SCHOOL OF ENGINEERING
MECHANICAL ENGINEERING
LRESE - Laboratory of Renewable Energy Sciences and Engineering

Renewable Energy: Solar Fuels Exercise

This exercise deals with assessment of solar fuels generation. In the first part, the production of hydrogen by photoelectrochemical water-splitting is investigated. In the second part, you use solar thermochemical route for the production of synthesis gas used in a fuel cell.

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1. The schematic of a photoelectrochemical cell is shown in figure 1.

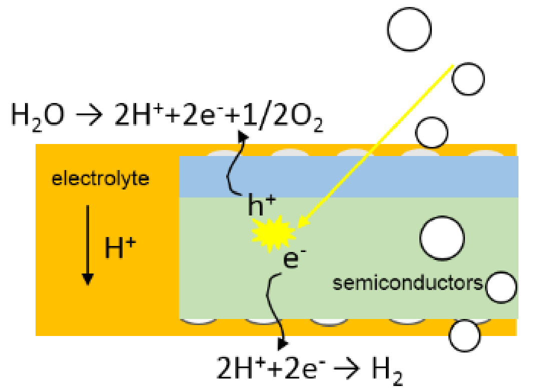

Figure 1: Schematic of the photoelectrochemical water splitting device

(a) The photoabsorber is a dual absorber made of Si (band gap 1.1 eV) and $BiVO_4$ (band gap 2.16 eV). Which of the two cells (Si or $BiVO_4$) will you put on top of your device?

(b) Calculate the fraction of incident light which is ideally absorbed in both cells.

(c) Assume that the resulting cell performance can be calculated by
$i = i_0 - i_1 \cdot \left(e^{\frac{qV}{nk_BT}} - 1\right)$
with $i_0 = 115$ A/m^2,$i_1 = 3 \cdot 10^{-42}$ A/m^2,$n = 1$, $T = 300$ K
Determine the short circuit current and open circuit voltage. What is the fill factor of this dual absorber cell?

(d) Assume that the load curve of the integrated electrochemical cell can be calculated by
$V = V_0 + i\rho l_p + a_1 log(\frac{i}{i_{0a}}) + a_2 log(\frac{i}{i_{0c}})$
with $V_0 = 1.23$ V, $\rho = 0.1\ \Omega m$, $l_p = 8$ cm, $a_1 = 0.035$ V/dec, $i_{0a} = 0.00001$ A/m^2, $a_2 = 0.03$ V/dec, $i_{0c} = 0.001$ A/m^2, $T = 300$ K
Describe the meaning of the four terms on the right hand side and calculate the overpotentials at a current density $i = 200$ A/m^2.

(e) Plot the two curves (i.e. for both PV an electrochemical cell) in a V-i-plot (x-axis: V, y-axis: i) and read the operating potential and current density. Is it operating at the maximum power point? How could we operate more close to the maximum power point?

(f) What is the efficiency of the cell, assuming an irradiation of 1000 W/m^2?

(g) Calculate how much hydrogen is produced per year and area assuming a continuous operation at the operating point for 1900 hours (high heating value of H_2 = 141 MJ/kg).

2. The solar steam-gasification of carbonaceous material for syngas production is represented by the net stoichiometric reaction:
CH_yO_z + (1-z)H_2O = (y/2 + 1-z) H_2 + CO

Each mole of CO in the syngas is further water gas-shifted to generate an additional mole of H2 according to:
CO + H_2O = H_2 + CO_2

The H_2/CO_2 mixture undergoes separation to H_2 and CO_2. H_2 produced is fed to a H_2/O_2 fuel cell, while CO_2 produced is released to the atmosphere. The process is schematically depicted in Fig. 2. The selected carbonaceous feedstock is wood, of elemental composition: 49 wt% C, 6 wt% H, and 45 wt% O.

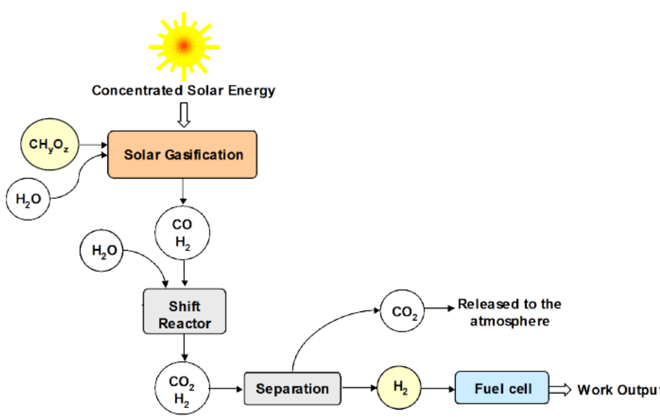

Figure 2: Schematic representation of the solar gasification process for H_2 generation

Assumptions:

- Solar reactor is a perfectly insulated blackbody cavity-receiver; only radiation losses are considered.
- Reactor operating temperature, $T_{reactor} = 1200$ K.
- Mean solar flux concentration ratio, $C = 1800$ suns.
- Normal beam insolation, $I = 1$ kW/m^2.
- Mass flow rate of CH_yO_z, $\dot{n}_{CH_yO_z} = 1$ mol/s.

- The net power absorbed by the solar reactor matches the enthalpy change per unit time of the reaction $\dot{Q}_{Reactor,net} = \dot{n}_{CH_yO_z} \cdot \triangle H$=210 kW.
- The water-gas shift reaction is carried out in an auto-thermal reactor.
- The H_2/CO_2 separation unit is based on the pressure swing adsorption technique (PSA) at 94% recovery rate.
- The H_2/O_2 fuel cell operates with a conversion efficiency of 62% of the high heating value of H_2.
- Heating value of carbonaceous feedstock, $HV_{CH_yO_z} = 570$ kJ/mol.
- High heating value of H_2, $HV_{H_2} = 285$ kJ/mol.

(a) Calculate y and z using the elemental composition of the carbonaceous feedstock. Calculate the number of moles of H2 and CO2 ideally produced for a mole of CHyOz gasified.

Hint: $\gamma_i = \frac{\nu_i/M_i}{\sum_n \nu_n/M_n}$, with γ molar fraction, ν weight fraction, and M molar mass of species i.

(b) Calculate the absorption efficiency of the solar reactor, $\eta_{absorption}$.

(c) Calculate solar power input, $\dot{Q}_{solar}$.

(d) Calculate the electric power output of the H_2/O_2 fuel cell, $\dot{W}_{out}$.

(e) Calculate the Energy Gain Factor (EGF), defined as the ration of the electric output of the solar process to that obtained when using the same amount of C as a combustion fuel in a 40% efficient Rankine cycle.

(f) Calculate the specific CO_2 emissions, in units of kg CO_2/kWh$_e$, for the solar process and for the 40% efficient Rankine cycle.