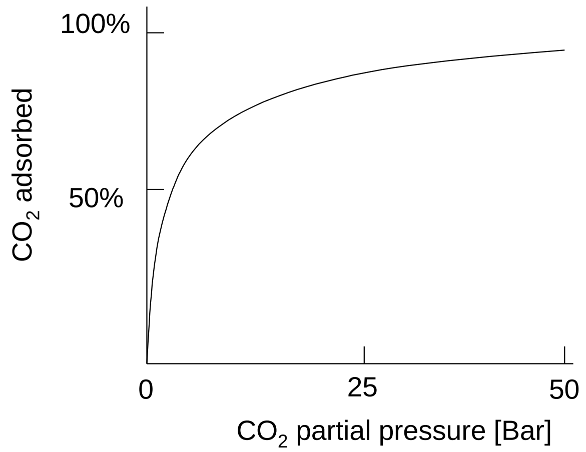
Sustainable Hydrogen and Electrical Energy Storage, SET3031
23 june 2008

Question 1.

a. Which technological factors need to be realized if an energy economy based on hydrogen as an energy carrier is to become a reality? Name 4.
b. What are main economical facts that have prevented the realization of a hydrogen economy?
c. Indicate what the current applications for hydrogen are.
d. For which current transport is hydrogen the fuel of choice and why?

Question 2.

a. How does the pressure swing adsorption method for the purification of hydrogen gas work?
b. Use the graph below. If one starts with a mixture of 50 mol% CO_2 and 50 mol % H_2. Estimate the H_2 concentration after loading such mixture in a pressure sweep vessel and applying a pressure sweep from 50 to 25Bar of the CO_2 partial pressure. What is the H_2 yield?
   Is a second sweep with 25 Bar CO_2 partial pressure technically feasible?



Question 3.

Consider the two half reactions $Ni^{2+}(aq) + 2e^- \rightarrow Ni(s)$ (standard potential -0.25 V) and $Fe^{3+}(aq)+e^- \rightarrow Fe^{2+}(aq)$ (standard potential +0.77 V). Assume that the $Fe^{2+}(aq)$ and $Fe^{3+}(aq)$ dissolved in the electrolyte cannot reach the Ni electrode. The $Fe^{3+}(aq)+e^- \rightarrow Fe^{2+}(aq)$ half reaction takes place at an inert Pt electrode (providing the electrons for the reaction).

a. Write down the total reaction in a battery configuration. In which direction will the reaction proceed spontaneously (Hint Fe^{2+} is more noble than Ni(s)).
b. What is the open cell potential under standard conditions, and how much chemical energy is converted to electrical energy per mole reacted Ni(s) ($\Delta G=-(\phi_C-\phi_A)zF$, F=96500 C/mol)?

Assume the starting concentrations are c_{Ni2+}=0.1, c_{Fe2+}=c_{Fe3+}=1 mol/liter and $c_{Ni(s)}$=1. Nernst law: (Nernst: $\varepsilon = (\phi_C - \phi_A) = \varepsilon^o - (RT/zF)\,[\ln \Pi c_j^{\nu}]$, for example applied to the half reaction $Fe^{3+}(aq)+e^{-} \rightarrow Fe^{2+}(aq)$ leads to $\varepsilon = \varepsilon^o - (RT/zF)\ln(c_{Fe2+}/c_{Fe3+})$. R=8.31 J/(mol K), T=293 K.

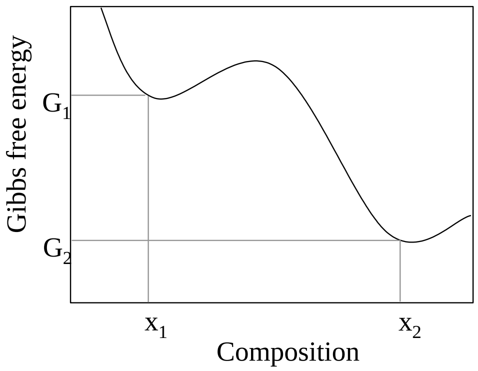
c. Calculate the open cell potential between the two electrodes under the given conditions?
d. When does the reaction stop?

Question 4.
The enthalpy of formation of iron hydride is +23.5 kJ/mol.
k_B= 1.38 10^{-23} J/K. 1 mole = 6.02 10^{23} particles

a. What concentration of H in Fe would one expect in iron at room temperature?
b. Hydrogen atoms in iron metal can move around. What happens if there is a crack or defect present in the iron? What happens if it is a carbon reinforced steel?

Question 5.

a. Give five required properties for rechargeable batteries.
b. Explain how a Li-ion battery works, what are the components, and what is their function?
c. What is the electrochemical double layer and what is its function in a supercapacitor?
d. Give the definition of the chemical potential, and its role in a battery.
e. Sketch chemical potential as a function of composition for the Gibbs energy shown in the graph, and explain its behavior.



f. Derive an expression in terms of G_1, G_2, x_1, and x_2 for the open cell potential between x_1 and x_2 given that $V_{OCP}=-\mu/F$.

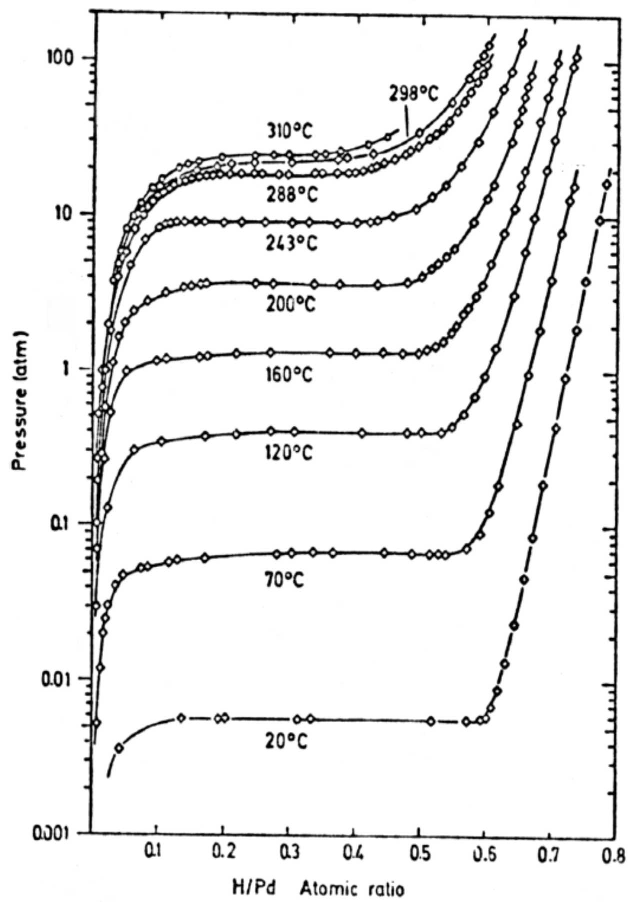
Question 6.
Hydrogen storage using surface adsorption attracts worldwide interest. The Langmuir isotherm describes the adsorption of molecules on a surface.

a. What are basic assumptions behind the Langmuir isotherm?

b. Derive a Langmuir isotherm for a process in which hydrogen is adsorbed on a surface and dissociates.
c. For which type of hydrogen storage materials would you expect to be able to measure an isotherm as in b? Name an organic and an inorganic material.

Question 7.
Below a pressure-composition graph is given for a hydride forming metal, Pd in this example, and H.
a. Describe what general thermodynamic features of the system can be read from the graph.
b. Estimate the enthalpy of formation using a van 't Hoff plot.

$$\frac{1}{2}\ln\left(\frac{P}{P_0}\right)=\frac{\Delta\bar{H}_H}{k_B T}-\frac{\Delta\bar{S}_H}{k_B}$$



Question 8.
$LaNi_5H_6$ is a hydrogen storage material. In practice commercial batteries use a modified compound: $MmNi_{3.55}Co_{0.75}Mn_{0.4}Al_{0.3}H_{5.18}$
Give three factors that necessitate the use of such modified compound.

Question 9.

a. What strategies are available to enhance the kinetics and reversibility of complex light metal hydrides? Shortly indicate how this works.
b. What strategies are available to improve the thermodynamics of light metal hydrides in order to bring operating temperature and pressures down to room temperature and pressure?

Question 10.

Hydrogen has a low natural abundance in the atmosphere: 0.5 ppm. Methane has a concentration of 1.8 ppm.

a. How do both gases play a role in the Greenhouse effect?
b. If a hydrogen economy is realized there will be some loss of H_2 in atmosphere. What do you expect to occur with the radiative forcing due to methane?

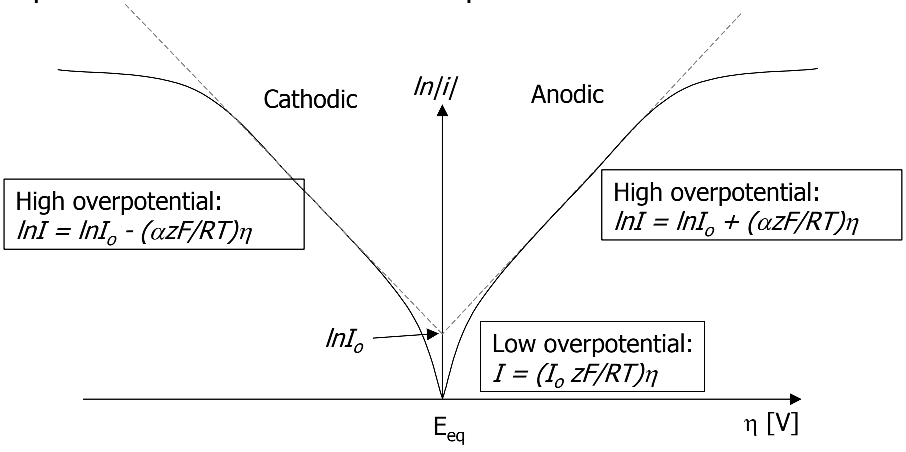
Question 11.

a. Describe which economic considerations play a role in the choice for hydrogen transport on large scales using liquid, or gaseous hydrogen.
b. Currently hydrogen is produced using fossil fuels mainly. How may the transition to renewable produced hydrogen take place and what happens with fossil fuel use and CO_2 reduction in the mean time?

Question 12.

a. Name three efficiency losses in the conversion of $H_2 + O_2$ towards H_2O in a fuel cell.
b. Explain what is meant by mixed potential?

Assume that for a certain fuel-cell the current responds on an applied overpotential looks like the "Tafel" plot shown.



c. What is the meaning of I_0 the exchange current density?
d. Which process dominates at low overpotentials, and what part of the fuel-cell should be changed to improve the performance at low overpotentials?

e. Which process limits the current at high overpotentials, and in which parts of the fuel-cell do you expect this to occur? Explain your answers.