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E DELL'INFORMAZIONE

EEG Track Macro Exercise for ETEPS

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1. Introduction

This report presents an electrolyzer's dimensioning and performance analysis designed to optimize hydrogen production for achieving a target H_2/CO ratio of 2.1. The exercise builds upon the thermochemical conversion of biomass and focuses on designing a system that balances efficiency and feasibility. Given technological limitations, the electrode size is constrained to 30 × 30 cm, with nickel selected as the material to minimize costs. The electrolyzer operates at 80°C and 5 bar, with cells connected in series and a maximum allowable current density of 400 A/m².

2. Methodology

2.1 Characteristics Plot and Required Power

In order to visualize the characteristics plot, it is necessary to calculate the characteristic variables. First, Nernst cell potential should be calculated using the equation below:

$$\Delta E = \Delta E^{\circ} - \frac{RT}{2F} \ln \frac{\left(P - P_{H_2O}^{\frac{3}{2}}\right)}{\frac{P_{H_2O}}{P_{H_2O}^{0}}} \qquad 2.1$$

Where ΔE° is the standard electrode potential, F is Faraday's constant (96,485 C/mol), P^{0}_{H2O} is the equilibrium water vapor pressure, and P_{H2O} is water vapor pressure.

The overpotential of anode and cathode is calculated using the following equation:

$$\eta = b \times \ln\left(\frac{i_{nom}}{i^{0}}\right) - b \times \ln\left(1 - \theta\right) \qquad 2.2$$

Where b is the Tafel slope, i_{nom} is nominal current density, i_0 is exchange current density, and θ is the gas bubble coverage fraction.

Bubbles are one of the key contributors to Ohmic overpotential, and this contribution is expressed as:

$$R_{el} = R_{bubble\ free} + R_{bubble\ el} = \frac{1}{\sigma_{KOH}}\left(\frac{\delta_{el}}{A}\right) + \frac{1}{\sigma_{KOH}}\left(\frac{\delta_{el}}{A}\right) \times \left[\frac{1}{\left(1-\frac{2}{3}\theta\right)^{\frac{3}{2}}} - 1\right] \qquad 2.3$$

Where $R_{bubble\ free}$ is the resistance of the electrolyte without bubbles, $R_{bubble\ el}$ is additional resistance caused by bubbles, σ_{KOH} is ionic conductivity of the KOH electrolyte, δ_{el} is the thickness of the electrolyte layer, and A is the electrode surface area.

The consumed power is calculated as follows:

$$P = I.\Delta V = I.A.\Delta V \qquad 2.4$$

All of the calculations have been done using MATLAB, and the exchange current density varies from 5 to 400 $\frac{A}{m^2}$ with step 5 $\frac{A}{m^2}$.

2.2 Calculation of the Required Water Flux and Produced H_2 for Single Cell

The electrochemical reaction in the electrolyzer follows:

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2 \quad 2.5$$

Using *Faraday's Law of Electrolysis*, the molar flow rate of a species produced or consumed in an electrochemical reaction is:

$$n = \frac{I}{n_e F} \quad 2.6$$

Where I is the current and n_e is the number of electrons transferred per molecule. The volumetric flow rate is then calculated as:

$$V = n.V_m \quad 2.7$$

Where V_m is the molar volume of the gas at standard conditions, the amount produced or consumed for each reaction component can be determined using the equations above.

2.3 Calculation of the Required Water Flux and Number of Cells

This section aims to calculate the number of cells to achieve a H_2/CO ratio of 2.1. First, it is necessary to determine the amount of H_2 generated to reach the desired final stream composition.

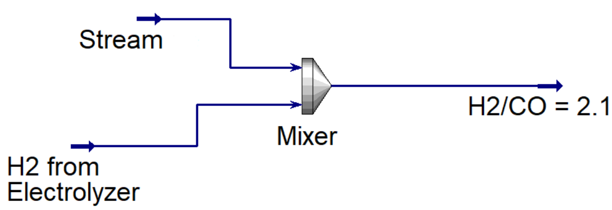

Figure 1- Schematic of Hydrogen Generating Mixing Flows

For the output stream from biomass conversion, three scenarios are considered. The stream properties and the required H_2 from the electrolyzer for each scenario are presented in the following table.

Table 1- Generated and Required Stream Flow and Composition

Scenario	Gas Flow [kmol/s]	H_2 Flow [kmol/s]	CO Flow [kmol/s]	Total Required H_2 Flow [kmol/s]	Required H_2 Flow from Electrolyzer [kmol/s]
1	1.54733E-05	4.05189E-06	5.43482E-06	1.1413122E-05	0.7361E-5
2	1.71033E-05	3.85476E-06	4.99964E-06	1.0499244E-05	0.6644E-5
3	2.3136E-05	5.85926E-06	3.56465E-06	7.485765E-06	0.1627E-5

The number of cells can be determined by dividing the total required H_2 by the amount produced by a single cell. Then, the total required water flux can be calculated by multiplying the water needed for a single cell by the number of cells.

3. Results and Discussion

3.1 Determination of the Number of Required Cells

The number of required cells for each scenario is shown in the table below.

Table 2- Number of Electrolyzer's cells

Scenario	Number of Cells
1	41
2	37
3	9

3.2 Characteristics Plot

The characteristic plots of the electrolyzer is shown in the figure below:

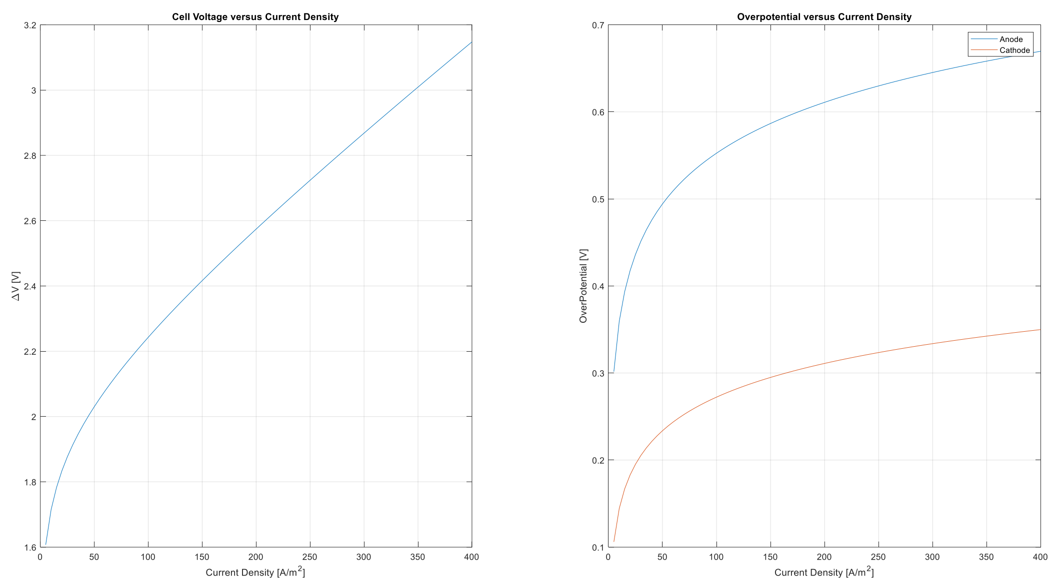

Figure 2- Characteristics Plot of a Single Cell

3.3 Consumed Power of System

The required power for the electrolyzer for each scenario is shown in the following table.

Table 3- Required Electrolyzer's Power

Scenario	Required Power [kW]
1	4.6461
2	4.1928
3	1.0199

The required power versus current density for each cell is illustrated as follows.

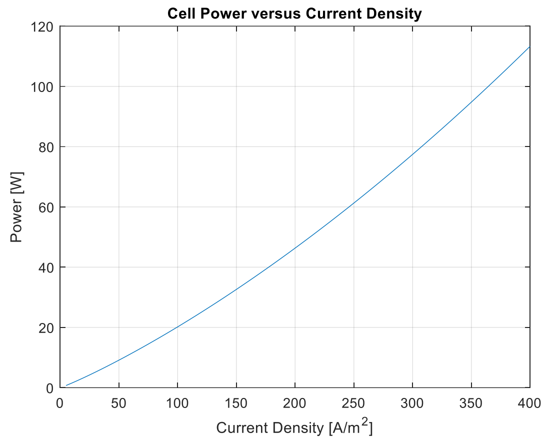

Figure 3- Consumed Power of a Single Cell versus Current Density

3.4 Required Flux of H_2O and generated Flux of H_2 and O_2

The required water flux for each scenario is shown in the table below.

Table 4- Required Flux of Water for Electrolyzer

Scenario	Required Flux of Water [L/h]
1	0.49748
2	0.44895
3	0.1092

The produced O_2 and H_2 for each cell versus current density is shown in the following picture.

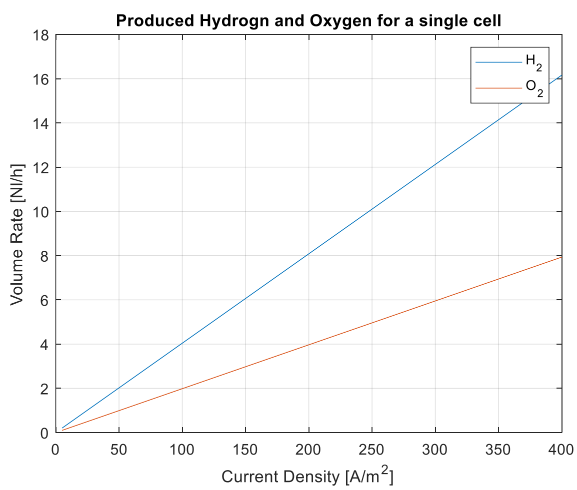

Figure 4- Produced H_2 and O_2 for a Single Cell

3.5 Evaluation of Cell Performance Improvement with Commercial Electrocatalysts

This section evaluates the impact of commercial electrocatalysts, Acta 3030 for OER and Acta 4030 for HER, on electrolyzer performance.

The figure below emphasizes on comparison characteristics plot between Ni electrodes and commercial electrocatalysts.

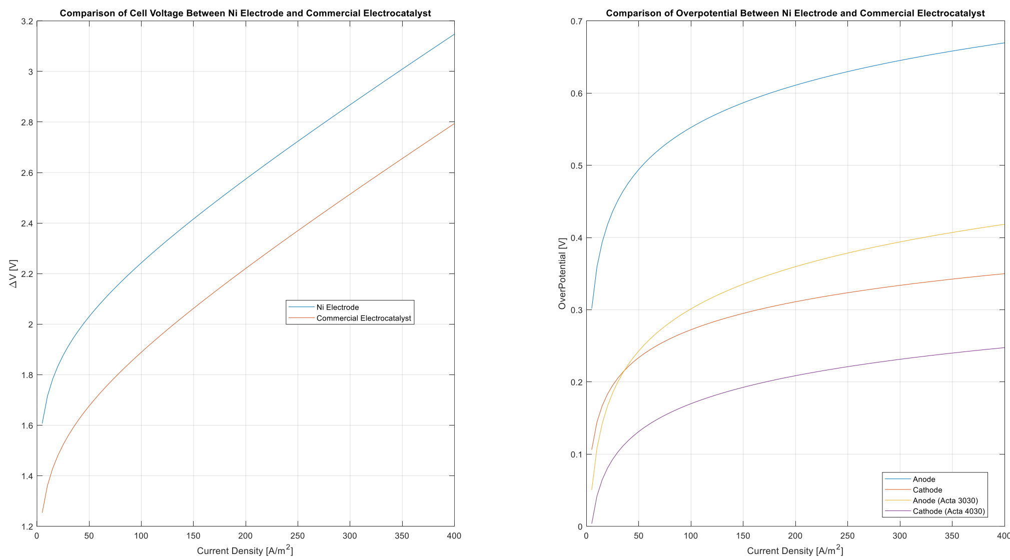

Figure 5- Characteristics Plot Comparison Between Ni Electrode and Commercial Electrocatalyst

The plots show that commercial electrocatalysts improve electrolyzer performance. The left graph indicates lower cell voltage (ΔV), meaning reduced power consumption. The right graph shows a significant drop in overpotential, especially with Acta 3030 and Acta 4030, improving reaction efficiency, which confirms that electrocatalysts enhance hydrogen production while reducing energy losses.

The comparison of the consumed power of the cell between Ni electrodes and commercial electrocatalyst is illustrated in the following figure.

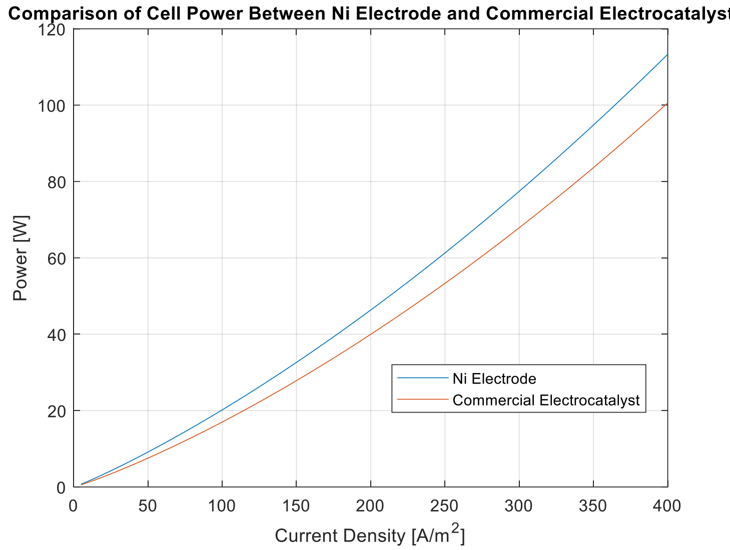

Figure 6- Consumed Cell Power Comparison Between Ni Electrode and Commercial Electrocatalyst

The commercial electrocatalyst consistently requires less power, indicating improved efficiency. The lower power demand means reduced energy losses and better system performance, making commercial electrocatalysts more energy-efficient for hydrogen production. The electrolyzer's required power by employing commercial electrocatalyst electrodes is mentioned in the table below.

Table 5- Required Electrolyzer's Power by Employing Commercial Electrocatalysts

Scenario	Required Power [kW]
1	4.1239
2	3.7215
3	0.90524

All the MATLAB code and materials are accessible via GitHub!
