Problem 5.5. Consider a fuel cell that uses methane ("natural gas") as fuel. The reaction is

$$CH_4 + 2O_2 \longrightarrow 2H_2O + CO_2.$$

(a) Use the data at the back of this book to determine the values of ΔH and ΔG for this reaction, for one mole of methane. Assume that the reaction takes place at room temperature and atmospheric pressure, and that the water comes out in liquid form.

(b) Assuming ideal performance, how much electrical work can you get out of the cell, for each mole of methane fuel?

(c) How much waste heat is produced, for each mole of methane fuel?

(d) The steps of this reaction are

$$\text{at } - \text{ electrode:} \quad CH_4 + 2H_2O \longrightarrow CO_2 + 8H^+ + 8e^-;$$
$$\text{at } + \text{ electrode:} \quad 2O_2 + 8H^+ + 8e^- \longrightarrow 4H_2O.$$

What is the voltage of the cell?

Phys 335: Problem 5.5

Methane fuel cell

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

assume 1 mole of methane, room temp, atmospheric pressure, and the final H_2O is liquid.

(a) ΔH and ΔG values

substance	$\Delta_f H$ (kJ)	$\Delta_f G$ (kJ)
CH_4	-74.81	-50.72
O_2	0	0
$H_2O(l)$	-285.83	-237.13
CO_2	-393.51	-394.36

for the whole reaction

$$\Delta H = \Delta H(\text{products}) - \Delta H(\text{reactants})$$
$$= 2\cdot(-285.83) + (-393.51) - (-74.81 + 2\cdot 0) \text{ kJ}$$
$$\Delta H = -890.36 \text{ kJ}$$

$$\Delta G = 2\cdot(-237.13) + (-394.36) - (-50.72 + 2\cdot 0) \text{ kJ}$$
$$\Delta G = -817.90 \text{ kJ}$$

(b) work? recall

$$\Delta G = (Q - T\Delta S) + W_{other}$$

If $\Delta S = Q/T$, then (the best you can do)

$$W_{other} = -817.90 \text{ kJ},$$

i.e. you get 817.90 kJ of work out for each mole of methane used.

(c) Waste heat? Recall $G = U - TS + pV$

$G = H - TS$

$\therefore \quad \Delta G = \Delta H - T\Delta S$ at constant temperature

Assuming ΔS is as small as possible so

$$Q = T\Delta S$$

$$Q = \Delta H - \Delta G =$$
$$-890.36\ kJ - (-817.90\ kJ)$$
$$Q = -72.46\ kJ$$

Q = heat added to the system

so $-72.4\ kJ \Rightarrow$ that is heat <u>leaving</u> the system.

(d) Voltage of the cell?

at − electrode: $CH_4 + 2H_2O \rightarrow CO_2 + 8H^+ + 8e^-$

at + electrode: $2O_2 + 8H^+ + 8e^- \rightarrow 4H_2O$

(note net effect is

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

and 8 electrons get moved from − electrode to + electrode.

For one mole of methane

$$W_{other} = 817.90\ kJ$$
$$\Delta q = 8\ \text{moles} \times (1.602\times10^{-19}\ C)$$
$$\Delta V = \frac{W_{other}}{\Delta q} = \frac{817.90\times10^{3}\ J}{8 \cdot 6.02\times10^{23} \cdot 1.602\times10^{-19}\ C} \times 1.02\ J/C$$

$$\boxed{\Delta V = 1.02\ \text{Volts}}$$