PINN for parameter identification of equivalent circuit models of PEM electrolyzer

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Introduction

In this work, PINNs are employed for parameter identification of equivalent circuit models of PEM electrolyzers. Physics-Informed Neural Networks (PINNs) is a scientific machine learning technique designed to solve problems that involve differential equations [1]. The PINNs integrate experimental data with differential equations to improve the neural network performance [2]. A hybrid loss function composed of data, boundary and physics terms is minimized during the training process. The loss function is $L_{total} = \lambda_d L_d + \lambda_p L_p + \lambda_b L_b$. For ordinary differential equations, variables only depend on time and we have:

$$L_d = \frac{1}{N_d}\sum_{i=1}^{N_d}|u_\theta(t_i) - u^{true}(t_i)|^2, \quad L_p = \frac{1}{N_r}\sum_{j=1}^{N_r}\left|N\left[u_\theta\left(t_j\right)\right]\right|^2, \quad L_b = |u_\theta(t_0) - u_{bc}(t_0)|^2 \qquad \text{(eq. 1)}$$

where L_d corresponds to the discrepancy between the measured and predicted variables, L_p enforces compliance with the differential–algebraic equations governing the dynamic system, and is given by a sum of squares of residuals of the equations at selected points in time (and space in the case of partial differential equations). Finally, L_b ensures that the solution satisfies the initial condition of the system, thereby constraining the network to remain consistent with the physical states of the system at specific points in time. N_d corresponds to number of experimental data points, $u_\theta(t_i)$ and $u^{true}(t_i)$ are respectively the PINN predicted values and measured values at time t_i. N_r is the number of points where the physics is enforced, $N\left[u_\theta\left(t_j\right)\right]$ is the residual of the governing physical equation at time t_j. Finally, $u_{bc}(t_0)$ is the known initial condition. In addition, the coefficients λ_d , λ_p and λ_b act as weighting parameters that balance the contribution of each component of the loss function.

Methodology

All of the data used for training PINNs in this study was synthetically generated in Matlab. The data contain 3 columns with time (t), current (I_{cell}), and voltage (V) at 601 time points. The variables time and current are used as the inputs to the neural network, while the "measured" voltage serves as the reference output. The objective is to solve the inverse problem, where the PINN framework is employed not only to find the optimal neural network parameters θ but also the parameters of the PEM electrolyzer equivalent circuit. Using both data and physics loss, the network is able to estimate the unknown parameters.

In the first phase of this study, the PEM electrolyzer is modelled as a very simple equivalent circuit [3], as shown in Figure 1a). The corresponding physical loss is shown in eq. 2a. In a second phase of the study, the equivalent circuit presented in Figure 1b) is considered [3]. The corresponding physical loss is shown in eq. 2b. In this case, two differential equations govern the process. $q_{a,i}$ and $q_{c,i}$ are the charge of capacitors C_a and C_c, respectivelly.

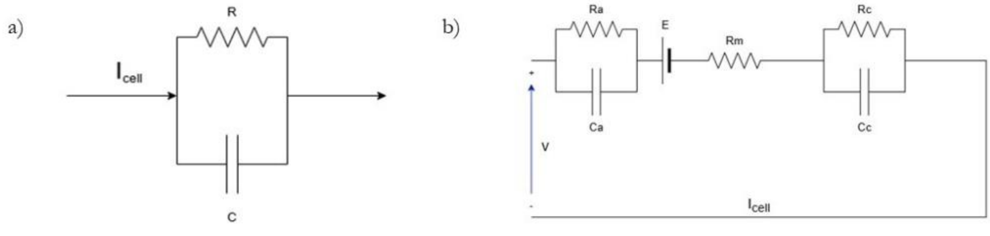

Figure 1. Equivalent Circuits of PEM electrolyzer

$$L_p = \sum_{i=1}^{601} \left(C \frac{\hat{V}_i - \hat{V}_{i-1}}{\Delta t} + \frac{V_i}{R} - I_{cell,i} \right)^2 \cdot \Delta t \qquad \text{(eq. 2a)}$$

$$L_p = \frac{1}{N} \sum_{i=0}^{601} \left(\left[\left(\frac{q_{a,i+1} - q_{a,i}}{\Delta t} - (I_{cell,i} - \frac{q_{a,i}}{R_a C_a}) \right)^2 \right] + \left[\left(\frac{q_{c,i+1} - q_{c,i}}{\Delta t} - (I_{cell,i} - \frac{q_{c,i+}}{R_c C_c}) \right)^2 \right] \right) \cdot \Delta t \qquad \text{(eq. 2b)}$$

Results:

For parameter identification of the simple circuit shown in Figure 1a), C and R were the unknown parameters. The PINN neural network architecture features used are shown in the first row of Table 1. For the equivalent circuit of PEM electrolyzer shown in Figure 1b), the PINN features used to estimate the unknown parameters are shown in the second row of Table 1. The identified parameters are C_a and C_c, which represent the capacitors of the two parallel RC branches. The performance of the PINN in estimating the parameters can be assessed by comparing the "real" values with the estimated parameters.

Model	Layers	Neurons	λ_d	λ_p	λ_b	Epochs	Real Value	Estimated Value
a	2	32	10000	10	10	59000	R=5.0, C=10	R=5.09, C=10.00
b	2	16	6	0.05	0	75000	C_a =37.26, C_c =37.26	C_a=37.09, C_c =37.25

Table 1. PINN features and estimated versus real circuit parameters for case studies a and b

Conclusion

This work is based on two PEM electrolyzer equivalent circuit models implemented in MATLAB, from which data was obtained synthetically. On the other hand, the equivalent circuits governing differential equations were used to include physics information for the neural networks training through their corresponding physical residuals. The circuits were then modeled using Physics-Informed Neural Networks (PINNs) that had the capability of identifying the unknown circuit parameters. For the simple equivalent circuit (model a), PINNs successfully estimated the parameters R and C with high accuracy. In the case of the more complex equivalent circuit (model b), the parameters C_a and C_c were also reliably estimated, with the predicted values closely matching the real ones. These results demonstrate the strong potential of PINNs as a powerful framework for parameter identification and modelling of PEM electrolyzers, even in increasingly complex circuit representations.

Acknowledgment:

This research was conducted at the ESAII Department of the Universitat Politècnica de Catalunya (UPC) and funded by the Gobierno de España through the competitive R+D+i project TSI-100930-2023-5 under the Agenda España Digital 2025 and the National Artificial Intelligence Strategy. Support from IDEAI-UPC and Siemens Energy is gratefully acknowledged.

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