

Renewable Energy: Solar Fuels Exercise

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

1. The schematic of a photo-electrochemical cell is shown in figure 1.

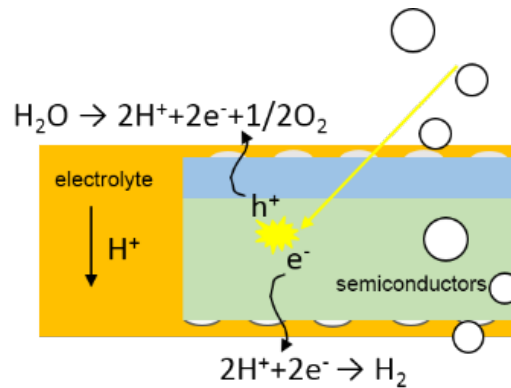
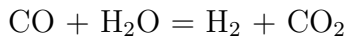


Figure 1: Schematic of the photo-electrochemical water splitting device

- (a) The photo-absorber is a dual absorber made of *Si* (band gap 1.1 eV) and *BiVO₄* (band gap 2.16 eV). Which of the two cells (*Si* or *BiVO₄*) 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
- $$i = i_0 - i_1 \cdot \left(e^{\frac{qV}{nk_B T}} - 1 \right)$$
- with $i_0 = 115 \text{ A/m}^2$, $i_1 = 3 \cdot 10^{-42} \text{ A/m}^2$, $n = 1$, $T = 300 \text{ K}$
 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
- $$V = V_0 + i\rho l_p + a_1 \log\left(\frac{i}{i_{0a}}\right) + a_2 \log\left(\frac{i}{i_{0c}}\right)$$
- with $V_0 = 1.23 \text{ V}$, $\rho = 0.1 \text{ } \Omega\text{m}$, $l_p = 8 \text{ cm}$, $a_1 = 0.035 \text{ V/dec}$, $i_{0a} = 0.00001 \text{ A/m}^2$, $a_2 = 0.03 \text{ V/dec}$, $i_{0c} = 0.001 \text{ A/m}^2$, $T = 300 \text{ K}$
 Describe the meaning of the four terms on the right hand side and calculate the overpotentials at a current density $i = 200 \text{ A/m}^2$.

- (e) Plot the two curves (i.e. for both PV and the 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 (lower heating value of $\text{H}_2 = 120 \text{ MJ/kg}$).
2. The solar steam-gasification of carbonaceous material for syngas production is represented by the net stoichiometric reaction:
- $$\text{CH}_y\text{O}_z + (1-z)\text{H}_2\text{O} = (y/2 + 1-z) \text{H}_2 + \text{CO}$$

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



The H₂/CO₂ mixture undergoes separation to H₂ and CO₂. H₂ produced is fed to a H₂/O₂ fuel cell, while CO₂ 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.

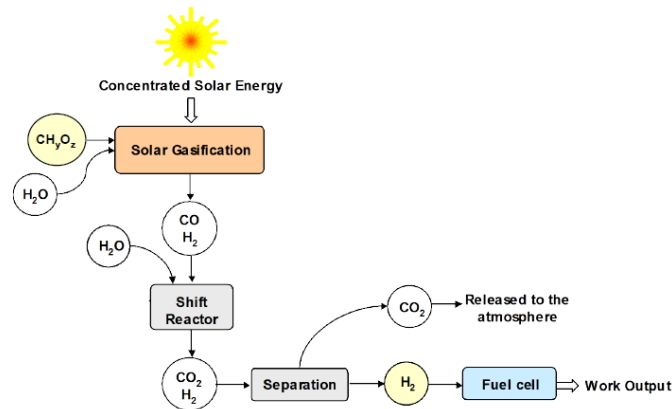


Figure 2: Schematic representation of the solar gasification process for H₂ generation

Assumptions:

- Solar reactor is a perfectly insulated blackbody cavity-receiver; only radiation losses are considered.
- Reactor operating temperature, $T_{reactor} = 1200 \text{ K}$.

- Mean solar flux concentration ratio, $C = 1800$ suns.
 - Normal beam insolation, $I = 1$ kW/m².
 - Mass flow rate of CH_yO_z , $\dot{n}_{\text{CH}_y\text{O}_z} = 1$ mol/s.
 - The net power absorbed by the solar reactor matches the enthalpy change per unit time of the reaction $\dot{Q}_{\text{Reactor,net}} = \dot{n}_{\text{CH}_y\text{O}_z} \cdot \Delta H = 210$ 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, $HV_{\text{CH}_y\text{O}_z} = 570$ kJ/mol.
 - High heating value of H_2 , $HV_{\text{H}_2} = 285$ kJ/mol.
- (a) Calculate y and z using the elemental composition of the carbonaceous feedstock. Calculate the number of moles of H_2 and CO_2 ideally produced for a mole of CH_yO_z 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, $\eta_{\text{absorption}}$.
- Hint: You can use the Stefan-Boltzmann-Law to account for black-body radiation losses.
- (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 ratio 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.