

Renewable Energy: Solar Fuels Solution

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.

1. (a) The solar cell with the larger band gap will be on top.
- (b) $E_g=2.16$ eV implies $\lambda_1 = 0.574 \mu\text{m}$; $E_g = 1.1$ eV implies $\lambda_2 = 1.127 \mu\text{m}$;
 $F_{0-\lambda_1 T} = 0.346$, fraction of top cell;
 $F_{0-\lambda_2 T} = 0.779$, fraction bottom cell: $F_{\lambda_1 T-\lambda_2 T} = F_{0-\lambda_2 T} - F_{0-\lambda_1 T} = 0.433$
- (c) Short circuit current density (i.e i @ $V=0$) is $i_{sc} = 115 \text{ A/m}^2$
 Open circuit voltage (i.e V @ $i=0$) is $V_{oc} = 2.59 \text{ V}$ (using $V = \ln\left(\frac{i_0}{i_1} + 1\right) \frac{nk_B T}{q}$)
 Fill factor (FF) = $P_{max}/(i_{sc} V_{oc})$
 P_{max} can be calculated using the plot below or numerically using $\frac{d(i \cdot V)}{dV} = 0$;
 $P_{max} = 284.76 \text{ W/m}^2$ and hence FF = 0.954

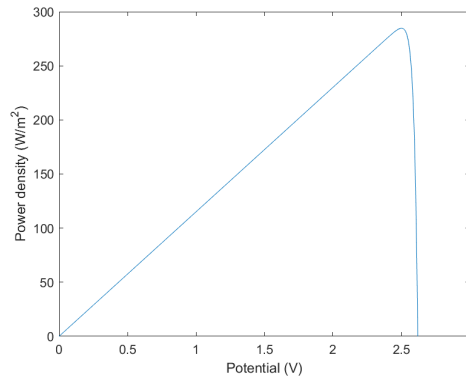


Figure 1: Plot of the power density vs. potential (V) of the solar cell

- (d) The first term is the equilibrium potential, second term is ohmic losses due to resistances in the solution, the third and fourth terms are the kinetic overpotential due to reaction, one for the anode and one for the cathode.
 $\Delta V_{ohmic} = i \rho l_p = 1.6 \text{ V}$ (@ $i=200 \text{ A/m}^2$)
 $\Delta V_{anode} = a_1 \log\left(\frac{i}{i_{0a}}\right) = 256 \text{ mV}$ (@ $i=200 \text{ A/m}^2$)
 $\Delta V_{cathode} = a_2 \log\left(\frac{i}{i_{0c}}\right) = 159 \text{ mV}$ (@ $i=200 \text{ A/m}^2$)
- (e) Operating point: $i_{op} = 112.1 \text{ A/m}^2$; $V_{op} = 2.525 \text{ V}$; implies $P_{op} = 283.1 \text{ W/m}^2$ which is smaller than P_{max}
 We need to reduce the overpotentials: i.e. by using better conducting solution, using catalysts that can support faster reaction kinetics, etc.

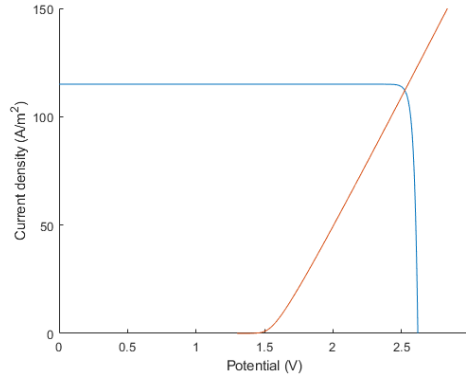


Figure 2: Operating curves of PEC cell

(f) Efficiency: $\eta = \frac{i_{op}V_0}{Q_{in}} = 112.1 \cdot 1.23 / (1000) = 0.14 = 14\%$

(g) $m = \frac{\eta Q_{in}}{LHV_{H_2}} t = \frac{(0.14 \cdot 1000)}{120 \cdot 10^6} 1900 \cdot 3600 = 8.0 \text{ kg/m}^2$.

Note: Strictly speaking, the hydrogen production should be calculated using the Gibbs free energy change (237 kJ/mol), since this corresponds to the reversible cell voltage of 1.23 V used in the efficiency definition in (f). However, in this case, assuming the lower heating value is sufficient.

2. (a) $\gamma_i = \frac{\nu_i/M_i}{\sum_n \nu_n/M_n}$, with γ molar fraction, ν weight fraction, and M molar mass of species i ; implies

$$x_1 = \frac{0.49/0.012}{0.49/0.012 + 0.06/0.001 + 0.45/0.016} = 0.317,$$

$$y_1 = \frac{0.06/0.001}{0.49/0.012 + 0.06/0.001 + 0.45/0.016} = 0.465,$$

$$z_1 = \frac{0.45/0.016}{0.49/0.012 + 0.06/0.001 + 0.45/0.016} = 0.218,$$

$$y = y_1/x_1 = 1.469;$$

$$z = z_1/x_1 = 0.689;$$

Total number of H₂ moles: $(y/2 + 2 - z) = 2.046$;

Total number of CO₂ moles: 1

(b) $\eta_{absorption} = 1 - \frac{\sigma T^4}{CI} = 1 - \frac{5.67 \cdot 10^{-8} \cdot 1200^4}{1800 \cdot 1000} = 0.935$.

(c) $\eta_{absorption} = \frac{\dot{Q}_{Reactor,net}}{\dot{Q}_{solar}}$; hence

$$\dot{Q}_{solar} = \frac{\dot{Q}_{Reactor,net}}{\eta_{absorption}} = 210/0.935 = 224.7 \text{ kW}$$

(d) $\dot{n}_{H_2, fuelcell} = (y/2 + 2 - z)\dot{n}_{CH_4O_2}\eta_{PSA} = (1.469/2 + 2 - 0.689)(1 \cdot 0.94) = 1.92 \text{ mol/s}$
 $\dot{W}_{out} = \dot{n}_{H_2, fuelcell} \cdot HV_{H_2} \cdot \eta_{fuelcell} = 1.92 \cdot 285 \cdot 0.62 = 339.8 \text{ kW}$

(e) $EGF = \frac{\dot{W}_{out}}{\dot{W}_{Rankine}};$

$$\dot{W}_{Rankine} = \eta_{Rankine} \cdot \dot{n}_{CH_4O_2} \cdot HV_{CH_4O_2} = 0.40 \cdot 1 \cdot 570 = 228 \text{ kW}; \text{ hence}$$
$$EGF = 339.8/228 = 1.49$$

(f) $\dot{m}_{CO_2} = \dot{n}_{C_xH_yO_z} \cdot M_{CO_2} = 1 \cdot 0.044 = 0.044 \text{ kg/s};$

$$Em_{solar} = \frac{\dot{m}_{CO_2}}{\dot{W}_{out}} = \frac{0.044 \cdot 3600}{339.8} = 0.47 \text{ kgCO}_2/\text{kWh}_e$$

$$Em_{Rankine} = \frac{\dot{m}_{CO_2}}{\dot{W}_{Rankine}} = \frac{0.044 \cdot 3600}{228} = 0.69 \text{ kgCO}_2/\text{kWh}_e$$