ME 446.671 Fuel Cell Science and Technology
Midterm Exam
2007 Apr 19 14:30~15:45

1. Explain following terms in a couple of sentences.
  a) Triple phase boundary
  b) Standard electrode potentials: STP condition
  c) Activation energy: Energy barrier
  d) Exchange current density
  e) Electroosmotic drag
  f) Limiting current density

Answer: Please refer to the textbook.

2. A hydrogen-oxygen fuel cell is operating under STP condition using hydrogen and air. The stoichiometric number of hydrogen and air is 1.1 and 2.0 respectively. At this condition, the fuel cell exhibits following characteristic.

$$V\ [\mathrm{V}] = 1.2 - 0.6j\ [\mathrm{A/cm^2}]$$

A compressor provides air to the fuel cell at the given flow rate. The power consumed by the compressor may be expressed as,

$$P\ [\mathrm{W/cm^2}] = 0.3 * p\ [\mathrm{atm}] * j\ [\mathrm{A/cm^2}]$$

Here, *p* and *j* denote the pressure of air and current density of the fuel cell. Answer the following questions

(a) Find the maximum power output from the fuel cell combined with the compressor.

Answer)

$$P_{FC} = 1.2j - 0.6j^2$$

$$P_{comp} = 0.3 \times 1 \times j = 0.3j$$

$$P_{output} = 1.2j - 0.6j^2 - 0.3j = 0.9j - 0.6j^2$$

$$\frac{dP}{dj} = 0.9 - 1.2j = 0, \ j = 0.75$$

$$P_{\max} = 0.3375 W / cm^2$$

(b) Repeat (a) if the air is provided at 3 atm. (you should consider the voltage change of the fuel cell. For simplicity, consider only the Nernst effect)

Answer)

$$E_0 = 1.23\,\text{at STP}$$

$$E = 1.23 - \frac{8.314 \times 298.15}{2 \times 96400} \ln \frac{1}{3^{0.5}} = 1.24$$

Only 0.01V increase due to Nernst effect.

$$P_{FC} = 1.21j - 0.6j^2$$

$$P_{comp} = 0.3 \times 3 \times j = 0.9j$$

$$P_{output} = 1.21 - 0.6j^2 - 0.9j = 0.31j - 0.6j^2$$

$$\frac{dP}{dj} = 0.31 - 1.2j = 0,\ j = 0.258$$

$$P_{\max} = 0.040W / cm^2$$

(c) Find the efficiency of the fuel cell system (combined with compressor) for the condition described in (a) (say, at maximum power output of the fuel cell). Use enthalpy for hydrogen oxygen reaction as 286kJ/mol.

Answer)

$$E_h = \frac{286000}{2 \times 96400} = 1.48V$$

At 0.75A

$$P_{in} = 1.48V \times 0.75 \times 1.1 = 1.22W / cm^2$$

$$\varepsilon = \frac{0.3375}{1.22} = 27.7\%$$

3. Bultler-Volmer equation has several simplified forms. Describe validity and usage of the following simplified equations.

a) Linearized BV equation

Answer) Valid 1) when activation overvoltage or current density is very small 2) when j0 (exchange current density) is very large. This form would be useful for very fast kinetic reactions such as hydrogen dissociations.

b) Tafel equation.

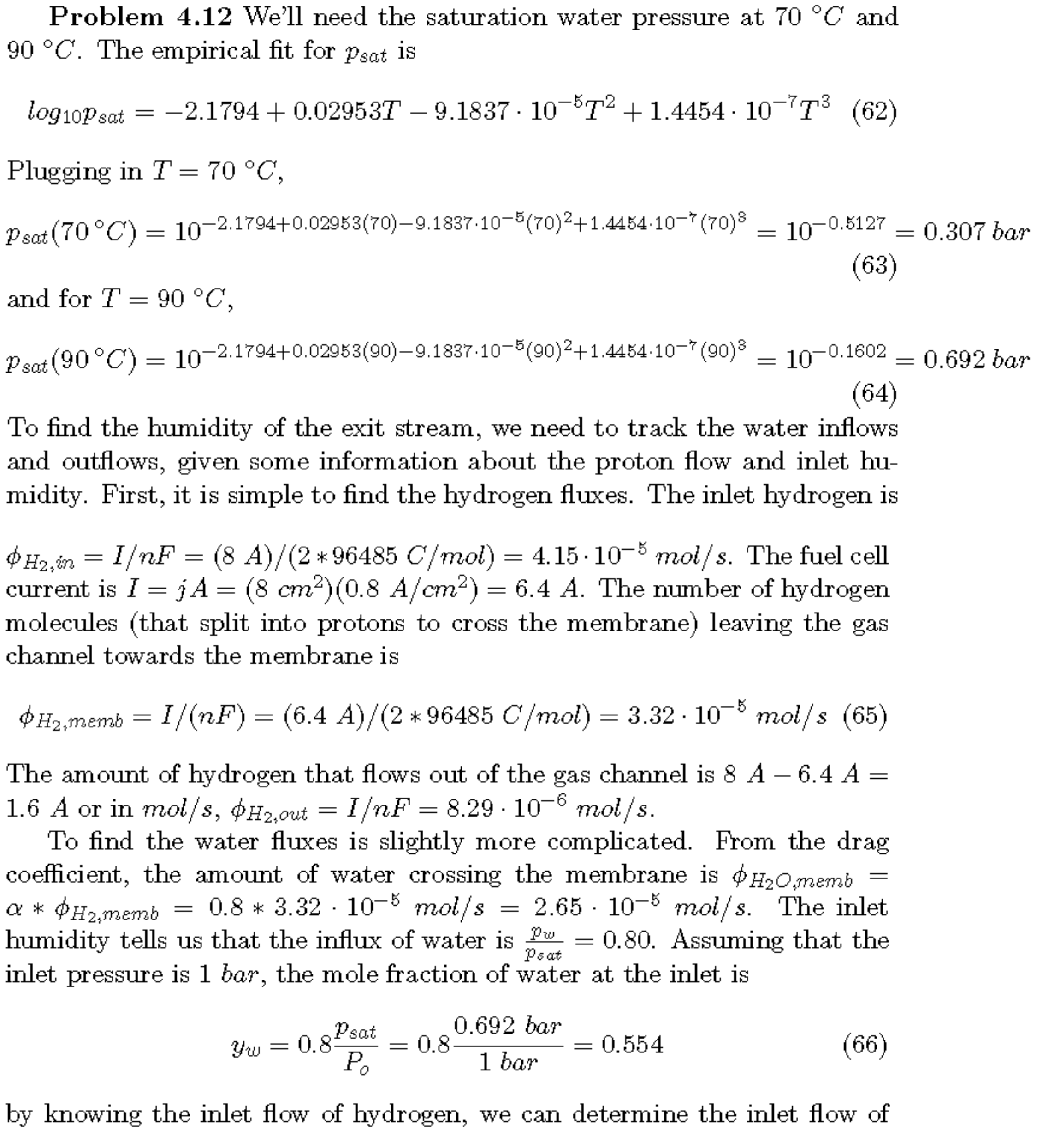
Answer) Valid when activation overvotltage or current density is very large. This form is useful for most fuel cell cases as fuel cells operate at decent current density level. The equation will explode at zero current density.

c) $j_T = j_0 \left[\exp\left\{ \frac{\alpha F \eta}{RT} \right\} - \exp\left\{ \frac{(1-\alpha) F \eta}{RT} \right\} \right] \frac{C_R^*}{C_R^0}$

Answer) To remedy the exploding issue of Tafel equation at zero current density, backward current flux term can be added. At zero overvoltage, the current density goes to zero unlike Tafel equation. This give the freedom to be used at any current density with good accuracy. However, the equation becomes implicit when you want to find overvoltage as a function of current density.

4. Consider a PEM fuel cell operating at 0.8A/cm^2 and 70C. Hydrogen gas at 90C and 80% relative humidity is provided to the fuel cell at the rate of 8 A. The fuel cell area is 8cm^2 and the drag ratio of water molecules/hydrogen, **α** is 0.8. Find the water activity of the hydrogen exhaust. Assume P=1 atm and assume the hydrogen exhaust exits at the fuel cell temperature, 70C.

Answer)



Problem 4.12 We'll need the saturation water pressure at 70 $°C$ and 90 $°C$. The empirical fit for p_{sat} is

$$log_{10} p_{sat} = -2.1794 + 0.02953T - 9.1837 \cdot 10^{-5} T^2 + 1.4454 \cdot 10^{-7} T^3 \quad (62)$$

Plugging in $T = 70\ °C$,

$$p_{sat}(70\,°C) = 10^{-2.1794+0.02953(70)-9.1837\cdot 10^{-5}(70)^2+1.4454\cdot 10^{-7}(70)^3} = 10^{-0.5127} = 0.307\ bar \quad (63)$$

and for $T = 90\ °C$,

$$p_{sat}(90\,°C) = 10^{-2.1794+0.02953(90)-9.1837\cdot 10^{-5}(90)^2+1.4454\cdot 10^{-7}(90)^3} = 10^{-0.1602} = 0.692\ bar \quad (64)$$

To find the humidity of the exit stream, we need to track the water inflows and outflows, given some information about the proton flow and inlet humidity. First, it is simple to find the hydrogen fluxes. The inlet hydrogen is

$\phi_{H_2,in} = I/nF = (8\ A)/(2 * 96485\ C/mol) = 4.15 \cdot 10^{-5}\ mol/s$. The fuel cell current is $I = jA = (8\ cm^2)(0.8\ A/cm^2) = 6.4\ A$. The number of hydrogen molecules (that split into protons to cross the membrane) leaving the gas channel towards the membrane is

$$\phi_{H_2,memb} = I/(nF) = (6.4\ A)/(2 * 96485\ C/mol) = 3.32 \cdot 10^{-5}\ mol/s \quad (65)$$

The amount of hydrogen that flows out of the gas channel is $8\ A - 6.4\ A = 1.6\ A$ or in mol/s, $\phi_{H_2,out} = I/nF = 8.29 \cdot 10^{-6}\ mol/s$.

To find the water fluxes is slightly more complicated. From the drag coefficient, the amount of water crossing the membrane is $\phi_{H_2O,memb} = \alpha * \phi_{H_2,memb} = 0.8 * 3.32 \cdot 10^{-5}\ mol/s = 2.65 \cdot 10^{-5}\ mol/s$. The inlet humidity tells us that the influx of water is $\frac{p_w}{p_{sat}} = 0.80$. Assuming that the inlet pressure is 1 bar, the mole fraction of water at the inlet is

$$y_w = 0.8\frac{p_{sat}}{P_o} = 0.8\frac{0.692\ bar}{1\ bar} = 0.554 \quad (66)$$

by knowing the inlet flow of hydrogen, we can determine the inlet flow of water

$$\phi_{H_2O,in} = \phi_{H_2,in}\frac{0.554}{1-0.554} = 5.14\cdot 10^{-5}\ mol/s \tag{67}$$

Knowing the inlet water and the amount that crosses through the membrane, we can find the outlet water flow

$$\phi_{H_2O,out} = \phi_{H_2O,in} - \phi_{H_2O,memb} = (5.14\cdot 10^{-5}\ mol/s) - (2.65\cdot 10^{-5}\ mol/s) = 2.49\cdot 10^{-5}\ mol/s \tag{68}$$

Finally, we can find the activity of water in the exhaust

$$a_w = \frac{p_w}{p_{sat}} = \frac{y_w \cdot P_{out}}{p_{sat}(T_{out})} = \frac{\phi_{H_2O,out}}{\phi_{H_2O,out} + \phi_{H_2,out}} \cdot \frac{P_{out}}{p_{sat}(70\ °C)} \tag{69}$$

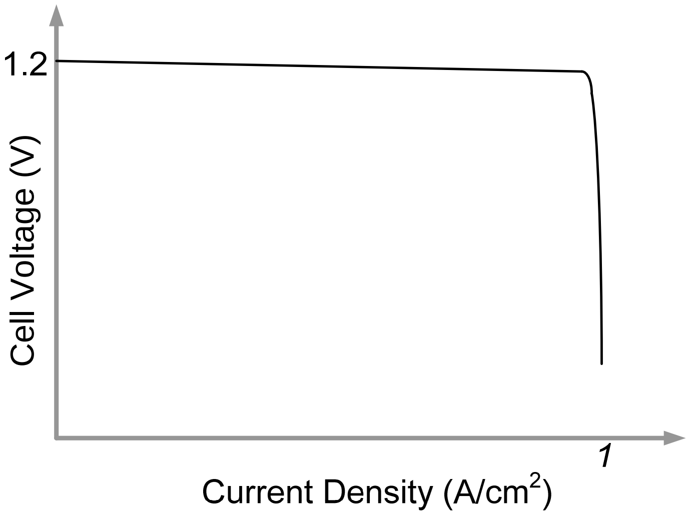
Assuming that the pressure drop along the gas channel is negligible,

$$a_w = \frac{2.49\cdot 10^{-5}\ mol/s}{2.49\cdot 10^{-5}\ mol/s + 8.29\cdot 10^{-6}\ mol/s} \cdot \frac{1\ bar}{0.307\ bar} = 2.44 \tag{70}$$

Since the activity is greater than 1, we have liquid water in the exhaust.

5. A hydrogen-oxygen fuel cell at STP condition has the IV characteristic as shown in the figure. 2 A/cm^2 worth of hydrogen and 1 A/cm^2 worth of oxygen is provided to the fuel cell.

Now, we mix 20% volume percent ozone, O_3, to the oxygen (which is 80% now) with all other conditions are same. Sketch the IV curve for this case including as much detail as you can. Explain your curve to justify your answer.



Answer) From Standard electrode potential table, hydrogen-ozone reaction gives 2.07V. 20% ozone give 0.2 atm partial pressure and according to Nernst equation,

$$2.07 - \frac{8{,}314 \times 298.15}{2 \times 96350} \ln \frac{1}{0.2^{1/3}} = 2.06V$$

The voltage change is minimal and could be ignored.

The original IV curve shows almost no diffusion limitation. 20% ozone is worth of 0.3A/cm^2 (=1A/cm2 * 0.2 * 3/2). These data will generate a first part of the IV curve. 80% oxygen is worth of 0,8A/cm2. Thus, the new limiting current will be 0.8+ 0.3 = 1.1A/cm^2. This gives the 2nd part of the IV curve. The final IV curve is shown in solid line. (In reality, the transition from the 1st curve to 2nd curve would be smoother.)