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Exhaustive Generation of the Complete Multidimensional Pareto Front for Multi-Objective Process Network Synthesis

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In sustainable systems design, optimizing complex process networks often involves multiple conflicting objectives, such as minimizing cost, reducing environmental impact, and maximizing performance. Traditional single-objective optimization methods frequently fail to address this complexity, resulting in suboptimal and inflexible solutions. This study focuses on a comprehensive approach to multi-objective optimization for a single fixed process structure, where all integer decisions are predetermined through a prior process synthesis phase, such as the Solution Structure Generator algorithm from the P-graph framework. The remaining task involves optimizing continuous parameters—specifically, the operational volumes within the network—to generate the complete Pareto front, representing all non-dominated solutions. Each objective function is assumed to be a linear function of operational volumes, allowing for a scalable mathematical formulation. An algorithmic framework is developed to address the challenges associated with generating infinite-point Pareto fronts in high-dimensional spaces, incorporating genetic algorithms, machine learning models, and the P-graph methodology. This hybrid approach supports dynamic adaptation to changing data and improves computational efficiency. The methodology is demonstrated through a case study. The example highlights how balancing cost and environmental criteria using Pareto optimal solutions leads to more sustainable system designs. Ultimately, this work underscores the practical importance of generating and evaluating the complete set of Pareto optimal solutions in sustainable system design. Moving beyond a single optimal configuration, the proposed methodology offers robust decision support across diverse industrial applications, bridging the gap between theoretical optimality and real-world implementation.

1. Introduction

The global transition to sustainable and resilient energy systems increasingly relies on integrating multiple renewable resources through hybrid renewable energy systems (HRES). These systems aim to mitigate the intermittent and variable nature of single-source renewables, such as solar and wind, by combining them with other energy sources and storage solutions to enhance system stability and reliability (Guo et al., 2018). However, the design and operation of HRES involve multiple conflicting objectives that must be simultaneously addressed through robust optimization techniques. Traditional single-objective models fail to capture the inherent trade-offs in such complex systems, often privileging one metric at the expense of others. In contrast, multi-objective optimization (MOO) techniques have emerged as indispensable tools in HRES planning and operation. They allow stakeholders to explore a spectrum of non-dominated, Pareto-optimal solutions in which improvements in one objective necessitate compromises in another.

Recent studies illustrate the growing sophistication of MOO frameworks in energy system design. Cheraghi and Jahangir (2023) developed a comprehensive MOO framework using NSGA-II and MOPSO algorithms to optimize an autonomous hybrid energy system that integrates PV, wind, heat pumps, fuel cells, and batteries. The optimization targeted four key objectives and demonstrated how varying trade-offs influence system composition and renewable energy fraction. Similarly, Jaszczur et al. (2020) optimized household-scale microgrids. They showed that cost-focused objectives favor smaller system sizes with lower investment, while environmental priorities lead to higher renewable penetration but increased costs. Zhou et al. (2020) introduced

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a building-vehicle energy sharing network that employed the Pareto archive NSGA-II to optimize cost, emissions, and energy flexibility. The study highlights the role of energy interactions in enhancing overall system robustness. In the commercial building sector, Ren et al. (2021) applied MOO techniques to optimize hybrid combined cooling, heating, and power (CCHP) systems for various building types. Their analysis incorporated solar PV, geothermal heat pumps, and thermal storage, showing that the optimal configuration and control strategy depend highly on building use profiles.

The field of multi-objective optimization (MOO) across diverse applications has been extended from energy systems to scheduling. Zhu et al. (2023) demonstrated the integration of solar, wind, and hydrogen storage with PEM fuel cells, optimizing cost, environmental benefits, and grid interaction in hybrid energy systems. Giannelos et al. (2024) analyzed Pareto frontier sensitivity in power systems, highlighting how operational characteristics shape economic–environmental trade-offs. Li et al. (2024) proposed a dispatch framework for integrated energy systems that incorporates regional time-of-use pricing and EV demand, advancing pricing-based multi-objective scheduling. Mahmoudi et al. (2025) introduced a gravitational search-based MOO approach, achieving improved Pareto convergence and evaluating carbon tax impacts on hybrid renewable energy systems. Babu and Girish (2024) addressed piecewise-linear trade-offs in scheduling, presenting methods to construct entire Pareto fronts rather than isolated points. Finally, Ehrgott et al. (2025) reviewed fifty years of MOO, emphasizing both mathematical programming and evolutionary approaches, with a focus on techniques that recover or approximate entire Pareto sets. Collectively, these works underline the methodological and practical importance of constructing full Pareto fronts, strengthening the motivation for the present study.

The present work introduces an algorithmic approach to integrated process synthesis and optimization, where alternative operations and equipment units are given as candidates in the design phase to construct the best energy supply system. Decisions are not only about including or excluding candidates but also about their optimal volumes. Due to complex process networks where alternative technologies can lead to the same goal, and the intervals of their feasible volumes or capacities result in infinitely many combinations of their parameters measured according to multiple objectives. The aim of the research presented is to provide a robust and computationally fast algorithmic solution resulting in the complete combined Pareto front for such process synthesis problems.

2. Problem statement

Typical optimization software usually offers a single optimal solution for a single objective function, often leaving other potentially viable solutions unexplored. As defined by Bertok and Bartos (2020), the process of generating locally optimal solutions involves constructing structures without any cheaper subsets, ensuring there are no useless elements. In contrast, the P-graph algorithm introduces a more nuanced approach by generating a complete set of locally optimal structures, specifically targeting cost optimization. These locally optimal solutions are defined as networks that do not contain any feasible sub-networks that could operate at a lower cost. This ensures that each solution is the best possible within the specific restrictions of the existing operational units.

The concept of local optimality is crucial in complex systems where interactions between different units can lead to multiple optimal solutions, each with its advantages and trade-offs. By broadening the scope beyond a single optimal solution, the P-graph algorithm accommodates the complexity of real-world systems, offering multiple solutions that are locally optimal. The current contribution aims at extending the solution generation to provide a complete set of Pareto optimal process structures and configurations according to multiple objectives, in addition to the previously available ranked list of N-best networks generated due to a single objective.

Pareto optimality is a fundamental concept in multi-objective optimization, particularly relevant in fields where decisions must balance conflicting objectives such as cost, emissions, sustainability, and reliability. A Pareto optimal solution is one where no other feasible solutions exist that could improve any of the given objectives without worsening at least one other. This means that each solution identified as Pareto optimal is incomparable to the others: better in at least one aspect and not worse in others, forming a set of equally optimal solutions under different criteria.

In practical terms, Pareto optimal structures are incredibly useful for scenarios where multiple factors need to be optimized simultaneously. For example, in environmental management, a Pareto optimal solution might balance the reduction of emissions with economic costs, providing a solution that minimizes impact without unsustainable expense. Similarly, in engineering, designing systems or networks that achieve Pareto optimality ensures that reliability and sustainability are maximized without incurring prohibitive costs or environmental damages.

The difficulty of Pareto front generation in engineering process design is due to the infinitely many feasible configurations of complex process structures to be explored algorithmically (Blaiech et al., 2023).

Table 1: Model parameters of the potential components of the electric energy supply system

Name	Capacity	*Investment cost [EUR/day]*		*Operating cost [EUR/day]*	
		Fix	*Proportional*	*Fix*	*Proportional*
Solar Panel	5 kWh/day	1,000	6,000		
Battery	5 kWh		2,500		
Generator	1 kW	1,500			18

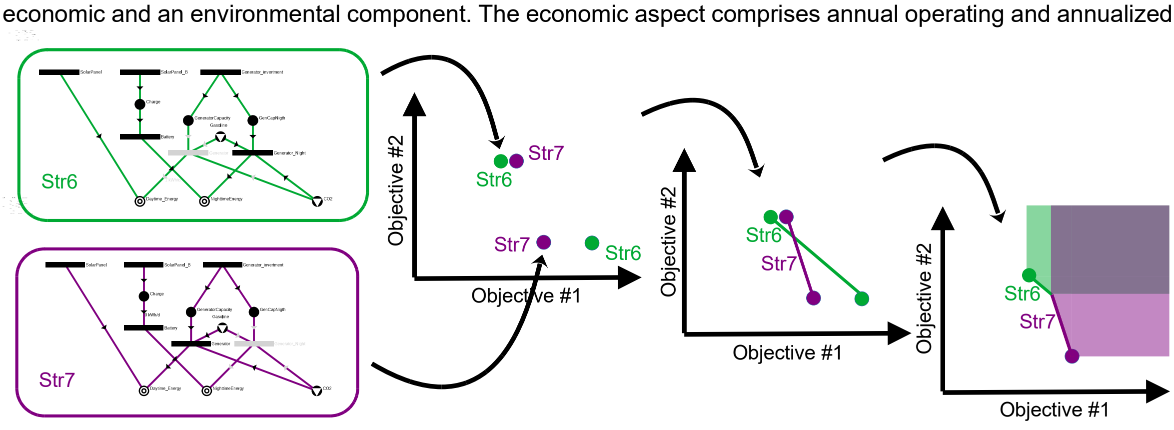
As a first step, a simple parametric model of the process network synthesis problem (Bertok and Bartos, 2020) is solved with two objective functions, i.e., an economic and an ecological. The illustrative problem of interest is the electric energy supply of a household, considering the cost and CO_2 emission of the operation of a combined energy system potentially consisting of a generator, solar panels, and batteries; see the model parameters in Table 1.

3. Method

In process synthesis, the design variables can be classified into two sets: existence variables expressing the involvement of components in a process structure and capacity variables defining the volumes of the operating units in a system configuration. The P-graph methodology is an effective tool to handle the structural part of the problem by providing a complete set of structurally feasible process networks by algorithm SSG for example; see Friedler et al. 2022. The advantage of parameter-independent model generation is that none of the potential structures is avoided. Each potential structure is to be examined due to each objective, while investment costs are paid as the price of flexibility.
The proposed process starts by generating all feasible structural combinations of components and connections within defined constraints; see Step a) in Figure 1. Next, each structure is optimized due to all possible orders of multiple objectives. This identifies optimal configurations under different goal combinations; see Step b) in Figure 1. Note that additional constraints are required to ensure that the optimization includes each operation selected during structure generation. Then, the optimal points are connected in a multidimensional space to cover the regions achievable by modifying the volumes of activities in the structure; see Step c) in Figure 1. Finally, only those parts of the achievable regions are kept that can contribute to the Pareto front, i.e., there is no other achievable region that is better from the point of view of all the objectives; see Step d) in Figure 1. As a result, the complete Pareto front is generated as a set of multidimensional regions achievable by at least one process structure. This provides insights into system behavior and supports strategic decision-making for maximizing performance.

4. Case Study

Figure 2 shows the relations among the potential system components depicted by P-graph. Daytime (5 kWh) and nighttime (2 kWh) energy demand is to be satisfied either by solar panels and batteries or by the utilization of the capacity of a generator. The two objectives follow the work of Isafiade and Short (2022), i.e., involve an economic and an environmental component. The economic aspect comprises annual operating and annualized



a) b) c) d)

Figure 1: Proposed steps: a) Structures b) Multi-objective extremes c) Feasible regions d) Pareto front

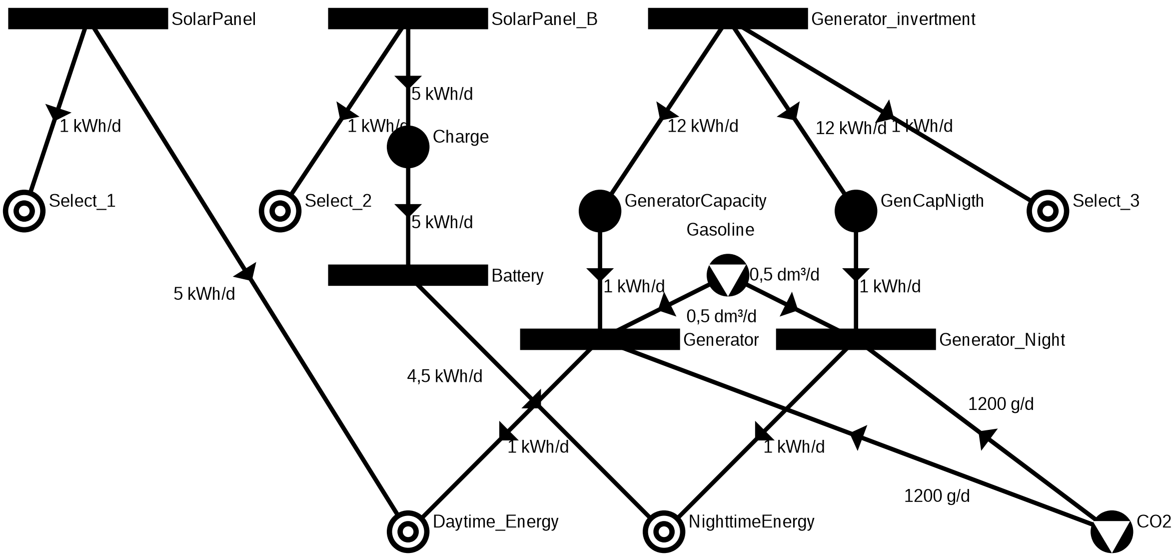


Figure 2: P-graph representation of the maximal structure for the case study

capital costs, while the environmental component is the CO_2 emissions. Cost parameters are defined as listed in Table 1. The CO_2 emission is modeled as a resource to be minimized in the network, since reducing greenhouse gas emissions is a primary sustainability objective in energy system design. Targets Select_1, Select_2, and Select_3 are potential targets during the structure generation, and are activated as required targets in the optimization phase only, to force the optimization algorithm to include all the operating units selected in the structure generation. Energy and material flows are represented in the initial network according to the reference capacities of the potential operating unit. The resulting cost–emission compromise represents a realistic basis for decision support in practice.

For the software implementation of algorithm SSG, a complete set of 9 combinatorially feasible process structures was generated, listed in Table 2. Each combinatorially feasible process structure has been optimized one by one according to both objective functions, i.e., to minimize the cost and the CO_2 emissions caused by the operation of the energy supply system. The optimization was performed using the free software P-graph Studio (P-graph.org, 2025). Initially, it was conducted based on cost parameters, and then, in a second round, a cost coefficient proportional to CO_2 emissions, which is three times higher than the cost parameters, was added to minimize emissions. The computation requires less than 0.1 s on a PC (Intel I5-8350U, 16GB RAM). Those structures providing a single option for daytime or nighttime energy supply have a single pair of cost-emission values. In contrast, complex structures with higher flexibility have the potential to be fine-tuned in a range of cost-emission value pairs; see Figure 3.

Table 2: The list of each combinatorially feasible process structure and the ranges of their objective values for the illustrative example

Structure	Gen. Night	*Gen. Day*	*PV*	*PV+Battery*	*Cost EUR/day*	*CO_2 g/day*
Str1	No	Yes	No	Yes	13.17	6,000
Str2	Yes	Yes	No	No	7.5	8,400
Str3	Yes	Yes	No	Yes	9 - 10	8,394 - 6,000
Str4	No	No	Yes	Yes	17.67	0
Str5	Yes	No	Yes	No	14.25	2,400
Str6	Yes	No	Yes	Yes	15.75 - 19.92	2,399 - 0
Str7	No	Yes	Yes	Yes	14.67 - 17.67	5,999 - 0
Str8	Yes	Yes	Yes	No	9 - 10	8,399 - 2,400
Str9	Yes	Yes	Yes	Yes	10.5 - 19.92	8,399 - 0

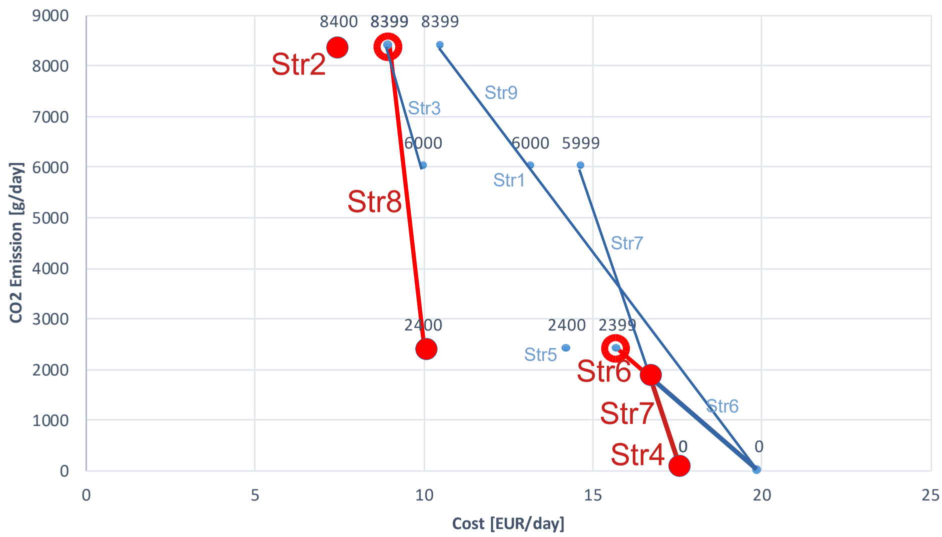


Figure 3: Ranges of cost-emission parameter value pairs of the feasible structures for the case study

Due to linearity, the cost and emission values as functions of volume changes of operating units in a fixed process structure, parameter ranges can be represented by line segments in the two-dimensional space of the cost-emission values. Structures Str1, Str2, Str4, and Str5 are represented by individual points, while structures Str3, Str6, Str7, Str8, and Str9 by line segments. Components of the Pareto front are highlighted in red, including structures Str2, Str4, Str8, and a limited set of configurations of structures Str6 and Str7. None of the configurations represented on the Pareto front has a better alternative from both objectives' point of view.

5. Results and discussion

The results reveal five distinct Pareto-optimal structures, each representing a different combination of available technologies. This illustrates that there is no single universal solution: depending on the relative importance of economic and environmental objectives, different structures may be preferred. Because both objectives are linear, the Pareto front consists of line segments, which makes the trade-offs transparent and facilitates decision support. The analysis further shows that the methodology can be generalized to more complex industrial networks, where multiple objectives would lead to higher-dimensional fronts, but the same principle applies. In the present case study, the explicit cost–emission compromise demonstrates how the method offers more insight than reporting only one optimal solution.

The illustrative example effectively highlights the importance of exhaustive generation of all the potential process structures in multi-objective optimization. Even for such a simple example, the single objective optimization would provide only the two extremes of objective values of structures Str2 and Str4. In contrast, systematic structure generation and optimization resulted in five structures with Pareto optimal configurations, each of which can be considered as a best choice under certain circumstances.

6. Conclusions

The proposed method utilizes P-graph algorithms in constructing the Pareto front of potentially achievable regions of the values of multiple objective functions during process synthesis. P-graph algorithms are demonstrated to be capable of both generating a complete set of alternative process structures and optimizing them according to multiple objectives while keeping in the structure all those operating units in the structure, which were selected in the first phase.

Complex structures, characterized by a high degree of freedom, typically cannot be fully optimized through single-objective approaches due to their inability to handle multiple competing variables and constraints effectively. Instead, these structures require an optimization process encompassing a wide range of possible decisions, captured through combinatorially feasible process structures. These structures account for the complete set of structural decisions, typically represented as integer variables, reflecting the various operational modes and configurations possible within the system.

By optimizing each structure across all possible combinations of objectives, one can determine the extreme points of operation. These points represent the optimal configurations under specific conditions and objective priorities, essentially capturing the best possible outcomes for each scenario. This multi-objective optimization ensures that all potential operational modes are explored, maximizing the structure's overall efficiency and effectiveness. The elements of the Pareto front, which are critical in multi-objective optimization, can then be algorithmically constructed from these extreme points. The Pareto front represents a set of solutions where no other solutions can improve one objective without worsening another, making it a vital tool for decision-making in complex systems. By analyzing these extreme points, one can algorithmically determine which configurations offer the optimal trade-offs among the objectives, outlining the Pareto front. It provides a clear visualization of how different objectives interact and what compromises must be made to achieve the best overall performance, guiding strategic decisions in complex systems optimization.
The illustrative example presented highlighted the efficacy and reliability of the proposed approach, rooted in the generation and then optimization of the complete set of each feasible process structure by P-graph algorithms. In contrast to only two best process structures of single configurations that could be provided by single objective optimization, the proposed method resulted in a complete set of five Pareto optimal structures with an infinite many feasible and Pareto optimal configurations among them, each of which is potentially achievable during their potential applications.

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