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Conditional Physics-Informed Neural Network Modelling of PEM Electrolyzer Voltage Dynamics

Nouhaïla Elkasmi*[a], Maria Serra Prat[a], Carles Batlle Arnau[b]

* corresponding author: nouhaila.elkasmi@estudiantat.upc.edu
[a] Institut de Robòtica i Informàtica Industrial, CSIC-UPC, Llorens i Artigas 4-6, 08028 Barcelona, Spain
[b] Universitat Politècnica de Catalunya, IOC and EPSEVG, Av. V. Balaguer 1, 08800 Vilanova i la Geltrú, Spain

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Abstract

Introduction:

Proton exchange membrane (PEM) electrolyzers are promising for green hydrogen production under variable renewable electricity, but their voltage dynamics must be predicted accurately for efficient simulation, optimization, and future control-oriented operation. Detailed electrochemical models can capture internal phenomena, but they are often too complex for frequent online prediction. Reduced-order equivalent electrical circuit models provide a practical alternative by representing the dominant transient voltage behaviour with a small number of dynamic states [1,2]. Purely data-driven neural models can be fast, but they usually act as black-box approximators, require representative training data, and may behave poorly outside the training domain.

Physics-informed neural networks (PINNs) reduce the dependence on data by embedding governing equations into the training process [3]. However, a standard PINN is usually tied to a fixed problem setup and does not naturally include the control input and initial internal state as conditioning variables. This is restrictive for control-oriented modelling, where the model must be queried from different states and under different input values [4]. In this work, a conditional physics-informed neural network (CPINN) is developed to represent a family of transient voltage responses of a PEM electrolyzer over a trained short-time interval T_{train}. The model is conditioned on the applied current and initial capacitor voltages, and it is extended to temperature-dependent voltage prediction by including the cell temperature as an additional input.

Objectives:

The purpose of this study is to develop a CPINN-based voltage model that combines physical consistency, fast evaluation, and suitability for sequential prediction. The objectives are to formulate the model from a second-order equivalent electrical circuit, train temperature-independent and temperature-dependent CPINNs conditioned on current and initial capacitor voltages, and evaluate their performance under sequential rollout, operation outside the training range, and direct long-window prediction. The effect of increasing the CPINN training period is also analysed in terms of accuracy and rollout efficiency.

Material and methods:

The physical prior is a second-order equivalent electrical circuit with two RC branches, a reversible voltage term, and an ohmic voltage contribution. The internal states are the capacitor voltages U_{c1} and U_{c2} . The terminal voltage is reconstructed as

In the temperature-independent formulation, U_{rev} and R_{Ω} are constant. In the temperature-dependent formulation, U_{rev} follows an affine temperature relation and R_{Ω} is scaled using a temperature-dependent conductivity-inspired expression.

The CPINN learns the mappings and for the temperature-independent and temperature-dependent cases, respectively. The model is trained over a short-time interval . During prediction, the trained CPINN is evaluated over a prediction window . For standard sequential rollout, , so each CPINN query remains inside the time interval used during training. A longer total simulation horizon is obtained by chaining several prediction windows of duration , where the terminal predicted state of one window is used as the initial condition of the next one. Direct long-window prediction is also tested to assess the behaviour of the model when evaluated beyond its trained time interval.

The physics loss includes the differential residuals of the two RC state equations and the algebraic residual enforcing voltage consistency with the equivalent-circuit expression. An optional data loss can also be added when reference voltage or state data are available. In this work, the internal states are reconstructed using a hard initial condition embedding, which enforces and by construction. This improves consistency during sequential rollout. Training is performed using Adam followed by L-BFGS.

Results:

The temperature-independent CPINN achieved stable voltage prediction across the evaluated rollout scenarios. In nominal cases within the training range, the terminal-voltage RMSE remained below , with an aggregated in-range RMSE of . This aggregated value represents the mean performance over rollout cases that remain inside the current, state, and time ranges used during training. Errors increased when the model was evaluated outside the training range or directly over a time window longer than the training interval, but the sequential rollout remained stable.

The temperature-dependent CPINN improved the prediction of voltage dynamics under current and temperature variations. For the model, the voltage RMSE remained below in the intended rollout tests, and the long-horizon sequential rollout reached an RMSE of . This shows that the model can be used repeatedly over several short prediction windows without significant error accumulation.

Direct long-window prediction produced larger errors. For the temperature-dependent CPINN, using increased the voltage RMSE to . The model reduced this direct long-window error to , showing that increasing can reduce the number of rollout calls needed for a total simulation horizon , at the cost of slightly lower short-window accuracy.

Conclusions:

The results show that CPINNs are suitable for modelling the dynamic voltage response of a PEM electrolyzer over short prediction windows. By conditioning the model on current and initial capacitor voltages, the CPINN represents a family of transient responses rather than a single fixed trajectory. Adding temperature as an additional conditioning variable extends the surrogate to temperature-dependent voltage behaviour. The proposed model achieved millivolt-level accuracy in nominal rollout scenarios. Direct long-window prediction produced larger errors, confirming that the CPINN should be deployed through sequential rollout instead of direct extrapolation beyond . The hard initial-condition embedding improves continuity between rollout windows, while the comparison between and highlights the trade-off between short-window accuracy and rollout efficiency. Overall, the proposed innovation is a physically structured, temperature-aware CPINN surrogate for PEM electrolyzer voltage dynamics. Since the model includes both the control input and the initial internal state as conditioning variables, it provides a useful modelling component for future optimization and model predictive control applications.

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