Techno-economic optimization and system integration of power-to-gas at different geographical scale in Europe

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ABSTRACT

Decarbonization targets and global political instabilities push the European Commission to elaborate strategies to ensure more affordable and secure energy. Within these strategies, e.g., RePowerEU, Power to Gas (P2G) is foreseen to become a key play for the successful transition towards a sustainable energy system. A rigorous methodology to investigate P2G plants' potential and optimize the techno-economic performances is therefore essential for an effective scale up and implementation of P2G plants. Therefore, this study aims to show how energy modelling tools can be used to support decision-makers to identify potential locations of P2G plants and furthermore estimate the techno-economic performance of the plants. In this study, three energy modelling tools were developed and adapted to investigate the P2G design and planning at different levels of detail in the Apulia region (Italy), considering the integration with the energy system in order to ensure a complete assessment.

KEYWORDS

Power to Gas, Sector coupling, Power to X, Hydrogen, Multi-Energy System Planning, Planning tool.

1. INTRODUCTION

Following the recent crisis due to Ukraine crisis, EU-27 leaders agreed to the need of speed up the still existing decarbonisation process aiming to achieve European energetic independence. For this purpose, the production and imports of larger volumes of green fuels, including hydrogen, are proposed in the RePowerEU plan to cut the dependence on Russian gas and oil [1]. In addition to strategic considerations, climate change requires the reduction of fossil fuels consumption by the transition to cleaner renewable fuels from many years [2]. A full review of alternative fuels such as those derived by Power to X (P2X) and their utilisation possibilities was proposed by [3]. Despite this consensus, P2X is still facing several challenges that hinder

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its implementation. For example, technical, economic, social and normative barriers still hinder the hydrogen economy penetration [4]. Among the barriers are the challenges related to the economic feasibility P2G plants which is, among others, depending on the size and location. System energy planning is a dated problem. The most recent review about energy systems optimization tools in case of a large penetration of renewable sources was published by [5]. Seventy-five modelling tools were identified based on the criterion to be used in at least one publication after 2012. A categorization approach was used dividing tools in accordance with key parameters defined on a four levels map structured as follow: 1) main information (developer, availability and software implemented), 2) general logic (approach, methodology and purpose), 3) spatiotemporal resolution and 4) technological and economic parameters included. Based on the results of the review, many of these account for the possibility to include hydrogen as a potential source of energy storage.

Among the existing energy modelling tools, the H₂RES model supports the integration of renewable sources and hydrogen into island or any isolated region that can be modelled as stand-alone system [6]. Based on an hourly temporal resolution, the model evaluates possible scenarios ensuring energy balancing. Balmorel, an open source bottom-up partial equilibrium energy system optimisation model, satisfies energy demand including renewable fuels ensuring the optimization of social welfare while minimizing energy generation, storage and distribution costs taking into account of technical, physical and regulatory constraints [7]. Since different time and spatial combinations can be investigated by the user, the model ensures a high level of flexibility. The open source Calliope model is an energy systems modelling framework that enables arbitrarily high spatial and temporal resolution allowing to scale analyses from single urban districts to countries and continents [8]. The Planet model supports policy makers and network operators in exploring, identifying and evaluating optimal grid planning and management strategies for future energy systems. Among P2X technologies, PEM electrolysers, hydrogen buffers and methanation units are comprised. In addition, based on Simulink environment, real-time simulations are possible [9]. Recently, Jie and Peng proposed a combined optimization planning method for an electricity-natural gas coupling system with P2G that aims to minimize the sum of initial investment and operative costs based on an hourly time step on a small-scale regional supply system [10].

The need of different tools derives from the fact that P2X implementations have to be optimized as a function of various factors that depends on the needs of stakeholders and end-users who require tools to realize these optimizations for benefitting from the techno-economic potentials of developing and operating multi-vector energy systems. However, no comprehensive and end-user-friendly tool is available at present allowing end-users to adapt and optimize the installation of these solutions to their specific needs, considering the following variables: location, size, technology, electric and gas transmission infrastructure, energy integration, energy production characteristics and other consumer specific demands.

For this purpose, we apply three tools in this study, to investigate and optimize decisions of P2X and P2G solution applied for different purposes, using a case study of a region of the South of Italy, Apulia. This paper summarizes preliminary results of this investigation and is structured as follows. The second section details the methodology of the three energy modelling tools used in this study by highlighting key parameters and describing the main functionalities as well as how the tools complement each out for a comprehensive analysis of the location and techno-economic performance of P2G plants. In the third section, we present results at different geographical scale and with different level of details. Finally, we summarize the conclusions and provide an outlook for future developments.

2. METHODOLOGY: ENERGY MODELLING TOOLS

2.1 Overview

There is a strong need for tools that can support P2G solutions to enable commercial implementation by contributing to the technical optimisation and system integration, the market access and uptake, as well as for development of solutions for adoption. Therefore, we aim to apply three tools, i.e. SpineOpt, SuperP2G-Italy and DBI-MAT, in order to analyze the implementation and integration of P2G systems in the future.

Spine [11] is a network optimization model that can represent any process and flows based on node-arc relationships, e.g., energy, economic and environmental. The model is built upon a bottom-up approach with the objective to minimize system costs, subject to system constraints. Therefore, for a given system consisting of processes (nodes) and flows (arcs), SpineOpt will identify the optimal, least-cost pathway among the hypothetical pathways in the network. While sources and sinks are provided with exogenous data, these can also be used to link SpineOpt to other energy system models, such as Balmorel. Overall, in this study, SpineOpt is used to optimize the techno-economic performance of the investigated network for green fuel production, including P2G, P2X and biomass-based fuels subjected to specific system constraints.

SuperP2G-Italy is a WEB-GIS tool that optimizes P2G plants' location and size minimizing total costs developed in the SuperP2G project. The conceptual approach of the tool is shown in Figure 1. Georeferenced data are uploaded in a structured database where they are collected for the future elaboration by an optimization engine. Based on the transhipment problem, the cost-optimization algorithm is executed, calculating the best P2G solution for the specific case study. Finally, the georeferenced results are shown in a web-based form.



Figure 1. SuperP2G – Italy tool's approach.

The DBI-MAT (Microgrid Analysis Tool) is a techno-economic simulation framework for the analysis, scenario exploration and system optimization of local energy systems, i.e.: the so-called "microgrids", with a focus on flexibility and scalability. For this purpose, the tool analyses and optimizes local energy systems by modelling energy and process streams between its components, i.e., elements of the microgrid that either provide, transform, store, or use energy or mass streams. Generally, the computation is based on the existence of balance groups that contain several components and in which mass and energy conservation balances apply. In Figure 2 three balance groups (power, hydrogen, and heat) are shown. The tool allows for

technical, economic and environmental analysis, i.e.: balancing of supply and demand, cost optimization and carbon footprint estimate.



Figure 2. Graphical example of a system solved by DBI-MAT tool.

2.2 Code structure

The energy modelling tools are developed on different code structures and mathematical formulation. The Spine tool [11] uses three different languages, i.e., Python, Julia and GAMS. The data analysis and processing is performed in the SpineToolbox, a Python-based Interface. The software makes it possible to interactively customize the data structure and model, allowing the user to easily create new units, nodes, connections, add relationships between them and manipulate parameters. The optimization model is provided in Julia language utilizing a predefined mathematical optimization code provided by its developers and that is based on a minimization model total system cost.

SuperP2G-Italy tool is developed on using two separated components, whose interface was developed through Python modules, i.e.: *Pandas* and *Geopandas* (Figure 3-right). The former manages the existing data through different frameworks, i.e. *QGIS* for the management of georeferenced data, *PostgreSQL* (integrated with the georeferencing add-on *PostGIS*) for the creation of a properly structured relational database, *GeoServer* for the implementation of maps and shape-files and *OpenLayers* for the visualization of the results (Figure 3-left).



Figure 3. The software used to develop the SuperP2G – Italy tool: representation of the data flows. In the left the raw data from different sources / to map visualization. In the right, the packages used for data pre-processing and transhipment problem resolution

The latter is entirely developed in Python using open-source packages (*scikit-learn* for plants clustering, *numpy* and *scipy* for fundamental calculation, *NetworkX* for routing path finding, and *pyomo* for logistic problem resolution) to approach the P2G plants positioning as a transhipment problem (i.e., energy and hydrogen flows distribution from power generators to hydrogen users through an optimized set of conversion plants), Figure 3-right. Because of the large amount of data (about 47000 generation plants), the generation plants were regionally subdivided by the K-means clustering methodology [12], as a set of clusters centroids on a Puglia meshed map. Once data pre-processing is completed, the optimum solution is calculated as the one that ensures the minimum cost. Once data elaboration is completed, the optimum solution is calculated as the one that ensures the minimum cost.

DBI-MAT is written in Python and built in an object oriented and modular structure. By using an object-oriented approach, technology specific calculations are implemented in the components that represent technical processes. The tool is modular in the sense that the user can easily add or remove components from a system, prioritize flows, and create links between them.

2.3 Data inputs and outputs

The tools used in this study involve different inputs and outputs, whose characteristics depend on the specific problem to be solved. A simplified schematization of the required inputs by the tools and of the resulting output are shown in Figure 4 and Figure 5. As can be seen, overlaps exist. However, the different temporal and spatial resolutions give the possibility to cover different needs with the tools. For example, the spatial dimension in SpineOpt is flexible and can be adopted to any location worldwide, however, in this study, the geographical representation is defined to represent the six provinces in Apulia. In SuperP2G-Italy tool, since data is georeferenced, the inputs and outputs are, wherever applicable, managed in a structured database with their coordinates, i.e., latitude and longitude. DBI-MAT, instead, does not include spatial resolution since it is expected that the transport of mass or energy within the microgrids is lossless.

Concerning the temporal resolution, SpineOpt is flexible, however, in this study, hourly time profiles are aggregated to allow computation of the comprehensive network of energy technologies and production pathways. The temporal resolution of the SuperP2G-Italy tool is limited to the year since, to date, the tool aims to balance the annual P2G plants production and the renewable plants electricity generation. DBI-MAT, instead, works with temporal resolutions that are defined by the load profiles that are set as an input of the system. Based on successful past projects, temporal resolutions can be reduced to fifteen minutes even if smaller time intervals down to one minute can be aspired. For these smaller time intervals, however, it should be stated that inertia, start-up and shutdown conditions of the components that are operated in the system are currently not fully implemented but may be essential for an accurate technical representation.



Figure 4. Schematic representation of the data required by the three tools. Colour code: Spine: red; SuperP2G-Italy: blue; DBI-MAT: green



Figure 5. Schematic representation of the results computed by the three tools. Colour code: Spine: red; SuperP2G-Italy: blue; DBI-MAT: green

2.4 The Apulia case study

In this study, the modelling framework that includes the three energy modelling tools were applied to a case study focusing on a region, Apulia, which is located in the South of Italy and has a high potential for P2G. In fact, almost 51,000 photovoltaic plants and 1,000 wind turbines were in service in Apulia in 2021 for a total nominal capacity respectively of 2.55 GW and 2.45

GW and an energy generation of 3.5 TWh/year and 4.5 TWh/year. In addition, up to 75,000 ton/year of agricultural residues are available in the region.

The three energy modelling tools are developed for different purposes, however, to show the benefits of their application, the modelling approach in this study is depicted in Figure 6.



Figure 6. The proposed approach for the application of the three SuperP2G tools in Apulia case study.

As shown, the SpineOpt tool is applied together with Balmorel to perform a high-level investigation of Power to X potential at province level, i.e. the boundary of the system. A sketch of the network adopted for the analysis is reported in Figure 7. Specifically, the target of the analysis performed by SpineOpt is to evaluate, for each province of Apulia, the utilization of resources and the P2X conversion technologies to be installed and operated in order to produce those fuels that ensure the best techno-economic performance of the investigated system.



Figure 7. SpineOpt network applied for the analysis.

SuperP2G-ITALY is applied to identify the optimum size and location for the installation of P2G plants at local level for sector coupling applications. For this purpose, georeferenced data about renewable plants, delivery infrastructures and local hydrogen demand were adopted in the tool. Figure 8 shows the simplified approach applied in the tool. In the figure, renewable plants are indicated as "P", P2G conversion plants as "W" and demand as "R". Specifically, based on the existing amount of hydrogen demand and the renewable electricity generation, the SuperP2G-Italy evaluates where P2G plants must be positioned but also estimates how the electricity and the hydrogen flows have to be distributed between generation, conversion and utilization plants in order to maximize the economic benefits.



Figure 8. The SuperP2G-Italy approach. Transshipment problem approach in the Italian SP2G tool. In the left a schematic representation is shown; In the right, instead, the complete graph connection from clusters centroids (generation plants aggregations) to users through all the potential mesh centroids.

Lastly, DBI-MAT tool is applied to a specific case study in the city of Taranto where an onsite P2G plant is assumed to be connected to a local end-user. Specifically, the installation in the existing steelmaking plant as possible green revamping solution is simulated. Because of the large amounts of waste heat available in a Basic Oxygen Furnace (BOF) steelmaking process, i.e. 0.034 MWh/ton of steel [13], two different P2G configurations are preliminary explored (Figure 9):

- Case A: the steam that is recovered by the steel making processes is supplied to the hightemperature electrolysis section aiming to maximum conversion efficiency. In the algorithm, a theoretical approach based on Gibbs energy (theoretical load-independent efficiency) and on the steam temperature and pressure was applied.
- Case B: mature technologies, i.e., alkaline and PEM electrolysers, are installed in the industrial site to produce the same amount of hydrogen calculated in case A. So the recovered steam is used to produce electrical energy in a local steam turbine. A load independent fixed efficiency was assumed.

Five scenarios characterized by a different nominal capacity of the electrolyser were investigated: 2.68 MW, 5.36 MW, 13.4 MW, 26.8 MW and 40.2 MW.

Regarding to the renewable plants that supply the electrolysis section, a wind park and photovoltaic plants close to the steelmaking industry were assumed. Concerning the wind park, a nominal capacity of 30 MW was assumed in accordance with the one that is going to be installed in an already approved project [14,15]. Relating to the photovoltaic plants, a research

in the public accessible database [16] was performed collecting only those plants installed in the area of Taranto and with a nominal capacity greater than 100 kW. A total nominal capacity of 37.4 MW was considered for the specific case. To simulate their performance, the pvlib python tool was applied [17].

Because of no technical data about the processes in the steelmaking are available to the Authors, the target of the application of the tool is only to investigate if and in which conditions the adoption of high temperature electrolysers over traditional ones is justified in industrial context characterized by large amount of waste heat. For the analysis, the performances of traditional electrolysers are in accordance with FCHJU key performance indicators [18], the high temperature electrolyser with the data declared by [19]. Instead, since insufficient information are available about the energy recovering system, a sensitivity analysis was performed to take into account of the uncertainty of steam to electricity conversion efficiency. For this purpose, efficiency in the range between 35% to 45% were considered.



Figure 9. The two simplified configuration investigated.

3. RESULTS AND DISCUSSION

3.1 SpineOpt application to Apulia: preliminary results

Several options for P2X configurations exist and can be applied in the Apulia region. In this study, we investigate four renewable fuel production pathways: straw-based methanol (ST_MeOH), wood-based methanol (WO_MeOH), ammonia (NH3) and hydrogen (H2). Figure *10* shows the optimized fuel strategy for Apulia based on available resource and potential end uses. As shown, Apulia could be an important hub for the production of methanol, ammonia and hydrogen. Based on the simulation, about 333 000 ton/year of ammonia could be produced in the hub, which resembles 30% of the current national production, based on the nominal capacity of the Yara Italia site in Ferrara. Regarding hydrogen production, up to 116 000 ton/year of hydrogen can be produced in the region, satisfying up to 20% of the national demand. It should be noted that effects of transport and delivery to end-users of renewable fuels are not within the scope of this paper. A high amount of excess heat is generated from the production processes and could potentially be used to supply district heating. However, since district heating is not present in the South of Italy, the excess heat could be used for low-temperature heating purposes in industrial clusters to reduce the consumption of fuels, e.g.: natural gas and consequently reducing the carbon dioxide emissions.



Unit: GWh/year

Figure 10. Sankey diagram of the Apulia case study – future perspectives for 2050.

The SpineOpt tool was also applied to identify the geographical localization of green fuel production and the results are shown in Figure 11. While the hydrogen was produced to satisfy end-use demands in each province, the production of green fuels is based on a market selling price. In this way, the least-cost production pathways in each province, which are subject to specific system conditions, e.g.: resource potentials, are computed and the model identify the production of green fuel within a province. The results illustrate that hydrogen is produced in the different provinces to satisfy projected hydrogen demands. Furthermore, the results show potentials for producing green liquid fuels for the hard-to-abate transport sector, by using local biomass resources i.e.: straw and the aggregation of woody-biomass. Based on these results, all regions are producing green fuels and hydrogen, and therefore all regions can be used for a more detailed analysis using, the DBI-MAT tool, which is chosen to be applied for the case of hydrogen production for steel making in Taranto.



Figure 11. Renewable fuel potential distribution in the Apulia region.

3.2 SuperP2G-Italy application to Apulia: preliminary results

SuperP2G-Italy tool was completely developed in the project. Therefore, Puglia case study represents the first development and test phase of the tool. For this reason, the results derived from SpineOpt geographical optimization were not considered but will be used for a later validation in the upcoming advanced phase. In addition, for the first runs, only the production (i.e., electricity conversion) of hydrogen was considered. Furthermore, because of the aim of this specific activity was limited to run the tool, hydrogen demand in the region was supposed by the Authors, above all due to the necessity of limiting the aggregated demand to the mathematical feasibility of the problem solution.

To compare results coming from a commercial and the in-house developed algorithm, the mathematical problem formulation of the SuperP2G-Italy tool was implemented in MATLAB and Python, assuming the same boundary conditions. P2G locations and overall cost function result more or less independently from the selected environment (about 5% discrepancy).

To show the complexity of the calculation, the complete graph layout (including all the possible connections/combinations in the meshed territory) is reported in Figure 12.



Figure 12. Main entities of the Italian tool: in the left generation clusters, in the middle, the selection of open facilities (P2G plants) and their capacities, while in the left, the users demand summary.

Once the cost functions were calculated for all the branches, the optimization started. In Figure 13, the renewable generation clusters centroids calculated by K-means method (blue dots), the selected P2G (black dots) and the hydrogen demand locations (red dots) are shown. As reported, the application of K-means clustering algorithm to all the existing renewable plants in Apulia results in 14 generation clusters that are located more or less uniformly in the region. This number was determined by separating 5 very big plants in "one-element" clusters and then having the remaining plants distributed (in 9 clusters ranging from 3000 to 6000 kW) by weighting the plants nominal power by the distance from the cluster centroid.

Based on the preliminary evaluation of regional hydrogen demand, the SuperP2G-Italy was also able to precisely localize the optimal/needed P2G plants without occurring any specific bug.



Figure 13. Optimum P2G plants location as calculated by SuperP2G-Italy tool.

3.3 DBI-MAT application to Apulia: preliminary results

The Taranto steelmaking plant produces approximately 4 million ton of steel annually that, assuming a constant production during the year, corresponds to an hourly production of 450 ton/h. Based on the required hydrogen consumption (81.2 kg per ton of steel [20]), 36,500 kg/h of hydrogen (approximately 1.2 GWh/h based on the Low Heating Value) would be required to revamp the process towards a complete green transition. The wind park and the PV plants generates up to 60.6 GWh/year and 55.5 GWh/year, i.e.: a total of 116.1 GWh/year. Simulation results are shown in the following figures. Annual total electricity consumption and hourly hydrogen production are shown in Figure 14 in five different cases. Each case is characterized by an increasing nominal capacity of the installed electrolysers as reported in Table 1. As can be seen, the SOEC technology is found to have the smallest sufficient nominal capacity with respect to the two alternative technologies, due to its greater electrical efficiency. Focusing on energy consumption, the local renewable energy generation is sufficient to supply power to the SOEC electrolyser in all the cases, while additional electricity purchased from the grid would be required to power supply alkaline and PEM electrolysers in cases 4 and 5. To reduce the amount of electricity purchased from the grid in these two cases, steam conversion is considered.



Figure 14. Annual electricity consumption and hydrogen production for the five cases.

	ELECTROLYSER' S NOMINAL CAPACITY [MW]				
ELECTROLYSER TYPE	CASE 1	CASE 2	CASE 3	CASE 4	CASE 5
SOEC – To Date	2.7	5.4	13.4	26.8	40.2
AEK – To Date	3.4	6.7	16.8	33.5	50.3
PEM – To Date	3.7	7.4	18.5	36.9	55.4

Table 1. Electrolyser's nominal capacity for the five analysed cases.

Figure 14 shows the surplus of electricity for the analysed cases. Two main findings result. Firstly, AEK and PEM configurations are characterized by a higher energy surplus than SOEC configuration only in the case that traditional cycle efficiency is greater than 39.2% and 59.3% respectively. Secondly, the investigated local renewable plants are sufficient to cover, 10% of the total green hydrogen demand to cover the steelmaking plant demand.



Figure 15. Energy surplus in the five cases for "To date" performances.

Figure 16 shows the energy surplus in the five cases considering electrolysers' efficiency in accordance with KPI suggested by FCHJU. As indicated, thanks to the technological improvement, a higher energy surplus is expected resulting in a potential increase of hydrogen production up to 8%, resulting in 30 tons per year. However, this amount would still be insufficient to cover the total demand.



Figure 16. Energy surplus in the five cases for 2024 (left) and 2030 (right) performances.

Although not shown, DBI-MAT gives the possibility to investigate other streams such as oxygen. For example, it could be utilized in the furnaces in oxy-fuel combustion processes. Furthermore, pure oxygen could be utilized in wastewater treatment, improving process efficiency.

4. CONCLUSIONS

In this study, we present a comprehensive modelling framework that consists of three energy models and that allow end-users to adapt and optimize the installation of P2X solutions to their specific needs. The three tools are each suitable for answering specific questions raised by the end-users and project developers, and essentially can be used to support the fast implementation of P2X and P2G projects, which is needed in the future. While SpineOpt is used to provide long-term assessments of potential locations for P2X and P2G projects in the future, the SuperP2G-Italy tool encounter high resolution geospatial data for a more in-depth analyses of the locations for P2G plants. DBI-MAT is applied when potential locations are identified and is applicable for a more detailed techno-economic investigation of the P2G plant performance at specified locations.

The results from this study show the benefits of each single tool but also how knowledge exchange between the tools enables a thoroughly assessment from identifying locations and throughout the supply chain to quantifying the techno-economic performance.

This study therefore provides a new methodology that can be applied to assess different needs of potential P2X stakeholders, e.g., project developers and industrial end-users that need to optimize plant design and investigate the resulting business plan to decide the feasibility of their projects, and towards policy and other strategic decision makers who develop strategies and roadmaps for the scale up of P2G in the future.

However, further efforts are required to make it possible to bond the workflow between the tools for a fully integrated approach towards all spatial and temporal levels of detail. For this reason, a future research step is to ensure a full linking of the tools' in- and outputs to ensure a coherent workflow.

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