TWINP2G: A DIGITAL TWIN ARCHITECTURE FOR OPTIMAL POWER-TO-GAS PLANNING

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ABSTRACT

Power-to-Gas (P2G) is an emerging technology aiming to contribute towards addressing the climate change and environmental degradation. Yet, numerous factors need to be taken into consideration to for practical P2G applications. Digital Twins (DT) are used for simulation and optimization purposes, allowing investigation and prediction of their short-, medium- and long-term results. This paper presents a DT architecture, namely TwinP2G, that aims to couple the electrical power and natural gas sector by enabling multi-resolution simulations and optimization relating to the integration of P2G plants and regenerative hydrogen fuel cells (RHFC) in the power grid. The suggested solution is meant to be applied initially in the Greek energy system enabling data- and simulation-driven P2G and fuel cells optimal planning and techno-economic analyses. This piece of work concludes with future application plans and application development perspectives.

KEYWORDS

P2G, Digital Twin, Hydrogen, Sector Coupling, Natural Gas, Simulation, Optimization

1. INTRODUCTION

Climate change along with the growing population, the increase in electrical energy consumption and the depletion of resources have led to a large-scale deployment of Renewable Energy Sources (RES), increasing their energy share worldwide (Lewandowska-Bernat & Desideri, 2018). Numerous RES technologies have significantly progressed in technical and economic maturity over the past few decades. Yet, their fluctuating and intermittent nature raised concerns related to the balancing and capacity adequacy of an energy supply configuration relying mostly on RES (Varone & Ferrari, 2015). The necessity of increasing the flexibility of the existing bulk system has led researchers to investigate new methodologies to fully exploit the production of RES in the context of water pumping stations (Sarmas, Spiliotis, et al., 2022), supply to the energy system (Karakolis et al., 2022; Mazza et al., 2018) and so on.

Towards that end, the P2G technology has arisen unveiling various possibilities. P2G uses renewable or excess electricity to produce hydrogen via water electrolysis (Robles et al., 2018). This hydrogen can be used directly as a final energy carrier for electricity, mobility (fuel cells powering electric vehicles) and heat, converted to methane, liquid fuels, or chemicals (Gahleitner, 2013) or even stored in fuel cells to be later reconverted into electricity. Thus, they would satisfy the need for long-term energy storage by converting it to other easily storable energy carriers, and at the same time reduce the load of the electricity grid by their controlled operation.

Hydrogen offers a great variety of alternatives in its production, transportation, and distribution. Its multi-dimensional benefits triggered the development of multi-energy systems' modelling approaches to assess the technical, economic, and system-level challenges of integrating hydrogen into the overall energy system (Fu et al., 2020). Terms such as HIGG (Hydrogen Injection into the Gas Grid) soon arose along with a variety of research, modelling and real-life demonstrator projects exploring the possibilities of Green Hydrogen (hydrogen produced by renewable excess) in conjunction with other energy systems (ENTSO-G & ENTSO-E, 2018; Gondal, 2019; Quarton & Samsatli, 2018).

Over the past decades, several P2G plants have been developed (Quarton & Samsatli, 2018), numerous hydrogen demonstration projects have been funded (Diaz-Londono et al., 2020; *Everywh2ere*, 2022; *H2Haul*, 2022), and several studies and research efforts have been documented, exploring green hydrogen's potential and variations. P2G optimization and simulation techniques and models have been used in many scenarios over Europe. This paper aims to present the methodological approach towards developing a P2G digital twin (DT) in Greece with short-, medium- and long-term optimization goals and perspectives.

This paper presents a conceptual DT architecture, namely called TwinP2G, aiming to promote hydrogen and accelerate the energy transition via P2G technologies. Section 2 presents a literature review aiming to shed light on the current state-of-the-art P2G approaches and methodologies, DTs, and relevant software. In Section 3, the case study details, and application architecture are presented. Finally, Section 4 concludes with a discussion relating to the challenges of P2G and future steps related to the research objectives of this.

2. LITERATURE REVIEW

During the last few years many studies have focused on developing several optimization models for P2G applications (Quarton & Samsatli, 2018). Most of them develop complex optimization models, while others focus on simulation. With respect to optimization, the most widely used methods are Linear Programming (LP) (Dodds & Demoullin, 2013), Mixed Integer Linear Programming (MILP) (Almansoori & Shah, 2012) and Non-Linear Programming (NLP) (Clegg & Mancarella, 2016). Simulation, on the other hand, is the process of modeling a scenario and finding the outputs of a system based on a given set of inputs. Such models may run several different scenarios, as in the case of (Abeysekera et al., 2016) which provided a simulation method for gas networks with injection of upgraded biogas and hydrogen. Usually, simulation models are tightly linked with DTs. The selection of the objectives for P2G optimization problems is another interesting aspect. Although most of the developed models target towards minimizing the total operation costs, there are a few focusing on minimizing CO2 emissions (Mesfun et al., 2017) or even fuel consumption (Tabkhi et al., 2008). Moreover, the decisions supported by most of these models focus on long-term policy, proposing the degree of penetration of each technology per year or decade. A thorough techno-economic analysis of P2G scenarios is conducted in (Fambri et al., 2022). It seems that the existing state of the literature shows the urgent need for designing modern, data- or simulation- driven applications and models for assisting the successful penetration of P2G technologies. In this direction, the PLANET project (Schröder et al., 2018) aimed to leverage energy conversion technologies for optimal grid planning towards full energy system decarbonization. Specifically, Diaz-Londono et. al develop a real-time platform for P2G integration in electrical distribution grids, enabling a quasi-automatic creation of case studies and using digital simulation technologies and proprietary software, such as eMEGASIM, RT-LAB, and Matlab / Simulink (Diaz-Londono et al., 2020). Although most studies have focused on the process of converting surplus renewable energy into hydrogen gas, the case of fuel cells should be considered as well. Fuel cells operate like a conventional storage system, differing in that they do not need recharging (Smith, 2000). Fuel cells can produce electricity if enough fuel is supplied, thus being one of the most promising storage solutions for the near future. The optimization models used in the case of fuel cells do not significantly differ from the aforementioned ones. Typical examples of exploited optimization models are multi-objective genetic algorithms (Ehyaei & Rosen, 2019) and multi-objective probabilistic analysis algorithms (Zhou et al., 2022), among others.

With respect to DTs, they comprise digital representations of physical objects (processes, or services) which facilitate the planning, management, and optimization of complex and new activities (Batty, 2018). DTs are recently gaining significant popularity in the energy sector for purposes such as smart grid development, RES management, and distributed generation control (Borowski, 2021). It should be noted that a DT does not make any decisions by itself, but rather generates insights through post-processing that support decision making. As more and more data are becoming available through advancements in IoT devices and smart sensors, the combination of a physical object and its digital mapping in virtual space can be combined with big volumes of data to facilitate informed decision-making in the energy domain. A series of recent studies on DTs for energy-related topics is presented by (Onile et al., 2021). Some of the most recent studies include the development of a DT for hybrid renewable energy systems (Andryushkevich et al., 2019), a regression-based DT for university campus' power supply (Francisco et al., 2020) and DT-based energy management systems (Brosinsky et al., 2018), (Zhou, Yan and Feng, 2019). Gerrard et al. (Gerard et al., 2022) focused on a data-driven DT, for mitigating the uncertainties and risks associated with green hydrogen facilities design as an investment, which also calculates financial indicators (e.g., internal rate of return) through stochastic simulations using the Monte Carlo method.

From a technical perspective, in the domain of P2G oriented optimal grid planning (simulation and optimization), several open-source tools are currently available and used within a multitude of related research studies. A rather extensive review of those tools can be found in the PyPSA whitepaper (Brown et al., 2017). Indicatively, open-source grid simulation tools include PyPSA, Pandapower (Thurner et al., 2018), MATPOWER (Zimmerman et al., 2011) and DPSIM (Mirz et al., 2019), while Pandapipes (Lohmeier et al., 2020) can serve in creating coupled power and natural gas systems (Lu et al., 2021; Qadrdan, 2012). Several of them, such as PyPSA also include cost-based optimization capabilities usually leveraging optimization techniques and specifically tools such as Pyomo (Bynum et al., 2021). Some well-known solvers for linear programming are GLPK, CPLEX, and Gurobi (Meindl & Templ, 2014) and they can be used in these scenarios. Regarding macroscopical and long-term modelling and optimization, a variety of energy system modelling tools that are usually disconnected from optimal power flow analysis and are most linked with national energy planning strategies, are available. Linear programming remains the dominant optimization method within this scope of these applications, such as OseMosys (Howells et al., 2011) (written in GNU MathProg), Nemo (SEI, 2020) (written in Julia), and EnergyPLAN EU (Lund et al., 2021) (written in Delphi Pascal).

3. CASE STUDY AND APPLICATION ARCHITECTURE

The proposed case study takes place in Greece in the context of the ENERSHARE (*Enershare | The Energy Data Space for Europe*, 2022) project funded by the EC and involves both the natural gas and electrical power national transmission and distribution networks managed by DESFA (Desfa, 2022 and IPTO (IPTO, 2022) respectively. The objective of the case study is to form a digital simulation and optimization platform, named TwinP2G, coupling the electricity transmission system with natural gas demands, leveraging a DT architecture that will enable multi-resolution simulations involving P2G technologies and regenerative hydrogen fuel cells (RHFC) (Pellow et al., 2015). TwinP2G will enable data- and simulation-driven P2G and RHFC optimal planning for using the RES surplus for green hydrogen production via electrolysis.

3.1 High-Level Architecture

The TwinP2G architecture is shown in Figure 1. A Platform-as-a-Service (PaaS) design is proposed. The architecture serves multiple user roles while it is composed of various subcomponents using a many state-of-the-art technologies that is further analyzed in the following sections.

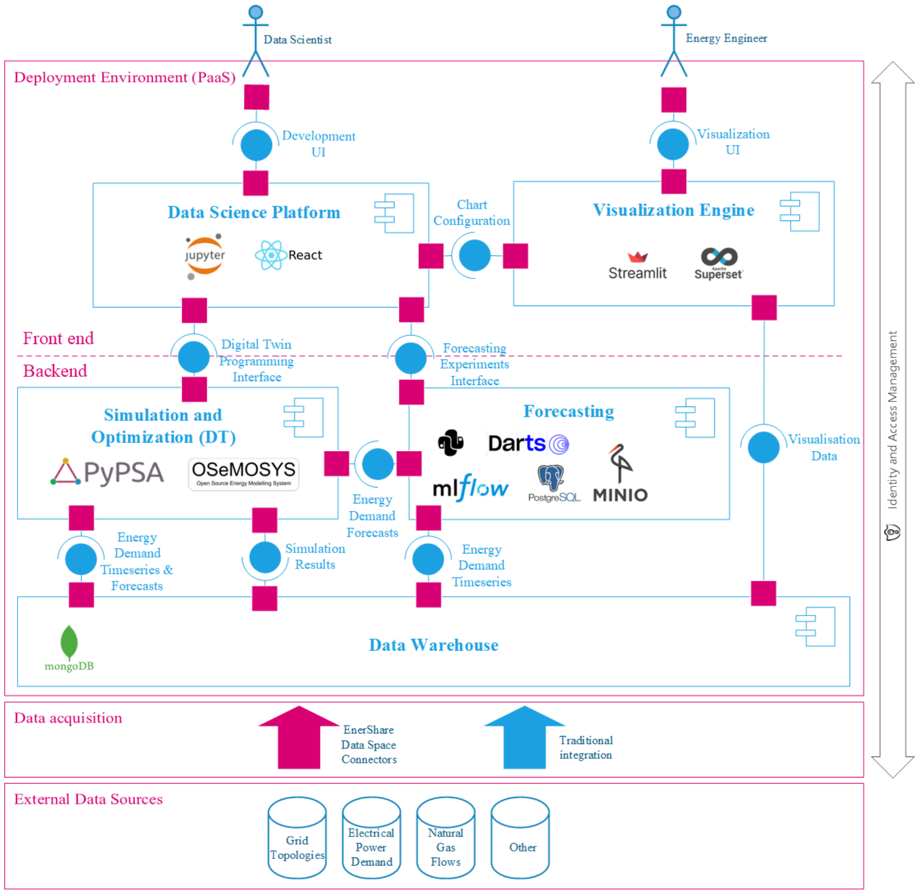

Figure 1. The high-level architecture of TwinP2G

3.1.1 Data Sources and Integration Process

For developing a DT application, data integration is a core process. It enriches the local data warehouse with new datasets that in turn improve the results of its main functionalities, therefore leading to up-to-date forecasts and simulation scenarios. TwinP2G mainly employs integration mechanisms based on Data Connectors (*IDSA Data Connector Report*, 2022; Qarawlus et al., 2021), as established by International Data Spaces (IDSA) (Otto et al., 2019) that will be further developed within the ENERSHARE project. In the conceptual architecture of Figure 1, TwinP2G receives data from IPTO (electrical power demand, RES generation, long-term grid planning, electrical grid topologies), DESFA (hourly / daily gas flows at entry and exit points, natural gas grid topologies) and other organizations (e.g. Eurostat, local and national grid topologies etc.) through Dataspace Connectors. Specifically, it acts as a data consumer, while the other organizations act as data providers. All the organizations involved need have a dataspace connector deployed in their infrastructure. Of course, traditional data ingestion methods are followed whenever the development of bidirectional Data Connectors is not feasible.

3.1.2 Multi-Horizon Simulation and Optimization

The Simulation core of the DT application involves physics- and data- driven simulation and optimization capabilities, allowing for extensive techno-economic analyses. In this context, the PyPSA open-source power system modelling tool is used as the short-term / mid-term simulation and optimization core of the DT. PyPSA can serve optimal power flow simulation based on network equations, security constraints and even least-cost (investment) optimization. Amongst the available models P2G and storage units with efficiency losses (suitable for RHFC) are of specific interest for the use case in question. Regarding multi-horizon dynamic investment optimization over several years (long-term projection), as PyPSA seems to have fallen behind, the OSeMOSYS open-source modelling system is selected, as it enables long-run integrated assessment and energy planning, also suitable for crisis modelling (Karamaneas A. et al., 2022). From a mathematical perspective, OSeMOSYS is a deterministic, long-term modeling framework based on linear optimization (linear programming and mixed-integer linear programming). The “Simulation and Optimization” component processes historical time series of renewable generation and production alongside power and gas demands originating from the data warehouse. It also uses forecasts produced by the “Forecasting” component creating projections within an optimization horizon. Local grid topologies in Greece with envisaged investments for P2G components is the main field of study within the “Simulator and Optimization" component. Pandapipes will also be considered if gas pipeline simulation is deemed necessary through the progress of the use case. With respect to optimization objectives, the following will be investigated in terms of optimal capacity and location: electrolysers (ENTSO-E, 2022), fuel cells, methanation reactors and hydrogen buffers (storage).

3.1.3 Forecasting

The forecasting component of TwinP2G is an MLOps (Sridhar et al., 2021) framework that has been developed within the I-NERGY H2020 project (Karakolis et al., 2022). The toolkit is based on a machine learning pipeline written in Python programming language that enables experimentation and evaluation of various machine learning and deep learning algorithms, such as XGBoost, Random Forest, NBEATS, Temporal Convolutional Networks (TCN) and Long Short-Term Memory (LSTM) networks as demonstrated in a recent work that dealt with a short-term load forecasting use case (Pelekis et al., 2022). The main technologies leveraged are MLflow (Alla & Adari, 2021) as the MLops platform, Darts (Herzen et al., 2021) as the time series forecasting framework, MinIO (MinIO, 2022) and PostgreSQL (PostgreSQL, 2022) as artifact storage and logging database respectively, FastAPI (*FastAPI*, 2022) as the API development framework, Javascript React (*React*, 2022) for developing the front-end. The forecasting platform in question can handle all type of time series and integrate new datasets with little to no extra development, hence allowing to easily handle the timeseries data ingested in TwinP2G (see Section 3.2.1) and providing forecasts of various (short-, mid-, long-term) horizons. Moreover, supplementing the existing forecasting models, novel practices in the field of machine learning can be used, including incremental analytics for periodically re-training existing models (Sarmas, Strompolas, et al., 2022), as well as transfer learning to handle cases with insufficient data (Sarmas, Dimitropoulos, et al., 2022).

3.1.4 Application Front-end and Security Framework

TwinP2G serves two main user roles/personas. The first persona is the “Data Scientist”, who is assumed to be an experienced user with scientific and coding background alongside modelling capabilities of P2G use cases. This user can enter the “Data Science Platform” provided by TwinP2G to interface with the “Simulation and Optimization” component to develop P2G experiments and visualize their results (simulation and optimization results, forecasting accuracies, etc.). Additionally, the “Data Scientist” can configure the desired types of interactive analytics visualizations to be displayed to the Energy Engineer persona. Specifically, Streamlit (*Streamlit*, 2022) is a candidate high-level technology for serving this purpose. However, more advanced technologies, such as Apache Superset (*Superset*, 2022) and MATRYCS (Pau et al., 2022) Visualization Engine (Kormpakis et al., 2022) are also under investigation. The second persona is the “Energy Engineer” who is considered an end-user with knowledge and understanding of energy systems but limited coding and modelling skills. This persona uses the “Visualization Engine” component to monitor simulation and forecast results and metrics leveraging them for decision support regarding future P2G investments.

Ultimately, an identity/access management mechanism is the basis of TwinP2G’s security. This has end-to-end processes, approaches, and technologies for user identification, authentication, and authorization. They ensure that the personas are allowed to access the appropriate resources. For this, the Keycloak (*Keycloak*, 2022) technology has been considered.

4. DISCUSSION

This work proposes a conceptual, innovative DT architecture, named TwinP2G to promote hydrogen and to accelerate the energy transition through P2G technologies. TwinP2G allows modelling multiple scenarios for green hydrogen production and storage as a flexibility provider and as an enabler for higher RES integration (directly through hydrogen fuel cells indirectly through the gas pipeline). The architecture has four main components, namely: i) a data warehouse that integrates open data mainly through IDSA technologies; ii) a simulation platform with state-of-the-art power and energy simulation and optimization technologies; iii) an MLOps-powered forecasting toolkit, for profiling, analyses and forecasts of electricity and gas quantities; iv) a front-end application that serves two user roles; a) a data scientist that can perform simulations and experiments by coding and b) an energy expert with limited coding skills that can inspect and visualize the high-level experiment results.

In conclusion, TwinP2G envisages addressing and overcoming some significant challenges posed in (ENTSO-G & ENTSO-E, 2018). Specifically, TwinP2G is expected to accelerate the learning curve effect within the P2G sector, allowing for experimentation with higher installed capacities at lower production rates of synthetic gas, hence contributing to the vision of much higher installed capacity by 2030. Finally, given that the current framework of regulations, market incentives and tariffs in Greece have not taken into account at all the opportunity of P2G, seasonal storage and other technologies. TwinP2G is expected to also promote the relevant national energy policies by establishing an innovative simulation platform that enables the experimentation with use cases that had been unfeasible until now.

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