International Journal of Sustainable Energy Planning and Management Vol. 41 2024 87–107

International Journal of
Sustainable Energy Planning and Management

Optimizing the Integration of Renewable Energy Sources, Energy Efficiency, and Flexibility Solutions in a Multi-network Pharmaceutical Industry

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ABSTRACT

In the contemporary landscape, roughly one-fourth of worldwide carbon dioxide emissions stem from industrial energy usage. In the industrial sector, improving the efficient and flexible coupling among different energy demands (electricity, heating, and cooling) and exploiting the integration of Renewable Energy Sources (RESs) and waste heat can lead to a drastic reduction in CO_2 emissions, which are also the goals of the EU founded Horizon Europe FLEXIndustries project.

This study aims to establish a cost-optimized decarbonization strategy for an energy-intensive industry, focusing on an Italian pharmaceutical company. It delves into the exploration of potential pathways and diverse energy mix configurations. The approach undertaken involves coupling a customized energy system simulation framework, specifically designed for the industrial site, with a Multi-Objective Evolutionary Algorithm (MOEA). The study, conducted with a focus on the year 2024, involves a comparative analysis of three distinct scenarios. Within the intricate and challenging constraints of the industrial demo site, 13 technologies are investigated. The outcomes of each scenario reveal a set of Pareto optimal solutions, which are thoroughly analyzed to discern the evolution of the energy mix along the Pareto front. These results shed light on the compelling potential of hybrid solutions, showcasing the feasibility of achieving substantial decarbonization with only moderate increases in costs. The availability of land for RES technologies, along with the existence of a biomass supply chain in the region, emerge as pivotal determinants.

Keywords

Pharmaceutical industry;
Multi-objective evolutionary algorithm;
Energy efficiency;
Energy system integration;
Flexibility

http://doi.org/10.54337/ijsepm.8167

1. Introduction

Climate change has been arousing attention internationally for decades and will continue to be a challenge for humankind. As the first major international effort to address climate change through targeted commitments, the Kyoto Protocol (1997) [1] established legally binding emission reduction targets for developed countries, later in 2015, the Paris Agreement [2] set the goal of limiting global warming to well below 2 °C, with efforts to limit it to 1.5 °C. Following this path, the European Union initiated the European Green Deal (2019), with one of the main goals being to reach climate neutrality by 2050 [3]. Achieving global environmental objectives, such as reducing fossil primary energy consumption and greenhouse gas emissions, is essential for authentic and sustainable development. This challenge demands the formulation of innovative and unequivocal strategies throughout the entire energy sector.

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Renewable energy technologies have garnered recognition as a potential alternative to fossil fuel-based energy systems among policymakers, scientists, and the public [4–6]. However, to address the persistent challenge of intermittency associated with variable Renewable Energy Sources (RES), such as wind and solar, it is imperative to embrace a holistic approach that integrates complementary technologies within advanced energy systems [5]. To tackle the intermittency of variable RES, a range of strategies can be deployed, encompassing both the supply and demand sides of the energy balance.

On the supply side, diverse solutions can be implemented [7]. These include leveraging different types of variable RES, recognizing their distinct characteristics and geographical distributions. Additionally, integrating dispatchable non-RES technologies, coupled with carbon capture, utilization, and storage (CCUS) capabilities, can provide a reliable backup to mitigate intermittency. Moreover, the deployment of storage solutions, such as batteries, pumped hydro or power-to-fuel offers the flexibility to store excess energy during periods of high generation and discharge it when demand peaks [5].

Addressing intermittency also involves exploring demand-side opportunities, known as Demand-Side Management (DSM), encompassing strategies such as load shifting and peak shaving. DSM enables consumers to adjust their electricity consumption patterns in response to supply variations [8].

The industrial sector highlights the criticality of flexibility in energy systems [9]. Industrial processes often require a consistent and uninterrupted power supply, rendering flexibility paramount yet challenging. Furthermore, industrial energy systems, acting as both consumers and producers, can enhance transmission and inter-sectoral flexibility. This dual role strengthens resilience against intermittency, amplifying the sector's impact on grid stability and overall energy system robustness.

To tackle the wide-ranging complexities, spanning technical aspects like grid control and management, to environmental, social, and financial considerations, the imperative for smart energy systems and intelligent modeling tools emerges as a crucial solution. The concept of a "smart energy system," as proposed and discussed by [10], stands out as a valuable response in mitigating these challenges and paving the way towards achieving net-zero emissions. This involves the seamless integration of various technologies and the formulation of energy usage strategies across all sectors [11,12].

As highlighted in [13], it is essential to shift away from a sole focus on electricity and embrace a holistic perspective of the energy system to uncover optimal solutions for integrating renewable energy. Employing an integrated cross-sector approach, the study advocates for efficient and cost-effective storage options across the entire renewable energy system. Therefore, in identifying optimal solutions, it is imperative to move beyond a simple smart grid approach and adopt a more holistic viewpoint, as suggested by some authors. This appeal to holistic approaches to smart energy systems has led to a proliferation of studies characterized by different spatial resolutions in the scientific literature. Examples include studies conducted at the national scale, such as the work of Singh et al. [14] focusing on India, and at the regional scale, as proposed for an Austrian region [15] or for the Bali Province of Indonesia [16]. There are also studies conducted at the municipal level, such as in the municipality of Bressanone-Brixen [17].

Current research has predominantly focused on optimization activities related to Generation Expansion Planning (GEP) and the optimal design of hybrid energy systems. GEP involves devising the most efficient long-term plan for constructing new generation capacity while adhering to economic and technical constraints [18]. Various approaches have been developed to address GEP problems. Some endeavors employ single-optimization processes, which are constrained to optimizing a single function. To overcome this limitation, researchers often transform multi-criteria considerations into a singular one by assigning weights. However, this a-priori method relies heavily on subjective judgments, which can lead to biases and disagreements among stakeholders. Conversely, the rising popularity of a-posteriori methods enables more objective considerations on multiple criteria, offering comprehensive approaches to addressing the complexities of GEP and design of hybrid energy systems.

The application of linear programming in addressing GEP problems was pioneered by Massê and Gibrat [19]. Subsequent research has explored various optimization techniques, including mixed-integer linear programming (MILP) [20], nonlinear programming (NLP) [21], and mixed-integer nonlinear programming [22], showcasing the versatility of these approaches.

Liu et al. [23] employed MILP to assess the integration of RES with large-capacity combined heat and power plants in the chemical industry. Their study centered on optimizing the design of a multi-pressure level steam network. In the study by Morales Sandoval et al. [24], a single-objective nonlinear program was created to evaluate decarbonization pathways for a healthcare facility. They assess the techno-economical performance of the proposed hybrid energy system on a typical day basis. Another study by Gabrielli et al. [25] developed a MILP methodology with dual objectives, focusing on annual cost and CO_2 emissions. This approach tackled a year-long time horizon with hourly resolution, effectively simplifying the optimization challenge. They applied this methodology to design a multi-energy system tailored for a neighborhood in Zurich, Switzerland.

In situations where creating a mathematical model is intricate, impractical, or overly time-consuming, the adoption of a dedicated framework for scenario evaluation becomes indispensable. This alternative approach enables a more practical representation of complex scenarios, addressing challenges posed by factors such as complex energy networks, the evaluation of multiple technologies of different nature, or the requirement for numerous decision variables, which can be cumbersome for traditional mathematical programming. This approach is reflected in various studies in the literature. Numerous works assess decarbonization by coupling an energy system-solving framework with an optimization algorithm. For instance, Mahbub et al. developed a framework [26,27] integrating models from EnergyPLAN, an energy system analysis tool [28] with NSGA-II, an evolutionary algorithm, to assess the decarbonization pathways of sub-regional energy systems [29–31]. De Maigret et al. [32] employed a similar approach to investigate the decarbonization strategy of a refinery. Another application lies in the study of Delgarm et al. [33], who adopted this coupling approach, integrating a building simulation software, EnergyPlus, with a particle swarm algorithm for the multi-objective optimization of buildings.

Several studies adopted multi-objective optimization to optimally design the so-called Hybrid Energy Systems [34] or Multi Energy Systems (MES) [25]. Among these works it is worth mentioning, the study of Sharafi & El Mekkawy [35], which proposed a three-objective framework (minimizing total cost of the system, unmet load, and fuel emission) for a case study including several technologies such as wind turbines, PV systems, batteries and hydrogen. Xu et al. [34] proposed a multi-objective optimization approach, considering the energy, environmental and economic performance of the energy system, and exploring different operating strategies for the cogeneration system and the ground source heat pump. The multi-objective optimization model proposed by Ren et al. [36] optimizes the performance of a hybrid energy system supplying the total building demand of energy services. This involves optimizing the variable output ratio of a ground source heat pump to match heat-to-electricity ratios, with scheme comparisons following electric, thermal, and hybrid loads in various operational modes.

This study takes root and emerges directly from the European Commission's dedicated effort to assist energy-intensive industries in designing and implementing the most effective decarbonization and energy efficiency measures, exploiting process flexibility methods within their industrial settings, with a positive influence on their integration into the electrical and heating networks. The FLEXIndustries project, which lasts from 2022 to 2026, is devoted to monitoring, analyzing, and optimizing the most energy-intensive industrial processes. This is achieved by adeptly handling emerging demand response mechanisms, providing plant and process flexibility, and contributing to grid services. This study aims to outline the potential routes for decarbonization, focusing specifically on one of the project's demonstration sites, SUANFARMA Italia, located in Rovereto, Autonomous Province of Trento (IT). The approach of this study was inspired by the framework created by Mahbub et al. while replacing EnergyPLAN with a customized Python framework developed by the authors of this paper due to some limitations of EnergyPLAN. Indeed, given the specificity and the complexity of the demo addressed in this study, as well as the intention to avoid strongly binding assumptions in modeling energy balances, and taking into account that the original destination of EnergyPLAN is a simulation model for regional and national energy systems, it was established to develop a dedicated techno-economic solver for the industrial case energy system. Moreover, it was chosen to leverage the powerful and adaptable architecture of evolutionary algorithms to search for optimal solutions without explicitly formulating the mathematical program. More specifically, the customized Python framework, coupled with the evolutionary algorithms, is used to characterize the solutions in terms of CO_2 emissions and total annual costs (therefore two objectives) and based on these two criteria there is an evaluation of the best solutions in each generation. Each solution is characterized by a specific mix of decision variables (size of energy technologies) and each decision variable is associated with some technical, economic and environmental data. Compared to the other mentioned studies, the innovations presented in this paper encompass several key areas for an industrial case energy system:

(I) development of a specialized hourly-based energy system solver capable of integrating multiple renewable energy technologies, simulating over an entire year of operations and with emphasis on prioritizing their integration and storage, particularly in addressing complex energy services demand (electricity, two levels of heating, and cooling);

(II) enhanced consideration of technology competition, including coupling with various storage forms and land utilization aspects;

(III) pioneering analysis of the energy services needed by an energy-intensive pharmaceutical industrial site, utilizing hourly-based historical data, and exploring active participation in local grids boosting sector coupling;

(IV) detailed characterization and discussion of the technologies emerging as crucial in the cost vs CO_2 emissions Pareto optimal set of solutions.

This approach provides the opportunity to incorporate greater modeling flexibility, allowing for the development of more customized and specific solutions compared to previous papers. It facilitates the exploration of possible decarbonization pathways and the evaluation of fossil fuel dependency for each energy vector adopted at the industrial site. Moreover, the proposed model allows the examination of the sensitivity of optimal solution Pareto-fronts to input parameters, including energy vector demand profiles, variable RES production profiles, and market-related specifications.

The challenge of this work is to answer the question: "Which technologies emerge when both economic and environmental aspects are taken into consideration for such an energy-intensive industrial site, i.e. SUANFARMA, and what strategies are consequent?". Since reducing both CO_2 emissions and costs has a mutually conflicting nature, a compromise has to be made. For this reason, this work intends to provide and assess multiple solutions which are all on the Pareto front, meaning that for any solution with a given cost, the CO_2 emission is minimized, and vice versa. Combining a large solution space, high temporal resolution and smart energy systems entails that searching optimal solutions is computationally challenging and that fast and efficient energy system models are crucial to identify energy transition pathways and characterize their impacts.

The remainder of the paper is organized as follows. In section 2 it is detailed the methodology, including the design of the energy system simulation model and how it is combined with the optimization algorithm. Section 3 introduces the case study, outlining the methodology for processing input data, modeling assumptions, and proposing various scenarios. Section 4 is dedicated to discussing and providing commentary on the results obtained. In section 5, conclusive remarks are provided.

2. Methods

This section discusses the methodology adopted to foster the integration of Renewable Energy Sources into an energy-intensive industry. In this study, a multi-objective evolutionary algorithm (MOEA) is coupled with a customized techno-economical energy system solver, which enables the evaluation of the integration of several utilities into a complex energy system. These utilities are responsible for supplying different energy vectors to production processes.

The adopted framework structure (Figure 1) is very well established in literature with several works that exploit the evolutionary algorithm architecture to search for optimal solutions in the energy system field, especially if it is capable of dealing with competitive objectives. A critical phase within the algorithm's routine is the "evaluate individuals" step, where each individual, defined by a set of decision variables, undergoes assessment. This involves the call of a simulation model that computes and assigns the values of objectives and constraints to each individual. In this study, the evolutionary algorithm utilizes the "evaluate individuals" function by passing the capacities of the considered technologies. Subsequently, the function computes and returns values for objectives and constraints.

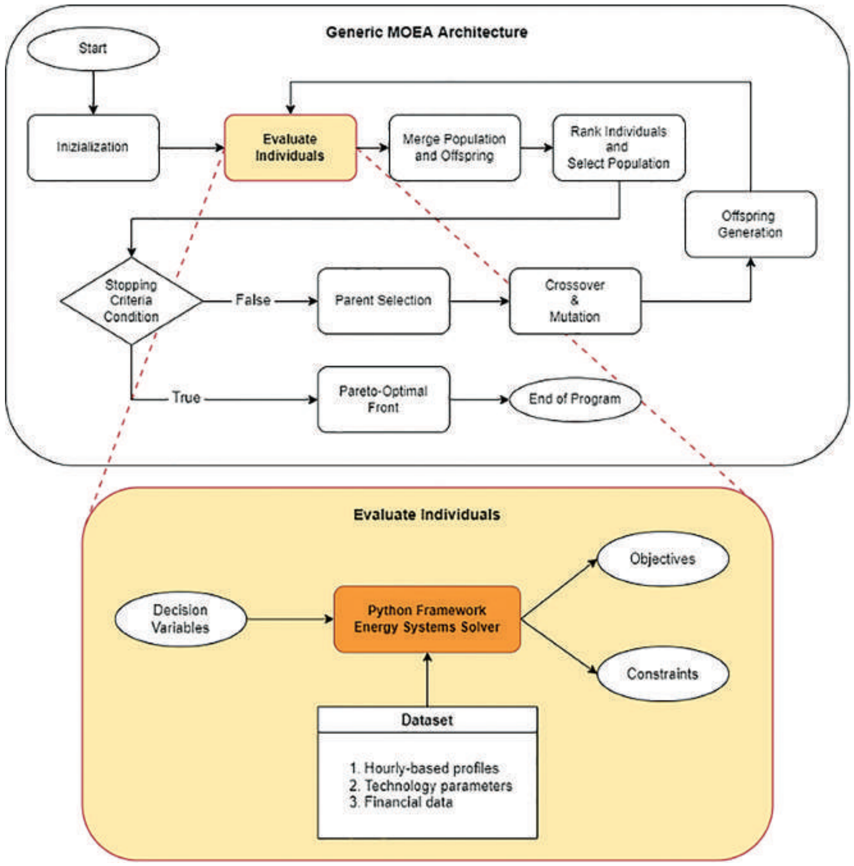

Figure 1: Flowchart of a Multi-Objective Evolutionary Algorithm (specifically NSGA-II) integrated with a Python framework for energy system optimization. The flowchart illustrates the energy system solver embedded within the 'evaluate individuals' step of the MOEA's execution flow.

2.1 Energy system techno-economic solver

The developed Python framework addresses the supply problem of serving energy vectors' demand in the system by simulating an entire year of operations. It takes a specific set of utilities' generation capacity as input and calculate the total annual cost and CO_2 emissions, along with constraints violation.

The model focuses on maximizing the self-utilization of renewable energy sources, it resolves the energy balance for every energy vector in the case study on an hourly basis. The structure of the program can be summarized as: (i) input data loading, (ii) hourly-based energy balance solver, and (iii) financial, technical and CO_2 emissions calculator.

The data loading step imports hourly sample profiles of RES production and the industry's energy demands. It then inputs the financial data related to the technologies and energy vectors and initializes the power capacity for selected technologies.

The core of the Python framework is the hourly-based energy balance solver presented in Figure 2.

The energy balance solver, operating on an hourly basis, functions as a simulation model with priority-based principles. It is mainly built upon endogenously defined priorities, which are derived from considerations of minimizing primary energy consumption while simultaneously ensuring adherence to the hourly energy balance.

The initial step involves computing the residual demand for each energy vector that needs to be satisfied. Following this, the production of RES is evaluated and subtracted from the specific residual demand. Normally, any production surplus that exceeds demand is unconditionally accumulated in energy storage systems. However, in the electrical domain, sector coupling necessitates the introduction of a logical condition. Consequently, the program execution flow is divided into two branches. In case of surplus production of

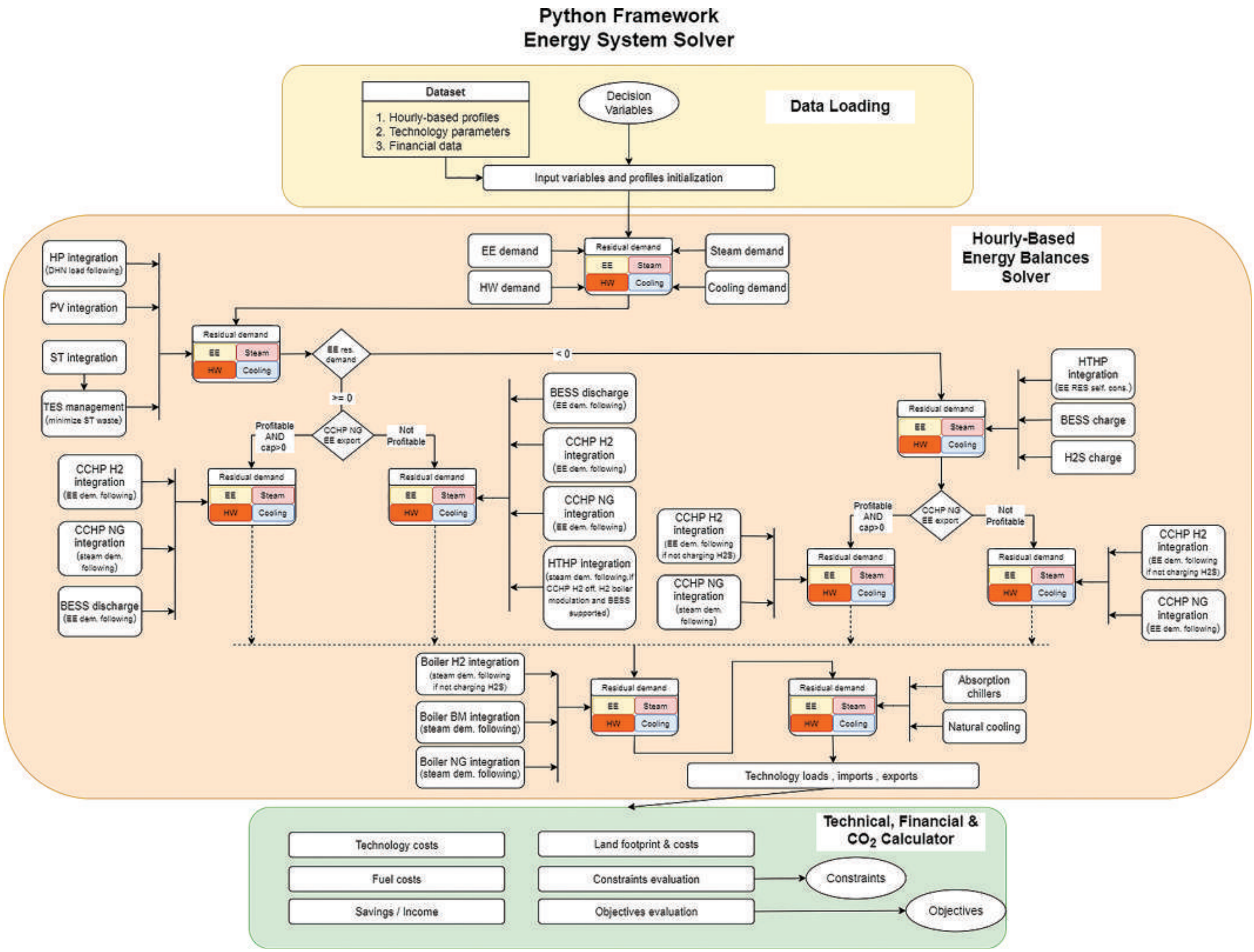

Figure 2: Solution flow of the proposed energy system simulation model. The process comprises three key steps: Input data loading, Hourly-Based Energy Balances Solver, and the Technical, Financial, and CO_2 Calculator.

electricity from RES, the following technologies are activated in sequence: (i) High-Temperature Heat Pump (HTHP); (ii) Battery Energy Storage System (BESS); (iii) electrolyzer and hydrogen storage system. Subsequently, the integration of the natural gas fired Combined Cooling, Heat and Power (CCHP) unit is evaluated according to the marginal cost of electricity production. Two operating strategies are defined for the natural gas CCHP: electricity self-production mode and maximum waste heat integration mode, allowing for electricity export. On the alternate branch, corresponding to persistent electricity demand from the industrial site, the program first evaluates if the natural gas CCHP has an installed capacity greater than zero and then determines whether it operates in electricity self-production mode or maximum waste heat integration mode. According to the operating strategy of the natural gas CCHP, the BESS is discharged in case of the existence of a residual demand, and the high-temperature heat pump (HTHP) for steam generation is activated under the condition that it is not fed by CCHPs' electricity (a condition derived from endogenous assessments on primary energy consumptions). In the final stage of the hourly-based solver, where the two program branches converge, technologies that operate in load-following mode and are not coupled with other energy streams, such as boilers and absorption chillers, are integrated. All the technologies investigated are assumed to operate with a constant efficiency across the full load range (from 0% to 100%), neglecting equipment technical limitations and considering the efficiency as its nominal value. In the last block of the program, the financial, technical, and CO_2 emissions calculator computes: (i) for each technology the annual equivalent cost from CAPEX, fixed O&M, variable O&M, and interest rate; (ii) the land footprint and its cost; (iii) energy vectors costs and emissions (electricity, natural gas, biomass, etc.) taking into account commodity cost, variable non-energy commodity costs, fixed costs, power or penalty costs and EU Allowances (EUAs) cost. Only the price of electricity is considered as variable on an hourly basis. For other energy vectors an annual mean value is used; (iv) revenues from the export of energy vectors and forms of incentive such as white certificates (TEE) for high efficiency CCHPs (CAR)[37].

2.2 Optimization

As illustrated in the previous subsection, the system contains numerous hierarchical and conditional rules, making it impractical to formulate a mathematical program. In this case a metaheuristic optimization algorithm is needed to generate solutions and select the optimum. In this sense, evolutionary algorithms are favorable not only because they are versatile and fast, but also because they naturally tackle multi-objective optimization problems, thanks to their population-based principle. Thus, one of the most developed genetic algorithms, NSGA-II [38] was adopted in this study.

In this application, individuals in the population are characterized by the installed capacity of each technology. In every iteration, a parent set is selected from the population to generate the offspring population, thanks to the crossover and mutation operators. The crossover operator takes two parent solutions (each representing an alternative, that is, a vector of nominal capacities) and creates an offspring that will share some features with one parent and some other features with the other parent, hopefully inheriting their good properties discarding the old ones. The mutation operator randomly applies some changes to some solutions to maintain population diversity. The solutions are then passed to the energy system model, which provides results indicating the CO_2 emission, the annual total cost and constraints violation for each individual. The set, consisting of the offspring and their parents, is later evaluated according to the concept of Pareto optimality. Within the proposed framework, a solution is considered to be Pareto-optimal if it cannot be improved in any of the objectives without degrading another. Graphically speaking, on the cost-emission plot, solutions located on the upper-right side of a given solution are dominated. Thus, for every set, consisting of parents and offspring, it is possible to establish a metric, rank every individual, and then select the best-performing individuals to form a new population. The algorithm advances by evolving the population until the stopping criteria is met and a set of non-dominated solutions emerges describing a Pareto front.

Table 1: Settings of the NSGA-II optimization algorithm.

Attribute	Method	Value
Population		500
Offspring population		500
Mutation	Polynomial Mutation	1.0/number of decision variables
Crossover	SBX Crossover	0.9
Dominance Comparator	Dominance with constraints comparator	
Stopping criteria	Number of generations	80

In this way, we expect to obtain a set of solutions that have the best confidence in answering the question raised in the Introduction: “Which technologies emerge for the energy-intensive industrial site SUANFARMA, and what strategies consistently emerge?”.

The settings of the NSGA-II solving algorithm are summarized in Table 1. The population size was determined through experimental procedures and fine tuning based on the authors’ experience with the framework [26,27,29,30], and with the goal of aiding the convergence of the algorithm towards the true Pareto front.

3. Case Study

SUANFARMA Italia S.p.A. is a leading company in the development, production, and distribution of active pharmaceutical ingredients for human and animal health. Equipment and processes are those typical of the pharmaceutical industry, the main energy intensive processes are fermentation, synthesis, solvents recovery, air compression, and refrigeration. The industrial plant under study is located in Rovereto, a valley town in the Autonomous Province of Trento, North of Italy (Figure 3).

3.1 Energy demand breakdown

The industrial site exhibits a notably high demand for electricity and natural gas, the latter being used as a fuel for electricity generation and for the production of heating and cooling.

Heat is delivered to the processes using mainly a saturated steam network at 165°C. Additionally, two other networks are used to satisfy the cooling demand, a low temperature at –7 °C and a medium temperature network with a delivery temperature of around 10 °C.

The 2024 baseline demand of each energy vector was established using historical data, along with a forecast analysis aided by industrial site experts. The need to select the year 2024 arises from already planned plant equipment upgrades (i.e. a new CCHP unit). Moreover, for the same year, the industrial site is planning to stipulate a new supply contract with the local District Heating Network (DHN) to export hot water (around 90°C). Table 2 summarizes the data used as a baseline in this study (year 2024).

3.2 Energy supply system

The industrial site is equipped with a combined cooling heat and power (CCHP) plant consisting of two twin natural gas-fired reciprocating internal combustion engines with a nominal electrical capacity of 4.5 MWel each. Additionally, a new CCHP unit is scheduled for installation in 2024, aiming to achieve a total electric generation capacity of 13.5 MW. CCHPs serve mainly internal electricity demand and, through heat recovery,

Table 2: Energy vectors demand provided by the industrial site.

Energy vector	Demand [GWh]
Electricity	87.66
Steam	95.08
DHN	3.83
Medium temperature cooling	100.77
Low temperature cooling	13.73

Source: SUANFARMA Italia S.p.A.

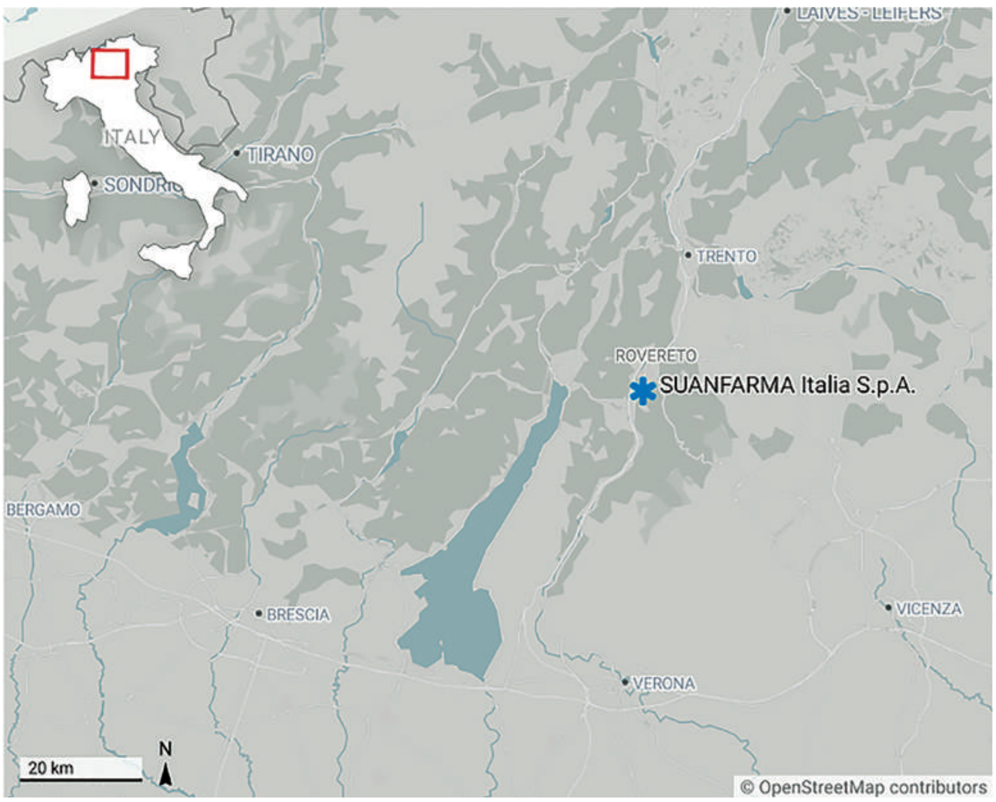

Figure 3: SUANFARMA Italia S.p.A. location.

steam and hot water can be produced. The latter is then converted into cooling for processes by means of absorption chillers. The medium temperature cooling demand is met by employing absorption chillers, complemented by the use of industrial water sourced from aqueducts and wells. A part of the hot water recovered from CCHPs can also be used to satisfy the Rovereto's DHN demand. Steam demand of the industrial site is mainly covered by three natural gas boilers with a total installed capacity of 26 MWth. The low temperature cooling demand is entirely satisfied by a dedicated, state-of-the-art solution, a refrigeration plant.

During the FLEXIndustries project, a 500 kW PV system, a 1 MW heat pump, and a 400 kWh BESS are planned to be deployed. More specifically, the heat pump is designed to simultaneously provide useful cold water to serve the medium temperature cooling network and useful hot water to be exported to Rovereto's DHN.

3.3 Modeling assumptions and decarbonization enabling technologies

A number of assumptions were made to simulate the SUANFARMA complex energy system and investigate decarbonization-enabling technologies.

3.3.1 Energy sectors considered

From the energy vectors' network point of view, all the quantities are converted and computed as equivalent power flow for each energy balance.

In the electricity sector, the interaction with the national grid and the electric market is considered, allowing for both import and export activities. However, it is important to note that the export capacity is assumed to be limited to the actual capacity of the network (30 MW). This limitation stems from the acknowledgment that it is beyond the scope of a pharmaceutical industry to adopt the business model of a large power plant actively engaged in operations on the electric market. The hot water demand from the DHN is considered like a demand from the production processes since it is constrained to be satisfied on an hourly basis. The low temperature cooling demand is not considered as an independent energy balance. Instead, it is counted as a load inside the electricity demand of the plant. Since the refrigeration plant is a state-of-the-art solution, no upgrades can be assessed. Under these assumptions, the normalized hourly sampled profiles considered for energy vectors' demands are shown in Figure 4.

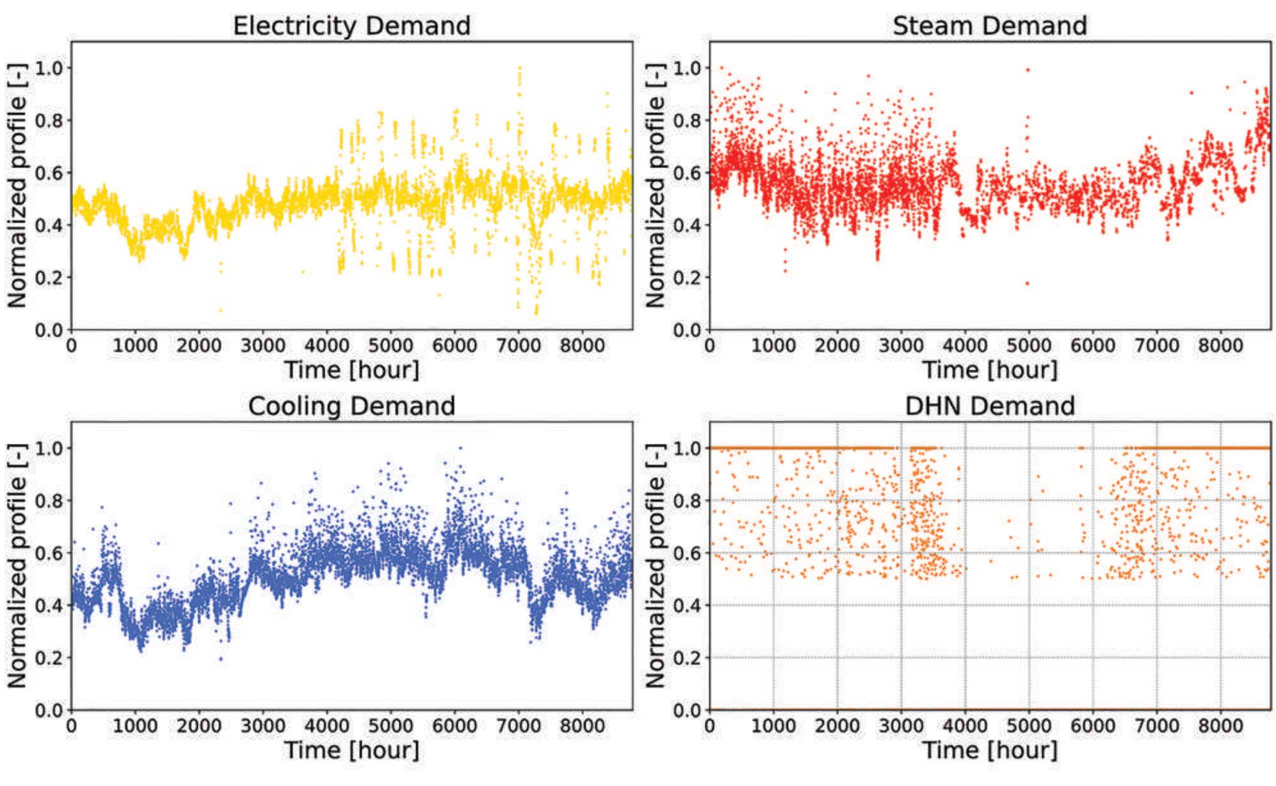

Figure 4: Normalized demands of the industrial site energy system.

3.3.2 Technology assessed for decarbonization

In addition to technologies already described (both existing and planned), the following technologies have been considered to evaluate decarbonization scenarios: (i) linear Fresnel solar collectors for direct steam production; (ii) high temperature heat pump for direct steam production, since no waste heat above ambient temperature is available, a two series-connected configuration is considered; (iii) biomass boiler; (iv) thermal energy storage dedicated to solar thermal integration; (v) alkaline water electrolyzer for green hydrogen production; (vi) pressurized vessel hydrogen storage; (vii) hydrogen-fired CCHP unit (viii) hydrogen-fired boiler.

It was decided to not investigate the integration of Organic Rankine Cycle (ORC) technology for power generation since the industrial site has no waste heat available at a useful temperature, which is by far the most promising application [39,40]. Furthermore, due to the site's energy-intensive nature across all energy sectors that could be potentially served by biomass-based technologies, the proposition of utilizing biomass for power generation has been dismissed. Instead, its application is restricted solely to steam generators.

Production profiles for solar technologies were generated by utilizing meteorological databases. The PV system's output was computed using the SAM model developed by NREL [41], resulting in an annual yield of 209 kWh/m^2. Additionally, for the linear Fresnel technology, the methodology outlined in [42] was employed, yielding an annual production output of 382 kWh/m^2 for a delivery temperature set at 200°C.

3.3.3 Land footprint considerations

The availability of free areas, both at ground and roof level, is a strong limitation for the deployment of decarbonizing solutions with high land consumption in the demo site. For this reason, it was decided to also consider the land consumption of the most impactful technologies, such as storages (e.g., thermal, hydrogen and battery), PV system, and linear Fresnel solar collector. The available area (Figure 5) is evaluated around 10,192 m^2 on the roofs and 3,800 m^2 on the ground. Moreover, it is assumed that SUANFARMA has the option to lease land in close proximity to the industrial site, with a maximum area of 20,000 m^2.

With the aim of not limiting and leaving the possibility to the evolutionary algorithm to explore scenarios with high penetration of PV systems and battery energy storage systems, an uncommon approach is proposed to expand the area available for these technologies. It is assumed that the PV system can be installed on a rented roof area and a BESS can be implemented on a ground rented area, both up to 1% of the total area served by the local high voltage substation, following the Italian approach for Renewable Energy Communities [43].

Figure 5: SUANFARMA aerial view and available area considered in the study.

A land competition among technologies is taken into account, with the following assigning order on the ground: (i) thermal energy storage, (ii) hydrogen storage, (iii) solar thermal, and (iv) BESS. Only the PV system is considered for the available area on the roof.

3.4 Input data for technologies and energy vectors

The reader is invited to refer to the supplementary material for details on efficiencies, costs, specific parameters and respective references considered for each technology. The industrial site did not provide any data on the installed technology, so data used in present work are derived from literature.

The industrial site provided costs of import of electricity and natural gas, export remunerations from DHN hot water export, white certificates from high efficiency cogeneration (CAR), again the reader is invited to refer to the supplementary material for details.

The price of electricity is the only energy vector value considered with an hourly based distribution, the profile was derived from the historical database [38] taking into account the shape and the dynamic of the price preceding well-known destabilizing events that inflamed prices and speculation on the electricity market. The profile is hence normalized with respect to the mean value and re-scaled according to the mean value adopted in the scenario. Figure 6 shows the adopted normalized profile.

3.5 Objectives, decision variables, constraints and scenarios

As described in previous sections, the objectives considered are one year of operational total cost and carbon dioxide emissions. The twelve decision variables are nominal capacities of the technologies described previously and they are summarized in Table 3.

To ensure security in supply, it is assumed that the capacity of the natural gas boiler is maintained fixed at the actual capacity installed in the plant. This choice will not affect the meaning of results since a certain capacity of a technology can be installed but not used, thanks to the proposed architecture of the energy system solver.

In this study the following conditions were restricted to have a value of zero: (i) DHN supply deficit, since it is a supply contract, it must be satisfied; (ii) electricity over-production, total amount of electrical energy that cannot be exported; (iii) steam over-production, the introduction of non-programmable RES into the system might lead to an excess of steam production, encouraging the adoption of energy storage solutions; (iv) hot water from CCHPs over-production, it must be limited to have access to the white certificate incentive scheme;

Table 3: Decision variables with their upper and lower bound.

Technologies considered	Decision variable capacity bounds	Status
Natural gas boiler (NG boiler)	26 MW, fixed capacity	Existing
Hydrogen boiler (H2 boiler)	0–26 MW, derived from NG boiler	Considered in all scenarios
Biomass boiler (BM boiler)	0–26 MW, derived from NG boiler	Considered in S_ALL & S_NOBM
Natural gas CCHP (NG CCHP)	0–30 MW, limited by cooling demand	Existing, planned, and considered in all scenarios
Hydrogen CCHP (H2 CCHP)	0–30 MW, limited by cooling demand	Considered in all scenarios
Heat pump (MTHP)	0–1 MW, limited by DHN demand	Planned and considered in all scenarios
PV system (PV)	0–120 MW, limited by area availability	Planned and considered in all scenarios
Linear Fresnel Reflectors (ST)	0–10 MW, limited by area availability	Considered in S_ALL & S_NOBM
High temperature heat pump (HTHP)	0–26 MW, derived from NG boiler	Considered in S_ALL & S_NOBM
Alkaline water electrolyzer (AEL)	0–120 MW, derived by PV system	Considered in all scenarios
Battery Energy Storage System (BESS)	0–2 GWh, derived from area availability	Planned and considered in S_ALL & S_NOBM
Hydrogen storage (H2S)	0–5 GWh, derived from area availability	Considered in all scenarios
Thermal Energy Storage (TES)	0–475 MWh, derived from area availability	Considered in S_ALL & S_NOBM

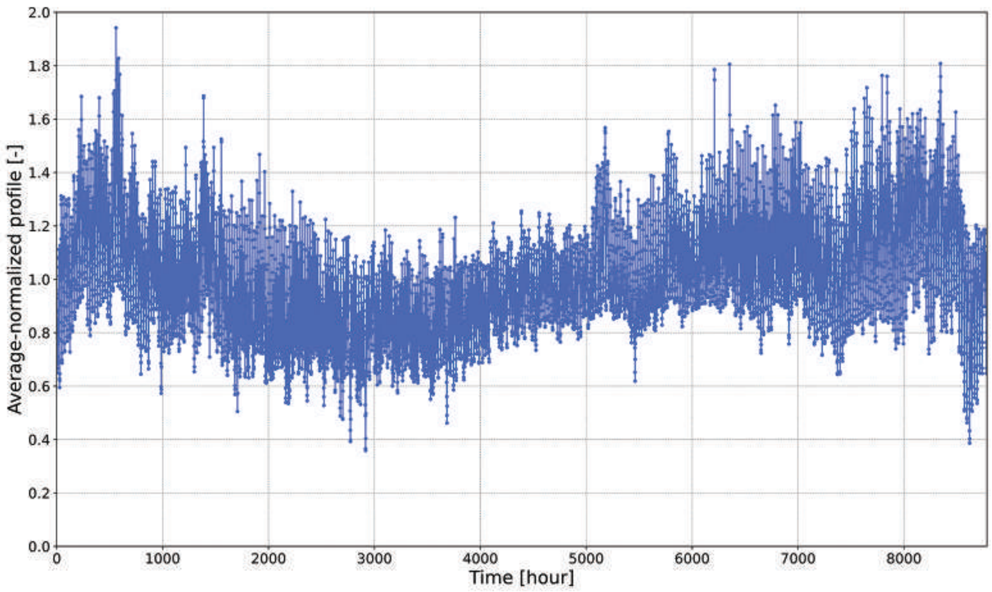

Figure 6: Electricity market price (PUN) normalized respect to the average.

(v) excess land area consumption with respect to the quantity available and purchasable.

Three scenarios were selected to analyze the role of the above-mentioned technologies to achieve decarbonization. Details on the decision variables range considered can be found in Table 3.

The chosen scenarios were deliberated with input from industrial experts of the case study, primarily reflecting their interest in investigating solutions leveraging a diverse array of technologies. The first scenario, shortened as “S_ALL”, represents a fundamental approach, incorporating the essential and most promising technologies for decarbonization [6]; the second scenario, shortened as “S_NOBM”, was chosen to test the set of solutions in case of limitations in regional biomass availability; the third scenario, shortened as “S_H2”, emerges from the aspiration to evaluate the feasibility, both technical and economic, of decarbonization solely through self-produced green hydrogen.

All the proposed scenarios will be compared with input data discussed in the previous section, referring to the year 2024. This decision is derived from the strong sensitivity shown by the proposed energy system model to the price of natural gas and electricity, and from the high uncertainty and volatility that still characterizes these markets. The assumed average price of the electricity market (PUN) for the year 2024 is 128.6 €/MWh. Additionally, the cost of the natural gas commodity is fixed at 40 €/MWh, and the assumed value for EU Allowances (EUA) is 100 €/tonCO_2. Additional parameters and cost references are collected in the supplementary material.

4. Results

This section presents and discusses the results obtained from the optimization problem at the core of this study. As a comparison, with all the Pareto optimal solutions for each scenario, it will be also shown the Business-As-Usual (BAU) solution, computed with the original assets described in the previous section, and the FLEXIndustries solution (BAU-FLEX), that also consider the implementation of technologies developed during the project. This section describes in the first place the analysis of convergence of the Pareto optimal solutions. Following this, the comparison of the Pareto front of each scenario with respect to the reference solutions is discussed. Furthermore, the detailed analysis of the evolution of the energy generation technologies’ breakdown, for each scenario, is presented. The last section compares and discusses the results obtained in this study with similar existing studies in the literature.

4.1 Pareto front convergence analysis

The stopping criteria adopted for the algorithm was chosen analyzing the convergence in the evolution of the Pareto front. Figure 7 shows the evolution of the Pareto front in the scenario S_ALL. Convergence is considered achieved after 80 generations, with a population of 500 individuals and a computational time of about 1 hour for each scenario.

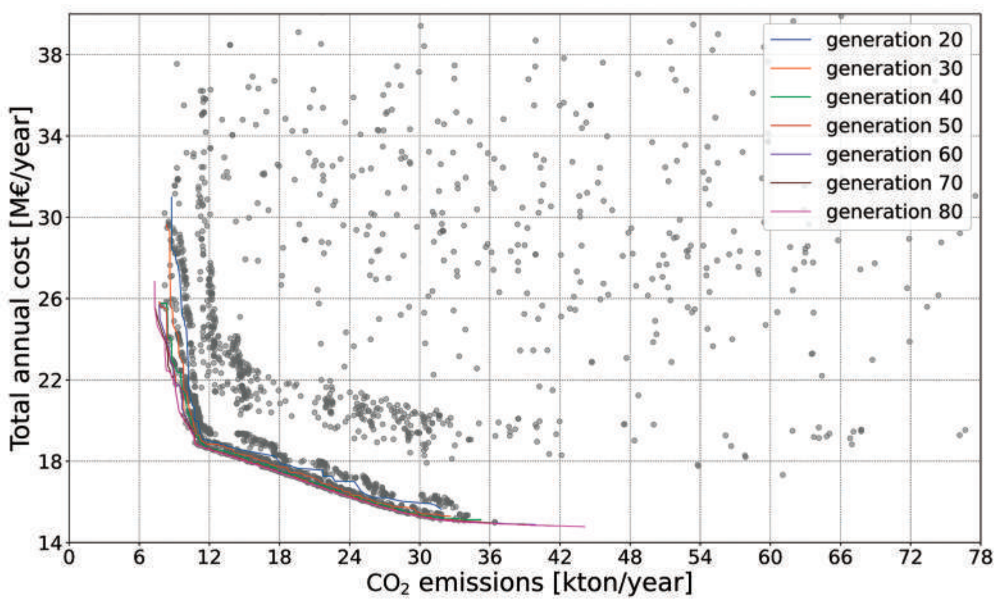

Figure 7: Evolution of the Pareto front in scenario S_ALL.

Among other things, Figure 7 shows that the Pareto front converges quite well already after 20 generations. Also, the computations were performed on a standard laptop computer with Intel(R) i7-12702, 2.2GHz, 12 core, 32GB RAM. These two facts open possibilities to quickly perform sensitivity analysis in the form of "if-then" analyses. These were used, for instance, to check whether and when small variations in the input parameters induce large changes in the adopted technologies and therefore check the existence of "jumps" in the use of technologies. Reporting a full-fledged sensitivity analysis would be beyond the scope of this paper, but we trust that its potential and its importance will be clarified by considering the following analysis of the scenarios "S_ALL", S_NOBM", and "S_H2". In fact, each scenario can be interpreted as an instance of an "if-then" analysis where some variables determining technology levels are subject to tighter constraints.

4.2 Scenario comparison

Figure 8 illustrates the comparison among the three Pareto optimal scenarios. Moreover, the diagram shows the annual results in terms of cost and CO_2 emissions necessary to meet the internal process demand of the industrial site.

One noteworthy observation that emerges from the comparison of various scenarios is the significant enhancement in performance with respect to the reference solutions. This improvement extends not only in terms of a substantial CO_2 emissions reduction but also in terms of total annual cost. It is crucial to underline that since the BAU and BAU-FLEX energy systems strongly rely on natural gas, the model shows a very high sensitivity with respect to the natural gas commodity price, leading to a notable enhancement in solutions based on alternative technologies.

Furthermore, observing the three Pareto fronts from a perspective of decarbonization, e.g. from higher to lower annual CO_2 emissions, three different phases emerge. The first phase is characterized by a linear evolution with a very limited slope of all three Pareto fronts (high emissions reduction and relatively low-cost increase). The second phase still shows a linear behavior in all three Pareto fronts, but they are steeper than the first phase. The third phase shows a distinct nonlinear slope increase trend unique to each scenario, influenced by the adopted mix of technologies.

With the proposed modeling of the industrial site, especially with the role played by the area availability for RES deployment, full decarbonization seems unreachable.

4.3 Scenario S_ALL

Figure 9 and Figure 10 show the evolution of the installed technologies and the resulting energy breakdown supplied to meet the industrial demand. The analysis focuses on the two sectors, electrical and thermal, which are responsible for most of the CO_2 emissions and the total annual cost. Each point along the Pareto front in Figure 8 corresponds to the annual outcomes in CO_2

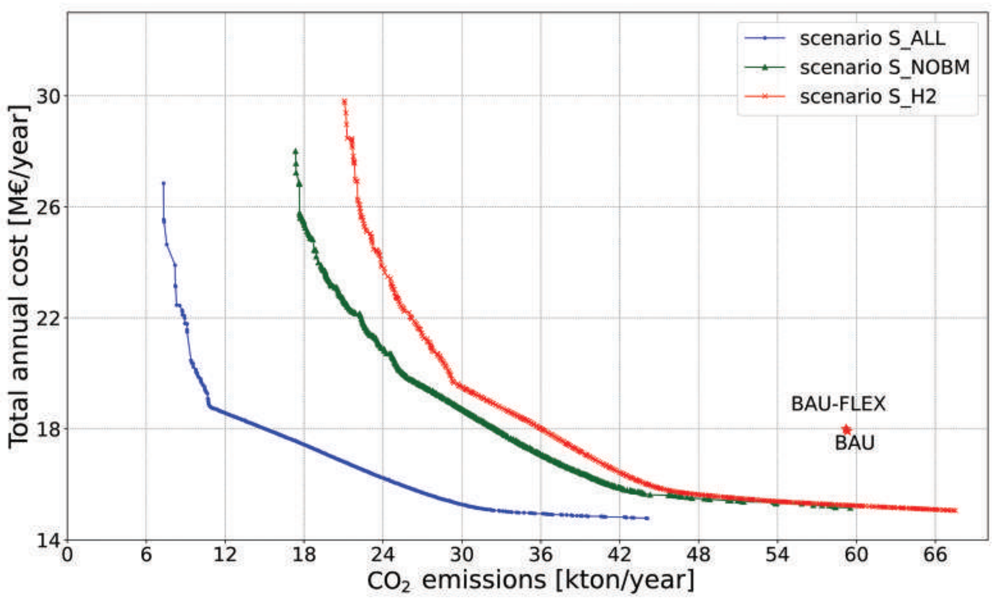

Figure 8: Comparison of Pareto fronts among scenarios and reference solutions.

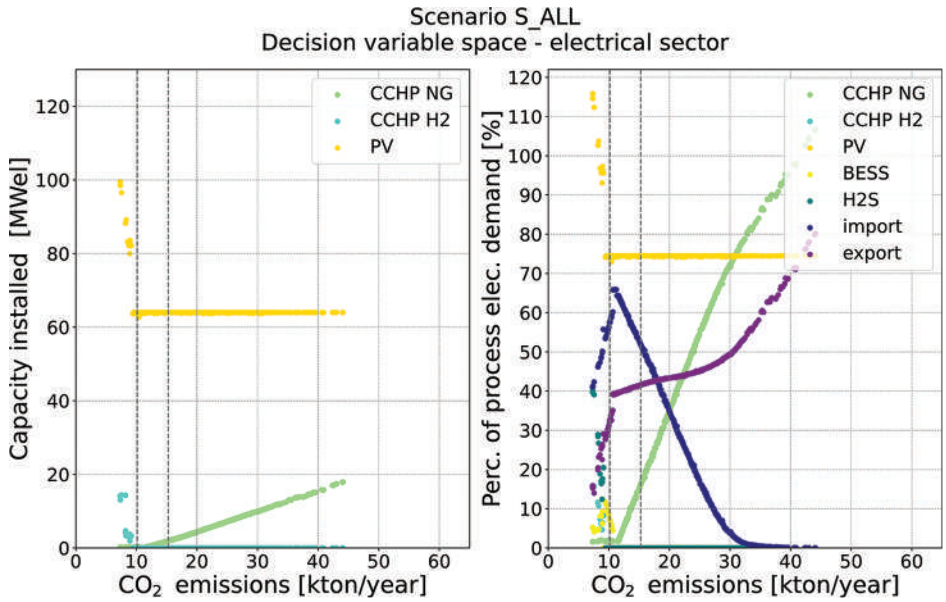

Figure 9: Analysis of the decision variables related to the electrical sector that characterize the Pareto-front solutions depicted in Figure 8. The left side shows installed capacities, while the right side displays weighted electrical energy quantities respect to the process industrial demand. Since export is allowed, total energy generation may not be equal to the industrial demand. The two vertical dotted lines highlight the annual CO_2 emission level where the Pareto optimal solutions show a change in the evolution trend.

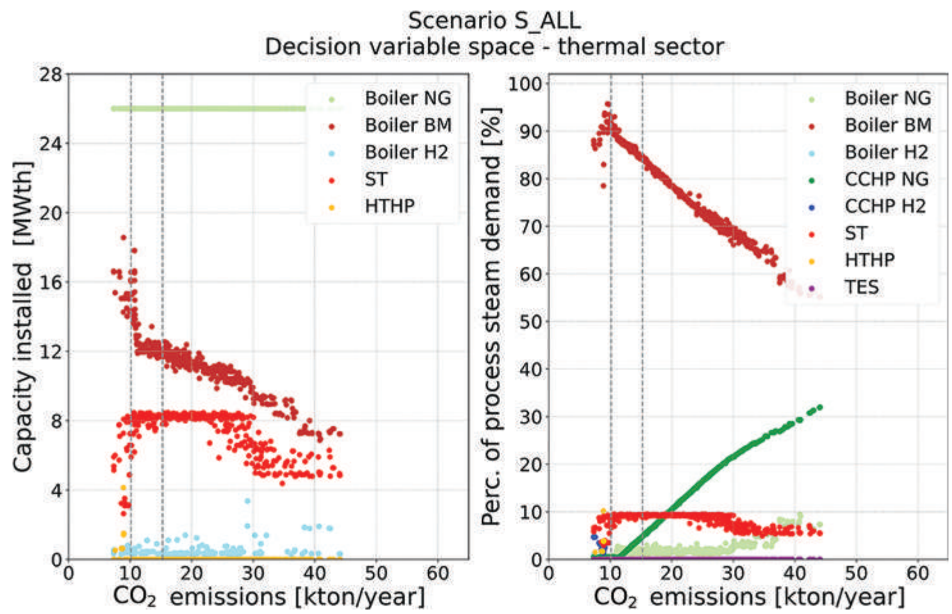

Figure 10: Analysis of the decision variables related to the thermal sector that characterize the Pareto-front solutions depicted in Figure 8. The left side shows installed capacities, while the right side displays weighted thermal energy quantities respect to the process industrial demand. The two vertical dotted lines highlight the annual CO_2 emission level where the Pareto optimal solutions show a change in the evolution trend.

emissions and costs for a specific configuration of technology capacities (i.e. decision variables). Consequently, understanding how the technology mix, and the related energy production, transforms with varying annual CO_2 emissions values is fundamental to the analysis.

The first stage of decarbonization can be interpreted as a "power plant mode", which involves a specific approach to the industrial site's operations. During this phase, the amount of carbon emissions decreases from 56 kton/year to 32 kton/year. The primary focus of the solutions is on maximizing electricity production, which exceeds by far the site's internal needs. The surplus electricity is then exported to the grid, generating profits. Although the capacity of the natural gas CCHP system decreases as decarbonization progresses, the capacity of the PV system remains unchanged. On the thermal side, there is a significant use of heat recovered from the natural gas CCHP, but the production of steam from a biomass source becomes increasingly dominant. Furthermore, solar thermal direct steam production consistently fulfills up to 6% of the demand. Thermal storage proves unnecessary, as all production can be seamlessly integrated into the relatively high demand with respect to the available area for solar thermal.

The second phase (between 32 kton/year and 11 kton/year) of the decarbonization evolution highlighted by the Pareto optimal solutions, shows the reduction of the capacity installed of the CCHP below the threshold of 10 MWel, which approximately coincides with the average process electricity demand. As a result, there is a notable decrease in the export of electricity compared to the previous phase. However, in this phase, the export remains almost constant, sustained by the PV system generating surplus electricity during production hours. It is worthwhile to mention that this set of solutions does not adopt any electrical energy storage. Instead, it addresses the electricity shortfall from CCHP by increasing the import from the network. Decarbonization also proceeds thanks to the lower emissions associated with grid electricity (with a RES and nuclear share of up to 54%, refer to supplementary material for details). During the same phase, on the steam domain side, measures were observed to compensate for the capacity reduction of the CCHP system. These measures include maximizing the solar thermal usage according to the available area and increasing the share of the biomass boiler.

The last phase of the decarbonization process is characterized by a notable acceleration in the cost increase compared to the progress made in reducing CO_2 emissions. This heightened cost trajectory is primarily driven by the introduction and escalating capacity of BESS, strategically installed to enhance the self-utilization of PV system energy, concurrently reducing both import and export.

The demand for steam is fulfilled through the synergistic use of solar thermal and biomass boiler, with a substantial contribution from the latter, satisfying up to as much as 90% of the demand.

4.4 Scenario S_NOBM

By forcing the framework to solve the optimization problem without relying on biomass-based steam generation, the second scenario is realized. Figure 11 and

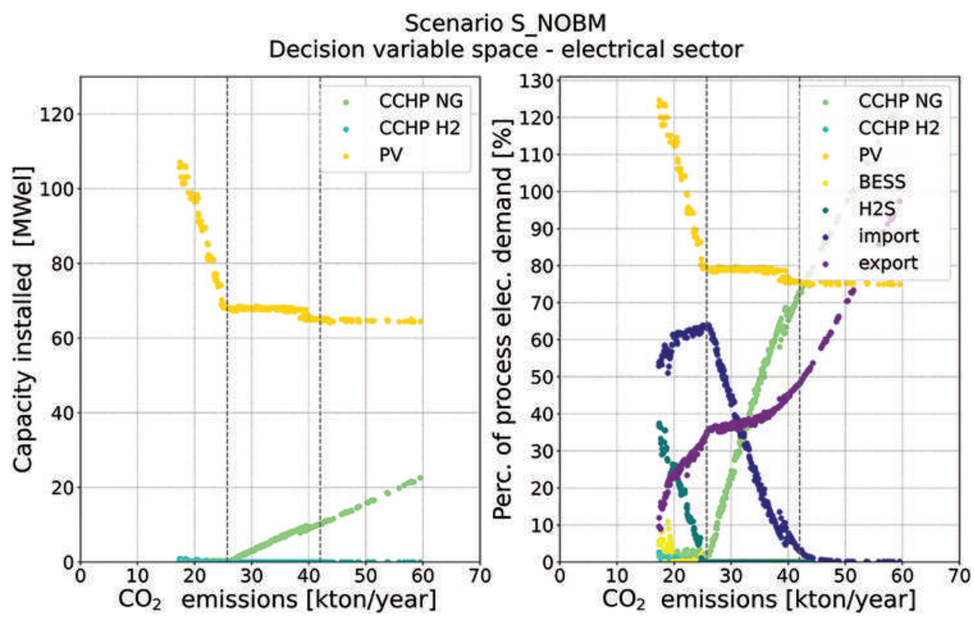

Figure 11: Analysis of the decision variables related to the electrical sector that characterize the Pareto-front solutions depicted in Figure 8. The left side shows installed capacities, while the right side displays weighted electrical energy quantities respect to the process industrial demand. Since export is allowed, total energy generation may not be equal to the industrial demand. The two vertical dotted lines highlight the annual CO_2 emission level where the Pareto optimal solutions show a change in the evolution trend.

Figure 12 show the technology breakdown and the energy production versus the annual CO_2 emissions.

The first phase of decarbonization in the electrical domain shows the same behavior described above for the first scenario. It's crucial to emphasize that this initial phase of decarbonization not only results in increased emissions but also incurs higher costs compared to the S_ALL scenario. This underscores the pivotal role of biomass-based decarbonization in the thermal sector.

The second phase of decarbonization evolves with very similar characteristics to those of scenario S_ALL. In fact, the CCHP phase out proceeds, reducing the export of electricity and increasing the import. A notable aspect of this phase is the slight increase in installed PV capacity, accompanied by a consistent decline in electricity export. In fact, the surplus electrical energy is used by the heat pump to increase its contribution to the production of steam in the thermal domain. After the step increase at around 38 kton/year of CO_2 emissions, the production of steam from the heat pump remains constant and the share covered by the CCHP's waste heat is replaced by the natural gas boiler. This result indicates that it is not advisable to increase the share of the HTHP in this region of the Pareto front. Decarbonization is carried forward by a more subtle detail. The combined evolution on the thermal and electrical sides results in an overall annual CO_2 emissions reduction, thanks to the fact that lower emissions are associated with the national energy mix.

In the third phase, after the phase out of the CCHPs, a more complex and coupled (between electrical and thermal domain) evolution of the technology mix is observed. The driving factor of this phase is the reduction of electricity import from the grid and its associated emissions. To achieve this goal a growing penetration of the storage is observed with a coupled rise of the PV installed capacity. Electricity export is also on decline, testifying a push to increase self-utilization of the PV electricity. This emission-free electricity fosters the decarbonization of the thermal sector by increasing the penetration of hydrogen boilers and high temperature heat pumps, proposing an intriguing hybrid solution. Bringing attention to the installed capacities in the thermal domain, the apparent local dispersion of solutions highlights the ongoing competition between technologies, with no singular solution standing out as the definitive choice for advancing decarbonization. This aspect showcases the complex interplay of efficiencies and costs in the trajectory of decarbonization progress.

It is also evident the priority given by the optimal set of solutions to heat decarbonization, with respect to the electrical domain, identifying it as a more cost-effective route.

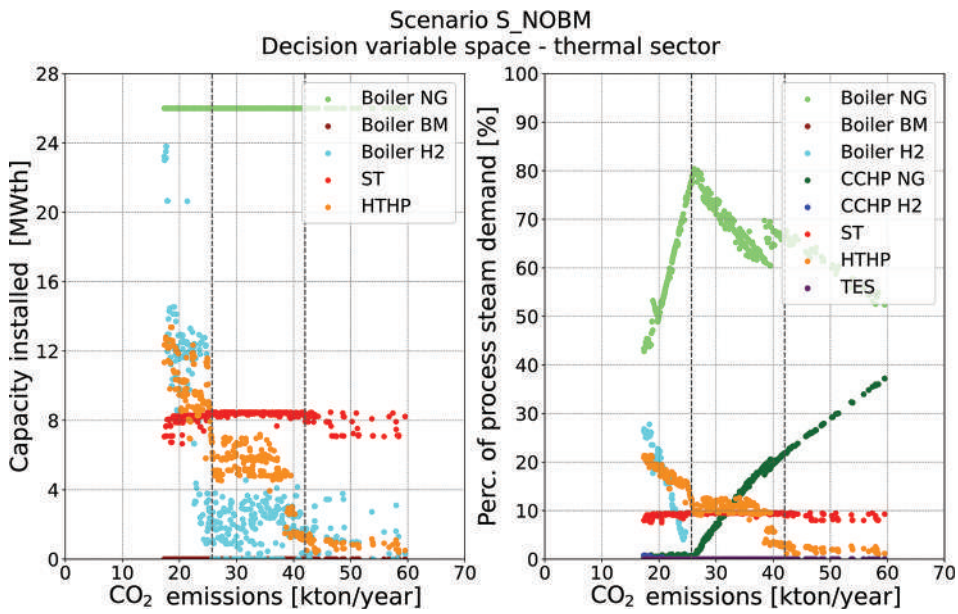

Figure 12: Analysis of the decision variables related to the thermal sector that characterize the Pareto-front solutions depicted in Figure 8. The left side shows installed capacities, while the right side displays weighted thermal energy quantities respect to the process industrial demand. The two vertical dotted lines highlight the annual CO_2 emission level where the Pareto optimal solutions show a change in the evolution trend.

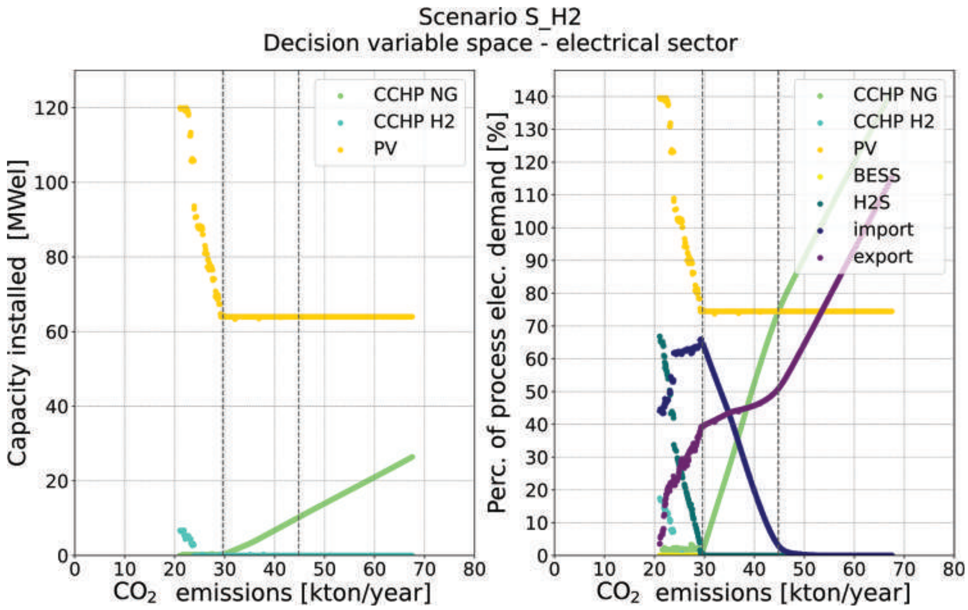

Figure 13: Analysis of the decision variables related to the electrical sector that characterize the Pareto-front solutions depicted in Figure 8. The left side shows installed capacities, while the right side displays weighted electrical energy quantities respect to the process industrial demand. Since export is allowed, total energy generation may not be equal to the industrial demand. The two vertical dotted lines highlight the annual CO_2 emission level where the Pareto optimal solutions show a change in the evolution trend.

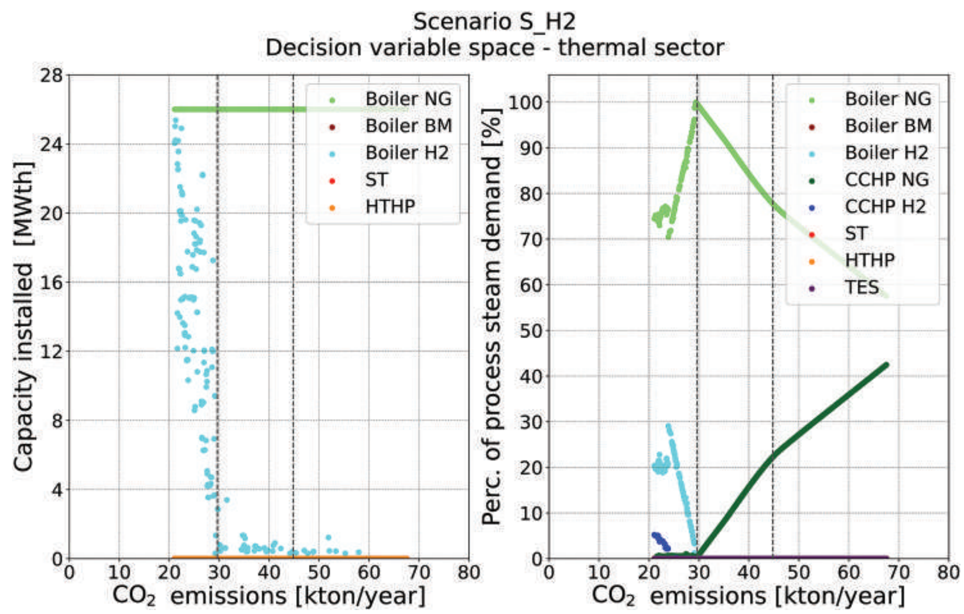

Figure 14: Analysis of the decision variables related to the thermal sector that characterize the Pareto-front solutions depicted in Figure 8. The left side shows installed capacities, while the right side displays weighted thermal energy quantities respect to the process industrial demand. The two vertical dotted lines highlight the annual CO_2 emission level where the Pareto optimal solutions show a change in the evolution trend.

4.5 Scenario S_H2

In order to analyze how a green hydrogen-based decarbonization performs, in this scenario the proposed framework is only able to implement hydrogen solutions to solve the decarbonization problem. The evolution of the technology mix versus the annual CO_2 emissions is given in Figure 13 and Figure 14.

Decarbonization phases one and two are characterized by the same “actions” described for the two previously commented scenarios, in fact there is the phase out of the CCHP accompanied by the increase of electricity import on the electrical side and in the natural gas boiler production on the thermal side. The third stage coincides with the attempt to reduce the import of electricity from the grid and avoid related emissions. Consequently, there is an observable trend to increase the installed capacity of the PV system and to store the excess electricity as hydrogen, reducing the export of electricity. Hydrogen is used in the first part of the third decarbonization phase to produce steam and in the second part it is also used as fuel for CCHP. Decarbonization advances with high total annual cost results that importantly deviate from the other two scenarios already described. However, the achievement of the maximum capacity for the PV system, derived from the area available, stops any progress toward decarbonization. In this scenario there is a pronounced need for space to integrate a very high-capacity PV plant, which can sustain the significant energy surplus demand resulting from the adoption of hydrogen-based technologies in both the electrical and thermal sectors.

4.6 Cross-scenario considerations

When examining the outcomes of the initial decarbonization phase it is evident that Pareto front solutions share a consistent operational pattern in their interaction with the electricity market. This operational mode can be accurately characterized as a “power plant” behavior, involving the significant export of both PV system and CCHP electricity production.

Comparing the results of the first decarbonization phase in all three scenarios, it can be observed that the industrial plant operates on the electric grid more like a power plant, exporting a gross part of PV and natural gas CCHP production. It is evident that in scenario S_ALL, in opposition with S_NOBM and S_H2, the crucial role played by technologies in decarbonizing the residual steam net of cogeneration and the strong impact of tackling that amount (pushing the Pareto front to the left). At this stage, only solar thermal proves to be economically advantageous for achieving emission savings, the other competing technologies result in too high costs and are implemented only in the following phases. Surely, it is essential to highlight the impact of electricity exports to the grid as an important source of revenue, especially from the PV system.

Advancing to the second phase, in conjunction with the phase out of the CCHP and the growing dependence on imports, it is evident from the Pareto front comparison (Figure 8) the impact that scenario-specific technologies on the thermal domain have on the total annual costs and on the decarbonization progresses. The absolute best performance according to the Pareto fronts is observed for biomass-based decarbonization, followed by heat pump-based solutions. The role of the storage emerges as a pivotal measure only in the third phase in all the scenarios, contributing to a very vertical development of Pareto fronts. The aim is to reduce the import of electricity and thus reduce its associated emissions, in order to advance in the decarbonization process.

4.7 Insights from literature comparison

This section deepens the comparison with existing research, highlighting both consistencies and areas of divergence, which shed light on the complexities and nuances inherent in this field, particularly when considering different scales of energy systems and diverse countries with varying energy vector prices.

Firstly, our findings corroborate several key observations made by previous studies regarding seasonal storage optimization [25], urban districts [35,36], a healthcare facility [24], and a refinery [32]. For instance, the importance of integrating RES, such as solar and wind, into the energy mix to achieve decarbonization targets while reducing operational cost is a consistent theme across various analyses. Similarly, the role of energy storage technologies, particularly battery systems and hydrogen storage, emerges as a solution that achieves significant CO_2 emission reductions, enhancing RES self-utilization, but comes with a substantial total cost increase.

Another noteworthy aspect is the efficacy of low and medium temperature heat pumps as a sector coupling cost-effective solution in decarbonizing heat demand up to 90°C [24,25,36]. This result also emerges in the SUANFARMA case study with the MTHP connected to the district heating of Rovereto. However, also HTHP plays a central role in highly decarbonized optimal solutions, such as in the S_NOBM scenario. Specifically, in our case study, for the HTHP dedicated to direct steam production at 165°C there is a noticeable cost increase due to a lower coefficient of performance, low local RES production, and high electricity vs gas price ratio. As observed by De Maigret et al. [32] and reaffirmed in our study, biomass plays a crucial role as a cost-effective solution for heat decarbonization. However, as previously discussed, verifying the existence of a large-scale biomass supply chain poses significant challenges.

Nevertheless, our study reveals certain discrepancies compared to earlier research. Specifically, our study considers four different energy demands from the demo site, including two heat loads. Here, the impact of high-temperature steam demand on overall emissions becomes evident, emphasizing the pivotal role of solutions and technologies capable of reducing such demand. Additionally, our study highlights the significance of solar thermal, a factor not considered prominently in previous research due to limitations associated with available area and geographical factors.

5. Conclusions

In this analysis for the decarbonization of a pharmaceutical industry, a sustainability assessment is conducted for SUANFARMA using the innovative framework proposed. The successfully developed energy system model simulates the integration of up to thirteen technologies over a full year of operation on an hourly basis and consequently, the optimization framework identifies a set of Pareto optimal solutions in terms of total annual costs and annual CO_2 emissions.

The study unfolds in three key steps. Initially, the focus is on data collection, with the FLEXIndustries project instrumental in enabling an in-depth analysis of processes and energy requirements. The project's diligent efforts have laid a robust foundation, fostering detailed examinations and the derivation of a coherent energy system model. Concurrently, a thorough analysis identifies the most suitable technologies, considering feasibility aspects and evaluating their compatibility and effectiveness within the industrial system. The second step involves designing and implementing the Python-based energy system simulation model for the industrial case study. In the final step, the energy system model is integrated with the MOEA.

Three scenarios are proposed to deeply investigate beneficial results in the integration of a hybrid energy system that relies on multiple generation and storage technologies. A key result of this work is the comprehensive design and subsequent implementation of the energy system simulation model, tailored to address the complexity of the industrial energy system, without losing generality by not considering sector coupling. Operating on an hourly basis, it intricately manages the interplay between various energy sources and demands. Upon scrutinizing the outcomes across various scenarios and figures comparisons, a discernible trend emerges. Firstly, it becomes apparent that achieving highly decarbonized scenarios is primarily feasible when there is access to a consistent source of biomass, as exemplified in the S_ALL scenario. In contrast, scenarios like S_NOBM and S_H2, where a reliable biomass source is lacking, show that alternative renewable sources of heat and electricity, such as PV, HTHP, hydrogen-based technologies, and concentrating solar thermal have a remarkable decrease in economic competitiveness as the process of decarbonization advances. In these scenarios, despite significantly increased costs, the pursuit of decarbonizing the thermal domain is underway, with hydrogen-based technologies and heat pumps taking the forefront. Intriguing synergies are emerging in hybrid scenarios. This dynamic is particularly elucidated by considering the tightening limit of availability of areas that burdens on the industrial site, forcing it to strongly rely on electricity from the national grid.

These critical considerations underscore the necessity of a more expansive perspective, capable of accommodating capital-intensive and land-intensive technologies. This underscores the significance of fostering a regional-scale approach to optimize the generation and storage of RES electricity. Equally important is the capability to test and demonstrate the resilience of these systems to their inherent variability. In navigating the complexities of achieving a carbon-free electricity landscape, collaboration and coordination across multiple entities within a region emerge as an implicit result.

This study does not claim to serve as a definitive solution to the intricate and multifaceted challenge of energy transition, especially within energy-intensive industries. Rather, it provides a tool for comprehending the optimal techno-economic-environmental solutions identified by the optimization framework. Undoubtedly, the limited analysis undertaken on factors such as demand variability, variable RES production, and techno-economic parameters results as a limitation of the present study. Nonetheless, it serves as a clear pathway for future research endeavors. Specifically, leveraging the adaptability and flexibility inherent in the developed model, there is an opportunity to bolster the robustness of the results. Furthermore, there exists potential for refining and enhancing a methodology to analyze the sensitivity and resilience of a set of optimal solutions.

Acknowledgements

This manuscript is an elaboration and extension of some preliminary results presented at the 9th International Conference on Smart Energy Systems, Aalborg (DK), 12-13 September 2023. This research has received funding from the European Union's Horizon Europe research and innovation program under the project FLEXIndustries, grant agreement N° 101058453. The authors would like to acknowledge the European Commission for the support granted to FLEXIndustries. The authors are grateful to SUANFARMA Italia S.p.A. for the support during the data gathering and modeling activities.

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