Mathematical modeling of re-electrification by green hydrogen storage through the PEM fuel cell integrating a 10-year economic study applied to a hotel

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Abstract. The energy transition to prevent global warming is the main concern. Climatic change effects show a catastrophic view to the word through the increase of temperature which promotes fire like in Siberia or ices melts by trigging the extinction of polar bears in the future, also adding the flooding in Norway. Thus, it is important to trait sectors the most polluters such as transport, industries, and residential tertiary sectors. In the perspective to reduce their dependence on fossil fuels. However, the frequently used sources of energy are unstable. They require an appropriate clean storage system and the technology of energy storage relevant as green hydrogen. In this article, we focus first on the creation complete of the model of production chain for green hydrogen by the fuel cell PEM. Then, the application of the model in one technical-economic study for energetic consumption HVAC for a hotel. We will consider the usage of thermic power resulting from the chemical reaction of the system, those powers allow us to demonstrate that the fuel cell PEM presents the brilliant performance compare to electrolysis. Through that thermic power from the fuel cells, we will expose the fact it is possible to avoid the utilization of natural gas and electricity structure for domestic hot water. This technical-economic study show that green hydrogen technology can be worthwhile for the short or middle term for the hotel industry.

1 Introduction

Use Energy transition is today a major stake for humanity to survive, in fact, global industrialization has caused the gradual degradation of our environment. The rate of greenhouse gases has dramatically increased throughout this decade [1] and today we can see the consequences. In order to fight against this phenomenon caused by our industrialization, several actions must be taken from now. As such, several conventions have been put in place to limit the increase in global average temperature to well below 2°C at pre-industrial levels, by limiting the increase to 1.5°C [2]. Among these actions, the principle of polluting pays by the carbon tax [3] was put in place and thus encourages the exponential growth that we can be observed in the development of renewable energies. Renewable energies represent an important factor in the energy transition, indeed, the increase of the world population [4] results in an increase of energy consumption and therefore induces an increase in greenhouse gases, especially in the transport, industrial, tertiary and residential[5], therefore the use of clean energies in these energy-intensive sectors will make it possible to achieve the objectives set knowing that their cost decreases year after year. However, the instability of renewable energies is a problem and transporting energy over long distances incurs high costs associated with wasted imports, from which energy storage plays an important role in bypassing these different problems. There are a multitude of studies on energy storage systems, however most of these technologies produce greenhouse gases although the LFP lithium-ion battery is one of the promising technologies because it emits a low amount of CO2 [7]. Never mind, Hydrogen storage by electrolysis of water remains the cleanest form of energy storage [8], and to face energy transition, it thus becomes one of the most promising solutions for the future of the energy sector in transportation which is the main polluter, but also in the industrial sector, tertiary and residential which occupy the second place in environmental pollution to date. Research on hydrogen is known nowadays, storage by proton membrane exchange (PEM) electrolysis contains several research articles[9-10], the main problem with this technology is its high cost compared to others. However, the increase in the carbon tax followed by the drop in the cost of renewable energies make that this solution becomes competitive. That is why, the main objective of this article is the mathematical modeling of the complete production chain of hydrogen storage by PEM electrolysis for re-electrification, starting from the electrolysis, storage tank, to the fuel cell PEM in order...
to simulate in real time the entire production chain, acting on all the possible parameters, thus allowing a global visibility on the system, but also, to apply this modeling to a technical-economic study in the residential-tertiary sector, in order to show the feasibility of the return on investment of the implementation of this technology when using these heat losses.

The document is organized as follows: In paragraph, the mathematical modeling of the electrolysis, the storage tank, followed by the modeling of the fuel cell. In section, we present a case study of re-electrification by PEM cell followed by all the results. A conclusion and a list of references complete the paper.

2 Mathematical modelling re-electrification by PEM fuel cell

2.1 Modeling of water electrolysis

The hydrogen storage chain by electrolysis of water begins in the electrolysis, several works about the modeling of water electrolysis exist in the scientific literature [11–15], and follows this equations are necessary for modeling the electrolysis.

\[
I(T,P) = \begin{cases} 
0 & V \leq E_{\text{rev}}(T,P) \\
\frac{V - E_{\text{rev}}(T,P)}{R_i(T,P)} & V \geq E_{\text{rev}}(T,P)
\end{cases} \tag{1}
\]

\[
V(T,P) = \frac{P}{\mu} I(T,P) + n_i E_{\text{rev}}(T,P) \tag{2}
\]

(1) and (2) the voltage and current coming from the production of solar panels.

\[
E_{\text{rev}}(T,P) = E_{\text{rev0}}(T,P) + \frac{R(273+T)}{2F} \ln \left( \frac{P}{P_0} \right) \tag{3}
\]

\[
R_i(T,P) = R_{i0} + kn_i \ln \left( \frac{P}{P_0} \right) + dR_i(T + T_0) \tag{4}
\]

(3) represents the reverse voltage and (4) the initial resistance of the PEM cells.

\[
V_i = \frac{\Delta G}{2F} \tag{5}
\]

\[
\Delta G = 285.84 - 163.2(273 + T) \tag{6}
\]

\[
v_H = \frac{6000v_m}{2F} \tag{7}
\]

\[
v_m = \frac{R(273+T)}{p} \tag{8}
\]

\[
P = V \times I \tag{9}
\]

\[
P_{H_2} = V_i I \tag{10}
\]

\[
N_{H_2} = \frac{I n_i}{2F} \tag{11}
\]

With (5) the ideal voltage responsible for producing hydrogen, (6) is the Gibbs free energy change of hydrogen gas, (7) the Average amount of hydrogen production, with (8) the molar volume. (9) and (10) representing the power absorbed and the power producing, (11) rate hydrogen.

The thermal power released by the reaction is

\[
P_{th} = \pm N_e \times (V - U_{tm}) \times I \tag{12}
\]

\(N_e\) number of cells in series; \(U_{tm}\) thermoneutral voltage of a cell = 1.48V.

2.2 Hydrogen storage tank

The storage tank intended to contain hydrogen at a certain pressure in liquid or gaseous form can be modeled according to [16]. Note that hydrogen storage is done according to three main methods, high pressure for stable systems 120 bars, for 250-700 bars mobile systems, in liquid form (-259 °C), then in hybrid metal form.

\[
P_t - P_{ti} = \frac{P V_m N_{H_2} R_t}{RT} \tag{13}
\]

\(P_{ti}\) Initial pressure of the storage tank(pascal)

\(P_t\) Pressure of tank (pascal)

\(R\) universal (rydberg) gas constant (J/kmol K)

\(T_t\) Operating temperature (K)

\(V_t\) Volume of the tank

\(P\) : Pressure

\[\begin{array}{|c|c|}
\hline
\text{Description} & \text{values} \\
\hline
T_0 & 20^\circ C \\
P_0 & 1 \text{ atm} \\
k & 0.0395 \text{ V/A} \\
R & 0.082 \text{ Latm}^{-1} \text{ K}^{-1} \text{ mol}^{-1} \\
F & 96487 \text{ C.mol}^{-1} \\
dR_i & -3.812 \times 10^{-4} \text{ C.mol}^{-1} \\
R_{i0} & 0.326 \Omega \\
\hline
\end{array}\]

2.3 PEM fuel cell

The re-electrification is carried out thanks to the PEM fuel cell, it is the reverse function of the electrolysis [17-19], in the electrolysis the water is broken down to remove the water in H2 and O2, here we use hydrogen and oxygen to produce a potential between the cathode and the anode, just as during electrolysis we get a great exothermic thermal power but also water. A series of equations is needed for this part. (Figure 1) shows the process used.
Fig. 1. Fuel cell PEM system.

\[ E_{\text{stack}} = E_{O_c} - E_{\text{act}} - E_{\text{com}} - E_{\text{ohm}} \]  

\[ E_{\text{ohm}}: \text{fuel cell output voltage} \]
\[ E_{O_c}: \text{open circuit voltage} \]

Cell voltage losses are composed of activation over-potential (Eact) due to the electro-catalyst layers, concentration over-potential (Econ) due to the limitations of mass transfer and ohmic overvoltage (Eohm).

\[ E_{O_c} = E_{\text{rev}} + \frac{RT}{2F} \ln(p_{H_2} \sqrt{P_{O_2}}) \]  

Partial pressure of hydrogen and oxygen, \( P_{H_2} \) and \( P_{O_2} \) pressure in the anode and cathode.

\[ p_{H_2} = X_{H_2} \cdot P_{an} \]
\[ p_{O_2} = X_{O_2} \cdot P_{cat} \]

The mole fraction of hydrogen, oxygen and water;

\[ X_{H_2} = \frac{n_{H_2}}{n_{H_2} + n_{H_2O}} \]  
\[ X_{O_2} = \frac{n_{O_2}}{n_{O_2} + n_{H_2O}} \]  
\[ X_{H_2O}^{an} = \frac{n_{H_2O}}{n_{H_2} + n_{H_2O}} \]  

The molar flow of hydrogen through the anode:

\[ n_{H_2} = \frac{N_{H_2}}{A} \]  

The molar flow of oxygen through the cathode:

\[ n_{O_2} = \frac{N_{O_2}}{A} \]  
\[ n_{O_2}^{H_2O} = \frac{n_{H_2O}}{P_{an}} \]

\[ 1 \leq \varphi_{an} = \frac{P_{an}}{P_{H_2, sat}} \leq 3 \]  

\( \varphi_{an} \): relative humidity, \( P_{H_2, sat} \): saturation pressure vapor, \( A \): area of membrane electrode assembly (cm²).

According to Faraday’s law, the molar flow rate of hydrogen and oxygen at the inlet is expressed:

\[ N_{H_2, i} = \frac{S_{H_2}}{2F} \]  
\[ N_{O_2, i} = \frac{S_{O_2}}{2F} \]

\[ E_{\text{rev}} = E_{\text{rev}}^0 + (T - T_{\text{ref}}) \times \delta \frac{\varphi}{n_F} \]

The theoretical minimum \( E_{\text{rev}}^0 = 1.229 \, \text{V} \). 

\[ I : \text{fuel cell output current (A).} \]

\[ \frac{\delta \varphi}{n_F} = -0.9 \times 10^{-3} \]

The speed of an electrochemical reaction is limited by the energetic acti-barrier:

\[ E_{\text{act}} = E_{\text{act}}^{\text{act}} - E_{\text{act}}^{\text{cat}} \]  
\[ E_{\text{act}}^{\text{act}} = \frac{RT}{2F} \ln \left( \frac{1}{\varphi_{an}} \right) + \frac{RT}{2F} \ln \left( \frac{1}{\varphi_{cat}} \right) \]

\[ i_{0,an}^{\text{act}} = \gamma M \times e^{-\frac{\varphi_{an}}{2}} \frac{1}{2} \frac{1}{\gamma_{ref}} \]  
\[ i_{0,cat}^{\text{act}} = \gamma M \times e^{-\frac{\varphi_{cat}}{2}} \frac{1}{2} \frac{1}{\gamma_{ref}} \]

\( i_0 \): effective density of the exchanged current; \( i \): current density (A/cm²).

\[ E_{\text{com}} = E_{\text{com}}^{an} - E_{\text{com}}^{cat} \]

\[ E_{\text{com}} = \frac{RT}{2F} \ln \left( \frac{C_{an}^{\text{mem}}}{C_{an}^{\text{all}}} \right) + \frac{RT}{2F} \ln \left( \frac{C_{cat}^{\text{mem}}}{C_{cat}^{\text{all}}} \right) \]

At the membrane-electrode interface, molar concentrations are expressed:

\[ C_{an}^{\text{mem}} = C_{an}^{\text{ch}} + \delta \frac{\varphi_{an}}{n_F} X_{H_2} \]
\[ C_{cat}^{\text{mem}} = C_{cat}^{\text{ch}} + \delta \frac{\varphi_{cat}}{n_F} X_{H_2O} \]

\( \delta_{an}, \delta_{cat} \): are respectively the anode and cathode thickness, molar concentrations of oxygen and hydrogen in the channels.

\[ C_{an}^{\text{ch}} = \frac{P_{an} X_{H_2}}{RT} \]  
\[ C_{cat}^{\text{ch}} = \frac{P_{cat} X_{O_2}}{RT} \]

The diffusion of a molecular species with an average free path through a porous medium with an average pore radius \( r \) is expressed:
\[
\frac{1}{\tau_{\text{eff}}} = \frac{\varepsilon}{\mu} \left( \frac{1}{D_{\text{eff}}^{\alpha,\text{cat}}} + \frac{1}{D_{\text{eff}}^{\beta,\text{cat}}} \right) \tag{40}
\]

Where \( D_{\text{eff}}^{\alpha,\text{cat}} \) is the effective binary diffusion coefficient; \( \varepsilon/\mu \) is the report of porosity on tortuosity.

\[
D_{\text{eff}}^{\alpha,\text{cat}} = \frac{4}{\pi} \int_{0}^{\infty} \frac{y}{\tau_{\text{eff}}} D_{H_{2}-H_{2}O}^{\alpha,\text{cat}} \, dy
\tag{41}
\]

\[
D_{\text{eff}}^{\beta,\text{cat}} = 0.00133 \left( \frac{1}{M_{\text{air}}} - \frac{1}{M_{H_{2}O}} \right)^{1/2} \int_{0}^{\infty} \frac{t^{3/2}}{\tau_{\text{eff}}} p_{\text{cat}} \, d\tau \tag{42}
\]

\[
\Omega_{D} = \frac{1.06}{\varepsilon_{\text{el}}} + 0.193 \frac{1.036}{\varepsilon_{\text{el}}} + 1.765 \frac{3.984}{\varepsilon_{\text{el}}} \tag{43}
\]

\( \Omega_{D} \) is a dimensionless diffusion collision integral; The mean molecular radii of species are express as following:

\[
\sigma_{H_{2}-H_{2}O} = \frac{\sigma_{H_{2}}-\sigma_{H_{2}O}}{2}
\tag{44}
\]

\[
\sigma_{O_{2}-H_{2}O} = \frac{\sigma_{O_{2}}-\sigma_{H_{2}O}}{2}
\tag{45}
\]

\[
\tau_{H_{2}-H_{2}O} = \frac{kT}{\epsilon_{H_{2}-H_{2}O}}
\tag{46}
\]

\[
\tau_{O_{2}-H_{2}O} = \frac{kT}{\epsilon_{O_{2}-H_{2}O}}
\tag{47}
\]

Lennard-Jones energies are expressed as follows:

\[
\epsilon_{H_{2}-H_{2}O} = \sqrt{\epsilon_{H_{2}} \epsilon_{H_{2}O}}
\tag{48}
\]

\[
\epsilon_{O_{2}-H_{2}O} = \sqrt{\epsilon_{O_{2}} \epsilon_{H_{2}O}}
\tag{49}
\]

The ohmic overvoltage, resistance of electrodes, plates and membrane respectively \((R_{\text{ohm}}^{\alpha}, R_{\text{ohm}}^{\beta} \text{ et } R_{\text{mem}})\):

\[
E_{\text{ohm}} = (R_{\text{ohm}}^{\alpha} + R_{\text{ohm}}^{\beta} + R_{\text{mem}}) I
\tag{50}
\]

\[
R_{\text{ohm}}^{\alpha} R_{\text{ohm}}^{\beta} = \frac{\rho_{\text{el}}}{(1-\varepsilon) \varepsilon}
\tag{51}
\]

\[
E_{\text{ohm}} = \frac{\varepsilon_{\text{mem}} I}{\sigma_{\text{mem}}}
\tag{52}
\]

\[
\sigma_{\text{mem}} = \frac{\varepsilon_{\text{mem}} I}{\sigma_{\text{mem}}}
\tag{53}
\]

The conductivity of the membrane can be empirically expressed as:

\[
\sigma_{\text{mem}} = (0.005139 \beta - 0.00326) \epsilon^{(\frac{1}{3} + \frac{1}{2})}
\tag{54}
\]

\[\xi = \frac{S_{\text{in}}}{c} = 1268 K \; ; \; \beta \text{ is the degree of humidification.} \]

Electrical power from fuel cell PEM is:

\[
P_{\text{stack}} = N \left( E_{\text{stack}} - I \right)
\tag{55}
\]

\[
\frac{p_{\text{in}}}{c_p} = P_{\text{in}} - \varphi_{\text{ext}} - \varphi_{\text{gas}}
\tag{57}
\]

\[
P_{\text{th}} = N \left( E_{\text{stack}} - I \right)
\tag{58}
\]

Table 2. Data PEM fuel cell.

| Description | Values |
|-------------|--------|
| \( \beta \) | 22     |
| \( S_{H_{2}} \) | 1.2 |
| \( A \) | 140 cm\(^2\) |
| \( T_{\text{ref}} \) | 303 K |
| \( \varepsilon_{\text{mem}} \) | 0.0254 cm |
| \( \alpha_{\text{an}} \) | 0.7 |
| \( \alpha_{\text{cat}} \) | 1.7 |
| \( \gamma_{M} \) | 47 |
| \( I_{0,\text{an}}^{\text{ref}} \) | \( 1 \times 10^{-4} \text{ A cm}^{-2} \) |
| \( I_{0,\text{cat}}^{\text{ref}} \) | \( 1 \times 10^{-9} \text{ A cm}^{-2} \) |
| \( \delta_{\text{cat}} \) | 0.008 cm |
| \( \sigma_{H_{2}} \) | 2.827 A |
| \( \sigma_{O_{2}} \) | 3.467 A |
| \( \sigma_{H_{2}O} \) | 2.641 A |
| \( \varepsilon_{H_{2}} \) | 59.7 K |
| \( \varepsilon_{H_{2}O} \) | 809.1 K |
| \( \varepsilon_{O_{2}} \) | 106.7 K |
| \( M_{H_{2}O} \) | 18.01528 |
| \( \tilde{\rho} \) | 0.06 |

3 Case study and results

3.1 Energy balance of the building studied.

This study will focus on data from a 3-star hotel in Paris [20]. We will focus on the consumption of the hotel's Heating Ventilation and Air Conditioning (HVAC) circuits, which represents a significant part of the consumption of energy within a residence [21]. In addition, this sector is the second energy consumer and second polluter to date [22]. Table 3 contains the data for this study, from electricity the blue in the Table 3 represents the natural gas, and Table 4 presents the cost over 10 years according to this consumption.

| Description | Consumption(KWh/year) |
|-------------|-----------------------|
| Heating pump | 20000 |
| Electric heater | 20000 |
| air conditioner | 50400 |
| Air renewal | 162000 |
| Kitchen extractor | 5600 |
| Hot water | 61000 |
| Hot water | 372000 |

Table 3. Hotel consumption.

\[ P_c = T_c \times GES \]  
\[ GES = C_a \times FE \times PRG \]  

With the global warming potential \((PRG) = 1\), \((T_c)\): carbon tax taken at 86.2 € / tCO2, \((FE)\): the emission factor, \((GES)\): greenhouse gases, \((C_a)\): consumption, \((P_c)\): carbon price.

**Table 4.** Spend over 10 years electricity and natural gas.

| FE(gCO2/KWh) | Pc(€/year) | Energy cost (€/year) | Cost (€/10 years) |
|--------------|------------|----------------------|------------------|
| 49 | 84,476 | 4318 |
| 49 | 84,476 | 4318 |
| 59 | 256,32 | 10881.3 |
| 59 | 823,89 | 34975.5 |
| 75 | 36,204 | 1209.04 |
| 58 | 304,976 | 13169.9 |
| 443 | 14205,41 | 704624,56 |

3.2 Simulation of re-electrification by PEM hydrogen storage and demonstration of the usable thermal power

3.2.1 Sizing of the isolated solar system

After calculation on PVsyst (Figure 2), we estimate a nominal power to be supplied by the field of 218KWp, the storage batteries must provide 24KW per day.

![Fig. 2. Solar power and battery capacity calculate on PVsyst.](image1)

Through the energy to be supplied by the batteries according to PVsyst we simulate the storage of hydrogen making it possible to supply 24kw per day.

3.2.2 Simulation of water electrolysis

In this simulation, we produce the rate of hydrogen to be stored in the flask (Figure 3). In addition, we highlight the evolution of powers in (Figure 4), we see that the thermal power can be endothermic or exothermic, the power absorbed becomes less than the thermal power and the real power consumed for hydrogen. (Figure 5) shows how the pressure increases in the tank according to the current coming from the photovoltaic field. Through the energy to be supplied by the batteries according to PVsyst we simulate the storage of hydrogen making it possible to supply 24kw per day.

![Fig. 3. Hydrogen production](image2)

![Fig. 4. Comparison of the power in electrolysis](image3)

3.2.3 Fuel cell PE result and simulation

In the (Figure 6) we show the evolution of losses during the production of electricity, the (Figure 7) shows the variation of the thermal power compared to the electrical power produced, we notice that the thermal power becomes more important than the electrical power produced after a while, which shows the importance of this power in this system.

![Fig. 5. Evolution of the pressure according to the current absorbed.](image4)
In (Figure 8), we compare the thermal power on the electrolysis side with that on the fuel cell side, in conclusion, cogeneration on the fuel cell side is more beneficial.

Figure 9, shows the numerical results of the simulation, we see that by producing 24 KW of electric power per day we obtain at the same time a thermal power of 31 KW at a temperature of 80°C.

By using this thermal power at this temperature, we are able to cover the sanitary water heating which was supplied by natural gas. This eliminates the cost of natural gas energy.

In the Table 5 we present an estimate of the cost of the PEM stack solution in this case study.
3.2.4 Cost analysis

The cost of solar installation and hydrogen production can be estimated according to [23-26]

| Description       | Energy (Kwh/year) | System cost (€) |
|-------------------|-------------------|-----------------|
| Electrolysis(599€/kw) | 210240            | 5 247240        |
| Fuel cell(40€/kw)   | 210240            | 350400          |
| Energy PV          | 1918440           | 284700          |

\[ P_{\text{stack}} = 0.15 \times \text{Cost}_{\text{PEM}} \quad (61) \]

\[ P_{\text{cleanPV}} = 26.42 \times \text{Area}_{\text{PV}} \quad (62) \]

In this part we present the evolution of the spending of the hotel over 10 years (Figure 10), we note that the calculation takes into account; (61) the cost of solar cleaning each year, as well as (62) the cost of changing the stacks every 5 years with the following equations [26-27].

Case 1: the red curve shows the evolution of the cost when the hotel is supplied with electricity and gas (the DHW circuit supplies with natural gas), against the curve in blue solar+hydrogen where we recover 31 kw of thermal power produced by the reaction when generating an electrical power of 24kw (Figure 9). This thermal power generated at 80°C can heat the 147 water circuits of hot water up to 71°C, by convection and thermal conduction.

Case 2: This is the solution where all the heating is based on electricity in green against the solar hydrogen system with heat recovery in blue. We see here a return on investment in three and a half years.

4 Conclusion

To perform one realistic study of a technical-economic base on evident data, we did the chain model and simulation of green hydrogen production for the re-electrification by fuel cell PEM. Through this simulation, we produce 24KW electric power per day by green hydrogen storage. That electrical production creates a thermic power of 31 KW at 80°C to fuel cell. The study demonstrates fuel cells present better results in thermic power for all the chains. However, this simulation indicates it is possible to warm up 147 circuits of hot water from the hotel study up to around 70°C, by convection and thermal conduction.

The economic study carried out shows us a short-term return on investment taking into account the fall in the cost of solar panels over the next 10 years as opposed to the increase in the carbon tax in this same period. A return on investment is estimated from the 5th year for the use of green hydrogen compared to the use of electricity + natural gas. This time is much shorter in the case of the use of electricity to cover all HVAC needs, from the three and a half years.

In conclusion, a techno-economic study shows the use of thermal power of the fuel cell for tertiary heating provides an interesting return on the investment. Thus, encouraging investors on this sector to use green hydrogen for a better preventive energy strategy.

In short, this techno-economic study shows that the use of the thermal power of the fuel cell for tertiary heating makes it possible to obtain an interesting return on investment thus making it possible to encourage investors in this sector to use the green hydrogen.

Note that this cost can be further reduced by using the water of the reaction in the fuel cell, indeed according to statistics, the cost of water has been increasing gradually for years and it will increase further in the years to come, therefore using this water for gardening needs would save money.

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