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A Comprehensive AI-Based Digital Twin Model for Residential Hydrogen-Based Energy Systems

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ABSTRACT As the urgency to mitigate climate change intensifies, the residential sector, a significant contributor to greenhouse gas emissions, calls for innovative solutions to foster decarbonization efforts. The integration of renewable energy sources and hydrogen-based technologies offers a promising pathway to achieve energy independence and so reduce reliance on traditional power grids. In this sense, digital twins, powered by artificial intelligence techniques, offer significant potential to enhance the performance of these systems, fostering energy self-sufficiency. This article presents a comprehensive architecture for a digital twin of residential hydrogen-based energy systems. We discuss the implementation of the digital replica based on both logical behavior and machine learning techniques. The resulting models are validated using real data collected from an electrically self-sufficient social housing in Spain, located in the town of Novales (Cantabria). The results evince that the behavior of the proposed solution accurately mimics the one shown by the physical counterpart, suggesting its utility as a valuable instrument for enhancing the efficiency of renewable hydrogen-based energy systems.

INDEX TERMS Digital twin, modeling, energy efficiency, hydrogen, neural networks, renewable energy.

I. INTRODUCTION

The urgency of mitigating the consequences of climate change has brought to the forefront the need for decarbonization of different polluting sectors, fostering the development of solutions to reduce emissions of CO_2 and other greenhouse gases, which are the main contributors to global warming.

Particularly, the residential and building sector is the third most polluting one, after industry, and agricultural and forestry activities [1]. This sector has received less attention globally, indicating untapped potential. The growing energy demand of this sector requires significant advancements and breakthroughs to ensure sustainable solutions, including, among others, the research and development of pilot projects. In this regard, self-supply systems, equipped with renewable energy sources (RES) and hydrogen-based technologies, offer a promising path to achieve energy independence, reducing the dependence on traditional grids and providing an attractive solution for remote areas or microgrids with restricted access [2]. However, significant economic and technical barriers remain, including the development of robust and cost-effective hydrogen generation and storage systems, as well as advanced energy management strategies, which present substantial challenges to optimize the overall system performance and efficiency. Integrated policies and regulatory frameworks are essential to catalyze innovation, aligned with governmental decarbonization goals, and to promote cohesive supply chain operations, as discussed in [3].

Although digital infrastructures may contribute to increasing CO_2 emissions, their potential to enable emission reductions through strategic applications is well known [4]. This article explores the application of the digital twin (DT) paradigm to an actual hybrid renewable energy-hydrogen system that is used to power a social dwelling located in the town of Novales (Cantabria, Spain). This was the first socially subsidized residence to achieve electrical self-sufficiency in Spain throughout the year. The DT serves as a virtual replica of the physical system, continuously ingesting real-time data on energy generation, consumption, and storage. This data is then processed through specific algorithms, which are deployed and validated on the digital replica to improve the performance of the real renewable hydrogen-based system (RHS). These novel methods unlock the potential of dynamic energy management strategies, which could be tuned based on weather forecast services and resources, consumption patterns and real-equipment data, to optimize the performance of the real system while seeking the most cost-competitive operation of the pilot plant [5]. This approach aligns with the United Nations Sustainable Development Goals (SDGs) [6], particularly SDG 7: "Affordable and Clean Energy". By enhancing the performance of self-supply systems, DTs can significantly contribute to increase the RES efficiency and reduce greenhouse gas emissions.

This work comprehensively describes the architecture of the DT, focusing on the digital model of the pilot plant. The article validates and discusses the performance of such digital replica, showcasing the benefits of applying artificial intelligence and machine learning (AI/ML) techniques compared to model-based approaches. The obtained results evince the potential gain of fostering data-driven techniques to mimic the behavior of real counterparts.

The main contributions of this work are:

- We design, implement and validate a complete Digital Twin of a fully operational hydrogen-based renewable energy system. The entire implementation is open-source, fostering accessibility, replicability and cost reduction. The source code is available at [7].
- The design of the DT follows a modular approach. This provides the proposed solution with a great degree of flexibility, since it can be adapted to different situations and conditions, opposed to more traditional monolithic approaches.
- The validation of each module and the whole DT is made by means of a large dataset (300,000 samples) from the real system. The results evince that the digital replica is able to accurately mimic the behavior of the real system.
- We compare the performance of different modeling approaches (algorithmic and based on neural networks). The results indicate that the most appropriate selection depends on the particular characteristics of the physical system.
- We show that pre-processing the data may yield significant benefits, and that the use of external variables can also significantly improve the accuracy of the cyber-physical system.

The rest of the article is organized as follows. Section II reviews the state of the art on the use of digital twins, in general, and in the renewable energy sector in particular, positioning our proposal. Section III depicts the architectures of both the real hybrid renewable energy-hydrogen physical system and the DT. Then, Section IV focuses on the models that we developed at the DT for the different modules, and how they were integrated. Section V discusses the results obtained with the proposed digital replica, assessing its feasibility. Finally, Section VI concludes the article, providing an outlook of our future work.

II. RELATED WORKS

The concept of DT, which entails the exchange of data between a physical system and its virtual replica in either direction, appeared for the first time at the turn of the century. In particular, it was first applied to the industrial realm, and the so-called Industry 4.0 paradigm [8], [9]. Nevertheless, its use has been extended to a broad range of sectors [10], [11], taking advantage of recent progress in digitization and the growing capabilities of communication and computing systems. As Qi and Tao discussed in [12], the increasing complexity of real processes can only be accurately replicated exploiting AI/ML techniques, whose relevance might be therefore rather strong when applied in DTs. Moreover, Zhang et al. highlight in [13] the effectiveness of ML and deep learning techniques in achieving high accuracy for predictive maintenance tasks of industrial equipment.

One of the few papers applying the digital twin concept to the energy domain is the one from Nguyen et al. [14]. The authors propose the use of a DT to improve the performance of power distribution systems, highlighting its ability to take optimal control decisions, based on analyses that are carried out in real time. Similarly, Agostinelli et al. discuss in [15] the potential benefits of DT in the management of energy distribution and consumption in buildings, and they highlight the role that artificial intelligence techniques could play. In the same line, Fathy et al. demonstrate in [16] that the application of a DT to improve decision-making of an energy system might significantly reduce energy demand dispersion, as well as per-household cost.

In [17], Ferdaus et al. present a comprehensive review of advanced digital technologies, and their role in enabling a sustainable net-zero energy. They highlight the role of AI and digital twin technologies for optimizing energy systems through real-time data analysis, enhancing efficiency, integrating renewable energy sources, and enabling informed decision-making to reduce carbon emissions. On the other hand, they also identify the challenges that need to be faced when applying these technologies, like high upfront costs and interoperability issues.

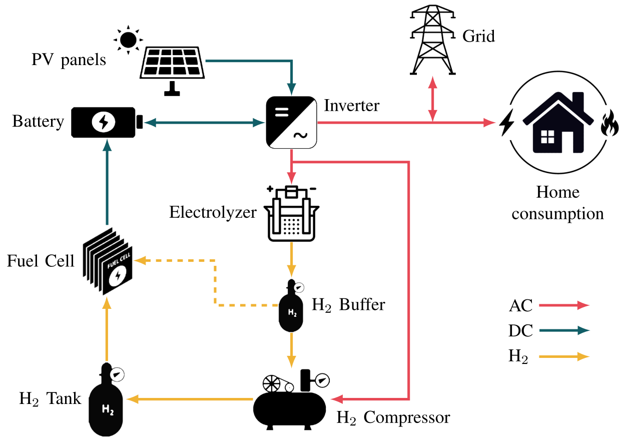


FIGURE 1. Schematic diagram of the hybrid RHS deployed in Novales (Cantabria, Spain).

One scenario of particular interest, due to the benefit it brings to the environment, is that of RES. In this line, [18] presents a short term predictive model to improve the efficiency of wind power. Within the AI domain, data-driven techniques have been successfully applied to forecast the electricity demand in [19], yielding high accuracy. This study has demonstrated the potential of such methods to achieve substantial cost reductions within the electricity supply chain. However, as Liu et al. and Tao et al. state in [20] and [11] respectively, there exist very few works that have tried to apply the DT concept to this type of systems. Moreover, Ebrahimi concludes in [21] that there do not exist any in-depth studies on the use of DT in this sector.

Focusing on the hydrogen production process, Gerard et al. propose in [22] the use of a DT to address the uncertainties associated with the investment and operating costs of the system. In another related work, Colmenares-Quintero et al. highlight in [23] the importance of using digital twins to validate and optimize the performance of green hydrogen production systems. Their work presents a conceptual and methodological framework for evaluating green hydrogen production as a foundation for a future digital twin development. In particular, the evaluation is conducted leveraging simulation commercial tools, so that the digital twin is model-based. Opposed to that, the digital twin proposed in this work is data-based, so that the behavior can be tailored to the real system.

As can be seen, despite their clear potential benefits, the use of digital twins in the green energy realm in general, and in renewable hydrogen-based systems in particular, is still very limited, and the few existing works are mostly theoretical-based.

This article introduces a leading-edge approach, modeling a comprehensive DT of a real renewable hydrogen-based system, which is currently in operation. We explore the advantages of applying the DT concept to improve the operational performance of the real system through the deployment of an open-source tool with a modular approach. This provides flexibility to the DT, facilitating the incorporation of improved models for other circumstances or to adapt the operation of the DT when some of the elements of the real system changes. It also permits focusing the analysis on a single element. In more traditional monolithic approaches, where the modeling of the whole system is proposed, this versatility is far more difficult to achieve. Moreover, the use of open-source code fosters vendor independence, while enhances accessibility, innovation, and transparency.

III. METHODOLOGY

This section describes the physical system which is replicated through the DT solution. Afterwards, the architecture of the DT is depicted, discussing its relationship with its physical counterpart.

A. REAL SYSTEM DESCRIPTION

The physical system corresponds to a pilot plant based on the hybridization of RES and hydrogen-based technologies to accomplish the 100% electrical self-sufficiency of a social dwelling, located in the town of Novales (Cantabria, Spain). The vulnerable tenants benefit from a completely decarbonized and efficient electricity supply, so reducing the risks of energy poverty. Fig. 1 depicts the configuration of the power system, providing a graphical visualization of the pilot plant with the interaction between the different modules that it entails [24].

Photovoltaic (PV) panels placed on the roof of the building harvest the solar energy that is supplied to the home through a hybrid inverter. The existing surpluses are initially stored in a lithium-ion battery pack that saves energy in a day-to-day basis, after covering the electricity demand of the social house. Afterwards, in case of further surpluses, the electricity is employed to store energy in the form of hydrogen, which is generated by an electrolyzer from deionized and demineralized water, yielding seasonal energy accumulation. This hydrogen is sent to a buffer tank composed of two steel cylinders until the maximum pressure the electrolyzer can deliver is reached. When the buffer reaches such maximum pressure, a compressor is triggered to accumulate the generated hydrogen in a high-pressure tank, up to 300 bars.

Finally, if additional electricity excesses exist, these are injected back to the grid, and sold to the utility grid company to obtain additional revenues.

Conversely, if there is not sufficient PV generation to meet the demand of the social dwelling, the batteries cover the electricity deficit in a first stage. If the energy stored in the battery pack is not enough to ensure the continuous electrical supply, the fuel cell is triggered, either with the hydrogen stored in the buffer tank or in the high-pressure tank. The fuel cell is activated when either of two different conditions are met: (1) if the state of charge (SOC) of the battery decreases below a defined threshold, or (2) if the peak demand is higher than the maximum battery discharge power. In both cases, the fuel cell can also charge the battery pack besides covering the electricity required by the home.

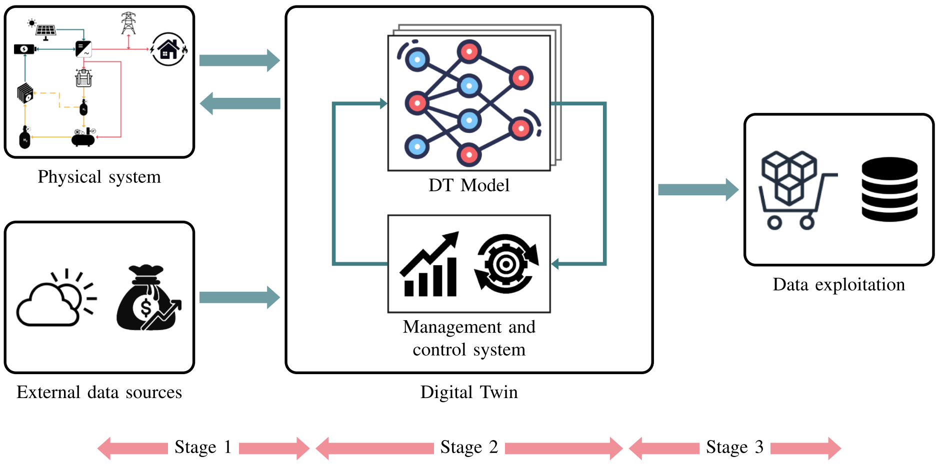


FIGURE 2. **Architecture overview of the RHS digital twin.**

The power system balance of plant (BoP) is completed with different safety, control and instrumentation devices that ensure the operation of the whole system and continuously monitor diverse parameters. All the gathered data is processed with a programmable logic controller (PLC) that allows the remote operation of the pilot plant, thanks to a tailor-made energy management strategy based on different battery state of charge thresholds, hydrogen deposits and energy flows within the system. Furthermore, the continuously recorded data is sent to a supervisory control and data acquisition system (SCADA) that enables the visualization and historic recording (trace generation) of all the desired parameters [25].

B. DIGITAL TWIN DESCRIPTION

Based on the pilot plant described above, we describe hereinafter the design and development of the DT where all plant components are included, and control solutions are developed to address the automatic improvement of the real system performance. To develop the DT, we propose an architecture with three main stages. The first one, focused on the physical-virtual interaction, is in charge of the collection of information from the real system, as well as the implementation of decision policies. As mentioned above, the pilot plant uses a SCADA system for monitoring the performance of the real devices. Thus, the DT is able to interact with the SCADA system through the PLC, to collect data and to apply the appropriate control actions.

Moreover, a module for the management and integration of data from external sources is also considered. At the time of writing, environmental temperature is collected from the Spanish meteorological agency, AEMET [26], open data portal. In a next stage, additional data, such as weather forecasts or energy prices, will be also collected, so that the control system can take into consideration current or future boundary conditions.

In a second stage, and taking advantage of the aforementioned modules, the DT model is implemented by a set of software libraries that replicate the behavior of the real system. In this regard, once the input/output and control variables of the main components of the RHS have been identified, we address their modeling. We will adopt a model-driven approach when the underlying behavior is well known, otherwise AI/ML techniques will be trained with the collected data in order to mimic the real operation of the RHS. Finally, the DT model is used to assess the performance of different control policies on the digital replica before configuring them on the real system, for example those based on weather forecasting. The logic of the digital replica thus stays within the DT model, which captures the behavior and performance of the real system.

The management system implements both control and performance improvement strategies. As shown in Fig. 2, the DT follows a loop-based approach to ensure that the behavior of the real counterpart is accurately captured: (i) the DT receives feedback from the physical system and external data sources (continuous monitoring) to train the DT for those cases where ML solutions are adopted; (ii) the DT replicates physical system behavior based on the received measurements; (iii) it performs the analysis of various control strategies to optimize the performance of the physical system; (iv) the DT finally implements the best strategy on the real pilot, by forwarding control commands that interact with the deployed SCADA system.

Finally, and although the design assumes the DT to run in a closed way, it is also envisaged that the data generated during its operation could be also exploited by other stakeholders. Thus, the data generated by the DT will be made available at a data marketplace [27] as well as at open access repositories. In this sense, open data models will be adopted, such as Smart Data Models (SDM) [28], which facilitates the interoperability and reuse of information by third parties. If there were not appropriate available models for the specific needs of the DT, new definitions will be proposed to extend the SDM repository.

The following sections delve into the DT behavior implementation and its validation.

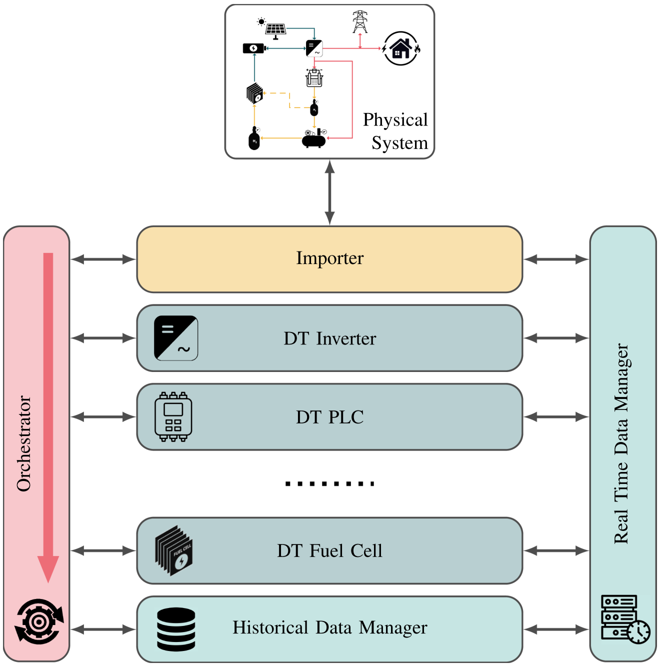


FIGURE 3. DT modules integration.

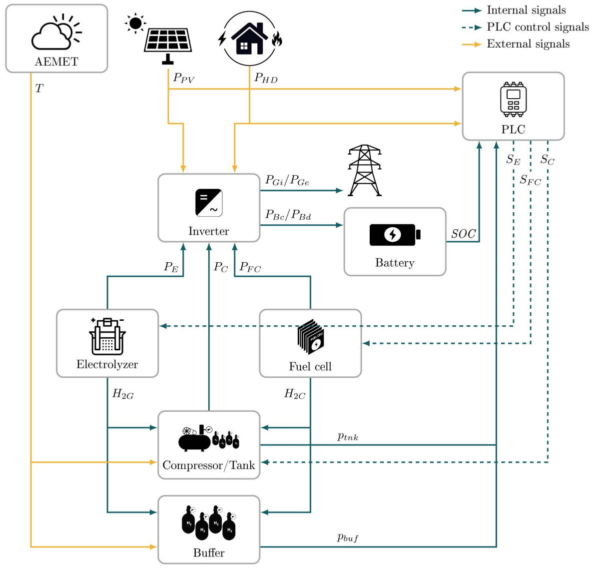


FIGURE 4. DT modular architecture, identifying the signals/variables exchanged between the different moodules.

IV. MODELING OF THE DIGITAL REPLICA

We describe in this section the implementation of the DT logic, following a top down approach. First, the overall solution is described, discussing how its constituent modules are interconnected. Afterwards, the details of each of the modules are nailed down.

A. MODULES AND INTERCONNECTION

The DT is implemented as a set of software modules, each of them modeling the behavior of one or more components of the physical RHS. This modular approach facilitates the validation and potential replacement of specific component models without disrupting the overall system. Furthermore, it enables the selection of the most suitable AI/ML model for each component's behavior.

As shown in Fig. 3, the DT modules are integrated through an orchestrator that is responsible, each time it receives a new set of measurements from the physical system, of executing them sequentially. In this sense, the execution follows a pre-established order so that the outputs of some modules feed, as input signals, other entities, as will be described in the next section.

The data acquisition from the physical system and external data sources is facilitated by an importer module. This is responsible for processing incoming data streams in real-time (RT) from the physical system and external data sources, or retrieving historical data from archived log files or databases. The input of external variables update a RT dictionary, hosted at the RT data manager.

Once the external variables are updated in the dictionary, the orchestrator runs the DT modules consecutively. Each module applies the required input variables provided by the RT data manager, runs the corresponding model, requests the RT data manager to update the dictionary with the estimated outcomes, and returns the control to the orchestrator to continue with the execution.

Finally, a historical data manager preserves the RT dictionary status before being updated by the next measurement batch. The historical data is also used to estimate the accuracy of the DT outcomes, by comparing them with the real measurements taken by the physical system. As depicted in Fig. 3, in further steps the historical data manager, together with the RT data manager, will be in charge of interacting with the data exploitation stage.

B. MODELS

Building upon the aforementioned concept, the DT employs a modular approach. This enables individual modules within the DT to leverage diverse models for replicating the behavior of the corresponding physical component. Each module is functionally encapsulated as an object, characterized by a well-defined set of input and output variables and whose behavioral model can be configured when executing the DT. Table 1 enumerates all the system variables/signals, along with their units and valid ranges. Besides, the table also indicates the inputs and outputs of each DT module. Furthermore, in order to show their interaction, Fig. 4 depicts the flow of variables and inter-module dependencies. The figure shows external input signals with orange lines, while green lines correspond to internal variables, and the dashed ones are the PLC control signals.

The models employed within the DT modules can be categorized into two main groups. The algorithmic ones leverage explicit algorithms, or mathematical formulae, to replicate

TABLE 1. Input/Output Variables and Parameters of the System

Variable Name	Symbol	Units	Values
PV panels power	P_{PV}	kW	$[0, 6.55]$
Fuel cell power	P_{FC}	kW	$[0, 2.66]$
Home demanded power	P_{HD}	kW	$[0, 5.40]$
Electrolyzer power	P_E	kW	$[0, 1.20]$
Compressor power	P_C	kW	$[0, 0.78]$
Charge battery power	P_{Bc}	kW	$[0, 3]$
Discharge battery power	P_{Bd}	kW	$[0, 5.41]$
Imported grid power	P_{Gi}	kW	$[0, 1.20]$
Exported grid power	P_{Ge}	kW	$[0, 5.92]$
Buffer pressure	p_{buf}	bar	$[0, 35]$
Tank pressure	p_{tnk}	bar	$[0, 300]$
Environmental temperature	T	ºC	$[5, 27]$
Time period with P_{Bd} under threshold	t_{FC}	min	5
State of charge	SOC	%	$[0, 100]$
Hydrogen flow generated	H_{2G}	Nl/h	$[0, 380]$
Hydrogen flow consumed	H_{2C}	Nl/h	$[0, 33]$
Electrolyzer on/off signal	S_E	n.a.	$\{0, 1\}$
Compressor on/off signal	S_C	n.a.	$\{0, 1\}$
Fuel cell on/off signal	S_{FC}	n.a.	$\{0, 1\}$
Battery capacity	C_{bat}	kWh	8.8
Buffer capacity	C_{buf}	bar	35
Tank capacity	C_{tnk}	bar	300
SOC threshold to switch on electrolyzer	th_E^{SOC}	%	85
P_{HD} threshold to switch off electrolyzer	th_E^{PHD}	kW	0.5
p_{buf} threshold to switch on compressor	th_C^{pbuf}	bar	34
P_{Bd} threshold to switch on/off fuel cell	th_{FC}^{PBd}	kW	2.50
SOC threshold to switch on fuel cell	th_{FCon}^{SOC}	%	20
SOC threshold to switch off fuel cell	th_{FCoff}^{SOC}	%	35

Inputs	Outputs
Inverter	
P_{PV}, P_{FC}, P_{HD}, P_E, P_C	P_{Bc}, P_{Bd}, P_{Gi}, P_{Ge}
PLC	
P_{PV}, P_{HD}, SOC, P_{Bd}, P_{Ge}, P_{Gi}, p_{buf}, p_{tnk}	S_E, S_C, S_{FC}
Battery	
P_{Ge}, P_{Gi}, P_{FC}	SOC
Electrolyzer	
S_E	P_E, H_{2G}
Hydrogen Storage	
S_C, H_{2G}, H_{2C}, T	P_C, p_{buf}, P_{tnk}
Fuel cell	
S_{FC}	P_{FC}, H_{2C}

the logical behavior of the real system. This approach offers control over the model's behavior through configuration parameters. Conversely, the data-driven approach exploits AI/ML models trained with historical data collected from the physical system. This approach aims to capture complex non-linear relationships, but it may lack control compared to algorithmic models.

The models developed for each component, according to these two groups, are detailed in the following subsections.

1) ALGORITHMIC APPROACH

The algorithmic models defined to replicate the logical behavior of real system components, based on their underlying physical phenomena, are described below.

a) Inverter: To replicate the behavior of its physical counterpart, the inverter module requires, as input variables, the power generated by the system, corresponding to the power produced by both the PV panels and the fuel cell, as well as the consumed power, which corresponds to the power demanded by the house, and the power required by both the electrolyzer and the compressor. The proposed model distributes the energy so that the power balance is met, see (1). This means that it compensates the power excess/deficit, calculated as the difference between the produced and the consumed power to/from the various energy storage modules, prioritizing the battery over the H_2 storage, and if necessary, to/from the grid.

$$P_{PV} + P_{FC} + P_{Bd} + P_{Gi} = P_{HD} + P_C + P_E + P_{Bc} + P_{Ge} \tag{1}$$

b) Battery: The battery module requires of the charge/discharge power provided by the inverter module to update its SOC. As can be inferred from (2), the variation in the SOC will also depend on the battery capacity (C_{bat}) and the sampling time (Δt). The output of this module, SOC, is fed back into the system, to be used by the PLC in its decision making processes.

$$\delta_{SOC} = \frac{(P_{Bc} - P_{Bd}) \cdot \Delta t}{C_{bat}} \tag{2}$$

c) PLC: The PLC module contains the overall management logic of the system. As indicated in Table 1, this module requires two external variables: home power demand and PV generated power. These variables, together with other signals that come from other system modules, such as the SOC and the H_2 storage systems pressure, are used as control signals for switching on/off the modules associated with the production, storage and conversion of hydrogen. The decision-making to switch on/off the electrolyzer, compressor or fuel cell (S_x) is based on the comparison of the system variables with a predefined set of thresholds (th_c), programmed into the PLC, as shown in Fig. 5. These thresholds can be dynamically adjusted, based on real time or expected boundary conditions to achieve optimal system performance.

The operation of the physical counterpart of this module is based on a series of logical instructions. Hence, its implementation follows an algorithmic approach. Initially, the digital PLC mimics the behavior configured in the real system, as described in Section III, to facilitate the validation of the different models. Subsequently, and exploiting the versatility of the DT, the implementation of different control policies will lead to the modification of this logic, improving the system performance.

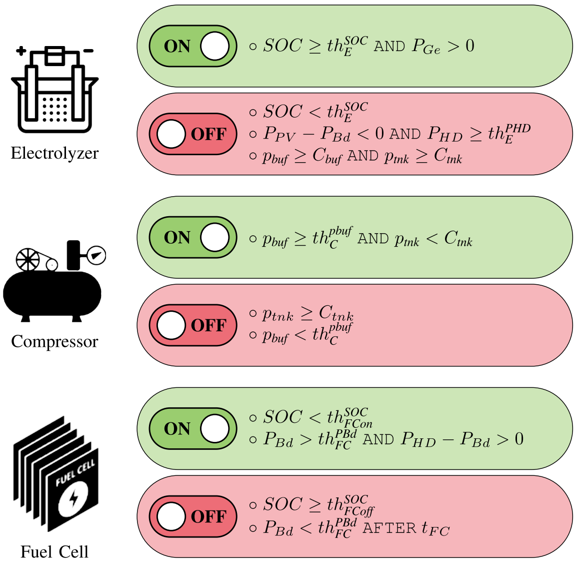


FIGURE 5. PLC decisions logic.

d) Electrolyzer: The electrolyzer module obtains the generated H_2 flow and the consumed power using, as input variable, the on/off signal provided by the PLC (S_E). These output variables are estimated by their mean values when the physical system is switched on. The outcomes of this module serve as inputs for the H_2 storage and inverter modules, respectively.

e) Hydrogen storage block: This module bundles the physical equipment that takes care of H_2 storage: H_2 buffer, H_2 compressor and H_2 tank. The compressor switching on/off signal, coming from the PLC, establishes whether the hydrogen generated by the electrolyzer should be stored in the buffer, or in the compressed hydrogen tank. In case the fuel cell is on, the consumed hydrogen will be updated in the storage system: first ingested from the buffer and later, when the pressure p_{buf} is below a configured threshold (th_C^{pbuf}), from the tank. The hydrogen stored determines the pressure on these blocks, according to the ideal gas law, considering the storage capacity, V_{buf} for the buffer and V_{tnk} for the high pressure tank, the temperature (T) and the gas constant (K), see (3). The pressure estimations will be fed back to the PLC for the control logic decision making.

$$p_{buf} \cdot V_{buf} = n \cdot R \cdot T \tag{3}$$

f) Fuel cell: This module receives the on/off signal from the PLC (S_{FC}) when the battery is below a certain threshold. It provides, as output variables, the consumed hydrogen and the generated power, which would then update the status of the hydrogen storage and battery modules. The H_2 flow consumed and the power generated are estimated by their mean values when the physical system is switched on.

2) DATA-DRIVEN APPROACH

While algorithmic models have the ability to capture different system configurations by simply modifying the underlying parameters, their effectiveness is limited when capturing more complex behaviors from real systems. In such scenarios, data-driven approaches leveraging AI/ML are beneficial. The solutions that have been considered are based on three types of neuronal networks that allow both the modeling of complex functions and the prediction of time series, as described below.

a) Dense Neural Network (DNN): It is a fundamental neural network architecture, characterized by multiple layers of interconnected neurons, where each neuron at a particular layer is fully connected to those in the subsequent layer, forming a dense connectivity pattern. Each neuron applies a non-linear function, known as activation, to a combination of inputs. In our case, Rectified Linear Unit (ReLU) functions, predominantly employed, are applied. This non-linearity allows to model complex relationships between input features and the desired output. The connections between neurons are represented by weights, optimized during the training phase, dictating the flow of information from input to output layers.

b) Convolutional Neural Network (CNN): CNNs are excellent at capturing spatial relationships within data, through a convolution operation where the network slides a filter across the input data. The weights associated with such filter are continuously updated. Unlike DNNs, each neuron output is a linear combination of the current input and a number of previous samples. This allows CNNs to find temporal dependencies within the data, making them suitable for tasks like time series forecasting.

c) Recurrent Neural Network (RNN): RNNs are specifically designed to handle sequential data, incorporating information from previous time steps into the current output. This inherent "memory" capability makes them well-suited for tasks involving time series analysis and prediction. In particular, we have used the well known Long Short-Term Memory (LSTM) neurons, which store and propagate relevant inputs sequences, enhancing their ability to learn long-term dependencies within the data.

Historical data of the input/output variables detailed in Table 1, captured from the physical system, were used for training, to learn the weight matrices that optimize the performance of the neural networks, but also for validation and testing each module. The choice of the most appropriate neural network for a specific model depends on the nature of the data and the desired functionality. DNNs are well-suited for general function modeling, while CNNs and RNNs with LSTM cells are particularly effective for tasks involving sequential data and long-term dependencies. Section V discusses the performance of these techniques when applied to the aforementioned DT modules.

V. VALIDATION

A validation process was conducted based on a dataset collected from the physical system over a time period of approximately 20 days. Measurements were taken at five-second intervals, to capture power consumption peaks by the dwelling, resulting in a dataset of more than 300,000 samples of each parameter. Subsets of these samples served as training data for the neural networks of the different DT modules and

TABLE 2. Output Variables NRMSE Per Model

Output variables	Alg.	DNN	CNN	RNN
Inverter				
Charge battery power	0.226	***0.023***	0.147	0.108
Discharge battery power	0.130	***0.010***	0.024	0.047
Imported grid power	0.014	***0.012***	0.028	0.035
Exported grid power	0.215	***0.015***	0.084	0.066
Battery				
State of charge	0.070	0.212	***0.020***	0.053
Electrolyzer				
Electrolyzer power	0.083	***0.066***	0.204	0.222
Hydrogen flow generated	0.103	***0.078***	0.369	0.193
Hydrogen Storage				
Compressor power	0.058	0.357	0.071	***0.054***
Buffer pressure	0.338	0.339	***0.062***	0.269
Tank pressure	0.288	0.357	***0.024***	0.135
Fuel cell				
Fuel cell power	0.067	***0.058***	0.062	0.060
Hydrogen flow consumed	0.083	***0.056***	0.059	0.058

for subsequent validation processes. In particular, 60% of the samples for used for training, while the remaining 40% were reserved for validation purposes. The dataset comprises samples collected between late March and early April, a period during which the fuel cell did not require any activation and so stayed idle. Consequently, the fuel cell was validated using a separate dataset, with samples collected during December and January, a period of higher fuel cell activity, but with a reduced number of samples ($\approx 90,000$). To assess the accuracy of the obtained results, the normalized root mean square error (NRMSE) is used, thus providing a standardized approach to asses the performance of the DT, by comparing predicted and observed values.

The system evaluation was conducted in two phases. Initially, an assessment of individual DT modules was carried out and the behavior of the whole digital replica was assessed afterwards. The PLC validation is not tackled in this article, as its behavior is absolutely deterministic and so the algorithmic approach perfectly reproduces its real operation.

A. MODULES VALIDATION

To validate the individual performance of the DT modules, the physical system measurements were used as input variables for each module, according to Table 1, where the different variables are described. Table 2 shows the NRMSE values obtained for each output variable when the models described in Section IV were applied to each module.

Table 2 evinces that there is not a single AI/ML model that best fits all the modules and variables, and we can thus conclude that tailored solutions are needed. The optimal AI/ML model to estimate a specific variable depends on its particular features and its relationship with other input variables. For instance, for variables exhibiting temporal dependencies, such as battery SOC or hydrogen storage pressure, models having a memory feature, capable of capturing sequential patterns, like RNN or CNN, exhibit better performance. In contrast, DNN are more suitable for variables that are primarily influenced by the current state of the input variables, like the inverter, electrolyzer and fuel cell. In any case, the optimal AI/ML models significantly improve the algorithmic estimation.

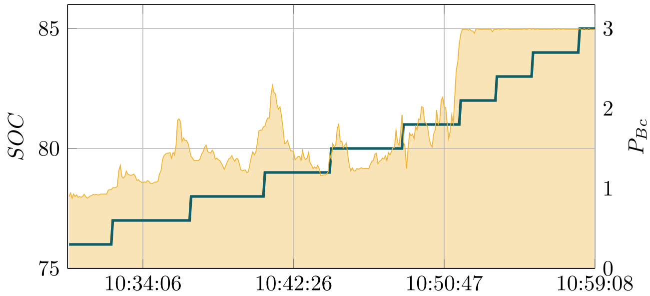


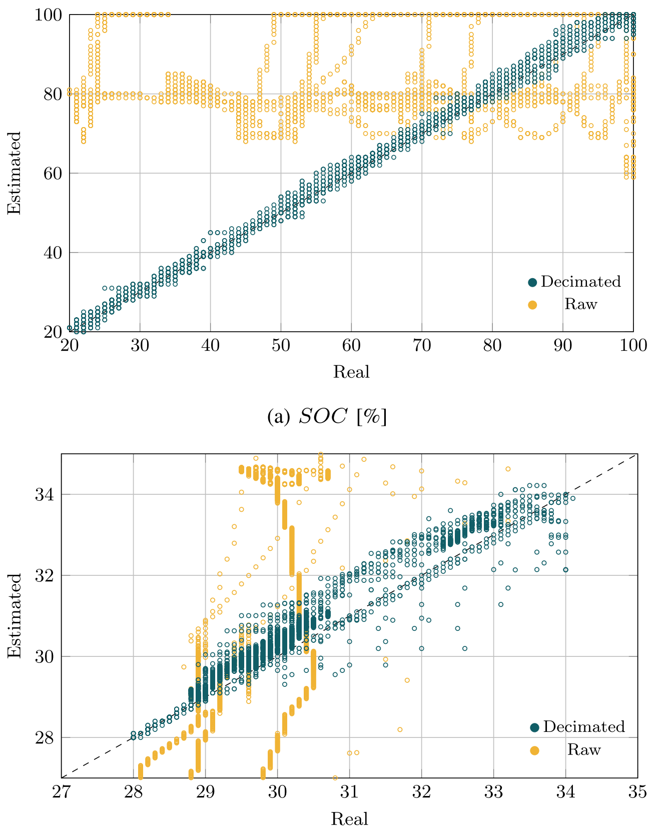
FIGURE 6. **Battery SOC [%] (green) vs. charging power [kW] (orange).**

One of the main challenges that we found when training neural networks for accurate estimation is data heterogeneity. Some variables, such as power and hydrogen flow, exhibit rapid fluctuations, requiring high-frequency sampling, while others, like SOC and hydrogen storage pressure, vary at a rather slow pace, due to their intrinsic nature or measurement limitations. Fig. 6 illustrates this disparity in the case of the battery, where charging power measurements (orange shadow) fluctuate rapidly, whereas SOC (blue line) remains constant over extended periods.

An issue arises when, training neural networks to estimate these slowly-varying signals over a series of samples, the output remains constant despite variations in the input signals. This lack of variation in the output hinders the network's ability to learn the underlying relationship, resulting in poor prediction accuracy.

To address this challenge, the sampling rate must be adjusted to accommodate the specific characteristics of the variable being estimated. This means that, for variables such as SOC and hydrogen storage pressure, decreasing the sampling rate by decimating the number of samples can significantly improve the accuracy of the estimated values. Consequently, the battery and hydrogen storage modules incorporate the decimation rate as a configuration parameter to facilitate the homogenization of input variables of these modules.

Fig. 7 shows the relationship between the measured values of the physical system and the estimated ones, using CNN, for the SOC (a) and the buffer pressure (b). The dashed line represents the ideal behavior, where the estimated values and the real samples are the same. Orange markers represent the accuracy of the estimated values when the complete samples set is used for training, while green ones correspond to the estimated values when a decimation rate of 1/60 is used, leading to 5 minute intervals between measurements. As can



(a) SOC [%]

(b) p_{buff} [bar]

FIGURE 7. Accuracy comparison with and without decimation. Raw data set (orange), decimated results (green). (a) *SOC* [%] (b) p_{buff} [bar].

be observed, the estimations improve remarkably when decimating is applied.

Another crucial consideration is the potential benefits of integrating external data sources, in this case environmental temperature. This input parameter is pivotal to ensure an accurate pressure estimation within the buffer and the tank, as dictated by the ideal gas law, see (3). However, the PLC that was used in the pilot plant (real system) did not have the capability to monitor this variable.

Fig. 8 shows the real buffer pressure values (green) measured within an interval of, approximately, one week. We then used a neural network, in this case CNN, which was trained exclusively with data from the PLC, without considering environmental temperature. As can be clearly seen, this approach completely fails to capture and precisely predict pressure fluctuations (red). The results show that at the beginning the prediction is correct, but when the temperature fluctuates the trained model is not able to follow the trend. On the other hand, when including temperature values from an external data source (in this case AEMET, Spanish Meteorology Agency) as an additional input variable, the CNN prediction significantly improves, yielding a very close approximation of the observed buffer pressure (orange).

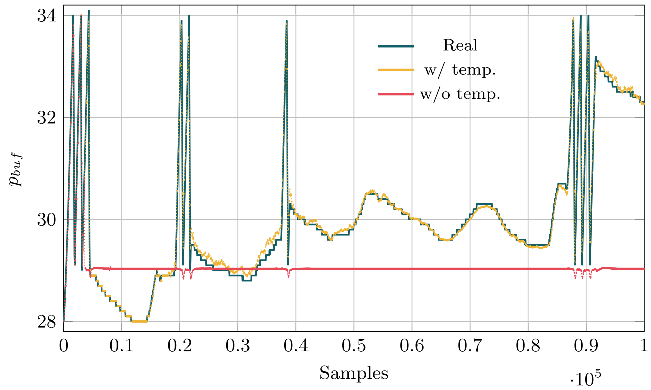


FIGURE 8. Comparison of buffer pressure [bar] with and without considering temperature. Real (green), estimated with temperature (orange) and estimated without temperature (red).

TABLE 3. Output Variables NRMSE of the DT

Output variables	Model	NRMSE 2-days	NRMSE 4-days	NRMSE 6-days
Inverter				
Charge battery power	DNN	0.022	0.023	0.022
Discharge battery power	DNN	0.011	0.010	0.010
Imported grid power	DNN	0.018	0.013	0.012
Exported grid power	DNN	0.015	0.014	0.014
Battery				
State of charge	CNN	0.017	0.022	0.022
Electrolyzer				
Electrolyzer power	DNN	0.071	0.056	0.066
Hydrogen flow generated	DNN	0.074	0.058	0.072
Hydrogen Storage				
Compressor power	RNN	0.105	0.082	0.087
Buffer pressure	CNN	0.093	0.119	0.117
Tank pressure	CNN	0.087	0.091	0.066

B. DIGITAL TWIN VALIDATION

The validation of the entire digital twin was conducted with the same dataset as the one used for the individual modules characterization. In this sense, we select for each module the neural network model that minimizes the NRMSE, as Table 3 illustrates, that is the one that better fits the behavior of its physical counterpart. In this case, the DT was initially aligned with the real system's battery state of charge and tank pressure measurements. On the other hand, only the PV panels power and the household demand measurements are used from the physical system; these, together with the environmental temperature from the Spanish Meteorology Agency, were used as external inputs. The remaining variables were estimated by the DT modules, with each module's output feeding the subsequent ones, as outlined in Table 1 and illustrated in Fig. 4, so that the evaluation consider the error propagation along the system.

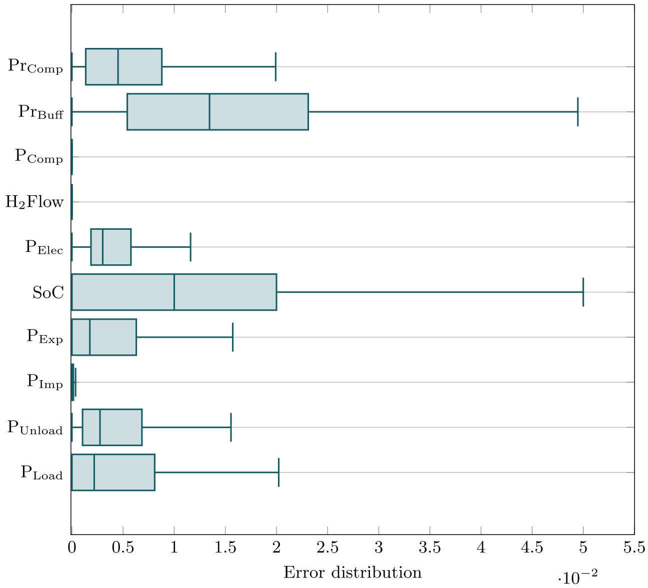


FIGURE 9. MME per output variable.

The DT results have been validated after running it for periods emulating 2 days (34,000 samples), 4 days (68,000 samples) and ≈ 6 days (100,000 samples). The NRMSE values obtained are presented in Table 3. As can be seen, errors in the estimation of a variable are propagated between the different modules, with an impact over the accuracy of dependent variables. An illustrative example is how the deviation in the hydrogen flow estimation directly impacts the estimation of the buffer pressure, increasing the error compared to those values obtained during individual modules validation.

On the other hand, there are no significant variations in the error induced by the DT along time, remaining within a narrow range and keeping a rather constant value.

Graphically, the error distributions for each variable are depicted in Fig. 9, using a box plot representation. Box limits correspond to the 25 and 75 percentiles, while whiskers represent the range where samples are not considered outliers ($1.5\times$ the inter quartile range). The line within the boxes corresponds to the median (percentile-50) of the error. In this case, for the estimation of the error of each sample we have used the maximum mean error, MME_i, see (4).

$$MME_i = \frac{|x_i - y_i|}{\max\left(|x_i|, |y_i|\right)} \tag{4}$$

As can be observed, the performance shown by the DT is very close to that exhibited by the real system, and the errors are rather low for all parameters, thus validating the performance of the whole DT.

VI. CONCLUSION

Smart building digital twins represent a significant paradigm shift to optimize building operations, thereby reducing their substantial energy consumption and emissions through digitization. The objective is to virtually replicate existing buildings' static and dynamic aspects, leveraging data, information, and models spanning the entire life cycle.

This work reports for the first time the digital twin of a photovoltaic-hydrogen powered dwelling. Digital twins represent a novel paradigm to optimize energy consumption and emissions through digitization. The objective is to virtually replicate the behavior of an existing pilot installed in a social dwelling. The DT can be later used for a number of smart functions, including real-time monitoring, autonomous control, and proactive decision-making to optimize energy operations.

Hence, this article discusses the architecture of a complete DT of a renewable hydrogen-based energy system, focusing on the implementation of its digital model, which follows a modular approach. The DT has been validated based on the real behavior of a real pilot plant, and sets a pioneering example of how such technologies can be applied in real-world scenarios to improve system efficiency, with the main goal to achieve electrical self-sufficiency.

The DT features functional modules that emulate the physical components of the real system. It uses, as external inputs, the household energy demand and the energy generated by the PV installation, both collected from the physical system, as well as the environmental temperature, obtained from the Spanish Meteorological Agency. The value of all the remaining system's variables are predicted by the DT.

Each module has been evaluated using both algorithmic and data-driven approaches. Results demonstrate that neural networks outperform algorithmic models, reducing prediction errors and capturing unexpected behaviors of the physical system.

The modular approach enables the selection of the most suitable AI/ML model for each module, aligning it with specific real-world behaviors and thereby enhancing the overall DT performance. Although errors accumulate from one module to another when assessing the behavior of the complete DT, they remain rather steady, within a narrow range, demonstrating the stability of the solution, and validating its performance. This allows the DT to operate regardless of the particular characteristics of the real system, requiring only energy generation and demand as inputs. In addition, this modular approach would allow the DT to adapt its operation to other systems, by simply changing the modules that are different. If a more monolithic approach had been followed this versatility would have not been possible.

Furthermore, it has been shown that appropriate preprocessing of input data for data-driven models, such as decimation to homogenize the nature of input and output variables, significantly improves the predictions made by neural network based models. Future research will explore the impact of applying different strategies, like moving average or interpolation techniques to tackle this data heterogeneity.

Validation results confirm the correct operation of the DT, presenting a promising tool for improving the efficiency of renewable hydrogen-based energy systems. Following the validation of the overall DT model, future efforts will focus on expanding its capabilities. This includes integrating external data sources, such as meteorological predictions or electricity rates, and developing control policies to optimize the real system performance. Furthermore, subsequent studies will focus on the DT behavior across diverse seasonal conditions, assessing its adaptability to particular contexts, as well as assessing the impact on the real system performance when different control policies are applied to the PLC.

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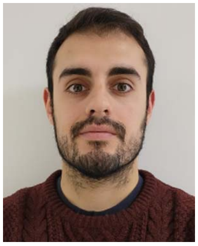

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