Data-Driven Control of a PEM Electrolyzer

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Abstract: Green hydrogen production has gained significant relevance in recent years to substitute fossil fuels in the coming years. One of the most promising technologies for attaining such a milestone is the PEM electrolyzer; nevertheless, some considerations related to controlling its temperature must be addressed, such as avoiding high temperatures to extend its useful life and improve its efficiency. Therefore, this study proposes a data-driven control strategy based on Gaussian Process Regression (GPR) and Nonlinear Model Predictive Control (NMPC). GPR is used to identify the system, while NMPC is used to regulate the output temperature of the PEM electrolyzer with the identified model. Simulations show a clear resemblance between the Gaussian Process model and the phenomenological model, as well as the effectiveness of the controller. Furthermore, error metrics and computational time are presented.

1 INTRODUCTION

The energy transition is a crucial step in the fight against climate change for a sustainable future. It involves substituting fossil fuels for renewable energy sources such as solar, wind, and green hydrogen. The significance of the energy transition has been recognized by international agreements to tackle environmental issues. For instance, the Paris Agreement exposes the need to limit global warming to 1.5 °C by the end of this century (United Nations Framework Convention on Climate Change (UNFCCC), 2015). In addition, countries in the European Union have launched specific strategies such as the one from Spain, ”Hydrogen Roadmap: A commitment to renewable hydrogen” (Ministerio para la Transición Ecológica y el Reto Demográfico (MITERD), 2020), to achieve net-zero greenhouse gas emissions by 2050 at the latest.

Electrolyzers play a pivotal role in green hydrogen production as they are able to use electricity from renewable sources to produce clean hydrogen (i.e. no presence of greenhouse gases), which is considered ”green” (Carmo et al., 2013). There are four main types of electrolyzers (Proton Exchange Membrane, Alkaline, Solid Oxide Electrolysis Cell and Anion Exchange Membrane), but only the Proton Exchange Membrane (PEM) electrolyzer stands out for its efficiency and ability to operate at high current densities. Additionally, it is particularly suitable for integration with intermittent renewable energy sources; nevertheless, its high cost because of the noble metals for being produced as well as its water management, could become downsides of operating it.

Green hydrogen production through PEM electrolyzers not only contributes to greenhouse gas emissions reduction, but also offers a feasible solution to store renewable energy and provides stability for the electricity transmission grid. A significant challenge in a PEM is overheating, which can cause material degradation and underperformance. The intermittency in renewable sources can induce rapid fluctuations in the supply energy to the electrolyzer, so that additional heat is generated because of its load/unload cycles. Moreover, operation in high current densities to maximize hydrogen production contributes to the increase in the internal temperature. The efficiency, economic feasibility, and useful life of the PEM electrolyzer can be compromised by overheating. Therefore, an implementation of a temperature control system is needed to mitigate such a problem. One of the most effective methods is to integrate a cooling system to prevent overheating by conserving its internal temperature in an optimal range. A refrigerant fluid through the electrolyzer absorbs heat during op-

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eration to dissipate it to the environment afterwards. Thus, efficient functionality is guaranteed, as well as the durability of the device is extended.

Different control algorithms have been proposed to regulate the internal temperature in PEM electrolyzers. (Keller et al., 2022) proposed a feedforward control strategy and a PID adaptive parameter to control the temperature of the PEM stack of a 100 kW water electrolyzer. An explicit Model Predictive Control (eMPC) was embedded in a microcontroller and implemented in a lab-scale PEM electrolyzer to preserve the water temperature across it (Ogumerem and Pistikopoulos, 2020). A heat management system composed of a water pumping circuit, an air-cooler and a PID controller has been developed in (Molina et al., 2024) to control the water temperature in PEM electrolyzers. (Barros-Queiroz et al., 2024) used a linearized model of a PEM to propose a closed control strategy based on MPC and a disturbance model to regulate the electrolyser output temperature. An intelligent controller based on Gaussian Mixture Model (GMM) and Gaussian Mixture Regression (GMR), was used to control the electrolyser output temperature (Becerra-Mora et al., 2024).

Renewable energy sources (solar, wind, or hydroelectric) can be used to power PEM electrolyzers and thus to produce green hydrogen; however, these types of sources are inherently nonlinear (behavior is not proportional to the input). Hence, the dynamics of the PEM electrolyzer can be considered nonlinear as well. Usually, a nonlinear mathematical model of the system is difficult to obtain. Even so, there are basically three options to know an approximate model: A simpler linearized model can be deduced; a learning method can be used to construct estimates from complex systems (Becerra-Mora and Acosta, 2024); or first-principles models can be employed. Although there already exists a phenomenological model for the PEM electrolyzer (Mora and Bordons, 2022), this paper presents an alternative way to build a machine learning-based model. Moreover, such a model is employed in a nonlinear controller. Therefore, a supervised learning method, such as Gaussian Process Regression (GPR) is employed to identify the complex dynamics of a PEM electrolyzer. Once the system model is identified, this is used in a Nonlinear Model Predictive Control (NMPC) strategy to regulate the output temperature of the system.

The paper is structured as follows. In Section 2, the dynamics of a PEM electrolyzer is presented. In Section 3, Gaussian Process Regression is explained to carry out the system identification. In Section 4, a Nonlinear Model Predictive Control strategy is addressed to perform set-point tracking. In Section 5, experiments are described as well as their analysis of results. Finally, in Section 6, conclusions and future research are summarized.

2 PEM ELECTROLYZER DYNAMICS

An electrolyzer contains an electrolytic cell with two electrodes, an anode and a cathode, which are in charge of providing an electric current across the water to perform the splitting process of the molecule (H_2 and O). Once the splitting process is performed, an amount of water still remains in the process, which is reused into the system to reduce wastewater and improve its efficiency. In addition, residual water and gases (Hydrogen and Oxygen) must pass through gas-liquid separators to guarantee high purity in them.

Some issues such as low purity in gases, electrical conductivity, and overheating are due to materials degradation by high temperature. Therefore, efficient operation and useful life in a PEM electrolyzer are highly dependent on the internal temperature; therefore, the cooling system is essential to preserve it within an optimal range.

Figure 1: Front view of the PEM Electrolyzer.

The electrolyzer dynamics is described in (Mora and Bordons, 2022). A first-order differential equation (1) represents the thermal model that arises from the simplified energy balance of the system:

$$C_t \frac{dT_{el}}{dt} = \dot{Q}_{gen} - \dot{Q}_{loss} - \dot{Q}_{cool} \tag{1a}$$

$$\dot{Q}_{gen} = I_{el}(V_{el} - n_c V_{tn}) \tag{1b}$$

$$\dot{Q}_{loss} = \frac{1}{R_t}(T_{el} - T_{amb}) \tag{1c}$$

where C_t is the stack thermal capacity (J/K), T_{el} is the electrolyzer temperature (K), $\dot{Q}_{gen}$ is the heat generated in the system as a consequence of overvoltages or irreversibilities (W), $\dot{Q}_{loss}$ is the heat loss by environmental interaction (convection and radiation) (W), $\dot{Q}_{cool}$ is the heat dissipated by the cooling system (W), I_{el} is the current applied to the system, V_{el} is the voltage applied to the system coming from the electrochemical system, n_c is the number of cells, V_{tn} is the thermoneutral voltage, R_t is the thermal resistance (K/W) and T_{amb} is the ambient temperature (K).

The nonlinear behavior of the PEM electrolyzer is due to the current I_{el} coming from a photovoltaic source and the ambient temperature T_{amb}. Therefore, (1) can be rewritten as a nonlinear first-order differential equation as follows:

$$\frac{dT_{el}}{dt} = \frac{1}{C_t}\left[I_{el}(V_{el} - n_c V_{tn}) - \frac{1}{R_t}(T_{el} - T_{amb}) - \dot{Q}_{cool}\right] \tag{2}$$

The data used in this study come from a phenomenological model of the Hamilton-STD SPE-HG 1 kW PEM electrolyzer (see Fig. 1). Some technical features of this system are operation voltage/current (V/A) $= 9 - 11/5 - 80$, nominal temperature (ºC) $= 60$, number of cells $= 6$, partial pressure H_2/O (bar) $= 6.9/1.3$, thermal capacity (J/K) $= 9540$ and thermal resistance (K/W) $= 0.11$.

3 MODELING OF PEM ELECTROLYZER WITH GAUSSIAN PROCESS

Initially, the Gaussian Process (GP) can be considered as a generalization of the normal probability distribution, and according to (Rasmussen and Williams, 2006), GP is a collection of random variables, any finite number of which have a joint Gaussian distribution. Therefore, it can be described by its mean and covariance functions.

According to Section 2, a phenomenological model of a PEM electrolyzer is defined; nevertheless, one of the goals of this study is to discover the electrolyzer dynamics through a complete dataset of inputs/outputs $\{x^I, x^O\}$ coming from the phenomenological model and a regression problem defined by

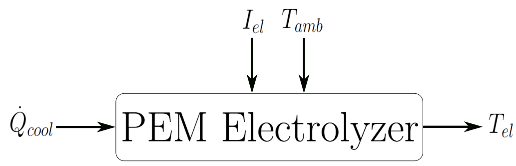

Figure 2: Inputs and Output of the System.

$x^O = f(x^I) + \eta$, where f is an unknown function and η an environmental noise. Hence, an output estimate x^{O*} can be calculated given unseen inputs x^{I*}. From this point on, x^I and x^O stand for input and output signals of the system (see Fig. 2), respectively, in our study. These can be written as follows:

$$x^I = [I_{el}, T_{amb}, \dot{Q}_{cool}]^T,$$
$$x^O = [T_{el}]^T$$

Note that x^{O*} is the estimate of the electrolyzer temperature $\hat{T}_{el}$. Thus, Gaussian Process Regression (GPR) is employed to estimate $\hat{T}_{el}$ given unknown data coming from x^{I*}. The dynamics of the system, as mentioned above, can be modeled as a multivariate Gaussian distribution $x^O \approx \mathcal{N}(\mu(x^I), K(x^I, x^I))$, where K, the covariance matrix, plays a fundamental role in GPs.

$$K(x^I, x^I) = \begin{bmatrix} k(x_1^I, x_1^I) & k(x_1^I, x_2^I) & \dots & k(x_1^I, x_N^I) \\ k(x_2^I, x_1^I) & k(x_2^I, x_2^I) & \dots & k(x_2^I, x_N^I) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_N^I, x_1^I) & k(x_N^I, x_2^I) & \dots & k(x_N^I, x_N^I) \end{bmatrix} \tag{3}$$

This matrix K is formed by a kernel function $k(x_i^I, x_j^I)$ that provides the covariance between two elements x_i^I and x_j^I. Similarity is a required property in a kernel function as two similar inputs (x_i^I, x_j^I) and their corresponding outputs (x_i^O, x_j^O) will have a higher correlation than for dissimilar inputs/outputs. One of the most used kernel functions is the Radial Basis Function (RBF), which is defined as follows:

$$k(x_i^I, x_j^I) = \sigma_1^2 \exp\left(-\frac{1}{\ell}(x_i^I - x_j^I)^T (x_i^I - x_j^I)\right) + \sigma_3^2 \delta_{ij} \tag{4}$$

where σ_1^2 is the signal variance, ℓ is the length-scale and σ_3^2 is the noise variance. In general, they are called hyperparameters. The posterior distribution stands for the estimate x^{O*} given some unknown datapoints x^{I*}, so that the joint distribution can be defined as

$$\begin{bmatrix} x^O \\ x^{O*} \end{bmatrix} \approx \mathcal{N}\left(\begin{bmatrix} x^I \\ x^{I*} \end{bmatrix}, \begin{bmatrix} K(x^I, x^I) & K(x^I, x^{I*}) \\ K(x^{I*}, x^I) & K(x^{I*}, x^{I*}) \end{bmatrix}\right) \tag{5}$$

The posterior distribution over x^{O*} is calculated with the conditional probability property of Gaussian distributions.Hence, mean and covariance become

$$\mu^* = \mu(x^{I*}) + K(x^{I*}, x^I)K(x^I, x^I)^{-1}(x^O - \mu(x^I)),$$
$$\Sigma^* = K(x^{I*}, x^{I*}) - K(x^{I*}, x^I)K(x^I, x^I)^{-1}K(x^I, x^{I*}) \quad (6)$$

A common assumption in practice is $[\mu(x^I), \mu(x^{I*})]^T = 0$. GPs can thus be expressed by their second-order statistics, the covariance matrix K, which is a positive semidefinite matrix.

4 NONLINEAR MODEL PREDICTIVE CONTROL STRATEGY

Although the PEM electrolyzer model can be linearized as in (Mora and Bordons, 2022), to consequently propose a linear controller (Barros-Queiroz et al., 2024), our approach is to deal with nonlinear dynamics, looking for improved performance. In fact, identifying a linear model is relatively easy; moreover, when the plant is in operation around the operating point, good performance can be achieved.

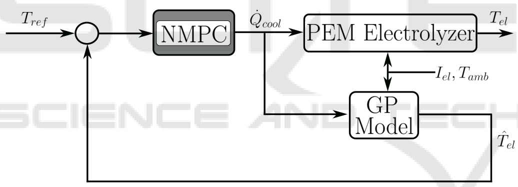

Figure 3: Block diagram of data-driven control system.

Nonlinear models may be very difficult in developing; nevertheless, learning methods such as the one presented in the previous Section, can help in this task. The electrolyzer model is identified off-line; hence, the control loop is less complex than in the case where the model shifts over time. A discrete representation of the nonlinear model can be expressed as:

$$x_{k+1} = f(x_k, u_k, v_k) \quad (7)$$

where x_k is the state/output (T_{el}), u_k is the manipulated variable ($\dot{Q}_{cool}$) and v_k is the disturbance (I_{el}, T_{amb}) at the instant k.

One of the better control strategies, both within the industry and within the research community, has been Model Predictive Control (MPC). This formulation integrates different control algorithms (e.g. robust, optimal, stochastic, adaptive, and so on). However, stability and robustness proofs have been difficult to obtain because of the finite horizon used (Camacho and Bordons, 1999). Despite having a nonlinear model, MPC concepts can be readily used. However, there are some issues with regard to nonconvexity in optimization problems and processing time.

Another goal of this study is to regulate the electrolyzer temperature T_{el} to maximize its hydrogen production without reducing its useful life. Hence, a Nonlinear Model Predictive Control (NMPC) strategy is proposed in this study. According to equation (7) and defining a reference temperature T_{ref}, the optimization problem to be solved at each instant k can be formulated as

$$\begin{aligned}
\min_{\dot{Q}_{cool}} \quad & J(\hat{T}_{el}, \dot{Q}_{cool}) := \delta \sum_{i=1}^{N_p} (T_{ref}(k+i) - \hat{T}_{el}(k+i|k))^2 \\
& + \lambda \sum_{i=1}^{N_u} (\dot{Q}_{cool}(k+i))^2 \\
\text{s.t.} \quad & \mathbf{\dot{Q}_{min}} \leq \dot{Q}_{cool} \leq \mathbf{\dot{Q}_{max}}
\end{aligned}$$

where N_p and N_u are the prediction and control horizons, respectively, δ and λ are weight factors to adjust the controller and $\mathbf{\dot{Q}}$ are the boundaries for the manipulated variable. Since the cooling system can operate only between a maximum and a minimal value, the input variable $\dot{Q}_{cool}$ must be constrained. Hence, the optimization problem attempts to reduce the error between the reference and the estimated temperature ($\hat{T}_{el}$) coming from the GPR model. The data-driven control system is depicted in Fig. 3.

5 EXPERIMENTS

In this Section, we present the results of performing two types of experiments to control the electrolyzer temperature T_{el}. First, we identify the nonlinear dynamics of the system using GPR; second, we propose a NMPC strategy to regulate the output temperature with the model initially identified. Indeed, the phenomenological model of the system is not used to develop the control strategy, but rather for testing the controller in it. The simulations are run in Matlab® on a laptop with an Intel® Core i9-13900H 2.6 GHz CPU and 32 Gb RAM.

5.1 Data Used in the Study

On the one hand, data related to ambient temperature T_{amb} were collected throughout the four seasons of the year in Seville, Spain. Actually, five different scenarios were used (i.e. autumn, winter, spring, summer and extreme summer). On the other hand, data related to photovoltaic cells to generate electrical current in the system I_{el} were collected on sunny/cloudy days. Therefore, ten different combinations were generated between T_{amb} and I_{el}. Additionally, data were sampled every second, which means 86400 samples per day.

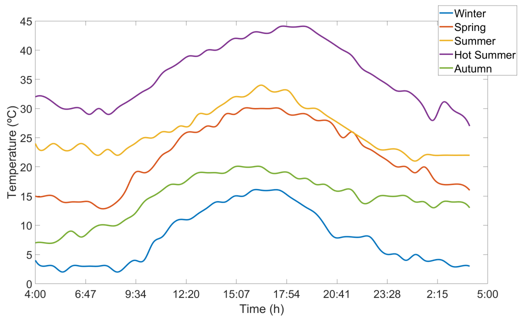

Figure 4: Ambient temperature.

The disturbances of the system correspond to the ambient temperature (Fig. 4) and the current applied to the electrolyzer (Fig. 5). The temperature of Seville T_{amb} varies from 3ºC to 44ºC throughout the year. The hottest months are July and August, as well as the coldest, January and February. The behavior of I_{el} comes from the photovoltaic system that shows the influence of irradiance on this variable. As expected in this kind of system, the electrical current on cloudy days is reduced compared to sunny days. Moreover, note that both disturbances have nonlinear behavior, which is the reason to use a nonlinear regressor (GPR) and a nonlinear control strategy (NMPC) to identify the system and regulate the output temperature, respectively.

In addition, the optimal operating range for this electrolyzer should be between 5 A - 80 A, therefore, I_{el} is saturated at 80 A approximately as the temperature of Seville can provoke higher levels of electrical current into the electrolyzer.

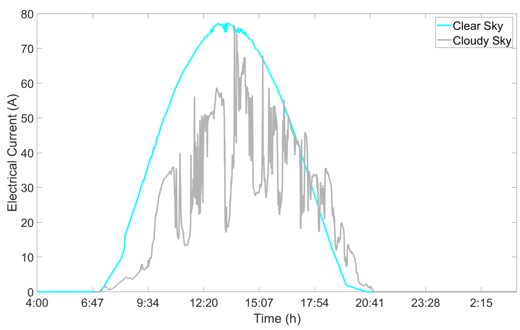

Figure 5: Electrical current from a photovoltaic cell.

5.2 Identification of the System

As stated above, the variables $[I_{el}, T_{amb}, \dot{Q}_{cool}]$ define the dynamics of the system. In Section 3 some fundamentals of GP are described as a method to construct an estimate of this dynamics. We have defined three inputs denoted as x^I and one output denoted as x^O to construct a dataset that describes such dynamics. The variables I_{el} and T_{amb} have been measured from the photovoltaic system and the climatological station, respectively. The PEM electrolyzer has been excited with step signals in the variable $\dot{Q}_{cool}$ to produce different levels of temperature at the output of the electrolyzer T_{el}.

One of the purposes of this study is to get as much data as possible to create a digital twin (Machado et al., 2023) of the system. Therefore, the step signals must be enough to reproduce the system dynamics; otherwise, the reproductions are poor, or the method is not capable of generalizing new inputs. Thus, we set 7 different levels of cooling capacity $(0, 25, 50, 75, 100, 125, 150)$ W. Note that GPR does not make distinction between disturbances I_{el}, T_{amb} and the manipulated variable $\dot{Q}_{cool}$, they are all inputs for this method.

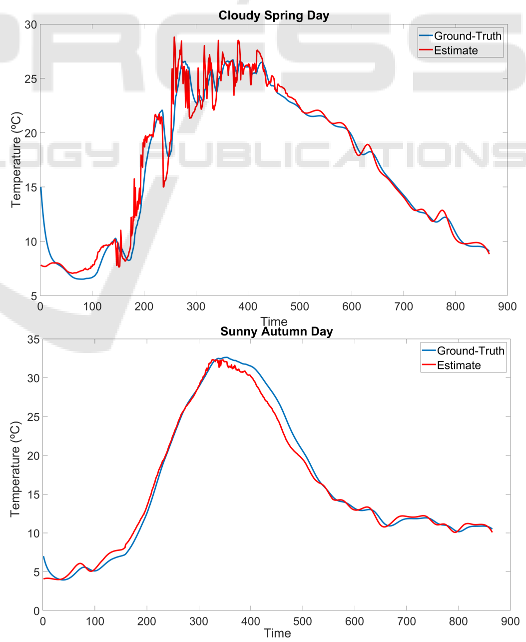

Figure 6: GP model of PEM electrolyzer.

The dataset comprises 6,048,070 samples, by grouping different scenarios (e.g. summer-cloudy-75 W, spring-sunny-25 W, winter-cloudy-150 W and so on) and collecting samples every second; nevertheless, it has been resampled to 100 seconds to reduce computational complexity without compromising the quality of reproductions. In this experiment, the reduced dataset (60,480 samples) is used as a training set to learn the complete behavior of the system throughout the year. The training time has been approximately 0.63 seconds. To validate a proper learning, new inputs x^{I*} associated with the variable $\dot{Q}_{cool}$ (heat dissipated) are used. In this case, we estimate the output x^{O*} (i.e. $\hat{T}_{el}$) with 2 different excitations (30 W, 70 W) in $\dot{Q}_{cool}$. During the training and validation process, the hyperparameters (σ_1^2, ℓ, σ_3^2) must be tuned to achieve better performance.

Two different scenarios (Cloudy spring day, Autumn sunny day) are used to compare ground-truth (phenomenological model) with estimates (GPR). The simulations have been conducted over a 24 hour period, starting at 4:00 a.m. Qualitatively, estimates (red line) are very similar to ground-truth (blue line) as can be seen in Fig. 6. Quantitatively, we have used the root mean squared error (RMSE) to measure the error between the ground-truth and the estimate. The scenario of a cloudy spring day shows an RMSE of 1.31ºC and the scenario of a sunny autumn day shows an RMSE of 0.93ºC, which means that an average low distance between the 2 curves is presented.

5.3 Nonlinear Control Strategy

The results in the previous Section show the behavior of the system in open-loop. In this Section a NMPC strategy (i.e. closed-loop) is implemented to preserve the electrolyzer temperature T_{el} below a reference temperature T_{ref} because of the reasons explained above. In Section 4 the input variable $\dot{Q}_{cool}$ (i.e. manipulated variable), the disturbances I_{el} and T_{amb} and the output variable T_{el} (i.e. controlled variable) are defined.

The optimization problem searches for the optimal value of $\dot{Q}_{cool}$ that minimizes the quadratic error between T_{ref}, which has been set to 30 ºC, and $\hat{T}_{el}$, which is the estimated temperature obtained from the GP model. Moreover, the constraint must be satisfied $\dot{\mathbf{Q}} \in \{0, 150\}$. The function *fmincon* from Matlab® along with the interior point algorithm are used to solve the optimization problem. The prediction N_p and control N_u horizons are set to 10 samples. The computational latency to solve the optimization problem has been approximately 415.81 seconds.

As in the experiment of the previous Section, two different scenarios are proposed to evaluate the NMPC strategy, the cloudy spring day and the sunny autumn day. The phenomenological model is used to test the performance of the control law; the blue line and the red line represent the behavior of the open-loop and closed-loop system, respectively (see Fig. 7 and Fig. 8). The two scenarios show a controlled temperature in the electrolyzer less than or equal to the reference temperature. Note that neither of them overcomes T_{ref}. The control signal effect (green line) is more intense in the cloudy spring day than in the sunny autumn day as the former reachs the set-point faster than the latter; therefore a higher correction is needed.

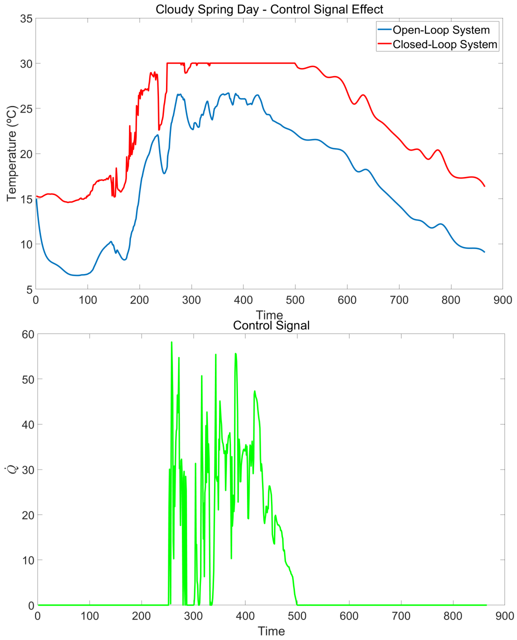

Figure 7: Control signal effect - Cloudy spring day.

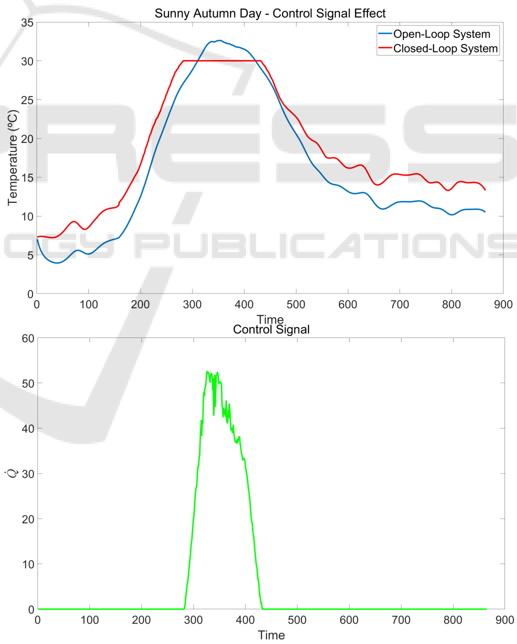

Figure 8: Control signal effect - Sunny autumn day.

6 CONCLUSIONS AND FUTURE WORK

In this study, we presented a data-driven control approach for a PEM electrolyzer. A dataset was built from a phenomenological model of the system. This dataset was used to build a GPR-based machine learning model. Furthermore, a NMPC strategy is proposed to control the output temperature of the electrolyzer from the machine learning model. The experiments corroborated a good system identification by providing a low RMSE between the ground-truth and estimate, as well as the use of such a machine learning model to develop a control strategy that preserves the temperature at the set-point.

The results suggest that a data-driven control strategy is useful when a phenomenological model does not exist or when it is too simple to represent nonlinear dynamics. Direct measures in the system are enough to build a dataset and develop a machine learning model.

Future work will implement the data-driven control strategy in the real system (PEM electrolyzer), besides, it will include a covariance analysis to represent confidence in the estimate, as well as a tuning of the weight factors to find a smoother control signal. Furthermore, a stochastic MPC approach (Hernández-Rivera et al., 2024) would be interesting to deal with measurement uncertainties. Finally, a stability analysis is considered to extend these results.

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