Reversible Proton Exchange Membrane Fuel Cells for Energy storage

AZZA MAMI, NIHEL CHEKIR, YASSINE BEN SALEM
National Engineering School of Gabes, University of Gabes,
Gabes, 6029
TUNISIA

Abstract: This paper describes the modeling, simulation, and optimization of reversible proton exchange membrane fuel cells (rPEMFCs) operating as both electrolyzers and fuel cells A MATLAB model has been developed to test the influence of operating variables such as temperature, pressure, and current density on system performance. Multi-objective optimization using a Genetic Algorithm (GA) identified optimal parameters that enhanced round-trip efficiency to 60%. The results demonstrate the potential of rPEMFCs for efficient hydrogen-based energy storage and their integration into hybrid solar-hydrogen systems for sustainable power generation.

Keywords: Reversible PEM fuel cell, Hydrogen, MATLAB, Genetic Algorithm, Energy optimization, Renewable energy.

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1. Introduction

The increasing penetration of intermittent renewable energy sources has intensified the demand for efficient and long-duration energy storage technologies. Hydrogen-based energy storage is widely recognized as a promising solution due to its high energy density, carbon-free operation, and suitability for large-scale and seasonal applications. In this context, reversible Proton Exchange Membrane Fuel Cells (rPEMFCs) have gained attention as a dual-function technology capable of operating as both a water electrolyzer and a fuel cell.

Nevertheless, existing studies predominantly model PEM fuel cells, electrolyzers, and hydrogen storage subsystems separately, or rely on simplified representations when integrating them at the system level. Such approaches limit the accurate assessment of reversible operation and fail to capture the strong coupling between electrochemical behavior, operating conditions, and overall system performance, particularly under realistic constraints and optimization requirements. To overcome these limitations, this work proposes a novel unified modeling and optimization framework for rPEMFC-based renewable energy storage systems. A physically based reversible electrochemical model, valid in both electrolyzer and fuel cell modes, is developed and implemented in MATLAB, then integrated into a hybrid PV–hydrogen energy system to enable comprehensive system-level analysis. In contrast to fixed-parameter or heuristic approaches commonly adopted in the literature, a multi-objective Genetic Algorithm is employed to optimize key operating parameters with respect to efficiency and energy autonomy. The framework is validated through both residential- and industrial-scale case studies, demonstrating its scalability and providing new insights into round-trip efficiency, hydrogen production, and practical integration limits of rPEMFC systems.

2. Methodology

2.1 Physical Problem Definition and Assumptions

A three-dimensional (3D) model of a reversible PEMFC was developed to simulate electrochemical reactions and transport processes within fuel/oxidant channels, the gas diffusion layer (GDL), catalyst layer, and proton exchange membrane. The model assumes isothermal operation at 80 °C and gases are treated as ideal and weakly compressible, which is reasonable within the limited pressure range (1–3 atm) considered, with a fixed current density of 0.8 A/cm². The GDL and catalyst layers are modeled as porous media, with electrochemical reactions confined to the catalyst layers. Transport phenomena include conduction, convection, and water movement across the membrane via electro-osmosis, diffusion, and pressure-driven flux. Governing equations for mass, momentum, species, and charge conservation are implemented. This 3D modeling framework enables detailed analysis of local electrochemical performance and species distribution, supporting subsequent energy balance calculations, efficiency assessment, and optimization of hybrid PV–hydrogen systems.

This figure (1) illustrates the dual operating modes of a reversible proton exchange membrane fuel cell (rPEMFC). In electrolyzer mode, an external power supply drives water electrolysis at the anode, producing oxygen, protons, and electrons. Protons migrate through the proton exchange membrane, while electrons flow through the external circuit to the cathode, where hydrogen is formed. In fuel cell mode, hydrogen is oxidized at the anode to generate electrical power; protons cross the membrane and electrons travel through the external circuit, reacting with oxygen at the cathode to produce water.

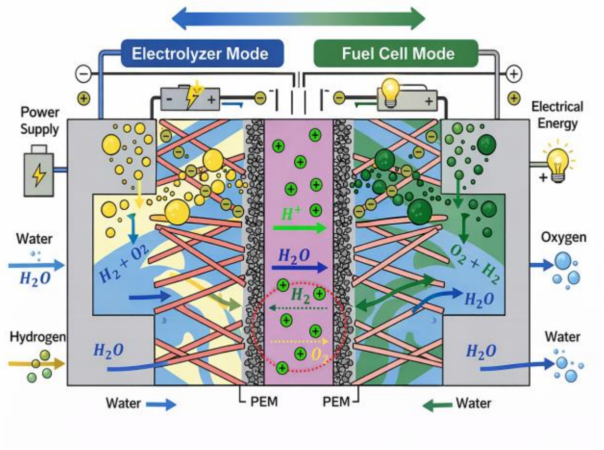

Fig. 1 Schematic diagram of rPEMFC

2.2 Electrochemical Reaction Kinetics

The electrochemical reactions governing rPEMFC operation are:

FUEL CELL MODE:

Anode: $H2\rightarrow 2H^{+}+2e^{-}$ **(1)**

Cathode: $\frac{1}{2} O_2+2H++2e^{-}\rightarrow H_2O$ **(2)**

ELECTROLYZER MODE:

Anode: $H2O\rightarrow \frac{1}{2} O_2+2H^{+}+2e^{-}$ **(3)**

Cathode: $2H^{+}+2e^{-}\rightarrow H_2$ **(4)**

CELL VOLTAGE MODEL:

The reversible cell voltage is expressed as the reversible (Nernst) voltage corrected by irreversible losses. In fuel cell mode, the cell voltage is given by:

$$VFC=E_{rev}-\eta_{act}-\eta_{ohmic}-\eta_{conc} \quad (5)$$

Where E_{rev} is the reversible voltage and η_{act}, η_{ohmic}, η_{conc} represent the activation, ohmic, and concentration overpotentials, respectively.

In electrolyzer mode, the required cell voltage is:

$$VEL=E_{rev}+\eta_{act}+\eta_{ohmic}+\eta_{conc} \quad (6)$$

2.3 Efficiencies in a Hydrogen-Based Energy System

ELECTROLYZER EFFICIENCY

The efficiency of an electrolyzer is the proportion of the amount of hydrogen evolved and the electrical energy input to produce it. That is, it is defined as:

$$Electrolyzer\ Efficiency = \frac{Mass\ of\ Hydrogen\ Produced\ (kg)}{Electrical\ Energy\ Consumption\ (kWh)} \quad (7)$$

FUEL CELL EFFICIENCY

The efficiency of a fuel cell is the inverse: it measures how much electrical energy is produced per amount of hydrogen consumed. Mathematically, it can be written as:

$$Fuel\ Cell\ Efficiency = \frac{Electrical\ Energy\ Produced\ (kWh)}{Quantity\ of\ Hydrogen\ Consumed\ (kg)} \quad (8)$$

REVERSIBLE SYSTEM EFFICIENCY

When we have a reversible system, where the same apparatus or a hybrid system can carry out both the fuel cell and electrolysis function, the overall efficiency is given by the ratio of the amount of electrical energy regained to the energy consumed during electrolysis in the first instance. It is written as:

$$CRT\ Efficiency = \frac{Electrical\ Energy\ Generated\ (kWh)}{Electrical\ Energy\ Inpu\ (kWh)}$$

(9)

A. *Governing Equations for rPEMFC Modeling*

The rPEMFC model is governed by conservation laws that describe the transport of mass, momentum, energy, and species in each component of the cell [2].

Mass Conservation: as shown in Equation (10) represents the balance between the accumulation and convection of mass within the control volume; S_m is the mass source term, non-zero only in catalyst layers.

$$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla(\varepsilon\rho\vec{u}) = S_m \quad (10)$$

Where ε is the porosity of porous medium, ρ is the fluid density, $\vec{u}$ is fluid velocity vector; $\partial(\varepsilon\rho)\ \partial t$ indicates non-steady state, $\nabla(\varepsilon\rho u)$ indicates convection, and S_m is the mass source term. In a fuel cell, S_m is zero everywhere except in the catalyst layer.

Momentum Conservation: Equation (11) describes the forces acting on the fluid, including pressure gradients, viscous effects, and momentum sources.

$$\frac{\partial(\varepsilon\rho u)}{\partial t} + \nabla.(\varepsilon\rho\vec{u}\vec{u}) = -\varepsilon\nabla P + \nabla.(\varepsilon\mu\nabla\vec{u}) + Su \quad (11)$$

Where P is the fluid pressure; μ is the viscosity of fluid, $\partial(\varepsilon\rho u)/\partial t$ indicates non-steady state, $\nabla.(\varepsilon\rho\vec{u}\vec{u})$ indicates convection, $-\varepsilon\nabla P$ *and* $\nabla.(\varepsilon\mu\nabla\vec{u})$ indicate diffusion, and S_u is the source term for momentum.

Energy Conservation: Equation (12) expresses the thermal energy balance considering conduction, convection, and internal heat sources.

$$\frac{\partial(\varepsilon\rho C_p T)}{\partial t} + \nabla.\left(\varepsilon\rho C_p \vec{u}T\right) = \nabla.\left(K^{eff}\nabla T\right) + S_Q \quad (12)$$

In this context, Cp represents the specific heat capacity of the fluid at constant pressure. K^{eff} denotes the effective thermal conductivity. The term $\partial(\varepsilon\rho Cp\ T)/\ \partial t$ reflects the transient (or unsteady-state) behavior, while $\nabla.\ (\varepsilon\rho Cp\ \vec{u}\ T)$ corresponds to the convective heat transfer. The expression $\nabla.(Keff\nabla T)$ accounts for the diffusive heat transfer, and SQ represents the energy source term.

Species Conservation: Equation (13) defines mass transport for each chemical species S_k, including convection, diffusion, and reaction-related source terms.

$$\frac{\partial(\varepsilon C_k)}{\partial t} + \nabla.(\varepsilon\vec{u}C_k) = \nabla.\left(D_k^{eff}\nabla C_k\right) + S_k \qquad \textbf{(13)}$$

In which Ck is the concentration of constituent $D_k{}^{eff}$ is the effective diffusion coefficient of constituent k, and S_k is the source term of constituent k (at the anode: H_2, H_2O; at the cathode: O_2, N_2, H_2O). The term $\partial(\varepsilon Ck)\ \partial t$ represents the transient (non-steady-state) term, $\nabla.(\varepsilon\vec{u}\ Ck)$ represents the convection term, and $\nabla.\ (D_k{}^{eff}\ \nabla Ck)$ represents the diffusion term.

Fick's Law: Equation (14) Simplifies species diffusion through porous layers as a function of concentration gradients.

$$q_y^k = -D_k\frac{\partial C_k}{\partial y} \qquad \textbf{(14)}$$

In which $q_y{}^k$ is the diffusion flux of constituent k along the y-axis, and D_k is the free diffusion coefficient of constituent k.

3. Results and discussion

The model uses real solar irradiance data from Gabes, Tunisia (average 6 kWh/m²/day) and assumes a PV efficiency of 18%. MATLAB simulations dynamically evaluate power generation, hydrogen production, and energy storage over a 24-hour period. The intelligent control algorithm governs the switching between electrolyzer and fuel cell modes based on real-time monitoring of load, generation, and storage conditions, ensuring continuous and balanced operation.

3.1 Residential System Simulation

It is proven through residential case studies that for an average home with an average daily electricity demand of 10 kWh, a 9 m^2 photovoltaic cell, or six panels with 350 Wp, is sufficient. It is observed from MATLAB simulation results in the residential model that not only is it feasible to meet the home's demand during peak sun hours, but there is also substantial surplus electricity to propel the electrolyzer, generating about 0.17 kg, or an average capacity to produce nearly 6 kWh of electricity, of hydrogen per day.

These outcomes make it clear that it is feasible to retain a full renewable energy cycle in 24 hours with the avoidance of conventional battery energy storage. By these means, hydrogen successfully performs the long-term energy storage functions, thereby maintaining stability in energy supply, even in scenarios with zero solar energy input. It again gets confirmed from these studies that such designs could result in domestic energy autonomy with low electrical grid dependence in regions with high solar irradiance levels.

To ensure consistency between electrical input and hydrogen production, an explicit energy balance is applied to the residential system. The electrical energy generated by the photovoltaic array is divided between direct load supply and electrolyzer input, while system losses are implicitly included through conversion efficiencies. The hydrogen production rate is calculated using Faraday's law and verified by comparing the chemical energy stored in hydrogen, based on its lower heating value, with the electrical energy supplied to the electrolyzer. This approach guarantees coherence between electrical and chemical energy flows and confirms the validity of the reported hydrogen production as shown in figure (2).

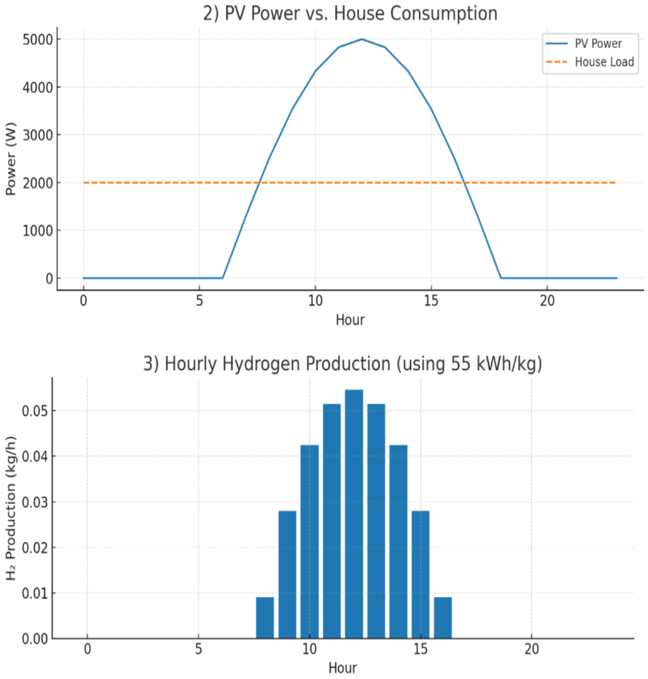

Fig. 2 Residential System Simulation

3.2 Industrial System Simulation

For large-scale applications (figure 3), the hybrid model was further developed to meet energy demand in an industry, requiring 274 MWh on a daily basis. It incorporates about 83,000 PV panels with 600 Wp capacity, assisted by a battery with energy capacity of 274 MWh, addressing short-term variations in energy demand, in addition to having sufficient storage for hydrogen on a long-term energy support perspective. Simulations in MATLAB show an estimated production level of about 10,000 kg hydrogen, while about 5,000 kg is used for meeting demand in nighttime/low irradiance conditions to support the industry.

The combined PV energy output, battery storage, and reversible fuel cell process enable stable power delivery. It is observed from the simulation outcomes that for any size, solar-hydrogen-based systems have the capacity to diminish dependence on the power grid, improve stability, and perform consistently throughout 24 hours. It proves the feasibility of such systems in handling high, fixed power demand while maintaining autonomy in energy.

At the considered industrial scale, the photovoltaic field would require a large surface area, potentially on the order of several hectares, depending on site conditions and module efficiency. In addition, the storage of significant quantities of hydrogen necessitates dedicated infrastructure and strict compliance with industrial safety standards and regulations. Although a detailed techno-economic analysis is beyond the scope of this study, capital costs, land availability, and safety requirements are expected to play a critical role in real-world deployment and should be addressed in future investigations.

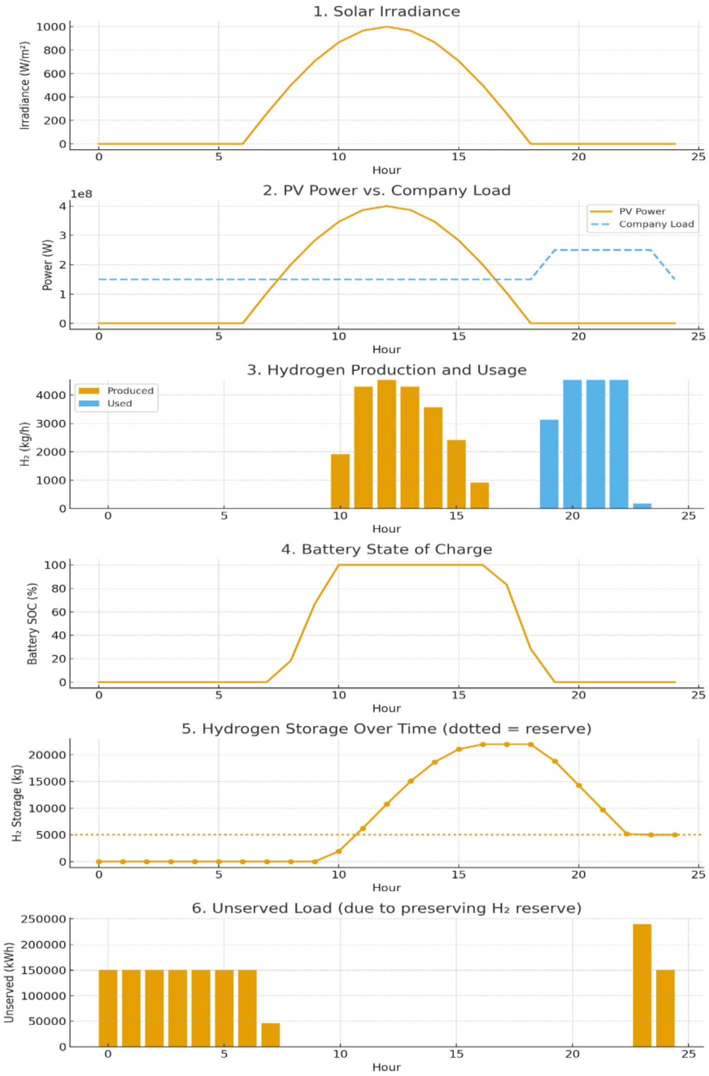

Fig. 3 Industrial System Simulation

3.3 Genetic Algorithm Optimization

Reversible Proton Exchange Membrane Fuel Cells (rPEMFCs) operate in two modes: fuel cell (producing electricity) and electrolyzer (producing hydrogen and oxygen). Optimizing both simultaneously is complex due to differing operating conditions. A multi-objective Genetic Algorithm (GA) was implemented in MATLAB to maximize round-trip efficiency

$$CRTE = (Output\ Energy/Input\ Energy).100\% \quad \textbf{(15)}$$

The GA optimizes four decision variables: operating temperature (60–85 °C), pressure (1–3 atm), relative humidity (30–100%), and hydrogen stoichiometry (1.2–2.0). These bounds were selected based on experimentally validated operating ranges reported for reversible PEM systems, ensuring membrane durability, stable electrochemical behavior, and practical system operation. The selected parameter bounds are consistent with operating ranges reported in experimental studies on reversible PEM systems, and were adopted to ensure membrane durability and realistic system behavior.

The GA was implemented in MATLAB with a population size of 50 individuals evolved over 100 generations. These values were selected following preliminary convergence tests, in which smaller populations or fewer generations led to premature convergence or unstable solutions, while larger configurations resulted in negligible improvement at significantly higher computational cost. For the present four-parameter optimization problem, the chosen configuration represents a balanced compromise between solution accuracy, convergence robustness, and computational efficiency. Tournament selection was used to favor fitter individuals, while single-point crossover and adaptive mutation were applied to preserve genetic diversity and avoid premature convergence.

The optimization converged consistently toward an optimal operating point at 75 °C, 2 atm, 80% relative humidity, and a hydrogen stoichiometry of 1.5. Under these conditions, the modeled rPEMFC system achieved a round-trip efficiency of approximately 60%. This value is consistent with experimentally reported efficiencies for state-of-the-art reversible PEM systems, supporting the validity of the proposed modeling and optimization framework. The results demonstrate that a single, well-defined operating point can ensure balanced and efficient reversible operation, which is essential for practical hydrogen-based energy storage applications.

4. Conclusion

This study examined the potential of reversible proton exchange membrane fuel cells (rPEMFCs) as an integrated solution for renewable energy generation and hydrogen-based energy storage. A comprehensive physical and mathematical model was developed to describe rPEMFC operation in both fuel cell and electrolyzer modes, accounting for electrochemical kinetics, transport losses, and operating constraints. The model was implemented in MATLAB and used to evaluate the influence of key operating parameters, including temperature, pressure, relative humidity, and current density, on system performance and stability.

To address the conflicting requirements of reversible operation, a Genetic Algorithm–based optimization framework was proposed to maximize the round-trip efficiency. The optimization identified an optimal operating point at 75 °C, 2 atm, 80% relative humidity, and a hydrogen stoichiometry of 1.5, resulting in a round-trip efficiency of approximately 60%. This value is consistent with experimentally reported efficiencies for current reversible PEM systems, supporting the validity of the proposed approach. The results demonstrate that GA-assisted optimization can effectively identify balanced operating conditions that ensure efficient performance in both modes, thereby enhancing energy autonomy in solar–hydrogen systems. Future work will focus on extending the model to dynamic operation, incorporating degradation mechanisms, and performing techno-economic assessments to evaluate long-term system feasibility and scalability.

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