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1D MODEL PARAMETER SENSITIVITY STUDY for LOW TEMPERATURE PEMFC

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ABSTRACT

Hydrogen plays a crucial role in advancing carbon-neutral energy systems, with Proton Exchange Membrane Fuel Cells (PEMFCs) offering high efficiency for applications in transport and stationary power. However, PEMFCs face commercialization challenges due to durability and economic constraints. Traditional models, especially zero-dimensional (0D) types, lack the depth needed for accurate performance prediction. This paper develops a one-dimensional (1D) PEMFC model to address these limitations, using Python to generate IV and power density curves. Validation against data from the PEPR PEMFC95 project at Lorraine University (UL) demonstrates the model's potential to improve PEMFC design and reliability.

Keywords: PEMFC, IV-Curve, Modelling, Power density curve, Sensitivity.

I. INTRODUCTION

Fuel cell systems, especially proton exchange membrane fuel cells (PEMFCs), have gained significant attention for their high efficiency, low environmental impact, and durability. These cells are a promising option for distributed generation (DG) applications. To effectively utilize PEMFCs, it is crucial to develop accurate mathematical models for steady-state and dynamic conditions, allowing for system optimization through simulation.

Many available models primarily focus on steady-state behavior [1]–[4], while only a few address the dynamic performance of PEMFCs [1]–[2]. Furthermore, many dynamic models lack validation with experimental data, relying instead on empirical methods [ref]. This study introduces a flexible simulation tool that integrates both electrochemical and thermodynamic principles to model the behavior of PEMFCs. Currently the tool simulates only the cell's electrochemical performance in the format of 0D steady state model.

The proposed model is validated against experimental data and considers key variables such as fluid dynamics, thermal dynamics, and feed system kinetics, though in a simplified manner for initial optimization. Built using Python, this model offers flexibility and can be adapted to various operational conditions, providing a robust framework for enhancing PEMFC systems and supporting the design of portable fuel cell stacks.

II. EXPERIMENTAL METHOD

The experimental setup in this study was assembled in-house and utilizes an IRD PEMFC95 as the Active Membrane Electrode Assembly (AME). The catalysts on the anode and cathode consist of Pt/HSAC 50 wt% (Tanaka TKK TEC10E50E), with loadings of 0.1 mg/cm² for the anode and 0.3 mg/cm² for the cathode. Nafion D2020CS is used as the ionomer in the catalyst layers, with an ionomer-to-carbon ratio of 0.8. A Gore 788.12 membrane, with a thickness of 0.0012 cm, serves as the primary proton conductor in the cell. Additionally, a Freudenberg H14CX653 gas diffusion layer (GDL), made of carbon fiber paper with a Teflon (Polytetrafluoroethylene PTFE) coating, features a single-sided microporous layer with an in-plane electric resistivity of 6 mΩ·cm². This GDL facilitates effective gas transport to the electrode surfaces.

The PEMFC cells utilized in this study have an active area of 25 cm², with channel geometries specifically designed to enhance gas distribution and mass transport. The design features 50 parallel straight channels, with channel depths of 0.15 mm on the anode side and 0.25 mm on the cathode side, carefully optimized to improve flow dynamics.

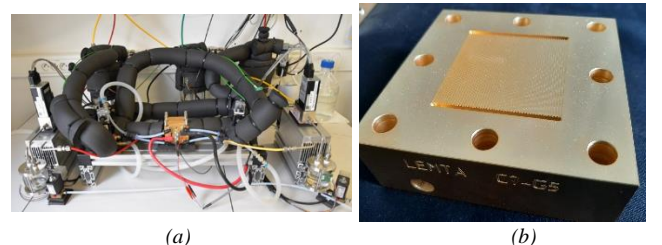


Fig. 1 (a) Benches for cells (non-)segmented, (b) Anode non-segmented bipolar plate (25 cm²)

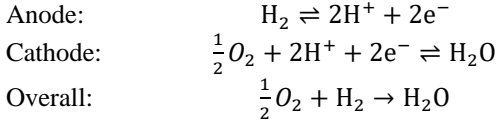
Table. 1 Controlled variables used in the experimental design of the test performed on the single-unit cell. ^a The proportion of the oxygen flow rate entering the system to the rate at which it is utilized.

Test. no	SR ^a	T(k)	Rh (%)	Inlet p _{air} (atm)	Inlet p _{H2} (atm)
1	2.5	343.15	0.3	2.961	2.961
2	2.5	343.15	0.5	2.961	2.961
3	2.5	368.15	0.3	2.961	2.961
4	2.5	368.15	0.5	2.961	2.961

The test bench setup includes tubing, temperature control, and flow regulation systems to maintain stable and consistent reactant flows and inlet pressures. This configuration supports testing under various operating conditions, enabling detailed analysis of current-voltage (I-V) characteristics and power density performance, in real PEMFC operations. Data collection is managed using LabVIEW software after 36min, and subsequent data processing and analysis are conducted using MATLAB and Python. A photograph of the testing system is presented in Fig. 1, and the controlled variables used in testing the single-unit cell are listed in Table I.

III. MODEL DEVELOPMENT

PEM fuel cells are composed of three primary components: the anode, which typically includes a catalyst made of platinum or a platinum alloy; a thin, solid polymer membrane serving as the electrolyte; and the cathode, which is also platinum-catalyzed. The principal reactions in a PEM fuel cell, operating with hydrogen-rich gas at the anode and oxygen-rich gas at the cathode, are as follows: [1]



1. GENERAL

The unit cell voltage (E_{cell}) is given by [1]–[6]:

$$E_{cell} = E_r - \eta_{act} - \eta_{ohmic} - \eta_{conc}$$

Where η_{act} activation over potential, η_{ohmic} Ohmic losses, η_{conc} concentration overpotential, and E_r represents the maximum reversible output voltage, expressed using the Nernst equation with temperature gradient and entropy change and it can only be obtained in the case of fuel cell is thermodynamically reversible [5],[6]:

$$E_r = E^0 - 8.5 \cdot 10^{-4}(T - 293.15) + 4.308 \cdot 10^{-5} \ln(P_{H_2} P_{O_2}^{0.5})$$

Where: 8.5×10^{-4} and 4.308×10^{-5} represents $\Delta S^0/nF$, and R/nF respectively, $E^0 = 1.229V$ Open circuit voltage (OCV) at standard state ($T_{ref}=25^\circ\text{C}$, $P_{ref}=101.325\text{kPa}$).

$$E^0 = -\frac{\Delta G}{nF}$$

ΔG : Gibbs free energy at standard state (=237316.5 J/mol), $n = 2$ represents number of transferred electrons, F : Faraday's constant 96487 (A·s/mol).[7]

P_{H_2} & P_{O_2} partial pressure ratios for hydrogen and oxygen respectively. Saturated pressure at the cathode found using the most common expressing given in [4]:

$$\log_{10} \left(\frac{p_{sat}(T)}{p_{ref}} \right) = -2.1794 + 0.02953T - 9.1837 \cdot 10^{-5} T^2 + 1.4454 \cdot 10^{-7} T^3$$

Where T in °C and p_{sat} in atm, $p_{sat,c} = p_{sat}$.

$$p_{H_2O} = RH \cdot p_{sat,c}$$

$$p_{Total} = p_{H_2O} + p_{dry\ air}$$

$$p_{dry\ air} = p_{Total} - p_{H_2O}$$

$$p_{dry\ air} = p_{N_2} + p_{O_2}$$

$$p_{N_2} = 0.79 \cdot p_{dry\ air}$$

$$p_{O_2} = 0.21 \cdot p_{dry\ air}$$

$$P_{O_2} = \frac{p_{O_2}}{p_0}$$

Similarly to find p_{H_2} and P_{H_2} to plug in the Nernst equation.

2. OVERPOTENTIAL & LOSSES:

In this preliminary model we took only the cathode side, with number of transferred electrons $n = 2$ as we took 1 mole of H_2 .

a. Activation Overpotential:

$$\eta_{act} = \frac{RT}{n\alpha F} \ln \left(\frac{i}{i_0} \right)$$

α : symmetry factor, 0.5, i_0 : exchange current density, A/cm², [1],[9]

$$i_0 = i_0^{ref} a_c L_c \left(\frac{P_r}{P_r^{ref}} \right)^\gamma \exp \left[-\frac{E_c}{RT} \left(1 - \frac{T}{T_{ref}} \right) \right]$$

Where: i_0^{ref} : reference exchange current density at reference temperature and pressure, $T_{ref}=25^\circ\text{C}$, $P_{ref}=101.325\text{kPa}$, per unit catalyst surface area, A/cm² Pt, a_c : catalyst specific area, cm²/mg, L_c : catalyst loading, mgPt/cm², P_r : reactant partial pressure, kPa, P_r^{ref} : reference pressure, kPa, γ : pressure coefficient (0.5 to 1), E_c : activation energy, 66000 J/mol for oxygen reduction on Pt, T_{ref} : reference Temperature, k [8].

b. Concentration overpotential:

$$\eta_{conc} = -\frac{RT}{nF} \ln \left(1 - \frac{i}{i_{lim}} \right)$$

i_{lim} : limiting current density, A/cm², [9]

$$i_{lim} = \frac{nFD_{N_2,O_2}^{eff} C_{O_2}}{\delta}$$

δ : electrode thickness, cm, bulk oxygen concentration (channels), mol/cm³, D_{N_2,O_2}^{eff} : effective diffusivity, cm²/s, using the following approximation [9]:

$$p \cdot D_{N_2,O_2}^{eff} = a \left(\frac{T}{\sqrt{T_{O_2,crit} T_{N_2,crit}}} \right)^b \cdot (p_{O_2,crit} p_{N_2,crit})^{\frac{1}{3}} \cdot (T_{O_2,crit} T_{N_2,crit})^{\frac{5}{12}} \cdot \left(\frac{1}{M_{O_2}} + \frac{1}{M_{N_2}} \right)^{\frac{1}{2}}$$

crit: represents critical pressure or temperature of species.

c. Ohmic losses:

Expressed as follows [1]:

$$\eta_{ohmic} = i \cdot R_t$$

R_t : internal resistance composed of both ionic and electron resistance, $\Omega \cdot \text{cm}^2$,

$$\eta_{ohmic} = i \cdot (R_{ionic} + R_{elec})$$

IV. PRELIMINARY RESULTS

We preliminary plotted both experimental and 0D steady state model predictions in a parity plot for all studied cases shown in Table I.

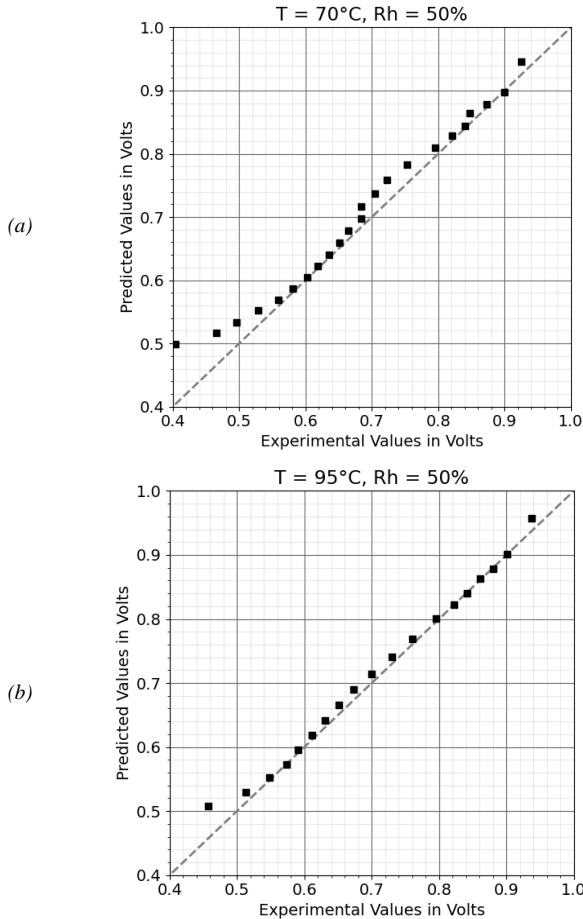
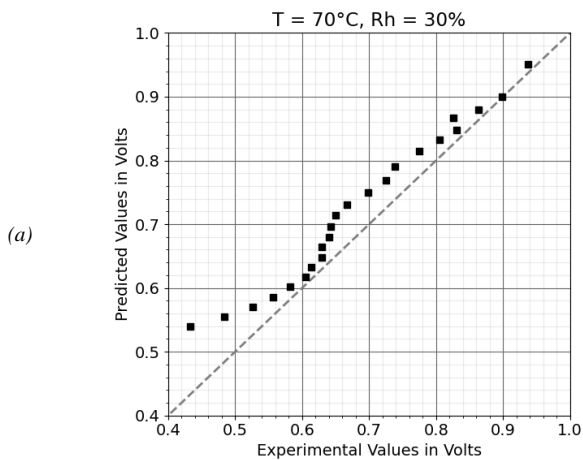
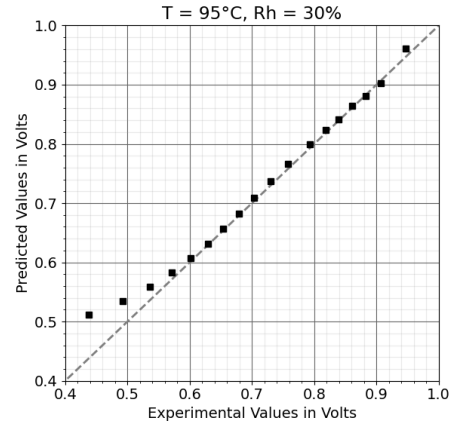


Fig. 2 Parity plot for cell voltage of experimental data as function of model prediction at 50% relative inlet humidity (a) operating temperature of 70°C , and (b) operating temperature of 95°C .



(a)



(b)

Fig. 3 Parity plot for cell voltage of experimental data as function of model prediction at 30% relative inlet humidity (a) operating temperature of 70°C , and (b) operating temperature of 95°C .

V. CONCLUSIONS

The developed model showed strong agreement with experimental data for a single unit cell operating at 95°C . However, deviations were most noticeable in the voltage range of 0.6–0.8 V and at higher current densities. To improve the model's precision, further refinement is required in optimizing the resistance R_t and concentration overpotential parameters, particularly the limiting current density i_{lim} .

Topic of paper : PEM fuel cell physics-based modelling

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