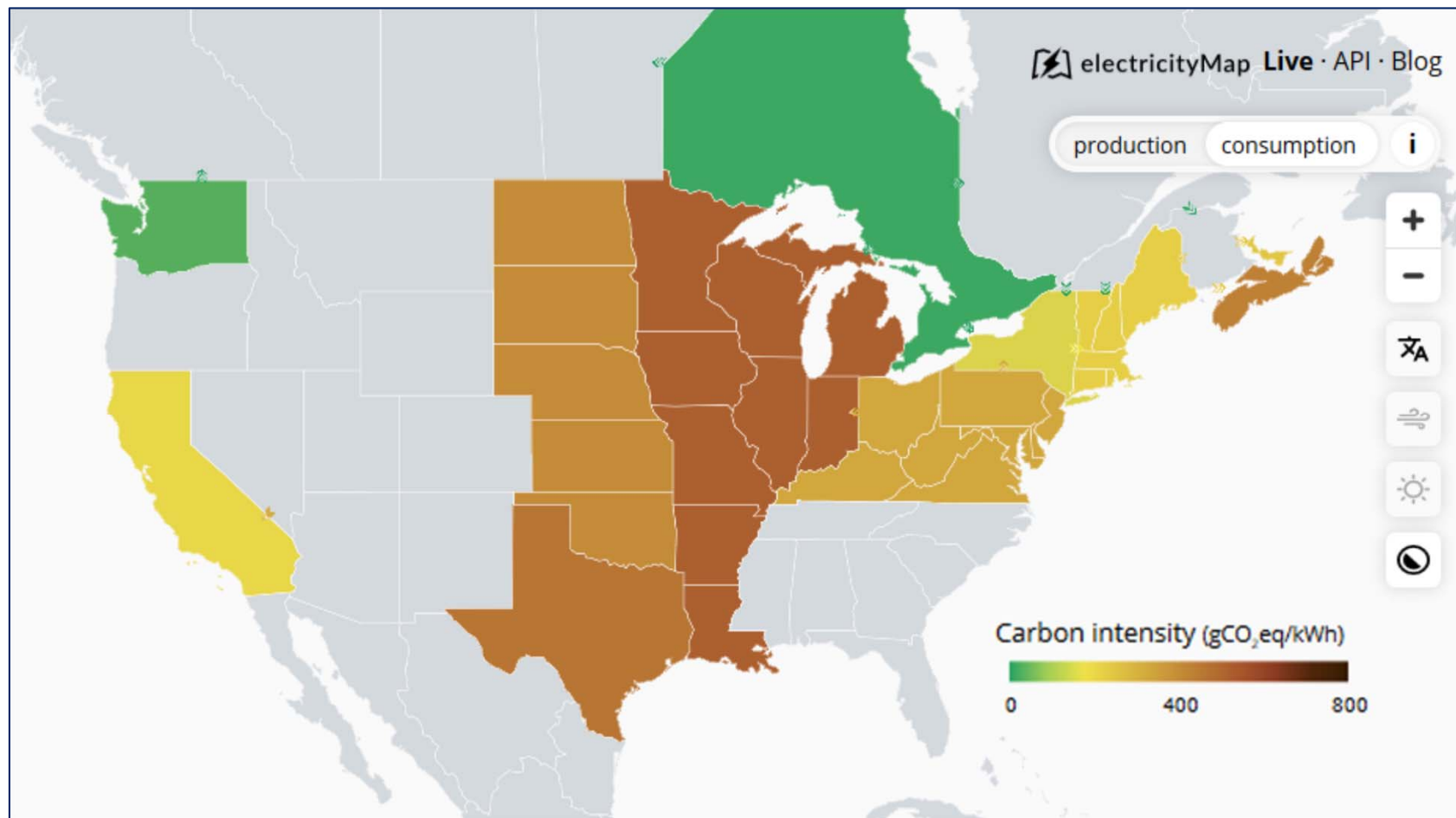
➤ Average Electrical Grid Carbon Intensity = $430 \text{ gCO}_2/\text{kWh}_e$

Carbon Intensity of Electricity: Europe



<https://www.electricitymap.org>

Carbon Intensity of Electricity: USA



<https://www.electricitymap.org>