

Systematic design and analysis of an industrial symbiosis: Integrating power-to-X technologies with bioprocessing systems

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ABSTRACT

This research presents a vital framework for designing and evaluating the feasibility of industrial symbiosis projects. By employing the theory of Metabolic Analysis, the framework systematically assesses the synergistic potential of integrating novel bioprocesses, such as single-cell protein production, with Power-to-X (Pt-X) and carbon capture technologies. A case study application demonstrates the framework's capacity to uncover critical trade-offs in energy and waste streams, thereby providing a clear, data-driven foundation for creating circular manufacturing networks. Finally, the study underscores the necessity for continued development of the tool itself, specifically to create pathways for integrating its complex output data into subsequent techno-economic and life cycle assessments.

1. Introduction

The current state of global circularity is at a critical juncture, as highlighted in the 2023 Circularity Gap Report by Fraser et al. [6]. Despite significant progress in sustainable manufacturing, the global economy's circularity has decreased to a concerning 7.2 %, down from 9.1 % over the past six years. Additionally, global material usage has tripled since 1970, underscoring the need for advanced circular manufacturing techniques, especially with the projected increase in material extraction to 170 gigatons (Gt) by 2050. Circular manufacturing aims to create a sustainable economy by minimizing waste and maximizing resource efficiency. Bioprocesses play a crucial role in promoting these practices, offering innovative solutions to environmental challenges [14]. However, transitioning to a bio-based economy faces significant hurdles, including economic viability and scalability issues [3]. For example, Unibio A/S, a pioneer in protein

production through fermentation, struggles with economic competitiveness in Europe due to high manufacturing and workforce costs and excessive regulations. This has prompted Unibio to explore establishing plants in regions like Saudi Arabia, where costs are less [21].

These challenges can be effectively addressed through the concept of industrial symbiosis, where different industries collaborate to gain competitive advantages by exchanging materials, energy, water, and by-products, often facilitated by geographical proximity [4]. Simpler examples of industrial symbiosis include wastewater treatment plants and biogas plants, where waste and bio-residues from various factories are collectively treated to maximize resource efficiency [22]. In contrast, a complex example of industrial symbiosis is the integrated biorefinery in Zeitz, Germany, which showcases the potential for synergistic production of food and fuels, enhancing economic viability [13]. These biorefineries demonstrate the practicality of combining multiple production processes to create more sustainable and economically

Abbreviations: BDF, Biodiesel; CCSU, Carbon Capture Storage and Utilization; EC, European Commission; Env, Environment; Exp, Exportations; F-Matrix, Flow matrix; GLY, Glycerol; iMAT, Metabolic Analysis Tools; Imp, Importations; IP, Intellectual Property; IS, Industrial Symbiosis; KIS, Kalundborg Industrial Symbiosis; LCA, Life Cycle Assessment; MA, Metabolic Analysis; MeOH, Methanol; PEM, Proton Exchange Membrane; Pt-X, Power-to-X; RE, Renewable energy; SCP, Single cell protein; S-matrix, Stoichiometry matrix; SRL, Symbiosis Readiness Level; TLR, Technology Readiness Level; Uloop, Fermentation Reactor Technology used by Unibio; WCO, Waste cooking oil.

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feasible solutions. Another excellent yet prominent example is the Kalundborg Industrial Symbiosis (KIS) in Denmark. Over its half-century legacy, it has fostered efficient local problem-solving and cooperation, significantly contributing to Denmark's employment, local economy, and infrastructure development. These achievements have given KIS the recognition to be at the forefront of industrial symbioses in the world [22]. Despite the innovative efforts of KIS, Denmark's circularity remains at a mere 4 % [6]. This highlights the urgent need to enhance and adopt more effective circular manufacturing practices at a global scale to create a sustainable and thriving economy.

In the region of Zealand, in Denmark, a recent focus within industrial symbiosis is Power-to-X (Pt-X). In this region this technology is being studied to be integrated with bioprocesses to address mutual challenges and establish future partnerships and investments [10]. A class of Pt-X technologies convert excess renewable energy into hydrogen through water electrolysis, which can be used directly as an energy source or converted into products like methanol, ammonia, and other derivatives. Although not yet economically competitive compared to traditional fossil-based products, Pt-X technologies hold promises for more sustainable production of commodities and effective utilization of surplus renewable energy [16]. Recently, these systems were suggested to leverage biogenic emissions from bioprocesses while supplying oxygen and heat to electrolyzers, enhancing sustainability and efficiency [16]. Integrating Carbon Capture, Utilization, and Storage (CCUS) with bio-manufacturing further improves environmental impact by utilizing captured carbon for bio-production [7]. Nevertheless, according to Mucci et al. [16] only a few studies have analyzed the integration of Power-to-X with such processes.

Despite its potential and several opportunities, industrial symbiosis faces challenges, including infrastructure and resource limitations, dependency on key actors, time constraints, and legal issues like antitrust and IP protection rules. Strategies to address these challenges include establishing knowledge hubs and adopting facilitator roles to bridge partnerships and promote long-term investments [15]. Various frameworks have been proposed to aid the establishment of industrial symbiosis, ranging from simple checklists to complex decision-support tools for waste stream utilization [15,19]. However, no framework currently supports the integration of advanced technologies like Pt-X and CCUS within industrial symbiosis networks. This study aims to address the above-mentioned gaps and challenges by presenting a framework using Metabolic Analysis. The proposed framework is illustrated through the case of Unibio, a novel sustainable protein company, to analyze the synergy of Pt-X and CCUS technologies with Unibio's upstream manufacturing process.

This study investigates how collaborative processes and innovative technologies, such as Pt-X and CCUS, can address physical barriers, like resource allocation and infrastructure limitations, in the development of an Industrial Symbiosis (IS). It seeks to identify a method or framework that could support the integration of these technologies within industrial parks. The research is structured around two theoretical questions: (1) exploring the impacts of technology integration within IS networks and their effects on various outcomes; and (2) evaluating the applicability of the proposed framework to other technologies for effective decision-making. The development of the framework culminated in its application in a case study, which tested its capabilities and limitations. The workflow applied in the current study is illustrated in Fig. 1. The initial step was the creation of a robust database from a hypothetical industrial park. The database was created through literature studies, inventory data from real-life processes (i.e. Unibio A/S), and process simulation tools (e.g. ProII or ASPEN). The data was then processed by a method (metabolic analysis), which created an output database used to analyze the integration of the novel technology (i.e. Power-to-X) and the hypothetical industrial park. From a Process Intensification (PI) perspective, the proposed framework contributes by enabling the identification and implementation of tightly coupled industrial interactions that reduce energy and resource inefficiencies. Specifically, it facilitates the reuse of

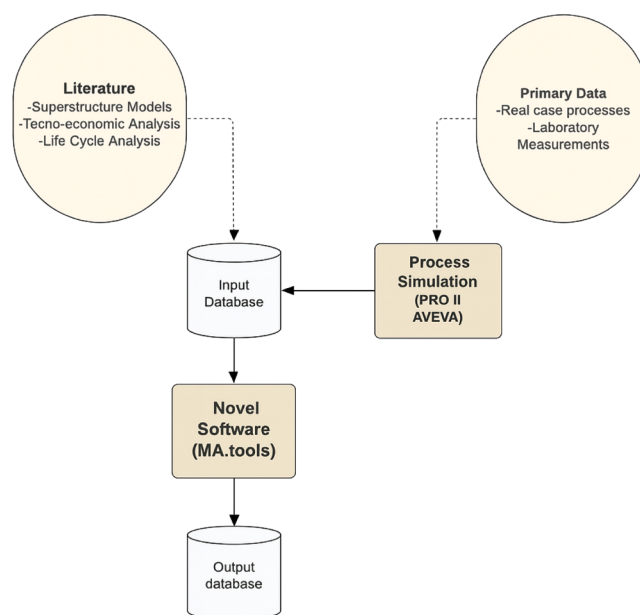


Fig. 1. Data flow diagram of current study.

by-products such as CO₂, heat, and oxygen within the industrial network, thus lowering the need for external utilities and enhancing circularity. The integration of Pt-X and CCUS technologies demonstrates that intensification can extend beyond equipment-level innovations to encompass system-wide improvements in material and energy flows. Additionally, the framework supports the generation of new symbiotic pathways, which minimize unit operations, promote multifunctional systems, and ultimately improve process performance and sustainability. The use of scenario analysis, decision gates, and simulation tools (e. g., MA.tools, ProII) within the framework allows for iterative exploration of alternative process configurations, providing actionable insights aligned with PI objectives. In this way, the study expands the scope of PI by proposing a structured methodology for network-level optimization that not only enhances operational efficiency but also supports strategic planning in industrial decarbonization and circular economy transitions.

2. The systematic framework

This work presents a simple decision-support framework to analyze the implementation of technologies in an Industrial Symbiosis (IS). The proposed methodology is generic, and it can be applied to different technologies with potential for enhancement of IS projects. The design of the framework took inspiration from the work of Silk et al. [19]. The framework is adaptable and can be applied to a range of technologies to enhance IS projects. An overview of the proposed systematic methodology is presented in Fig. 2.

The framework is explained in detail through four interconnected stage emphasizing strategic decision-making and implementation in the context of IS.- The framework starts with the selection of an industrial park and at least 1 technology that will be implemented within its boundaries. The purpose of the initiation step is to understand what challenges are occurring among the different stakeholders of the industrial park and how state of the art technologies might minimize them. Once novel technology is selected, the first interval is activated. The present case-study initiates on the step “*Technology Process Design*” considering the previous 2 steps were developed in a previous study [10].

Stage I: Needs Identification

The framework starts with a problem formulation definition. The problem needs to refer to a specific industrial park and new technology (new process) that will be incorporated within its geographical area. A

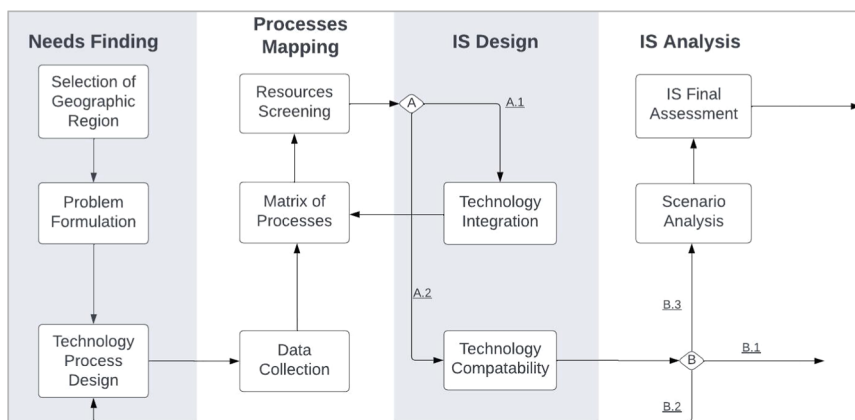


Fig. 2. Proposed Framework to analyze the integration of new technologies in industrial parks.

well-defined problem statement will allow us to select relevant technology and focus on important processes within the boundaries of the industrial park.

Step 1.1: Selection of Geographic Region

Here the geographic region is defined, in other words the actors that are involved and the system boundaries are stipulated.

Objectives: A certain geographic region is selected, all the industrial companies are mapped and tracked. The system boundaries are also defined, and certain *actors* within these boundaries will be added (i.e. companies, factories, and any kind of manufacturing organisms).

Notes: During the selection of the involved actors consider public entities or facilitator enterprises like Kalundborg Industrial Symbiosis (KIS), Symbiosis Center of Denmark, or any other relevant entities that can have relevant information about all the industrial actors of the region.

Step 1.2: Problem Formulation

The core function of the framework is to formulate and structure the problem. This involves clearly defining the objectives and scope of the design challenge.

Objectives: Description of a problem faced by one or more companies that can be solved through a certain technology available in the market. More than one technology can be selected.

Step (1.2.i): Technical problems of one or more companies are outlined.

Step (1.2.ii): The possible solutions available in the market are analyzed. Available technologies, or even companies that are preparing to invest in new facilities are scoped.

Notes: Consider that not all technologies are relevant and suitable for this framework. Their technology readiness level (TRL) needs to be considered, as well as its capacity to be integrated in multiple processes simultaneously. The best example are wastewater system facilities, which normally are connected to multiple firms/processes.

A group of companies can have a problem in common that can be approached here. Consider that step (i) is not mandatory and can be ignored. For instance, a new technology can be initially selected without any knowledgeable benefit to the system. Eventually the framework will dictate what benefits this company/technology/process can have to the previous selected geographic region.

Step 1.3: Technology Process Design

After the technology is selected several design options are available. Initially, a certain process design should be selected, which will be changed later.

Objectives: Here the design of the novel technologies should be chosen initially based on the highest TRL available. There are several options on how to design a process, including the order of its steps, or even the portfolio of products that are produced.

Step (1.i): During the first iteration of the framework the process design with the highest TLR should be chosen.

Notes: The framework will come back to this step on interval IV. Here, a different design of the process can be selected.

Stage II: Processes Mapping

Step 2.1: Data Collection

Objective: Collection of data for all the processes, which will be dependent on its availability.

Step (2.1.i): Primary and secondary data is collected for each actor within the system boundaries. Within a certain industrial system different process simultaneous exist

$$\text{processes} \leq v_i > \quad (1)$$

Where v_i is a vector containing the total number of processes present in the selected system boundaries (i).

Each process has a pre-determined functional unit, which is their main product(s).

$$\text{products} = p_m \quad (2)$$

Each process v_i has a vector p_m with the size of the total number of products that exports.

Usually, a facility has one main product, however its possible a certain facility/actor to have multiple products.

For each process all the input and outputs, which we call 'qualities' due to their diverse nature (substances and energy) have to be estimated. This includes importations, exportations, by-products and wastes/emissions.

$$\text{qualities} = q_n \quad (3)$$

Here n stands for all the qualities in the system. Every process has a vector q_n which in total comprise all of qualities present and turned over in the system.

Step (2.1.ii): Identify what of these processes (v_i) are obviously affected by the technology that will be incorporated within the system.

Notes: In a perfect world all data would be collected directly from companies, however this is never the case, making direct mapping of the whole industrial park unreachable. The flexibility of the framework allows the user to surpass IP protection barriers and use secondary data instead (e.g similar processes found in literature).

In this phase the industrial park is studied, and each factory/process is mapped. All the processes are analyzed based on primary or secondary data. Simultaneously, a literature search is performed on the selected technology and on its capabilities to be integrated with some of the processes within the industrial system.

Step 2.2: Matrix of Processes

For a comprehensive analysis of each section, various qualities are categorized into five groups: importations, energy, exportations, waste, and collocations. Detailed definitions of these groups can be found in the **Supplementary Material**. Each quality will be either exchanged within

the park (collocations), or with the reservoir outside the system boundaries (waste, importations, exportations and energy). Alluding to the network character of the system, we use the term **node** as the entity in which processes happen, i.e. *process nodes*, or virtual entities with which qualities are being exchanged, i.e. *reservoir nodes*.

Objectives: Organization of the collected data considering the environmental networks within and between nodes. Including the qualities that are exchanged across the system boundaries with the background system (reservoirs and suppliers outside the system boundaries).

Step (2.2.i): transfer the data from process v_i into a matrix.

Every numerical value of a certain quality (q_n) used in a certain process (v_i) is register in a matrix. Defined as stoichiometric matrix $S_{j,k}$.

$$j = 1, 2, \dots, n \quad (4)$$

$$k = 1, 2, \dots, i \quad (5)$$

Here, j refers to the qualities and k to the different kinds of processes within the system.

Step (2.2.ii): continue with process v_{k+1} until all data is stored and organized in the matrix. Once all the data is stored the user has completed the first data group defined as **S0** (the reference system structure). It is defined as:

The **S0** represents the industrial park without the integration of the new technologies.

In the first iteration the framework is run without any technology integration. Here, none of the processes have interactions with the new technology.

Step (2.2.iii): In this step the user will document the flow of qualities for every node. All qualities need to be assessed and their flows documented. Environmental networks between each process are documented and their flow needs to be tracked. Importations, exportations, and waste production must be tailed.

For instance, if a certain process consumes local methane from a biogas plant this will be tracked numerically between the two nodes and is defined as a transboundary flow. Similarly, if a certain quality comes or goes out of the system it's also considered a transboundary flow. All of this is documented, and each transboundary flow (t) should be differentiated considering if it's between nodes (t_w) or outside the system, which includes exportations (t_1), importations (t_2) or waste (t_3).

$$t = (t_1, t_2, t_3, \dots, t_w) \quad (6)$$

t is a vector with different types of transboundary flows. The value t_w can also be defined as an environmental network. In other words, it's a transfer of a certain quality between two nodes that are inside the system boundaries. Each quality will have w transboundary flows, depending on the integrability level of the process node which is part of.

Overall, its relevant to specify what type of transboundary flow each quality suffers within a specific process v_i . For instance, a certain quality q_n can have different applications within the industrial system: part can be wasted, exported, or even exchanged as an environmental network. This means each quality within a certain process v_i , will have a specific vector t that respects the following operation.

$$\sum_{t=1}^w t = 1 \quad (7)$$

The vector t in Eq. (7) represents the **proportions** or **fractions** of a specific resource q_n allocated to different pathways. The condition expressed in Eq. (7) is a fundamental mass balance requirement. It ensures that all fractions of a resource are fully accounted for. For example, if 60 % of a resource is imported ($t_2 = 0.6$), 10 % is wasted ($t_3 = 0.1$), and 30 % is exchanged internally ($t_w = 0.3$), the sum is 1.0. This guarantees that 100 % of the resource's flow within that process is documented, preventing any artificial loss or creation of the resource in the model.

Step 2.3: Resource Screening

From the previous organized data collection, specific processes and qualities are identified among the whole park as relevant to increase the circularity of resources within the system.

Objectives: Selection of the processes to be integrated with the novel technology.

Step (2.3.i): The processes of the control scenario (S_0) and the novel technology are characterized in terms of resource mapping.

Step (2.3.ii): The 2 groups are then compared for all types of qualities (i.e raw materials, waste, energy). This allows the user to list all the relevant qualities used and wasted by the newly selected technology and S_0 .

Step (2.3.iii): Move to decision gate A based on step (ii) findings. In this gate it will be sorted what processes from S_0 need to be integrated with the new technology (see next section).

Notes: This step is critical to differentiate the different processes and qualities. Their relevance for the integration of the novel technology and potential to enhance the circularity within the park needs to be fully accessed. Only this way, process and quality hotspots can be identified within the complex system that embeds them.

Stage III: IS Design

This framework section encompasses three distinct groups: the industrial park itself, the integrated technologies, and the background system (reservoirs), which includes all qualities entering and exiting the system. The goal of step III is to construct the new system based on all previously collected data.

Decision gate A is created to decide how technology integration will be conducted. From all the available processes some should be integrated through process simulation tools, while others could simply be based on previously conducted literature studies. Thus, the decision is based on the novelty of integrating the technology with the other processes.

Step 3.1 (Decision Gate A.1) - Technology Integration

After a complete resource screening is performed, the user has identified what qualities can be integrated between the technology and the industrial system.

Objective: Integration of the technology with the industrial system.

Step (3.1.i): Considering the results from the *Resource Screening* step, the relevant processes v_i are selected.

Step (3.1.ii): The selected processes v_i are analyzed in terms of changes to be integrated with the novel technology (see notes).

Step (3.1.iii): After the technology is completely integrated with the industrial system a new data group is formed and stored in a new similar matrix (similarly as the control group). This group is the initial scenario (S_1), defined as the group that has

The obvious environmental networks between the technology and the industrial park

Notes: The integration of the novel technologies with the different processes can be done based on previous conducted literature studies. In case the type of integration is not available in literature the user should use simulation software that will generate the necessary data.

This step can also be used to create environmental networks between processes within the system that are not the novel technology, which were unknown before the framework was used.

Step 3.2 Decision (Gate A.2) - Technology Compatibility

Once the initial scenario (S_1) is constructed, new symbiotic network links are designed and implemented. This means new collocated interactions were incorporated in the park, while the total park imports and probably waste production decreased. Based on the new designed collocated links the compatibility between the new technology and the industrial park is constructed qualitatively.

Objectives: Assess the impacts of the technology integration.

Step (3.2.i): If possible, substance budgets and mass and energy balances of the integration between the processes and the new technology are analyzed in detail.

Step (3.2.ii): The last step is the analysis between the technology and the whole system. Here an analysis is performed on the effects that

the technology has on the total importations, exportations, collocations, and waste generation.

Notes: The compatibility of the technology was analyzed in two aspects. One related to specific processes, and another related to the whole park. The last step of interval III allows the user to broadly know the potential of the novel technology. Here the user has reached a STOP/GO point. This is assessed in the next interval in the decision gate B.

Stage IV: IS Analysis

The last section initiates with a decision gate (B). Gate B has 3 alternative exits, that are based on the new technology's capacities to generate IS networks. If the outputs suggest a lack of potential for the designed IS park, exit the framework (Gate B.1).

If the results show good performance indicators, the user has two options: to change the design of the newly selected technologies and create a new arrangement between the park and the technology (**Gate B.2**) or move to the next stage of the framework (**Gate B.3**). The purpose of the next 2 steps is to analyze the IS system considering metrics based on the initial problem statement.

Step 4.1 Decision (Gate B.2) - Scenario Creation (Re-run of the framework)

Objectives: The creation of different technology-park rearrangements, defined here as scenarios.

Step (4.1.i): Evaluate how many scenarios can be created based on the following points:

- A. Modifications to the design of the novel technology;
- B. Changes in the capacity of relevant processes and the novel technology;
- C. Changes in the industrial pathways;

Each scenario will be created by re-running the framework. They will have their own datapoints stored in individual groups of data, similarly to interval III groups (S_0 and S_1). Here, every new scenario will be defined as

$$S_{u+1} \quad (8)$$

Where u is the total number of scenarios created in interval IV.

Step (4.1.ii): Considering the previous 3 options to create scenarios, consider the following aspects:

- A. There are multiple ways to implement a certain technology. There are several process design options available, and the most developed and suitable options, for the industrial park region, can be compared. For instance, differences in resource use, energy consumption or even the final products portfolio can be iterated.
- B. The total capacity of a process can depend on multiple factors: market trends, supply chain bottlenecks and many more. By changing the capacity of specific processes or the novel technology its possible to quantify resource' availability limits, which can compromise the relevance of the technology to the park and vice-versa.
- C. Changes on industrial pathways are not always possible. This case is only relevant for cases where multiple environmental networks are available for a specific quality (q_n). For instance, a specific industrial park might have different methane sources.

Notes: In this step several scenarios can be created if they are comparable and relevant to the problem statement. This step is extremely relevant for technologies that have several process design options with different types of raw materials, waste, and final products portfolio (An example in the case-study is given for this specific case).

In this step newly designed rearrangements for the novel technology are proposed. Each new process design will be analyzed as individual scenarios.

Step 4.2 (Decision Gate B.3) - Scenarios Analysis

This section delves into a general analysis of the different scenarios

emerging within the potentials of the industrial park. The performance and integration of these scenarios within the industrial park are examined both individually and in comparison, to each other.

Objectives: To compare the different scenarios and determine the best option considering the initial problem statement. The primary objective of this analysis is to understand how different scenarios affect symbiotic exchanges within the park. This involves evaluating their impact not only in terms of resource flow and utilization but also considering how they enhance the overall efficiency and sustainability of the industrial ecosystem.

Step (4.2.i): Based on the Resource Screening step select part or all the relevant qualities and compare how their consumption/emission changes between the different scenarios.

Step (4.2.ii): Do the same analysis but for the total energy consumption of the park.

Notes: This analysis should highlight the interdependencies within the industrial park. It should specify which pathways can significantly alter the dynamics of resource flow, thereby impacting the park's overall symbiosis readiness and efficiency. Each scenario has a unique structure to be integrated into the industrial park. While some may contribute additional resources, others may discover co-benefits with existing processes in the park.

Step 4.3: IS Final Assessment

The final step of the framework is described below.

Objectives: To analyze the capacity of the technology and the sensitivity towards the industrial park performance parameters (importations, exportations, waste generation and collocations).

Step (4.3.i): Select one scenario to perform the final assessment.

Step (4.3.ii): Select different capacity values for the technology. They could be selected based on the problem statement or on future market predictions for the technology which can reveal limits and development potentials of the interacting industries. Careful consideration of the scope is advised, to keep the analysis within practical limits.

Step (4.3.iii) Perform iterations to the pathway vector accordingly to the selected capacities. Keep in mind bigger capacities of the technology might create changes to some processes. For instance, vector t (interval II – Matrix of Processes) must be updated according to the changes in the environmental networks.

Step (4.3.iv): Similarly, to the previous section select qualities to be compare among the different technology capacities. They should be based on the results of the *Resource Screening* section.

Step (4.3.v): Conclusions based on the different scenarios and capacity analysis, if the studied technology has the potential and capacity to influence the industrial park's and the region overall sustainability and economical metrics.

Notes: When enough data is compared and consolidated the framework reaches the end. A final decision must be made based on the results: what decisions, tools and methods are needed to proceed with the analysis to the IS network. Eventually LCA, TEA or other methods could be applied to the output data generated from this framework.

3. Software implementation

To facilitate the modeling and analysis of industrial symbiosis networks, a novel software tool, MA.tools, was developed in the R programming environment. This tool implements a Metabolic Analysis (MA) framework that conceptualizes industrial systems as stoichiometric networks of material and energy flows, analogous to metabolic pathways in biological systems. MA.tools automates the construction of stoichiometric matrices (S-matrices) and flow matrices (F-matrices), the definition of pathway vectors, and the generation of process- and quality-specific flow diagrams. These diagrams visualize how materials such as CO₂, H₂, O₂, and electricity are exchanged among industrial nodes and environmental reservoirs. Users input data through structured Excel files, detailing the functional unit of production and allocation of inflows and outflows. The tool allows for screening of

symbiotic exchanges, integration scenario development, and comparative evaluation of configuration alternatives. While MA.tools is currently under internal development, it has proven effective in identifying and quantifying exchange opportunities across PtX, CCSU, and bioprocess systems in this study. The software successfully performed a life cycle assessment of the environmental networks at the Kalundborg Symbiosis industrial complex [11]. Readers may inquire having access to the software by contacting the corresponding author.

3.1. Motivation for metabolic analysis

To analyze the complexity of biological organisms, specialists in the area of bioinformatics have emphasized the relevance of using mathematical models and computer-aided frameworks for the analysis of network-based pathways [18]. Just as for biological organisms, it is also useful and relevant to analyze the metabolism of industrial processes. Industrial ecology books have emphasized the relevance of such applications to understand the possible interactions between separated industrial systems [9]. The similarities between industrial and biological organisms shouldn't be interpreted as having a similar complexity for the applications of metabolic analysis. The industrial applications are focused on the substance, mass and energy flows of the system, while the biological gives more importance to the changes on metabolic pathways. Nevertheless, the industrial ecology field envisions the development of tools that map and control the dynamic use of resources of an industrial process and the surrounding industrial ecosystem.

Industrial pathways, such as the ones in KIS, can be modelled with a relatively low computational power compared to biological metabolic pathways happening inside microorganisms and between different cells. Overall, MA application in industry, translates into understanding and mapping the processes happening inside an industrial system and across its boundaries with the environment.

MA. tools facilitates quantitative analysis of substance, material and energy flows from diverse sources, aiding in identifying potential materials for reuse in industrial networks. It offers a quick means for quality screenings of extensive process databases. In this study MA. tools models various industrial pathways emerging from integrating Pt-X and CCSU technologies. Its flexibility allows for simulating different combinations of pathways and analyzing their impacts on individual nodes, the environment, and overall park performance.

3.2. Theory and overview

According to Graedel and Allenby, an industrial pathway is "the sequence of transformations that convert resources into final products". In other words, they represent the different processes required to produce a product or service. Similarly, a "metabolic pathway" occurs with the same purpose: to deliver a service to the cell or organism that embeds it. Taking Unibio production as an example, fermentation, recovery, purification, and packaging processes are required in order to obtain single cell protein (SCP). Ideally, if an industrial organism has to be studied through such theory, all inputs/outputs, including the material composition of the transformation processes (i.e. transformation from raw substances to product substance) must be simulated. This set of information can create the metabolic diagram of the industrial system.

For simplicity the metabolic diagrams developed in this study are organized in a stoichiometric matrix (S-matrix). To quantify the capacity of the industrial system's processes a pathway vector is required (p). Each row of the vector quantifies the desired product.

Fig. 3 presents a simplified example of a stoichiometric matrix (S-matrix) used in the metabolic analysis framework to represent the exchange of materials and energy—referred to as "qualities"—between industrial processes. Each column corresponds to a specific process, and each row corresponds to a quality, such as CO₂, electricity, O₂, or steam. The values within the matrix are stoichiometric coefficients indicating the magnitude and direction of the exchange:

$$s^T = \begin{bmatrix} A & B & C & D & E \\ -1 & +1 & 0 & 0 & 0 \\ 0 & -2 & +1 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & -1 & +1 & 0 \\ -1 & -2 & +2 & -1 & 0 \end{bmatrix} \cdot p = \begin{bmatrix} p1 \\ 2 \\ 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Fig. 3. Transposed stoichiometric matrix and pathway vector example.

- Negative values denote consumption of a quality (i.e., input to the process).
- Positive values denote generation of a quality (i.e., output from the process).

To enhance visual clarity, the matrix is shown in transposed form, placing qualities on the rows and processes on the columns, which makes it easier to observe how each resource is distributed across the different processes. This is a common convention in industrial ecology and metabolic network analysis when the reader is interested in the flow of specific substances.

The pathway vector defines the level at which each process is activated or scaled in a given scenario (e.g., normalized production of 1 ton of final product). When multiplied by the S-matrix it yields the flow matrix (F), which quantifies the net amount of each quality consumed or produced by the entire network.

$$S \cdot p = F \quad (8)$$

This formulation allows the systematic evaluation of multiple scenarios by varying process capacities and configurations, and provides a robust platform for identifying synergies among industrial actors based on shared resource flows.

To clarify the application of the pathway vector and the S-matrix in metabolic analysis, we provide a simplified example. Assume Process 1 uses 1 unit of quality A to produce 1 unit of product B. This transformation is reflected in the S-matrix with a -1 in the column for quality A (consumption) and a $+1$ for product B (production). If the pathway vector indicates that Process 1 is operating at a capacity of 2 units, then the resulting flow of each quality is obtained by multiplying the pathway vector by the S-matrix. In this case, the flow of quality A is -2 (2×-1), and the flow of product B is $+2$ ($2 \times +1$), which represent the total system-wide consumption and production. This allows tracing how much of each resource or quality is used and produced throughout the network. We have added a supplementary table with this numerical example to guide the reader step-by-step.

3.3. Implementation: MA.tools in interval II in the "Matrix of Processes" step

Since completing a metabolic matrix (S-matrix) for an industrial system might be an arduous task, the program should be designed to ease the data collection. Here, the data can be collected in digital systems like excel workbooks, that individually organize the information for each industrial organism/node. In other words, every company can have its own workbook with information about the transformations require to produce the service. The user will be required to fill in the sheet with information about each company: the v_i processes and the q_n qualities that are needed to deliver the final service. A table is individually constructed for each company, which the software should read and transform the data into one initial S-matrix. Below an example is given for a hypothetical table constructed for the company Unibio and their U-loop process to produce single cell protein, which is further explained in the case-study. Fig. 4

Notice the data is collected in terms of one functional unit, which

node	process	quality	flow	unit	reference	donor1	receiver1	f1	donor2	receiver2	f2	fsum
UNIBIO	uloop	protein	1.0000	kg	Unibio A.S	UNIBIO	exp	100.00%	-	-	-	1.00
UNIBIO	uloop	O2	-3.1373	kg	Unibio A.S	ELEC	UNIBIO	100.00%	-	-	-	1.00
UNIBIO	uloop	natural_gas	-1.5466	kg	Unibio A.S	BAS	UNIBIO	100.00%	-	-	-	1.00
UNIBIO	uloop	NH3	-0.1506	kg	Unibio A.S	imp	UNIBIO	100.00%	-	-	-	1.00
UNIBIO	uloop	electricity	-3.9812	MJ	Unibio A.S	imp	UNIBIO	100.00%	-	-	-	1.00
UNIBIO	uloop	heat	-0.0157	MJ	aveva	imp	UNIBIO	100.00%	-	-	-	1.00
UNIBIO	uloop	CO2	2.4783	kg	aveva	UNIBIO	CCSU	50%	UNIBIO	env	50.00%	1.00
UNIBIO	uloop	wastewater	8.8902	kg	NOT FOUND	UNIBIO	env	100.00%	-	-	-	1.00
UNIBIO	uloop	sulfuric acid	-0.9108	kg	NOT FOUND	imp	UNIBIO	100.00%	-	-	-	1.00
UNIBIO	uloop	phosphoric acid	-0.7622	kg	NOT FOUND	imp	UNIBIO	100.00%	-	-	-	1.00
UNIBIO	uloop	water	-6.1220	kg	NOT FOUND	imp	UNIBIO	100.00%	-	-	-	1.00

Fig. 4. Example of a possible input database table for the software.

should be the final product. In this case it's specify the flow of each quality. For instance, 50 % of the CO₂ of the process are treated to the node "CCSU" while the rest is emitted to the environment defined as "env" (highlighted in yellow) respecting the previously mention Eq. (7). This workbook needs to be updated to any changes on the industrial pathways, for instance if the CCSU node has a bigger capacity, more than 50 % of the CO₂ can be treated.

A similar workbook is also developed for the pathway vector. The pathway vector will be the vector p_m previously described in interval II. The total production capacity for each process will be defined in this vector.

3.3.1. Possible outputs of the software

The software collects the data from the matrix of processes and gives several outputs that the user can sort based on the objectives of the problem statement. The outputs are the following:

A complete an organized transposed form of the S-Matrix. Flow diagrams can also be generated for every process and quality showcasing the interactions between them and the rest of the industrial system (an example is given in Fig. 5). However, the main output of the program should be the flow matrix of the whole system (F-matrix), which is estimated based on the product of the pathway vector and the S-matrix.

These software outputs would engage with the framework in specific sections, mainly running the steps "Resources Screening" and "Scenario Creation".

Resources Screening

The identification of critical qualities and processes for the integration of the new technology and the park is possible by analyzing the flow diagrams. In Fig. 5 the two types of flow diagrams are showcase. The diagrams are both created for each quality as well as for each process. In other words, it gives the user a visual understanding of the flow of a specific quality, in the example below it showcases the flow of the

quality "succinic acid", and the qualities interacting with the node "UNIBIO" (more information available in the case study).

In Fig. 5 nodes correspond to industrial processes (e.g., SCP processes as "UNIBIO", PtX units as "ELEC"), utility providers (e.g., electricity grid), or environmental sinks (e.g., external reservoirs as "env") and importations (described as "imp") or exportations (described as "exp"). Connectors (arrows) represent the exchange of qualities—material or energy flows—between nodes. The directionality of each connector reflects the supplier–consumer relationship, allowing users to visually track how resources move through the network. This type of diagram supports the identification of material reuse opportunities, critical resource dependencies, and serves as a diagnostic tool for assessing the initial design of the industrial symbiosis system on stage III.

4. Application example

The case study examines two specific technologies, highlighted in a report by the European Commission, deemed essential for IS implementation [20]. The analyzed problem is based on the project "Power-to-X(PtX) Cluster Zealand" conducted by a consortium of companies based in the region of Zealand, Denmark [10]. The process capacities selected for the Pt-X technologies are based on the future electrolysis plant "Green Fuels for Denmark" in the region of Greater Copenhagen [5].

The initial phase of this Pt-X facility, projected to commence in 2025, has a planned capacity of 10 MW. The analysis also considers future projections, where electrolyzers with 250 MW and 1.3 GW capacity are expected. In this case-study the technology design of the Pt-X process is inspired in the plans detailed in the official project documentation. Initially, the focus is on hydrogen production for direct fuel applications (10 MW), followed by an increased capacity for methanol production (250 MW), and eventually introducing methane, although the official project aims to produce e-kerosene (1.3 GW).

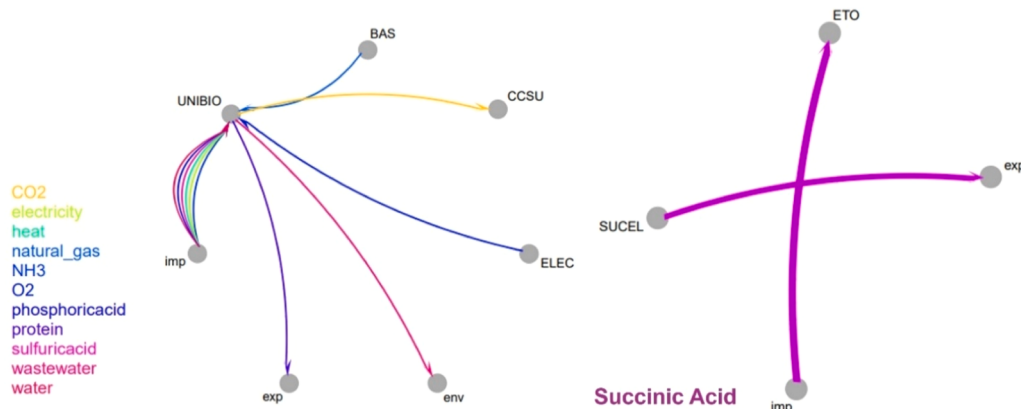


Fig. 5. Visual representation of the industrial symbiosis network generated using MA.tools. (Left: flow of all the qualities in 'GAS' node. Right: All the nodes that exchange the quality succinic acid).

Given the Intellectual Property (IP) concerns of companies about sharing process data, this study models an industrial park using data derived from literature. Detail descriptions of the selected processes, along with their data sources, are available in the supplementary material (Appendix B). In the following section the framework is applied in the case-study with the purpose to analyze its strengths, opportunities, and weaknesses.

Stage I: Needs Identification

The Needs Finding aspect was addressed in the “*Pt-X Cluster Zealand*” project, which led to the identification of a core problem: the competitiveness of bioprocesses and Pt-X technologies against fossil-based alternatives [10]. The selection of CCSU and electrolyzer technologies was pre-determined on this report. The oxygen delivery for protein production through electrolysis coupled with post-combustion CO₂ recovery is initially modeled in this work.

Step 1.1. Selection of Geographic Region

The current case-study does not have a specific geographic area since no interviews and data collection were performed to companies. The only exception is the company Unibio A/S that agreed to share information about its current process and technology. For this reason, most of the processes are based on literature studies. While more processes could have been selected, the purpose of this case study is to serve as an initial test for the framework’s capabilities and limitations.

Upon the successful integration of various technologies with the Unibio process, a comprehensive symbiotic network encompassing all the processes was methodically constructed and designed. The complete network is depicted in Fig. 6, illustrating a systematic approach to service delivery within the network. The diagram assigns distinct color codes to different industrial pathways. The methanol production route is indicated in orange, a bio-methanation route is in green, and the blue selects the original processes of the park connected to the initial proposed technologies (PtX and CCSU units). These color-coded streams represent strategic pathways for the utilization of pure hydrogen and capture CO₂ within the network. Further details on the various industrial pathways are provided during Stage IV as part of the scenario creation process.

The processes shown were selected based on their relevance for carbon valorization, green hydrogen use, and compatibility with Unibio’s microbial gas fermentation process. Arrows indicate material and

energy exchanges (e.g., CO₂, CH₄, H₂) between nodes. This overview reflects a synthesis of process simulation (from AVEVA PRO/II) and stoichiometric modeling via MA.tools, supporting scenario construction for evaluating integration alternatives.

Flowrates and scenarios in Table 1 were defined using a reference basis of 9009 ton of protein, and correspond to different configurations of process activation, captured through variation in the pathway vector p_m . The required flows for key services were determined as follows: hydrogen production was based on the oxygen consumption of the Unibio process, and pure CO₂ production was based on the purification of all exhaust gases. The remaining processes for Scenario 1 are based on the capacities of typical plants in Denmark. For more details, refer to Appendix B in the supplementary material. The process capacities for Scenarios 2 and 3 are explained in Stage IV.

Step 1.2. Problem Formulation

The current market of green hydrogen is facing issues to scale up the technology and compete with fossil fuel-based hydrogen. The *Pt-X Cluster Zealand* project suggests that bioprocesses and Pt-X technologies should be integrated and mutually benefit from a cost reduction. In what

Table 1
Process-Node pair and their capacity on the different scenarios (0-3).

Node Name	Process (v_i)	Scenarios				Units
		0	1	2	3	
SUCEL	Biodiesel	87,500				
SUCEL	Succinic acid	1,000				
GAS	Biogas	91,400				
BAS	Methane Scrubbing (CH ₄ production)	35,900	22,633	35,900		
ETOH	Wheat production	71,500				
ETOH	Ethanol	17,900				
ELEC	Electrolyzer (H ₂ production)	-	3,520			
CCSU	Amine Scrubbing (Pure CO ₂ production)	-	56,500			
MEOH	Methanol	-	-	-	17,700	
BAS	Biomethanation (CH ₄ production)	-	-	20,000	-	

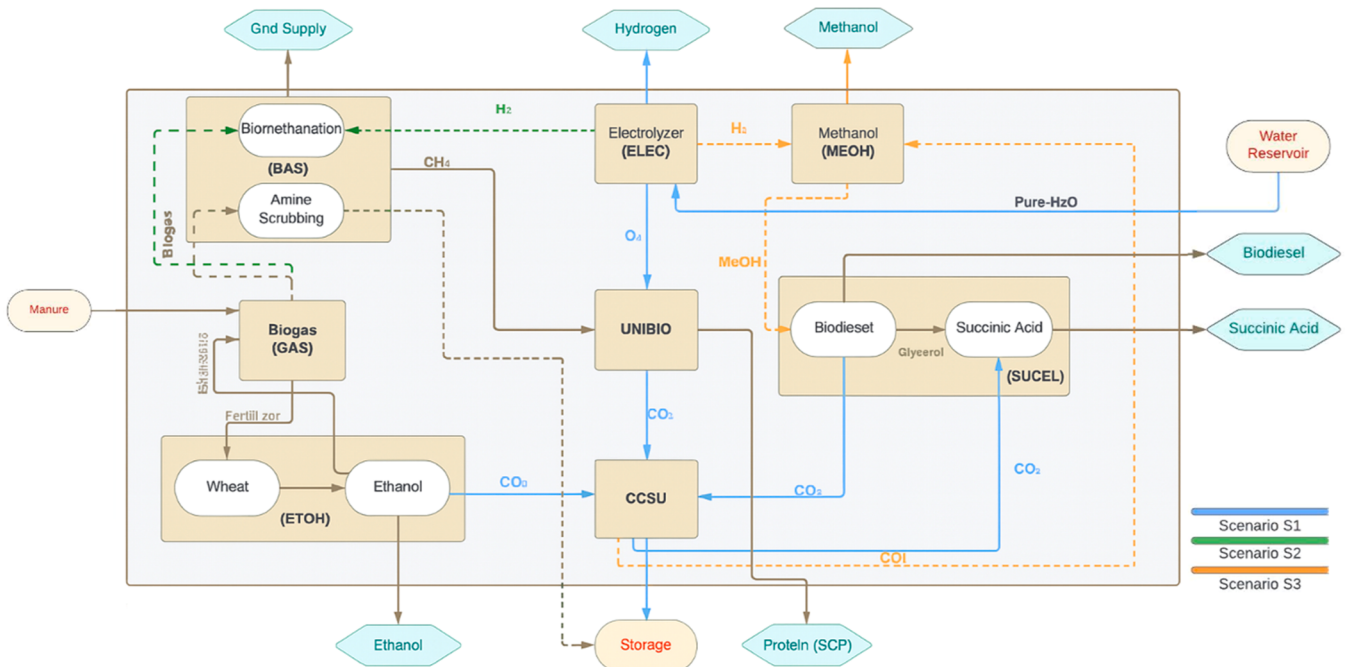


Fig. 6. Conceptual diagram of the integrated industrial symbiosis network considered in this study.

ways can this integration be performed in the previous presented industrial park? Can the previously proposed framework find ways from different alternatives to optimally integrate the Pt-X process within the industrial system given a predefined goal?

An in-depth analysis will be conducted on the process used by Unibio for protein production, assessing how Pt-X and Industrial Symbiosis (IS) might positively influence its efficiency. Here, Unibio benefits from oxygen supplied by the electrolyzer and contributes steam and captured CO₂ to the symbiotic system.

Considering the hypothetical park described in Fig. 6, several constraints were applied to the previous problem statement to make the case study more realistic:

- The park aims to be self-sufficient in methanol.
- The supply of methane to the local grid cannot be decreased.
- Maintaining the park's CH₄ self-sufficiency while also supplying Unibio.
- There is a renewable energy limit to the electricity consumption of 24.5 MW, indicating the need for additional energy sources for high electrolysis capacities.

Step 1.3. Technology Process Design

A Proton Exchange Membrane (PEM) electrolyzer was selected, considering its wide operational range and its capability to quickly respond to fluctuations in Renewable Energy (RE) excess [16]. This selection is supported by the increasing use of PEM technology in several power-to-hydrogen projects, indicating its potential [2]. For CO₂ capture, absorption of amine technology was chosen, as it is the most studied method and is suitable for large-scale applications [1,17].

The Power-to-X product portfolio is rich and several combinations between hydrogen and carbon dioxide can be designed. For simplicity reasons this study only considers the following set of products: pure hydrogen and carbon dioxide, methane through biomethanation, and methanol through direct synthesis. Nonetheless products such as ammonia, DME and many more could have been analyzed.

Stage II: Processes Mapping

Step 2.1. Data Collection

In the supplementary material a condensed overview of each process segment is provided (see appendix B). Part of the data input to the software can be checked in the supplementary material as well (appendix C), Examples for each scenario are provided.

Step 2.2. Matrix of Processes

The matrix of each one of the processes is given in the supplementary material. For each process a specific scenario is selected as example.

The Flow-Matrix (F-Matrix) in this study encompasses all material and energy requirements of the system, representing the model's desired output. The matrix in this analysis reached a maximum dimension of 28 × 216 data points, from which comprehensive data about the system could be extracted for analysis.

Step 2.3. Resources Screening

The analysis begins by examining relevant qualities and their flows

across different nodes and the technologies. In this study it is obvious qualities such as electricity, CO₂, H₂ and water are relevant. Water and CO₂ are the primary inputs for both technologies, while H₂ is the main quality responsible for the creation of different industrial pathways.

Through the flow diagrams generated by the software, it is possible to match the obvious needs between the novel technology and industrial. Initially (Scenario 1), both technologies have a minimal set of qualities. Evaluating the park's qualities reveals that the only potential benefit it can offer the technology, aside from the pre-existing CO₂, is wastewater, which can be converted into quality water.

In Fig. 7 the flow of matched resources is depicted. Negative flow indicates consumption, while positive flow signifies production.

Positive values indicate net production (i.e., the system releases this quality), while negative values represent net consumption (i.e., the system requires this quality as an input). Values are computed from the flow matrix F. The analysis includes both material flows (e.g., CO₂, O₂, biomass) and energy flows (e.g., electricity, steam), all expressed in normalized units per functional output (e.g., per ton of protein). This representation supports identification of potential symbiotic exchanges and critical resource dependencies within the network.

Considering the flow diagrams (such as the ones in Fig. 5) and the different technology design options described in stage one, the following qualities are highlighted: methanol, methane, and oxygen. UNIBIO emerges as a node with significant collocation potential, consuming three matched qualities at substantial levels. This suggests a promising symbiotic connection between UNIBIO and the technologies. The quality methanol (MeOH) is concentrated at the SUCEL node, primarily from biodiesel production. Conversely, ammonia consumption is widespread across several nodes, but its significance is lessened due to low consumption volumes. This highlights how capacity differences often obstruct quality flow matches between potential symbiotic partners.

Water consumption is also a key factor, with both new technologies requiring water inputs. Interestingly, their water consumption is not higher than ETOH node, while the biogas production process is the primary contributor to wastewater generation (Fig. 8). Notice the data for the "scrubber" and "electrolysis" is an accumulated value. The

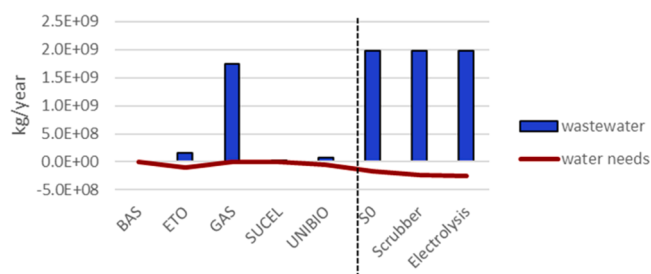


Fig. 8. Total quantity of exchanged water and wastewater per process in the evaluated scenario (S0) and the accumulated scenario for each implemented technology (Scrubber and PEM Electrolysis).

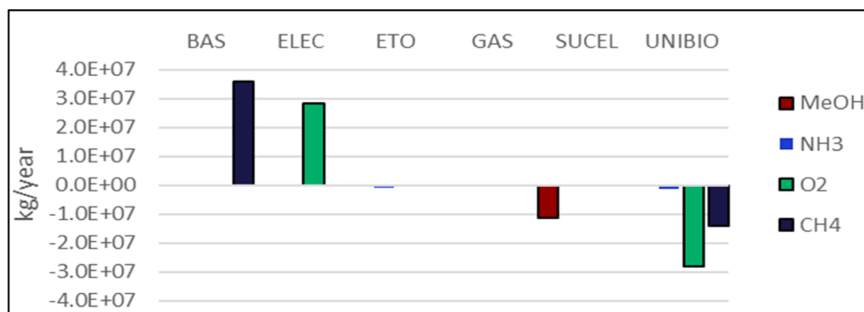


Fig. 7. Net exchange of selected qualities across the industrial symbiosis network under the evaluated scenario (S1).

addition of the scrubber or the electrolysis system does not impose a significant increase in the wastewater production, while it slightly increases the water consumption.

In Fig. 8, bars represent the net volume (absolute value) of material and energy flows associated with each process, as calculated from the flow matrix F (for simplicity only the 2 qualities are showcase). For scrubber and electrolysis units, the values shown correspond to the accumulated exchange of multiple flows (e.g., H_2 , O_2 , electricity, and water for electrolysis; CO_2 , residual biomass, and water for the scrubber). This aggregation provides a consolidated view of each unit's resource intensity. Detailed breakdowns are available in the supplementary flow tables.

Stage III: IS Design

The results from the metabolic analysis are utilized to examine the interactions between the technologies, each process, and the industrial park as a whole. The two technologies and their interactions within the industrial park are assessed across 4 scenarios simulations performed on the MA.tools software: S_0 (control, no integration performed), S_1 (technologies integration using primary process simulation data for UNIBIO node environmental networks, and literature secondary data for the rest of the integrations), S_2 and S_3 (integration using secondary data from literature for the newly added environmental networks).

Step 3.1. Option gate A.1: Technology Integration

Considering the results of the previous step it's clear that the following processes show potential to be integrated with the technology: UNIBIO, SUCEL and BAS. After the technology integration is performed, the new generated data is updated in the matrix of processes so a new iteration to the system can be performed.

Integration of UNIBIO node with ELEC and CCSU nodes (Scenario 1)

Since no literature studies were conducted for the integration of protein fermentation processes and Pt-X a software simulation tool was used to generate the necessary data. The thermodynamic behavior of the streams and mixtures throughout the process was analyzed using distinct cubic equations of state. The Soave-Redlich-Kwong Modified (SRKM), Pen-Robinson Modified (PRM), and Soave-Redlich-Kwong (SRK) equations were employed in different sections to accurately model the interactions and properties of the substances involved.

The process flowchart, depicted in Fig. 9, presents a clear numbering of streams and equipment, facilitating the association of these elements with their physical and thermodynamic properties (available in SM appendix A). The flowchart aids in understanding the process's operational dynamics and the interaction between various components.

The process simulation is based on a set of assumptions, which might impact its results. These assumptions were initially made to simplify the process design and data generation, they can be revisited and mitigated based on the sensitivity of the output to them. It is important to note that the modeling incorporated a significant number of uncertainties, reducing the precision of its results.

Option-Gate A.2: Technology Compatibility

For simplicity only scenario 1 is analyzed in this step. Nevertheless, the user can use it for multiple scenarios to compare the compatibility of the different technology designs.

Step 3.2. Technology-Process Compatibility

In Fig. 10 an overview of the total energy consumption within the system is provided. It is evident that the electrolyser is the most energy-intensive component, accounting for 9367 kW, which constitutes 97.0 % of the total electrical energy demand. The figure details the thermal energy requirements for each step of the process. The combustion of exhaust gases supplies the necessary heat for the CCSU system.

Fig. 11 compares the energy efficient of two technologies ("PEM Electrolysis" and "Air Separation Unit") that can supply the required oxygen to run the UNIBIO node. The "Air Separation Unit" is part of the current Unibio baseline system with an efficient energy consumption, while the proposed electrolysis system consumes more energy than the baseline Unibio process. Nevertheless, the new integrated technology

also produces hydrogen and integrates emerging technologies such as CO_2 uptake, scrubbing and reinjection to enable resource recovery and emission minimization.

The PEM electrolyser selected for this study can supply the necessary oxygen (977 kg/h) to a single Uloop reactor (Unibio bioreactor), while also producing 119 kg/h of hydrogen and generating a heat surplus of 4.6 MW. For simplicity, the focus of this analysis is on the oxygen supply rather than the generated heat. The oxygen stream, with a purity of 97.0 wt %, is cooled and supplied to the Uloop reactor at a high pressure of 8.5 bar, aligning with the reactor's design parameters. The efficiency of oxygen delivery by this process is approximately 9.6 kWh/kg O_2 , a value significantly higher than the typical energy requirement for O_2 production via air separation units, which is around 0.4 kWh/kg O_2 [8]. In Fig. 11 there is an comprehensive view of the total energy requirements for Methane SCP manufacturing. This chart compares the total energy requirements for methane SCP production from literature with those of the modeled PEM electrolyser. The electrolyser's high energy demand presents a significant challenge for its future application in the Unibio process, as the unit alone consumes more energy than the entire existing protein production process ("Methane SCP production").

Step 3.2 Technology-Industrial Park Compatibility

Assessing this technology requires an holistic park-wide perspective, as its benefits affect the entire industrial system rather than a single process. An F-matrix analysis comparing the baseline (S_0) and integrated (S_1) scenarios reveals a significant drawback: the new technologies decrease the park's overall energy efficiency. As shown in Fig. 12, for every megajoule (MJ) consumed, the park's exports are reduced by 73-75 %.

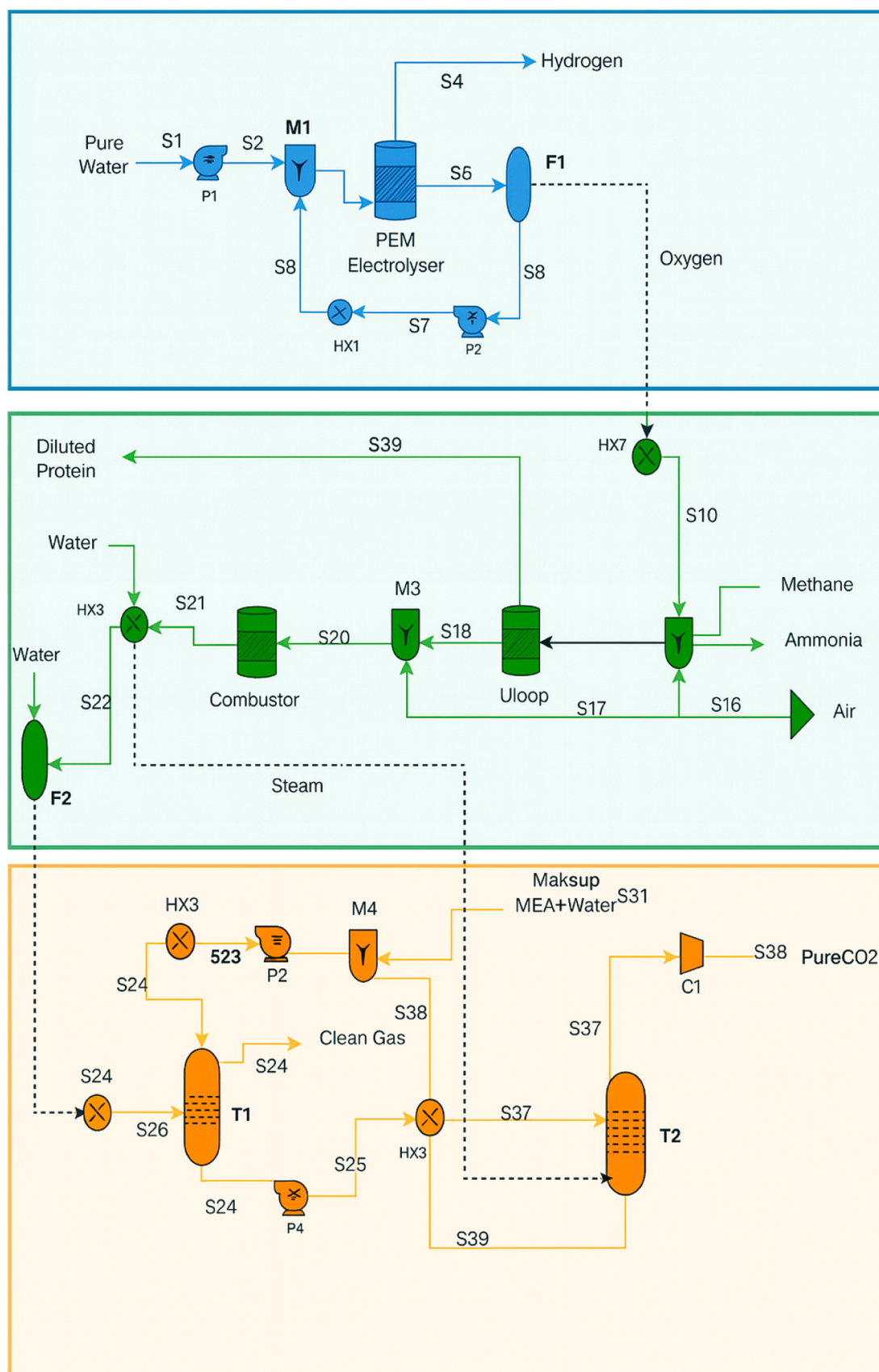
The Y-axis represents the absolute amount of each material categorized in groups (e.g., exportations, collocations, importations, and waste – see table 7 in the appendix for the definition of each group). "Performance" in this context refers to the resource exchange intensity, derived from the F flow matrix. Higher values indicate greater involvement of a group in the scenario, which may reflect either increased efficiency or higher resource dependency, depending on the context of integration. This performance metric does not reflect economic or financial output, but can offer a systems-level indicator of how deeply the technology engages with circular resource flows.

Overall, while the integration of Pt-X technologies appears to add a burden to the park's energy efficiency, this assessment does not account for the potential cost savings and environmental benefits arising from the newly created collocations, such as oxygen production and reduced CO_2 emissions. A future techno-economic analysis must address a key question: Do the benefits generated by integrating the ELEC and CCSU nodes justify the substantial energy cost of the proposed technologies?

Stage IV: IS Analysis

Option Gate B.2- Scenarios Generation

Following the *Resources Screening* in Step 2.3 methane, methanol, and oxygen are the selected resources for process integration. Although ammonia was also a candidate - offering an opportunity to reduce imports by producing it with hydrogen from the on-site electrolysis unit - it was ultimately excluded due to the park's low demand. Consequently, the scenarios were developed to focus exclusively on oxygen (Scenario 1), methane (Scenario 2), and methanol (Scenario 3). The generation of scenarios allows to consider different industrial pathways: the biomethanation upgrade of biogas, the production of e-methanol through CO_2 hydrogenation, and a combination of the two. Scenario S4 is unique in altering the electrolyser processing capacity, whereas the other scenarios maintain consistent process capacities. For this reason scenario S4 is not comparable with the other scenarios. Nevertheless, it showcases the modelling flexibility of the software. A dedicated path vector is developed for each scenario with the information on Table 1. The pathway vector values for scenario S4 are provided in the supplementary material (appendix C table 21). In this case-study each scenario is characterized by its unique industrial pathway, as illustrated in Fig. 6. This section delves into a detailed analysis of three new industrial



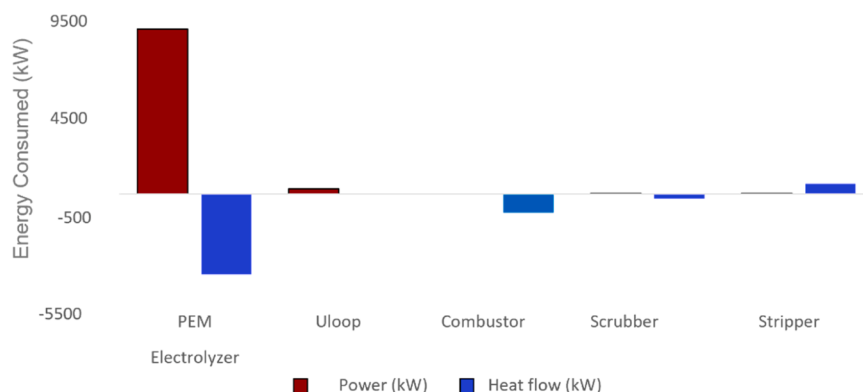


Fig. 10. Energy balance for main unit operations of Unibio-Pt-X system.

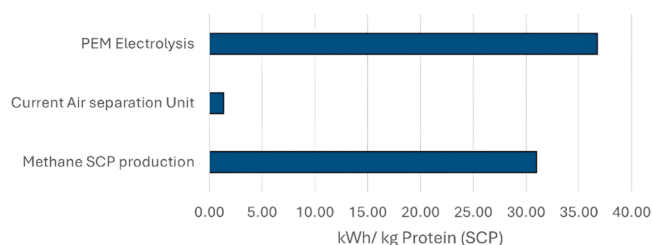


Fig. 11. Comparative overview of the baseline (current) Unibio configuration and the proposed PEM electrolysis technology.

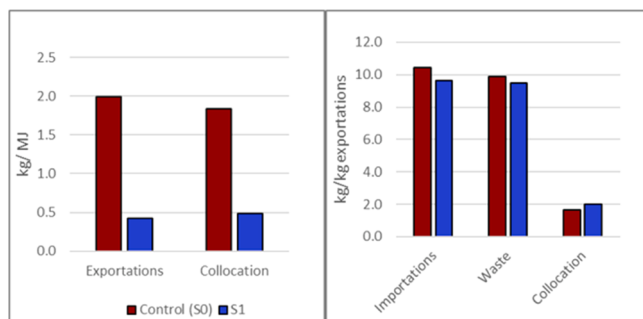


Fig. 12. Comparative performance of integration scenarios based on total quantity of exchanged qualities.

pathways emerging within the industrial park, thanks to the newly available sources of hydrogen (H_2) and carbon dioxide (CO_2).

Integration of BAS with ELEC node (Scenario S_2)

This step happens after the decision gate B.2 is chosen. It is defined as scenario 2 (S_2).

The first modification explored is the use of CO_2 and H_2 in methane production through a biomethanation process, as detailed in SM appendix B. Here 100 % of the hydrogen is utilized to convert carbon dioxide into methane. This pathway is visually represented in green in the network diagram (Fig. 6).

Key qualities such as ammonia, methane, CO_2 , and fertilizer are identified as having direct or indirect influence on the park's performance. Analysis of the F-matrix qualitatively shows that the biomethanation pathway contributes to increased methane production within the park, higher importation of NH_3 , generation of fertilizer as a by-product, and a reduction in CO_2 storage capacity.

Integration of SUCEL with ELEC, BAS and CCSU nodes (Scenario S_3)

This step happens after the decision gate B.2 is chosen. It is defined as scenario 3 (S_3).

The second modification is modeled on the methanol direct synthesis process, where the pathway, represented in dashed orange, utilizes 100 % of the produced hydrogen (H_2) to synthesize methanol in combination with CO_2 captured by the CCSU and BAS facility. The network diagram illustrates the node and relevant flows between the node, the park, and the environment. It is evident that the methanol process is highly symbiotic, engaging in four collocations with other nodes: SUCEL, BAS, CCSU, and ELEC.

A detailed examination of the F-matrix and diagrams reveals that three qualities are significantly impacted by this new pathway: CO_2 consumption, methanol collocation, and increased wastewater production. The SUCEL node, particularly its biodiesel process, is the only plant within the park consuming methanol. The high capacity of the MEOH plant renders the park self-sufficient in methanol needs, with 36 % of the produced methanol contributing to park exportations.

Scenario 4 (S_4)

This scenario activates all available pathways, presenting a comprehensive analysis. This scenario studies the 4 constraints previously mentioned in the *Problem Formulation* step.

Given these constraints, simple mass balances indicate that the existing hydrogen (H_2) production capacities are insufficient to support the selected pathways. To address this, two potential solutions are identified based on the industrial park network system: a. Increasing electrolysis capacity, supplemented by energy from the local grid or any available Combined Heat and Power (CPH) plant within the park. b. Expanding the biogas capacity by increasing the feedstock supply, potentially sourcing more biowaste from other entities within the park, like SUCEL or UNIBIO.

The first option is selected for detailed analysis in this section, though all identified pathways warrant evaluation and comparison.

Option Gate B.3: Scenario Analysis

Fig. 13 displays the normalized total production of key resources (e.g., pure CO_2 , H_2 , O_2 , methane) for various integration scenarios modeled in MA.tools. Each stacked column represents a different scenario, defined by its level of PtX and CCSU technology integration, allowing for a direct comparison of resource intensity. The values are calculated from the system-wide F-matrix. Methane (CH_4) and carbon dioxide (CO_2) are highlighted due to their critical roles. The chart is designed to reveal how technology integration impacts the system: lower CO_2 production signifies more effective internal upcycling, while higher methane production indicates greater park self-sufficiency. Interestingly, the park's electricity consumption remains relatively stable across different pathways, suggesting that the production of a specific commodity "X" won't substantially impact the park's energy consumption.

The height of each bar reflects the overall volume of exchanges, while the composition reveals which qualities dominate the system. This provides a multidimensional view of trade-offs, synergies, and system transformations across scenarios.

Despite S_3 consuming significant amounts of captured CO_2 for e-

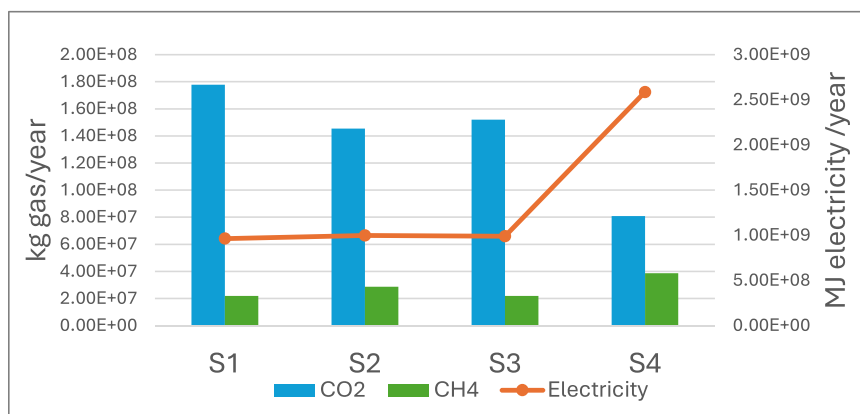


Fig. 13. Comparative scenario performance based on cumulative exchange of key material and energy flows.

methanol production, the storage capacity remains higher than in S₂. This illustrates how different pathways can influence the park's outputs and storage reserves. Coexistence of both pathways (Scenario S₄) might strain CO₂ storage, potentially limiting methanol production capacity. The capacities of various processes within the park will dictate its ability to adapt to different pathway scenarios, particularly in terms of CO₂ emissions and methanol production. Interestingly, the park's electricity consumption remains relatively stable across different comparable pathways, suggesting that the production of a specific commodity "X" won't substantially impact the park's energy consumption.

The purpose of this comparative figure is not to rank scenarios by a single optimal metric, but to visualize trade-offs and inform decision-making based on process integration priorities—whether environmental, operational, or infrastructural.

Ste 4. IS Final Assessment

The final assessment is performed with scenario S₃. This allows to have a complete overview of the technologies capacities and how they effect the *node* UNIBIO (central sub-system for the problem statement of this case-study).

The analysis centers on the UNIBIO node, examining how the varying capacities of Pt-X affect the availability of oxygen. Based on the previous *Resource Screening* for Scenario S₃, the F-matrix outputs for O₂, H₂, CO₂, MeOH, and CH₄ are analyzed across the mentioned capacities. The analysis shows that to fully meet UNIBIO's oxygen needs, a capacity at least 2.5 times greater than the initial 10 MW is required. Conversely, the 250 MW capacity projected for 2027 results in a surplus of oxygen, which might be exported or released as non-hazardous waste. This surplus indicates that future capacities of electrolyzers will significantly

influence the availability of both oxygen and hydrogen, potentially eliminating the need for UNIBIO to import oxygen. See Fig. 14 for the fluctuance of each quality towards different technology capacities. Expanding the park to include more bioprocesses that consume oxygen, like Unibio, could enhance the reliability and profitability of future Pt-X projects.

5. Discussion

5.1. Framework performance analysis

The framework developed in this study efficiently maps a network of multiple industrial pathways, offering a comprehensive overview of process interactions within an industrial park. Its effectiveness is not diminished by data scarcity or intellectual property concerns, as literature can be used to address gaps in data. Data availability has always been a limitation to the quantitative analysis and design of industrial Parks (REF). On the positive side, the framework offers numerous opportunities for application and development. It can be used in conjunction with LCA and Techno-Economic Analysis (TEA) methods. Optimization methods could refine the framework's outputs. The possibility of integrating this framework with other existing models presents additional opportunities for expanding its utility. Despite extensive research, no directly comparable frameworks have been identified in the literature, suggesting both a unique niche and potential vulnerability for this framework in the context of industrial symbiosis and technology integration.

However, the framework is somewhat limited in scope, primarily

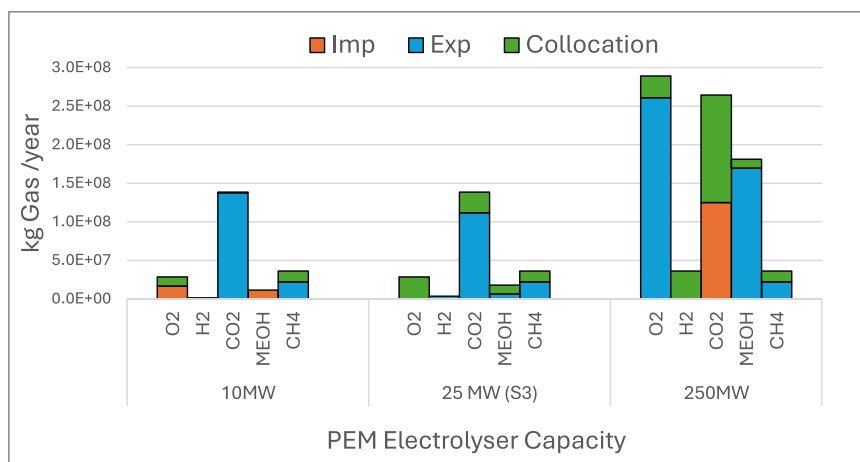


Fig. 14. Industrial Park Performance Sensitivity Towards Pt-X Capacity Growth model for scenario S₃.

suited for technologies that enhance Industrial Symbiosis. It may not be applicable to technologies that don't foster industrial synergies, thereby limiting its use to a small set of technologies.

Furthermore, the framework's value depends on the willingness of companies to share technologies and infrastructure. Regarding practical implementation, reluctance or skepticism from companies regarding investment in shared assets could pose a challenge for its use in industry.

Nowadays there are many alternatives to the fossil production of commodities (such as methanol, hydrogen, or methane). Perhaps, it could be relevant to analyse the integrability of such options with the geographic region where the factory will be located. The proposed framework could facilitate such decisions.

5.2. Analysis of the current implementation of metabolic analysis to the industrial network

The operational implementation of the methodology was performed in a very basic form. We are sure that the results are correct, but the software is far from being fully developed and ready for publication as a scientific tool. There are a number of limitations, of the software, but the most critical are introduced in the limited accuracy of the input data. The analysis does not differentiate between the chemical compositions and heat contents of various waste streams: solid, liquid, or gaseous. Uncertainty could be treated but is not part of this study.

Some of the integration of technology is highly dependent on the specificity of waste streams. For instance, capturing CO₂ from power plants poses different challenges than purifying exhaust gases from the modeled fermentation process. Purifying flue gas from such sources requires additional energy, particularly for removing impurities like H₂S, CO, SO₂, NO_x, and possibly trace hydrocarbons. But the framework that is suggested in this study does not require details for qualities that would never present symbiotic potential, such as small fractions of H₂S. In fact, in this case study all the exhaust gases streams had mainly CO₂, water and energy as relevant qualities. This means in early assessments of symbiotic projects, sometimes there is no interest on giving the software the exact composition of these streams. Nevertheless, the assessment should always be done from case to case.

In the case-study, any liquid stream containing organic matter was classified as wastewater. According to the techno-economic assessment (TEA) from which the data was sourced, the biogas process produces wastewater with an organic matter composition of 2.7mol %. Therefore, the term wastewater is somewhat reductive in this context, as detailed conclusions cannot be drawn from the F-matrix outputs alone. In this case the following questions were unanswered: What components are within this 2.7 % organic matter? Could any member of the industrial park benefit from its use? Is its quantity relevant?

5.3. Analysis of application example

Considering the diversity of facilities present in IS parks like the one in Kalundborg, the limited number of processes included in this case study affects the range of potential symbiotic interactions. A bigger database, with a bigger diversity of companies, would increase the potential of the study and consider more options for more realistic and relevant scenarios.

This study also explored various alternative utilization pathways for the primary products of the studied technologies, hydrogen, and CO₂. However, numerous other applications exist besides the use of CO₂ in succinic acid production, upgrading biogas with hydrogen, or synthesizing methanol from these products. Additional possibilities include producing ethylene, ammonia, or dimethyl ether (DME), indicating a wide array of potential industrial applications for the new two qualities. Potentially, they could be integrated in the best way with the park, by minimizing waste streams (CO₂ emissions) and importations (methanol), and maximizing collocations (a pathway similar to scenario S4 but rationalize based on a detail assessment).

The focus of this study was on integrating oxygen, with less emphasis on hydrogen supply and pressurization. Hydrogen pressurization is a critical aspect for efficient process integration, with requirements varying based on the application. For pipeline transport, a pressure of 85 bar is needed, while direct use in chemical synthesis may require up to 250 bar. Addressing this aspect could significantly enhance the study's applicability and results. Furthermore, the infrastructure required to support the integration of these technologies, particularly for hydrogen and CO₂ storage, was not fully addressed. Necessary components like storage tanks and pipelines, integral to the system's functionality, were outside this study's scope but are crucial for practical implementation. For example, activating both pathways in a model park would require a comprehensive pipeline system, akin to the Smart Delta Rivers project, entailing considerable investment [20]. Also, it is acknowledged that in scenarios involving larger processing scales or the integration of streams from multiple plants, temporary storage might be required to enable flexibility and synchronization. This limitation is recognized in the present model.

Analyzing the impact of technologies like Pt-X and CCSU on Industrial Symbiosis projects requires considering the availability of RE excess, which fluctuates annually and varies regionally. For KIS, a study estimated the potential for hydrogen production to be about 337 tons per year, only 10 % of what is required for the scenarios modeled in this study [12]. The variability in RE supply necessitates the development of storage reserves for oxygen and hydrogen, highlighting RE excess as a significant limitation of this study.

While the increased energy consumption associated with the electrolyser is notable, it's important to also consider the range of products delivered by each oxygen production technology. In contrast to air separation units, which additionally produce nitrogen that can be utilized in other industrial facilities within the IS park, the electrolyser generates hydrogen and heat as by-products. The trade-off is clear: more possibilities for creating environmental networks come with higher energy costs. The answer for such a question will be dependent on the geographic location of the IS park, which will dictate the availability of resources and energy.

The oxygen quality is a critical factor for Unibio's manufacturing process, significantly impacting its productivity [8]. Given the variability in oxygen quality across different electrolysis technologies, selecting a technology should be informed by the specific needs of the user. Presently, electrolysers are primarily designed for hydrogen production, focusing on cost-efficiency in H₂ generation. This often relegates oxygen quality to a secondary consideration. This could pose a challenge for symbiotic interactions between Pt-X processes and operations like Unibio, where the requisite oxygen quality might not be met.

A more general process library would increase the value of the approach. It would accelerate the responsiveness of partners in an industrial park to new partners and technologies coming in and altered boundary conditions forced by market dynamics and new regulations.

6. Conclusions

This study explores how Power-to-X (Pt-X) and Carbon Capture, Utilization, and Storage (CCUS) technologies can foster Industrial Symbiosis (IS) by enhancing resource reuse, reducing emissions, and creating new connections between collocated industries. The proposed framework, built around metabolic analysis, enabled the assessment of these technologies within a hypothetical industrial park. While the integration of Pt-X and CCUS was effective in generating essential resources—like oxygen and recycled CO₂—it also introduced challenges, particularly regarding energy intensity. The results underline the need for further studies to assess the sustainability and economic viability of these intensified configurations. From a Process Intensification perspective, the framework contributes by promoting system-wide improvements rather than unit-level changes. It facilitates the development of new symbiotic pathways, reduces process redundancy, and

identifies opportunities for multifunctional integration of technologies, such as using wastewater or excess energy to support other processes within the park. Moreover, by enabling the production of diverse commodities (e.g., methane, methanol) from hydrogen and CO₂, the study highlights the flexibility of Pt-X and CCUS as platforms for intensified and circular manufacturing strategies. However, evaluating such diversified outputs requires integrating Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA) tools to ensure environmental and economic robustness. Although this research does not provide a fully optimized solution, it establishes a flexible and scalable framework for early-stage decision-making in circular industrial systems. The modular design allows adaptation to different objectives, such as evaluating new companies joining a park or integrating emerging technologies. With further development—including better access to industrial data and simulation enhancements—the framework could support facilitators like KIS or the Symbiosis Center of Denmark in promoting IS across regions. In this way, it offers a promising foundation for advancing Process Intensification and sustainability in real-world industrial ecosystems. While this study focuses on the material and energy feasibility of industrial symbiosis scenarios, future work will incorporate techno-economic analysis to assess the economic viability and ensure that proposed exchanges are mutually beneficial for all participating entities.

CRediT authorship contribution statement

Guilherme Esteves Oliveira Frizado: Writing – review & editing, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **César Ramírez-Márquez:** Writing – review & editing, Writing – original draft, Validation, Supervision. **Rofige Dickson:** Writing – review & editing, Visualization, Validation, Methodology. **Juan Gabriel Segovia-Hernández:** Writing – review & editing, Validation, Supervision. **Andreas Ibrom:** Writing – review & editing, Writing – original draft, Formal analysis, Data curation. **Sayed Soheil Mansouri:** Writing – review & editing, Writing – original draft, Validation, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.cep.2025.110505](https://doi.org/10.1016/j.cep.2025.110505).

Data availability

Data will be made available on request.

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