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Report

Continuous training program: Process engineering for the decarbonization of the Swiss industry

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CONTENT

SUMMARY

Cross-cutting and sector-specific measures will be necessary to decarbonize the industrial sites, which include the improvement of component-wise energy efficiency, heat and mass recovery intensification, and integration of more advanced energy technologies. However, industrial plants are generally not aware of the upgrading potential due to limited technical information about the existing and newly developed processes, or simply due to the lack of motivation, time or skilled personnel to conduct thorough energy audits. Limited financial resources is also a constraint, especially in small and medium-sized enterprises. Thus, only few companies that could afford in-depth energy audits have been hitherto able to deploy pathways that improved their competitiveness, allowing them to reduce the energy bill and minimize their environmental burden.

In this regard, a more inclusive and sustainable energy transition will require the formation of highly qualified engineers within firms to effectively implement the complex technical and technological improvements required by the industry. They will need to be well-versed in energy audit, process modelling and design, and energy integration techniques (e.g. pinch analysis), whereas having an excellent knowledge of decarbonization technologies and their application. To this end, this Continuing Education Program has been developed to synthesize the principal energy integration and decarbonization concepts and support engineering decisions with advanced calculation and reporting tools. Although various decision-supporting methods and tools already exist, they are rather dispersed, barely used or not available in open access. For that reason, aside from the training course, the project provides advanced decision-supporting tools to be used by the future decarbonization engineers for the Swiss industry. Unlike other available tools, the developed tool can be tailor-made to meet the needs of specific industrial sectors and can be adapted to sectorial applications.

Three work packages on energy audits, utility supply and decarbonization superstructure design have been set for the preparation of the training program. First work package (WP1) focused on energy audits, composed of the description of process flowsheet, definition of the mass and energy needs, documentation of the process constraints and the validation of results together with industrial partners. Selected enterprises belonging to strategical economic sectors for Switzerland, such as distillery, malting, tanning, explosives, dairy, brewery, as well as aluminium and watchmaking have been involved in the demonstration of the versatility of the methods and the tools proposed. Due to confidentiality agreements, audits are only briefly presented, but two case studies on brewery and dairy processes are analyzed more in depth. The second (WP2) and third (WP3) working packages focused on building and documenting the energy integration tool and a database of the energy technologies and decarbonization models needed to assess the decarbonization pathways for the Swiss industry.

Finally, synergies between patronal associations, universities, industries and other actors have been identified, and the contact details are provided at the end of this report. The products developed in this research project will be used in the recently launched Master of Advanced Studies of the École Polytechnic Fédérale de Lausanne (EPFL). The open source code of the developed tool and database can be consulted in the tool repository:

https://gitlab.epfl.ch/ipese/mas/masbook

1. PROJECT OVERVIEW AND RELEVANCE

The computer-aided continuing education module on industrial decarbonization has been conceived in the frame of the Sustainable Energy Systems Engineering program of EPFL. The aim is to provide the engineers of the recently launched Master of Advanced Studies with the state-of-the-art methods and data on industrial decarbonization, as well as with decision-supporting tools, to promote the energy transition of the Swiss economic sectors. In this project-based education module, engineers will be trained in the generation of optimal solutions based on multi-criteria analyses to compare different decarbonization technologies using the advanced tools and models developed by EPFL in various Swiss and EU projects. Other models can be tailor-made to relevant Swiss industrial sectors and will be validated by their application to real-life case studies.

The tools developed in the current project include the documentation on the modelled energy systems and the methods for carrying out energy audits, creating new blueprint models of industrial processes and decarbonization technologies, as well as for proposing sustainable development goals metrics. This process capitalizes on more than two decades of research, resulting in various models and databases containing rigorous pinch-based calculation methods, as well as valuable information on energy demand, environmental impact mitigation and economic features of the Swiss industry. The support from experts is a crucial feature of the training program and the knowledge transfer, which ensures an accompanied application of the methods and a correct adaptation to the circumstances of each sector.

Even if many offers of tools concerning the pinch method application are available, there is no similar training offer in Switzerland giving access to different skill levels, databases and also the corresponding tools. Thus, thanks to this project, the consolidation of the advanced engineering methods and supporting tools, as well as their adaptation to solve real-case studies, can be achieved, which will approach academia to the actual industry conditions. By the end of the training program, the specialists will be able to use the tools provided to carry out themselves energy audits, perform process integration (Pinch Analysis), assess and compare the different carbon capture and mitigation technologies, and integrate renewable energy resources into real-life case studies of industrial energy systems.

As a result, engineers will be able to certify their training on the procedures, methods and tools to analyze the process systems towards higher energy efficiency and decarbonization, whereas the major economic sectors, responsible for 80% of the gross domestic product of Switzerland, will benefit from the participation of highly specialized professionals in their energy transition plans. In addition, with each new sectorial application, the database of decarbonization options can be enriched by former participants of the training course, thus creating a network of open source database and modular functionalities than can be updated by sharing the most recent experiences of the various experts in each sector. The energy conversion and decarbonization database include, but it is not limited to models of (i) conventional and advanced heating systems, (ii) carbon management and abatement technologies, (iii) storage units, (iv) power-to-fuel-to-X systems, (v) cogeneration units, (vi) biomass energy conversion processes (thermal and biological), and (vii) renewable energy harvesting, among others.

2. METHODOLOGY

The preparation of the training module builds on the expertise of the IPESE research group at EPFL, whose participation in Swiss and EU research projects resulted in a comprehensive knowledge of the most relevant decarbonization pathways for different industrial sectors. The models and databases developed by the group thus far provided the starting point around which the Continuing Education Program was developed. These models, called blueprints, come accompanied by documentation, recommendations and metrics for the relevant industrial sectors, and can be further adapted by the trained engineers. Three work packages have been internally set for the preparation of this training module and focus on (*i*) realization of energy audits, (*ii*) definition of a utility superstructure and (*iii*) development of a decarbonization superstructure. The methodology followed in each working package is described in the next sections.

2.1 Procedure recommended for the energy audits

Energy auditing is the practice of inspecting, evaluating and diagnosing the efficiency of the energy infrastructure and resources utilization. The energy audits help enterprises to understand how, when, and where they are using their energy resources, which allows to explain the energy bill and to identify opportunities for energy and emission savings. A summary of the steps taken during a typical industrial energy audit is depicted in Figure 1, encompassing preparation, execution, and reporting.

In the audit preparation steps, the criteria and scope of the audit is selected. Audits can take many forms, varying in scope, depth, and purpose. Some may be applied to single-unit processes, while others can be applied on entire facilities. In addition, regardless the scope, a good selection of the audit team is essential to properly assign the number of experts to collect, interpret and document the energy bills, and perform the preliminary analyses. Depending on the time and resources allocated, an audit can be a sweep for identifying general areas of improvement and analyzing energy use patterns. They are a cost-effective approach to pinpoint main production inefficiencies, thus prioritizing the most important actions and measurements. More detailed audits narrow down on certain key identified elements. It results in an interplay between data collection, benchmarking, assessment and re-evaluation. Although an energy audit begins with an energy-oriented scope, it can also evidence flaws in planning and management, instrumentation, technological lags, and other corporative approaches. Finally, but not least important, the reporting and post-audit activities are necessary to issue the recommendations and preparing the action plan. Audits must transcend beyond an archived report, so that the implementation and action plans can be executed, and the benefits be obtained.

In this regard, it is important to inculcate to both new and experienced engineers the idea that only by a thorough energy audit is possible to assess the energy performance of an industrial plant and develop the energy management programs to decarbonize the energy systems. In fact, by skipping this step and solving localized issues that appear due to the unidentified malfunctioning of other sections of the plant, industries incur the installation of costly equipment generally ill-suited for the definitive solution of the problem and, in the worst case, trigger an avoidable increment of the energy inefficiency.

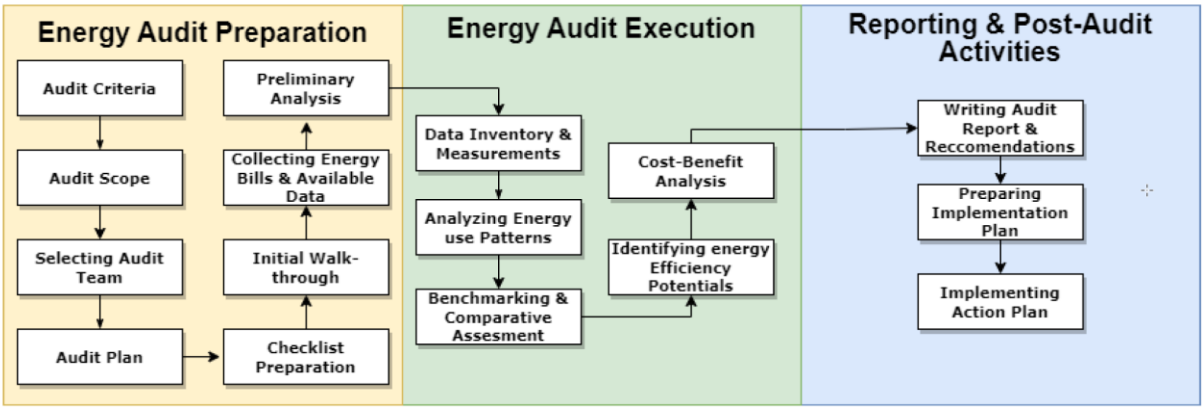


Figure 1. Steps of a typical industrial energy audit [1, 2].

In WP1 of this project, good practices for performing the energy audits have been applied, including: (i) strategies of data collection, benchmarking and management; (ii) inventory and detailed description of process units and interactions with the existing utilities systems in terms of mass and energy flows; (iii) definition of the process needs and interfaces, and analysis of the energy bills; (iv) validation of the results together with industrial partners; (v) documentation of process constraints, results of plant surveys and system measurements; and (vi) issuing of recommendations on opportunities for increased energy efficiency and decarbonization. As this point, the industries were responsible for undertaking post-audit activities at their convenience.

The following steps were followed in the construction and validation of the blueprints of the different industrial sectors, based on the mentioned audits [1, 2]:

- Data collection on the main onsite services and processes and construction of datasets. Any available documentation, such as process flow diagrams (PFD), piping and instrumentation diagrams (P&ID), or any other tabulated data on the design parameters of the process equipment and the operation units were critical to get an overview of the industrial processes structure and the interconnections between flows. Data treatment and check for consistency and coherence was also performed.
- Selection of the system boundaries and level of details for the internal streams of the specific industrial sector. Particularly, information about: energy and materials flows crossing the battery limits of the processes; nature and number of products, byproducts, and wastes; and thermal streams for heating and cooling requirements were inventoried whenever available.
- Standardization of the interfacing streams that directly interact with models of other utility systems and decarbonization technologies. A proper definition ensures a consistent integration process of the blueprints during the subsequent tasks.
- Rigorous modelling approaches were also implemented whenever needed to solve the set of equations that represents the mass and energy balances of the unit operations of the industrial process. Equation oriented or sequential modular simulators, along with Mixed Integer Linear programming (MILP) algorithms were used to determine the minimum cooling and heating requirements (MER).

Several enterprises of the Swiss industrial sectors with applications on distillery, leather, malting, explosives, aluminium, and watchmaking were approached and detailed energy audits of their processes have been performed. Patronal industrial associations and other sectors, such as hospitality and luxury brands, also demonstrated interest in establishing links between their organizations and EPFL's *continuing education program*, either for starting or advancing their decarbonization projects. These collaborations with engineers and managers of Swiss enterprises allowed to hear about the goals, risks perceptions, expectations and challenges on sustainability and competitiveness. As a result, the developed ex-ante models of the industrial sectors make up a database of models validated by case studies that can be used to analyze decarbonization roadmaps and industrial symbiosis. Each model comprises a series of thermal and electrical energy profiles, material profiles and other relevant information. However, due to data confidentiality, only general details of the energy audits are discussed in this report. Two typical processes of the Swiss industrial sector, namely dairy and brewery sectors, were examined more in depth and used to exemplify the functionalities of the tools developed in this project. The information of the previous energy audits has been adapted in the form of educational material to be used by engineers in the project-based *continuing education program*. The students will implement the computational tools and the models developed to draw their own recommendations as part of the certification process.

2.2 Development of the models of the utility systems

In addition to the models of the industrial processes, a library of energy technologies (ETs) is supplied for studying the energy integration and industrial decarbonization strategies during the training program. Utility systems are fundamental for all the industrial activities, as they deliver the supporting material and energy flows that drive the processes within the industrial plants, thus enabling efficient, safe and reliable operation and production, and environmental impact mitigation control.

In WP2, the blueprint models of utility systems were developed based on the experience of the research group in various projects on energy integration and industrial decarbonization. The documented library has the relevant information about existing and advanced energy technologies. The models are able to simulate and predict the performance of the integrated energy systems for different operating conditions. The database is flexible enough, so that it can be easily adapted to the different industrial applications. Together with the industrial sectorial blueprints, these utility systems models reproduce the key energy features of the most relevant industrial Swiss sectors, so that students and future experts will be provided with documented applications adapted to their specific branch, allowing them to start with a predefined didactic framework.

The database is documented in a computational shareable format, in such a way that users can select one technology from the library and integrate it into their own scenario to evaluate the effect of its integration and compare it with the choice of other approaches. After the training program, practitioners will be able to model, propose and implement further innovative and feasible solutions to reduce the carbon footprint of their processes. Although a predefined collection or energy technologies may seem generic and applicable to a broader spectrum of sectors, the main objective of the training course will be to provide the skills to adapt them to the specific branch and conduct made-to-measure cost-benefit analysis. The database of utility systems is briefly described next.

The most common utility units are thermal cycles, such as gas and steam turbines, internal combustion engines, heat pumps, refrigeration cycles, mechanical vapor recompression units and organic Rankine cycles. These cycles are used for combined power, heating, and cooling applications. More advanced cogeneration units not classified as thermal cycles are the fuels cells technologies.

Steam networks are important utility systems, especially in large installations with large amount of waste heat, since they facilitate its distribution through various applications, including electricity generation, heating, and mechanical work. Steam generators and hot water boilers are utilized mainly for heat supply at lower temperatures and pressures. Air and water cooling systems also play a crucial role in dissipating excess heat generated in industrial processes, whereas refrigeration systems supply the cooling requirements that cannot be achieved using simpler cooling methods at ambient temperatures.

In addition to waste heat management, utility systems encompass air separation units and oxycombustion furnaces, which are utilized in processes involving syngas, synthetic natural gas (SNG), and natural gas combustion. These units enable efficient combustion and easier CO_2 separation, contributing to the emissions reduction and environmental sustainability. Other types of furnaces also can burn hydrogen, whereas more specialized technologies rely on plasma torches. These furnaces utilize different energy sources and combustion techniques to meet specific process requirements, thus demonstrating the versatility and adaptability of the utility systems in diverse industrial settings.

The integration of renewable energy harvesting systems, such as photovoltaic panels, is drawing more attention, offering sustainable solutions for industrial energy generation and consumption. Photovoltaic panels harness solar energy to generate electricity, reducing reliance on conventional energy sources and mitigating environmental impact. Moreover, they can be used to transform typical consumers of electricity from grid into prosumers, which can interact with the energy systems to balance the electricity and gas grids. Overall, utility systems play a critical role in industrial processes by providing essential energy services, thermal management, and environmental controls. The continuous development and integration of innovative technologies contribute to enhanced efficiency, sustainability, and resilience in industrial operations.

All the models are available in the Gitlab repository of the developed tool and can be found in the Appendix 1 of this report.

2.3 Development of the models of the decarbonization technologies

Decarbonization technologies can encompass from single equipment up to a group of complex energy conversion systems aimed at reducing or eliminating the CO_2 emissions associated with industrial activities. These technologies are crucial for achieving global climate goals by mitigating the impacts of greenhouse gas emissions on the environment. The importance in the energy transition lies in their capacity to enable the shift towards a low-carbon economy, while ensuring the energy security and sustainability.

Carbon capture, utilization, and storage technologies are at the forefront of decarbonization efforts. They involve capturing CO_2 emissions from industrial processes or power plants, then either storing it underground or utilizing it for other industrial processes. Electrolysis is another crucial technology, particularly in the field of renewable energy integration and renewable energy storage. Electrolysis and co-electrolysis allows the hydrogen and syngas production for later serving as clean fuels for various applications or as intermediates for producing other fuels and chemicals.

Biomass utilization is another pathway for decarbonization, where organic materials such as agricultural residues, forestry by-products, or dedicated energy crops are converted into biofuels or used for power generation. Both biochemical and thermochemical biomass conversions can be applied to reduce the consumption of fossil fuels. In addition, the production of biogenic carbon enables the supply of a sustainable source of CO_2, largely required in the plastics and chemicals products, otherwise derived from fossil resources. Electrification also plays a vital role in the decarbonization process by replacing fossil fuel-based technologies with electric alternatives, such as electric heating, heat pumps, plasma torches, and electric induction furnaces for industrial processes.

The cost of decarbonization strategies vary depending on the technology and the scale of implementation. Initially, decarbonization technologies incur higher costs compared to conventional fossil fuel-based counterparts, primarily due to technological immaturity and economies of scale. However, as these technologies mature and deployment scales up, costs tend to decline, thus making decarbonization steps more economically feasible.
The integration of decarbonization technologies into existing energy systems and grids is crucial for an effective deployment and operation. This integration requires careful planning and coordination to optimize synergies between the different technologies and industrial sectors, and ensure the stability and reliability of the energy supply. It involves upgrading existing infrastructure, developing new grid management strategies, and implementing policies and regulations that incentivize the adoption of low-carbon technologies. Overall, the successful integration of decarbonization technologies into energy systems is essential for achieving long-term sustainability and combating climate change.

All the models of the utility systems are available in the Gitlab repository of the developed tool and the description can be found in the Appendix 2 of this report.

2.4 Computer-aided industrial process integration using ROSMOSE tool and the documented database of ex-ante models

After the audits have been performed and the necessary data for constructing the ex-ante models of the industrial processes and energy technologies has been collected; next, the language for writing the shareable blueprints and the tool for handling the modeling and simulation, heat and mass integration, cost optimization, and reporting tasks have been developed. The report and documentation is written in Markdown language using the Quarto tool that have various referencing and visualization options, and can be readily deployed in web-based format or shared as portable document format. The optimization solver of the open-source tool is based on mixed integer linear programming (MILP). Hence, an extensive list of process integration scenarios, based on decarbonization strategies such as electrification, mineralization, heat recovery intensification and efficiency improvements can be already undertaken and compared by the users.

Other tools reported in literature for studying process integration include Aspen Energy Analyzer®, gPROMS®, i-Heat®, and hiTRAN®. Aspen Energy Analyzer® is an Aspentech® energy management software used to perform optimal HEN design to minimize process energy consumption [3]. This software is compatible with flowsheeting simulators, like Aspen HYSYS® / Plus®. Another suite fully incorporated within Aspentech® flowsheeting simulators is Aspen Exchanger Design & Rating®, which produces options for optimal heat exchanger network designs with specifications of different types of heat exchangers, such as shell-and-tube, plate, or air-cooled exchangers [4]. i-Heat® is a proprietary software from Process Integration Limited® for the design, retrofitting and optimization of HENs, which allows identifying operating conditions for reduced energy consumption [5]. A common limitation in using these software is their commercial license-based features with rigid user interfaces (UI) and hidden algorithms, which hinders the data exchange with other software and prohibits modifications to the source code. Open-source accessibility and communication among software are major challenges in using process integration tools for designing and optimizing the overall energy consumption of industrial systems [6, 7].

To tackle this issue, a flexible and integrated open-source tool for the synthesis and design of complex energy systems has been devised at EPFL [8]. The tool undergoes continuous development, capitalizing on 20 years of research to expand its capabilities, robustness and versatility [9]. Lua programming language is used to write the source code of OSMOSE, as it features a fast and extensible architecture [10]. OSMOSE engine was integrated into the Quarto environment to conceive a high-level language called ROSMOSE. This is a first of its kind open-access integrated platform that combines modelling, simulation, data analysis, and rigorous process integration methods, and a versatile visualization and documentation functionality to write reproducible dynamic reports, while imbedding code chunks and generating results all in one platform [11]. The output files can be either static (portable document format – PDF) or interactive (hypertext markup language – HTML, to be used in web-based reports) and can be accessed through typical web browsers [12]. Next, a detailed explanation of the mechanisms of ROSMOSE is presented. Illustrative examples showcasing how it can aid the decision making for the synthesis, design, and optimization of industrial and urban energy systems is presented.

2.4.1 ROSMOSE language for handling process integration databases and reports

ROSMOSE platform is a combination of Rmarkdown tool and OSMOSE engine. RMarkdown is an extension to Markdown which includes the ability to embed code chunks and several other extensions useful for writing technical reports. On the other hand, OSMOSE is a process integration tool developed at IPESE group from École Polytechnique Fédérale de Lausanne (EPFL) and stands for "**O**ptimi**S**ation **M**ulti **O**bjectifs des **S**ystèmes **É**nergétiques Intégrés" (Multi-Objective Optimization of Integrated Energy Systems). It has been used for over two decades in many research projects and teaching activities in EPFL and undergoes continuous development of new features [13–17]. As a computational platform, OSMOSE can make use of a combination of metaheuristic (genetic algorithm) and deterministic (MILP) optimization approaches for combined heat and mass integration. This framework aids in decision-making for the design and operation of a variety of energy systems, either industrial or urban, while considering thermodynamic, environmental, and economic targets. Moreover, the OSMOSE platform exhibits flexibility in integrating various software and tools, such as database handling routines (CSV and JSON files), process modelling and simulation suites (Aspen Plus, Belsim Vali), optimization solvers (AMPL/Pyomo), and data visualization (GNU Plot, D3.js). Meanwhile, ROSMOSE tool was developed to simplify the utilization of the complex OSMOSE language, which operates in the backend, thus making it more accessible to scientific community. ROSMOSE extends OSMOSE functionalities by including a complete reporting suite built in the Quarto ecosystem capable to render Quarto (.qmd) and Rmarkdown (.Rmd) formats, which allows users to directly convert their work into a powerful report or presentation. Figure 2 illustrates the dynamics of the ROSMOSE web-based tool, highlighting the mechanisms of data transfer and interactions with various platforms, starting from the model parametrization down to the results visualization and report generation into multiple output formats.

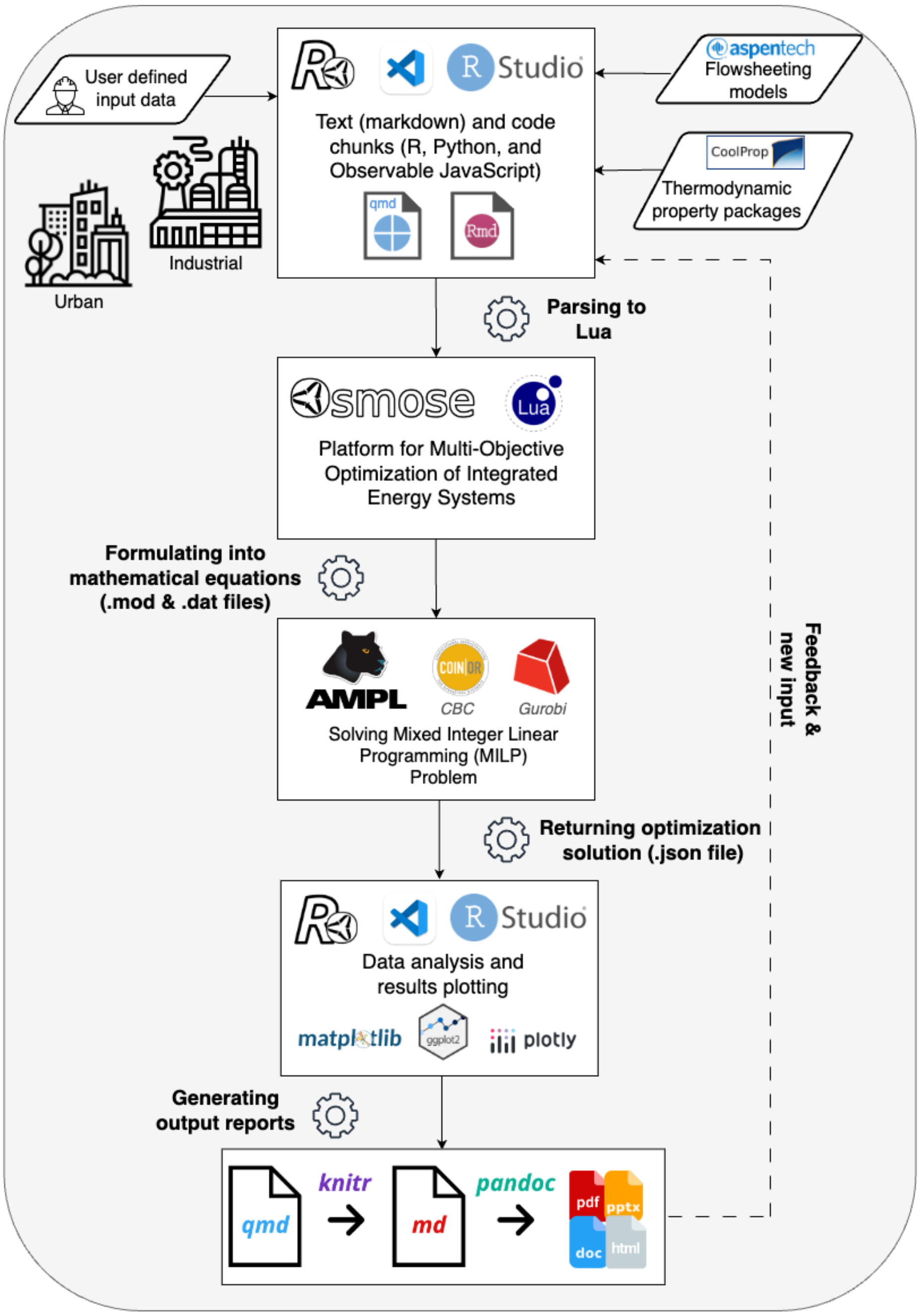


Figure 2. Schematic illustration of the working mechanism of ROSMOSE.

The aim is to make science reproducible by creating an ecosystem where programming can be embedded into reports [11, 18]. Compared to conventional reporting tools, in which data is stored as characters and figures are deployed as static images, a Quarto-generated report includes in the same document, text, raw data, processing, and the plotting instructions to generate the figures. The report is generated based on the raw data and figures can be updated automatically as soon as the raw data undergoes any changes. Multiple languages can be used to inject code chunks into a Qmd document including Python, R, Julia, and Observable JS. For example, Python could be used along with the open-source library Coolprop to calculate thermodynamic properties of various substances involved in energy systems like the milk production process (used as a case study), but also to simulate full heat pump and refrigeration cycles or a steam network [19].

Apart from its multiple applications in research projects [20–24], the ROSMOSE framework developed in this project is used for teaching different engineering courses at EPFL, which proves its suitability at both industrial and academic levels. In fact, sharing the ROSMOSE open-source code and derived reports with industry partners and collaborators from the scientific community is as simple as uploading the code to a remote repository online (Gitlab, GitHub, etc.). In ROSMOSE language, a variable is defined as a *tag*, which is an object containing a name, a value, a physical unit, and a description. The values can either be user defined or calculated based on other tags. The tags are used to specify inputs, outputs, or parameters of a specific model. The building blocks of an ROSMOSE project are the *energy technology (ET) models*. Each ET can have multiple input and/or output tags, as well as other attributes, such as *layers* and *units.* The layers in ROSMOSE can be interpreted as the pipelines through which similar streams flow and are defined by a name and a physical unit.

2.4.2 Mixed integer linear approach (MILP) optimization

For a given process, there could be various energy integration routes composed of multiple competing utility systems with numerous possible operating conditions, which entails many potential scenarios. For example, when utilizing a cogeneration utility unit in an industrial process, there is a possibility of importing fossil fuel or using the biogas produced locally in an anaerobic digester to satisfy entirely or partially the heating requirements of the system. Another alternative could be to import electricity and avoid the inefficiencies in a cogeneration unit. However, synergies may arise from the combined heat and power integration and the demands of ancillary technologies, such as refrigeration, cooling water, and heat pumps. Moreover, as the production routes can be different, the systems needed to satisfy their energy demands may also change. For this reason, the OSMOSE engine is used to first calculate the minimum energy requirements (MER) of the process by applying pinch analysis techniques. OSMOSE can then provide the best combination(s) of energy technologies and their corresponding operating conditions that can reduce the total cost. This is done by handling and solving the MILP problem in Eq. (1). Other thermodynamic and environmental indicators can be also calculated to rationally compare different scenarios and represent them in non-dominated Pareto plots. A weighted combination of multiple objective functions such as costs and impact factors may also be used to parametrize the optimization problem.

$$min\ Cost_{tot} = \sum_{u \in Units} \left[\sum_{t \in Time} \left(Cop1_u \cdot Y_{u,t} + Cop2_u \cdot M_{u,t} \right) \cdot \Delta t + Cinv1_u \cdot Y_u + Cinv2_u \cdot M_u \right] \quad (1)$$

where:

- $Cost_{tot}$ is the total annual cost of the industrial energy system (€/year),

- $Cop1_u$ is the fixed operating cost of unit u (€/h),
- $Y_{u,t}$ is the integer variable related to the presence or absence of each unit u at time t (-),
- $M_{u,t}$ is the corresponding continuous load of that unit u at time t (kg/hr or kW),
- $Cop2_u$ is the variable operating cost of unit u (€/kg or €/kWh),
- Δt is the operating time of unit u (hr/y),
- $Cinv1_u$ is the fixed annualized investment cost of unit u (€/year),
- Y_u is an integer variable related to the presence or absence of a unit u in the system; the maximum value of $Y_{u,t}$ (-),
- $Cinv2_u$ is the specific annualized investment cost of a unit u (€/kg) or (€/kWh),
- M_u is the corresponding maximum load of the unit u in (kg/y) or (kWh/y).

This objective function is subject to multiple constraints including unit existence and load boundary conditions:

$$Y_{u,t} \cdot Fmin_u \leq M_{u,t} \leq Y_{u,t} \cdot Fmax_u \; ; \qquad \forall u \in Units, \; \forall t \in Time \tag{2}$$

$$M_{u,t} \leq M_u \tag{3}$$

$$Y_{u,t} \leq Y_u \tag{4}$$

Mass and energy balance constraints:

$$\sum m_{Input\ streams} = \sum m_{Output\ streams} \; ; \qquad \forall\, Layer, \; \forall\, t \in Time \tag{5}$$

Power production or consumption constraints:

$$\sum_{w=1}^{N_w} M_w \cdot w_{w,utilities} + \sum_{Processes} W + W_{import} - W_{export} = 0 \qquad \forall t \in Time \tag{6}$$

Heat cascade constraints, balance at the temperature interval *r*:

$$\sum_{w=1}^{N_w} M_w \cdot q_{w,r} + \sum_{i=1}^{N} Q_{i,r} + R_{r+1} - R_r = 0 \; ; \qquad \forall\, r = 1 \ldots.. N \tag{7}$$

And solution feasibility:

$$R_1 = 0, R_{N+1} = 0, \; R_r \geq 0 \quad ; \quad W_{import} \geq 0, \; W_{export} \geq 0 \qquad \forall\, r = 1 \ldots.. N \tag{8}$$

where

- *N* is the number of temperature intervals based on the supply and target temperatures of all streams (-)
- *Q* is the heat exchanged between process streams (kW),
- *R* is the heat cascaded from higher (r+1) to lower (r) intervals of temperature (kW),
- N_w is the number of utility units available,
- $q_{w,r}$ is the specific heating or cooling flow supplied by any utility unit w within an interval r (kW_{heat}/kW or kW_{heat}/kg),
- *W* is the power produced or consumed by the utility systems, the unit processes, or imported from or exported to the grid (kW).

Thus, the units, either processes or utilities, can have multiple attributes including:

- Specific operating (EUR/$kg_{product}$) and investment costs (EUR/$(kg/h)_{product}$),
- Environmental impact factors (kg_{CO2}/$kg_{product}$),
- Sizing factors, i.e. continuous optimization variables in the case of utility units, and
- activation factors, i.e. binary optimization variables, also for utility units.

Moreover, depending on the main purposes of the energy conversion processes (heating, cogeneration, power production, waste treatment, mechanical processing, separation, storage, etc.), two types of streams may be assigned to each unit:

- *Resource streams*, which are linked to a respective *layer* and require indication of the direction with regard to the unit, namely *in* (for consumption) or *out* (for production).
- *Heat streams*, which correspond to the thermal energy flows and require information such as inlet and outlet temperature, inlet and outlet enthalpy (also heat capacity or heat flowrate), minimum temperature approach, and heat transfer coefficient.

Based on this information, ROSMOSE launches the execution of the routines in OSMOSE engine that write the respective *.run*, *.mod* and *.dat* files in AMPL® language, which contain the optimization problem equations and the parameters of the energy technology (ET) models (i.e. Industrial processes, Utility systems, and Decarbonization technologies). The mathematical formulation of the problem can be solved using any open-source mixed integer linear programming solver, such as CBC [25], compatible with AMPL® community edition. The costs of all input and output streams of the industrial application can be adopted based on current European markets.

Once the optimization problem is solved, results are recovered from the solver output file (.JSON format) and parsed to extract and structure the data. Post compute functions are next used to:

- Calculate the performance indicators (e.g. costs, environmental impact, energy efficiencies, etc.).
- Display graphical representations of relevant results (e.g. composite and integrated curves).
- Calculate objective functions for multi-objective optimization scenarios.
- Carry out post-optimization analyses and issue recommendations.

2.4.3 Key Performance Indicators (KPIs)

Thermodynamic, economic, and environmental performance indicators are proposed in order to compare the different process alternatives. Firstly, the energy consumption per unit volume of main product produced in the industrial system (φ) evaluates the overall energy efficiency of the system. It can be differentiated as fuel consumption efficiency φ_{fuel}, and electricity consumption efficiency φ_{EE} , based on Eq. (9) and Eq. (10) respectively.

$$\varphi_{fuel} \; \left[\frac{kWh_{fuel}}{kg_{product}}\right] = \frac{m_{fuel} LHV}{m_{product}} \quad (9)$$

$$\varphi_{EE}\ \left[\frac{kWh_{EE}}{kg_{product}}\right] = \frac{W}{m_{product}} \tag{10}$$

where,

- W is the power consumption in the overall system (kW),
- Q is the fuel consumption in the overall system (kW),
- $\dot{m}_{product}$ is the yield of product (kg/h)

The total CO_2 emissions ($kg_{CO2}/kg_{product}$), encompassing both direct and indirect emissions, are calculated per unit of product according to Eq. (11).

$$CO_{2,Spec} = \left[m_{fuel}LHV \cdot 3600 \cdot \left(\frac{I_{CO2,fuel}}{LHV_{fuel}} + \frac{r_{CO2,fuel}}{1000}\right) + \frac{r_{CO2,EE} \cdot W_{total}}{1000}\right] \cdot \frac{1}{m_{product}} \tag{11}$$

where

- $I_{CO2,fuel}$ is the direct emissions factor for the fuel ($kgCO_2/kg_{fuel}$),
- $r_{CO2,EE}$ is the indirect emissions factor of electricity (gCO_2/kWh),
- $r_{CO2,fuel}$ is the indirect emissions factor of fuel (gCO_2/kJ),
- LHV_{fuel} is the lower heating value of the fuel (kJ/kg),
- Q_{fuel} is the total fuel energy consumption (kW),
- W_{total} is the total electric power consumption in the system (kW).

Finally, total revenue ($Eur/kg_{product}$) is calculated by discounting the incremental annualized investment costs of the utility systems and the total annualized operating costs from the annualized revenues of the product streams, as shown in Eq. (12):

$$Revenue = \left[\sum_{products}(m_{product,i} \cdot c_{product,i}) - \sum_{input}(m_{input,i} \cdot c_{input,i}) \pm W_{total} \cdot c_{electricity} - m_{fuel}LHV \cdot c_{NG} - \sum_{u \in Units}(Z_u \cdot F_{annual,u} \cdot 1/8760)\right] \cdot \frac{1}{m_{product}} \tag{12}$$

where

- c_i is the specific cost of *i-th* input or product (€/kg or €/m^3 or €/kWh),
- Z_u is the investment cost of *u-th* industrial process, utility system or decarbonization technology (€),
- $F_{annual,u}$ is the annualization factor based on lifetime and annual interest rate (1/y).

3. RESULTS AND DISCUSSION

The objective of this project was the preparation of the computational tools and energy technology database to be used during the impartation of lectures and practical sessions of the recently approved Master of Advanced Studies of the École Polytechnique Fédérale de Lausanne (EPFL). Therefore, the content of this Continuing Education Program is firstly described. Next, the energy audits and other case studies, in which the ROSMOSE tool has been used, are overviewed. However, due to the industrial confidentiality of the results, only two typical examples related to the dairy and brewery processes are analyzed in detail using the developed computational tool. Finally, communications with enterprises interested in participating in the decarbonization strategies promoted by EPFL's MAS programme are presented later on this report, together with the recommendations and path forward.

3.1 Description of the CAS/DAS program launched at EPFL

Industrial plants are becoming more concerned about the evolution of policies, processes and technologies that will drive their transition towards more sustainable energy systems. The reason is that a shift to more efficient and environmentally friendly energy practices not only will impact their assets, but also redefine the skills required by their qualified staff, which will need a new learning cycle to update their expertise in new tools, processes and methodologies. In this context, the Extension School of EPFL has broaden its offering of Continuing Education Programs in three key areas: *(i)* digitalization and technological design, *(ii)* industrial transformation and health, and *(iii)* sustainability and ecological transition. Regarding the third area, a newly created Master of Advanced Studies (MAS) on Sustainable Energy Systems Engineering (SESE) is taught jointly with HES-SO Valais. The programme consists of four class modules imparted over two years and it requires each participant to complete a project. The CAS (Certificate of Advanced Studies) of 10 ECTS (education credits) is organized based on three major learning activities, namely *(i)* distance learning to understand the state-of-the-art around the thematic of the module, *(ii)* flipped classes to make the link between the theoretical elements and the practical project, and *(iii)* workshops to realize the project. The DAS (Diploma of Advanced Studies) of 30 ECTS consists of CAS + 20 ECTS for the individual project performed together with the industry.

In particular, the fourth module is supported by the advanced computer-aided tools that have been developed in the current project, which are delivered to the participants as part of a wider open science and industrial development effort from the Industrial Processes and Energy Systems Engineering (IPESE) group. The fourth module aims to develop a systematic approach to the enhanced energy efficiency and decarbonization of industrial processes. This approach encompasses:

- Understand, analyze and measure the energy features of an industrial process by using energy audits that consider thermodynamic, economic and environmental impacts of the production processes when integrated to the environment.
- Identify options for process efficiency improvement by technological changes, heat recovery and optimization of energy supply.
- Optimize the heat revalorization by the integration of advanced utility systems, such as those described in the previous sections (e.g. heat pump, steam networks, etc.).
- Integrate waste-water-energy management options to minimize the use of water, whereas valorizing waste streams as materials or energy resources.

- Organize and manage the integration of renewable energy resources.
- Integrate CO_2 capture, sequestration (e.g. mineralization) and reuse technologies.
- Integrate the industrial process to the main energy system infrastructure and the surrounding urban system, in order to favor the industrial symbiosis.

At the end of the module, the participants will be able to make a fact-based and data-driven energy audit of an industrial process to identify, design and assess energy savings and renewable energy options with quantitative and qualitative approaches. For a given process in a certain location, the participants will be able to identify, design and assess industrial symbiosis options, including the waste-water-energy nexus integrated within the energy infrastructure and the decarbonization technologies. To this end, participants will be faced with a real-world project-based training module that will demand:

- *Research and documentation*: Participants will delve into an extensive research to gather data about the energy systems, the environmental factors, and the specific region assigned for the project. This phase involves studying the existing energy infrastructure and demands, environmental impacts, and socio-economic factors.
- *Expert opinions*: Participants will seek out expert opinions, through interviews with professionals in the field, namely energy engineers, policymakers, environmental scientists, and stakeholders, who can provide valuable insights.
- *On-Site investigation*: Participants will visit industries, institutions, cities or regions to assess its energy needs, available resources, and local conditions. This hands-on experience will inform the development of sustainable solutions tailored to the unique characteristics of the region.
- *Solution proposal*: Based on research, expert opinions, and on-site observations, the participants will formulate a sustainable energy solution, including renewable energy integration, energy efficiency measures, environmental considerations, and economic viability.
- *Calculation and optimization*: Participants will use modeling and analytical tools to calculate the potential energy performance, costs, and environmental benefits of the proposed solution. Optimization strategies to maximize the sustainability and impact of the project will be also implemented.
- *Holistic approach*: Participants will need to consider not only the technical feasibility of the proposal, but also its social and environmental impacts, emphasizing a holistic approach (local communities, ecological system, long-term sustainability goals, etc).
- *Report*: Participants will prepare a dynamic and referenced report presenting the sustainable energy proposal highlighting key findings, methodology, and potential impact.
- *Assessment*: The assessment of the module will be implemented by an oral exam in which each participant will individually present the result of the project and answer theoretical questions asked by the experts.

The project is designed to cover the following topics, which are structured consistently with the working packages (WP1, WP2, WP3) established in the current research project:

Topic 1: Energy audits of industrial processes for the sustainable development:

The energy audit approach is applied to develop and quantify the sustainability metrics of the industrial processes. The typical operating conditions of the process are defined by measurements and data reconciliation to calculate the energy needs. It allows to identify the main energy drivers, key sustainability performance indicators, base load conditions and other relevant information to select suitable ex-ante models of energy technologies for the process and energy system integration analysis.

Topic 2: Heat recovery and energy conversion in industrial processes:

Definition of the energy requirements in a process and identification of heat recovery potentials by applying the pinch analysis, methods of heat exchanger network design, modification of operating conditions to maximize the heat recovery, integration of industrial heat and combined heat and power technologies, as well as waste and water use minimization and recovery.

Topic 3: Industrial symbiosis for process decarbonization by renewable energy integration and CO_2 capture, use and sequestration (mineralization):

Integration of renewable energy, storage, fuel cells and electrolysis, biomass conversion, waste valorization, CO_2 capture technologies, industrial symbiosis and regional energy systems integration, energy infrastructure and grids, and district energy systems.

3.2 Ex-ante models of selected industrial sectors derived from energy audits

Although it is costly and technically challenging to count on a comprehensive, real-time representation of an industrial sector, it is possible to build simplified ex-ante models that comprise typical unit operations and information on the main material and energy (i.e. thermal and electrical) streams, without disclosing any confidential data. They are clearly not intended to be an accurate description, but rather used to provide an insight into which resources are available and needed in a given industrial plant. These models, also known as ex-ante models, can be used to define a standard for the knowledge and information exchange between the industrial sectors, which can in turn reveal symbiotic interactions with other energy systems. In this way, the concept of ex-ante model emerges as a solution to overcome the challenge of sharing information, which is one of the main barriers to the dissemination and adoption of best available practices. A blueprint of an industrial process can be also a support for pointing and hierarchizing the main inefficiency sources when carrying out energy audits. Vice versa, information gathered in the course of audits can be used to improve and create new blueprints, or can be adapted to other plant setups. All in all, ex-ante models can be considered as good representatives of a given industrial sector, thanks to their identifiable units, the use of verifiable data and the provided information on the flows of the resources available in that typical industrial plant. A secondary objective of this project is to develop, document, validate and report the ex-ante models (blueprints) of the relevant industrial sectors. The blueprints should be flexible and sizeable so as to provide a good overview of the performance of the industrial plant.

The concept of ex-ante models (blueprints) has been also used in other projects in which the IPESE group from EPFL has participated as both project leader and contributor. The use of this concept has proved to be a powerful innovative approach to assess the energy integration potentials and to propose decarbonization roadmaps for the industrial sectors. Table 1 shows selected projects that preceded and inspired the development of ROSMOSE tool, and provided experience to the research group in the definition of best energy audit practices, process modelling and simulation, process integration, as well as mathematical optimization, documentation, validation and reporting strategies.

Table 1. Selected projects that preceded and inspired the development of ROSMOSE tool.

Project	Description of outcomes
AIDRES - Advancing industrial decarbonization by assessing the future use of renewable energies in industrial processes [26].	Generation of a database to support EU-27's long-term goals of achieving a fully integrated industrial strategy. It is a valuable resource for the European Commission and industries that offers insights into effectiveness, efficiency, and cost of potential innovation pathways to achieve carbon neutrality in key sectors, such as steel, chemical, cement, glass, fertilizer, and refinery by 2050. It considers geographical distribution of annual production for these sectors at the EU-NUTS3 regional level.
SCCER EIP – Efficiency of industrial processes [27].	Comprehensive techno-economic information of existing and new technologies, new integration methods and tools on company and/or site level to facilitate the application of energy efficiency measures and novel technologies.
SCCER BIOSWEET – Biomass for Swiss energy future [28].	Development and implementation of concepts of biomass valorization technologies that promote alternative energy carriers for mobility or heat and power applications in order to support the energy policy and market development.
EPOS – Enhanced energy and resource efficiency and performance in process industry operations via onsite and cross-sectorial symbiosis [29].	Development of a cross-sectorial Industrial Symbiosis (IS) platform for identifying cluster opportunities, bringing together global process industries from five industrial sectors, namely minerals, steel, cement, chemicals, and engineering. The development of blueprint models allowed to characterize in a simplified way the material and energy needs of the energy conversion systems.
METHAREN - Innovative biomethane system integration boosting production while managing renewable energies intermittency [68]	Optimize biomethane production from biogenic CO_2 to increase the overall production capacity of biomethane, while reducing overall production costs. Demonstrate the system efficiency to manage renewable energy systems intermittency by transforming electrons into biomethane as a flexible renewable energy carrier, using rSOC (reversible solid oxide cell) systems.
NETZEROLAB VALAIS – Enabling carbon neutral production at Novelis aluminium plant in Sierre Switzerland [73]	A systemic study has been launched aiming at increasing the inherent efficiency of the process units and reusing waste heat of aluminium plants, as well as increasing the use of renewable energy resources. Different key performance indicators, such as energy efficiency, CO_2 emissions, costs, and technology readiness levels, are used to evaluate various decarbonization technologies.
IEA ANNEX 58 HTHP – Integration of High-Temperature Heat Pumps in the Swiss Industry [72]	The overall objective of the Annex is to provide an overview of the technological possibilities and applications as well as to develop concepts and strategies for the transition towards heat pump process heat supply. The goal is to improve the understanding of the technology potential among manufacturers, potential end-users, consultants, energy planners and policy makers.
TASK XXIV IEA IETS – On the role of the process integration in the industry decarbonization [74]	Develop a documented open-source database of ex-ante models of selected industrial processes and energy technologies to assess the decarbonization potential, considering the ontologies and the infrastructure for sharing and executing the reporting tool.

The blueprints are constituted of a series of profiles providing insights into the key inputs and outputs of a given industry in terms of thermal and electrical energy, materials and services. Thus, a blueprint is not a detailed model of process operations and it is unsuitable for advanced process supervision or control, or to study dynamic systems. The validity domain is restricted to nominal operations and stationary regimes. The study of specific situations, such as start-up and shut-downs, requires specific and extended ex-ante models. The ex-ante models will be rather used for high level multi-objective optimization of the resources and energy networks utilization. The models constituting blueprints can be linear or non-linear, depending on the compatibility needed by mixed integer linear or nonlinear programming solvers used to optimize the internal performance.

The conceptual framework for producing blueprints is divided into (i) data gathering and (ii) processing, (iii) configuration of the models, and (iv) reporting (i.e. documentation and visualization). Data gathering is the most important step and one of the most time-consuming during the creation of ex-ante models, especially for large industrial processes. Also, its accurate realization directly affects the models response. In many datasets, materials and energy flows are decoupled from one another and there are few works that simultaneously embrace the integration of materials and energy networks. For this reason, the data processing is used to screen the information coming from different conflicting sources, as well as for suggesting the procurement of missing or incorrect data. During the models configurations, experts in major industrial sectors evaluate the level of detail necessary for each industrial activity.

Three levels of representation can be used to represent the industrial plants layout, namely global balance (black box), site map (grey box) or process units (white box). The black box level is the one with the least number of details, which basically includes the main external material and energy streams (fuels, feedstock, products and wastes), giving an insight on the main input and output flows crossing the system, but without any details of the internal needs of the process. A grey box model decomposes the plant into production units, utility systems, and waste treatment units; all interconnected via distribution networks. This layout identifies the main energy consumers, cold and hot utility distribution profiles, and efficiency of the energy conversion units. Yet, it still does not give any insight either on the process energy requirements (temperature levels, heat loads) or on the different production steps. To tackle this issue, the white box model contains information that enables the visualization of the internal transformation processes (e.g. pretreatment, reaction, separation and purification). In this case, the use of flowsheeting software, such proprietary (e.g. Aspen®) or open source simulators (e.g. DWSIM) can give access to thermodynamic databases and can calculate the thermodynamic properties of the substances involved in the industrial plants. Equations solvers aiming to execute mass and energy balances, and estimate the performance of the conversion processes, are also available in the ROSMOSE tool.

It is worth noticing that, oftentimes, open source literature is the only source of information available to initialize, generate and validate simulation-based results. Moreover, if industrial information is too detailed, data exchanges across industrial sectors may be hindered due to confidentiality issues. Thus, in this project, a compromise between the quality of the information needed for building the ex-ante models and the complexity of compiling the required data has been achieved. A summary of the energy audits is presented; but only the results of the dairy and brewery audits will be used in the next sections to exemplify the working principle and functionalities of ROSMOSE tool, prepared for the MAS programme.

3.2.1 Explosives production plant

This audit dealt with the industrial production of explosives, such as PETN (pentaerythritol tetranitrate), and ANFO (ammonium nitrate fuel oil). An overview of the plant flowsheet with the main mass and energy flows of the process is given in Figure 3.

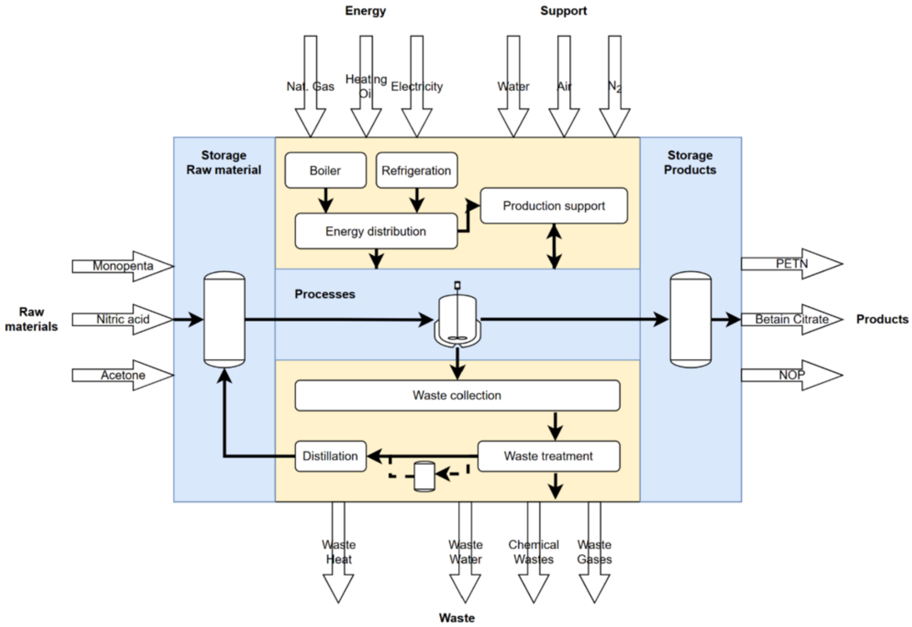


Figure 3 Mass and energy flows of the main units in the explosives production plant.

3.2.1.1 Process Description

To produce pentaerythritol tetranitrate (PETN), a batchwise nitration of pentaerythritol (also called monopenta) is performed in a stirring reactor, with a ratio between monopenta to nitric acid of 1:5 [30]:

$$C_5H_{12}O_4 + 4HNO_3 \rightarrow C_5H_8N_4O_{12} + 4H_2O \quad \text{(R1)}$$

The reaction is very exothermic and the temperature is maintained at 20°C to avoid thermal runaway. The enthalpy of formation of PETN is $\Delta H_f^0 = -1703\ kJ/kg_{PETN}$ [31], but according to measurements done on-site, only $506\ kJ/kg_{MP}$ or $1176\ kJ/kg_{PETN}$ of heat are effectively evacuated. After nitration, PETN is filtered out and sent to a second reactor, while the acid is sent to a recovery step in a distillation column. Next, the PETN (acid content < 25%) is washed out with water to drop the acidity to around 1%. The ratio of used water to rough product is about 11:1. PETN is mixed with a 1% sodium carbonate solution and heated up to 85-90°C to neutralize the remaining acidity. The ratio of Na_2CO_3 solution to PETN is around 8-10:1. Next, the PETN is dissolved in acetone in a ratio of 1:2.2 at a temperature of 58°C. The mixture is slowly cooled down, allowing the PETN to crystallize.

Afterwards, PETN is filtered out and the residual acid is washed out with a small amount of ethanol. Acetone and washing water are sent to a rectification column for separation and reuse. The rectification column is heated with steam and cooled with cooling water. Finally, PETN is dried at around 40°C, and it is ready for packaging or for the production of detonation cords. Nitric acid enters an equipment used for purification and concentration of inorganic acids, called plinke, and is mixed with 55% HNO_3 and sulfuric acid. The acid is stabilized, concentrated and bleached and leaves with at a purity of 99%. H_2SO_4 is then concentrated separately and reused again. The purification process generates NO_x, which is treated and released with the purified air, while the resulting 55% HNO_3 is reinjected into the process. It is worthy to note that the plinke is not connected to the steam network, but it has a separate burner that delivers heat to the processes using a thermal oil.

3.2.1.2 Energy consumption

The production of PETN requires heat at relatively low temperatures, rarely exceeding 200°C. To supply this heat, 3 boilers, fueled with natural gas, produce steam at around 15 bar, which is delivered through a steam network at 3, 9 and 14 bars to the different buildings and processes. In addition, a thermal oil system, also fueled with natural gas, is used for the recycling of nitric acid. Although electricity is mostly bought from the local grid, about a third can be produced with a hydro turbine driven by a nearby water flow. The total energy consumption and costs are presented in Table 2. Accordingly, natural gas accounts for about 86% of the total energy consumption, whereas 30% of the consumed electricity is produced by the hydro turbine. Due to the higher price of electricity, natural gas accounts for 77% of the energy costs, while the remaining part is made up by the electricity bought from the local grid. The energy bill can be calculated based on the monthly profile of energy consumption (natural gas and electricity), as shown in Figure 4.

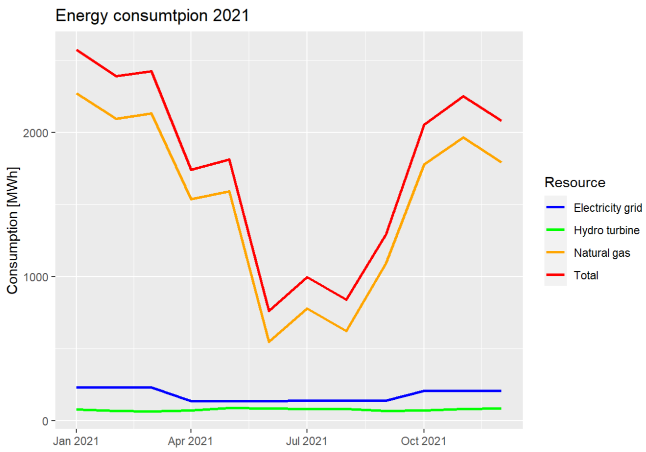


Figure 4 Energy consumption (2021).

Table 2 Total energy consumption and costs in the explosive production plant.

Type of energy input	Total consumption in 2021 (GWh)	Total cost in 2021 (kCHF)
Natural gas	18.2	970
Electricity from grid	2.1	280
Electricity produced	0.9	—
Total electricity consumed	3	—
Total energy consumed	21.2	1250

Figure 5 shows the energy consumption per process and per type of energy in the explosives production plant. Electricity breakdown is represented in the outer ring, whereas heat breakdown is shown in the inner pie plot. The total heat consumption is slightly larger than that shown before, because only natural gas was counted; but in Figure 5, the heating oil used for space heating in the PETN production building is also included. As it can be seen, penta and chemie processes account for more than half of the electricity and heat consumption. Buildings are also large consumers of both electricity and heat. Obsolete or non-existent insulation explains the relatively high heating demand. These building energy losses together with the heat losses during the production and distribution of the main product, as well as the intercooling of the air compressors can explain around 85% of the heating and electricity needs.

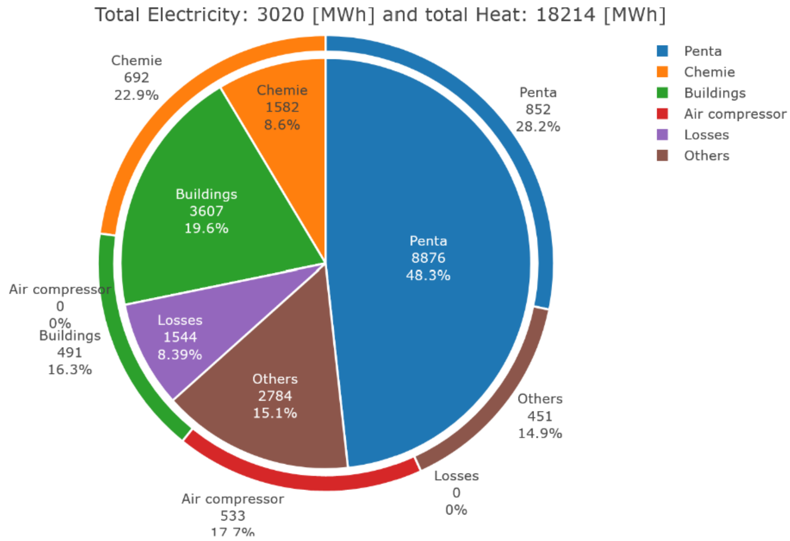


Figure 5 Breakdown of the energy consumption per energy type (electricity in outer ring and heat in inner pie plot) and per consumer.

Finally, Figure 6a-b shows the typical composite curves and Grand composite curve of an explosives production plant. Notably, a large potential for heat pumping is evidenced, which has the potential to recover around 1.8 MW of waste heat that otherwise is released to environment. By integrating heat pumping technologies, up to 80 % of the total plant energy consumption can be provided, whereas only a fraction of the heating is necessary above 100 °C. This is one of the several pedagogical examples used for exemplifying the potential if cutting down the natural gas consumption by electrifying the low temperature heating demands, while capitalizing on the process heat from exothermic reactions.

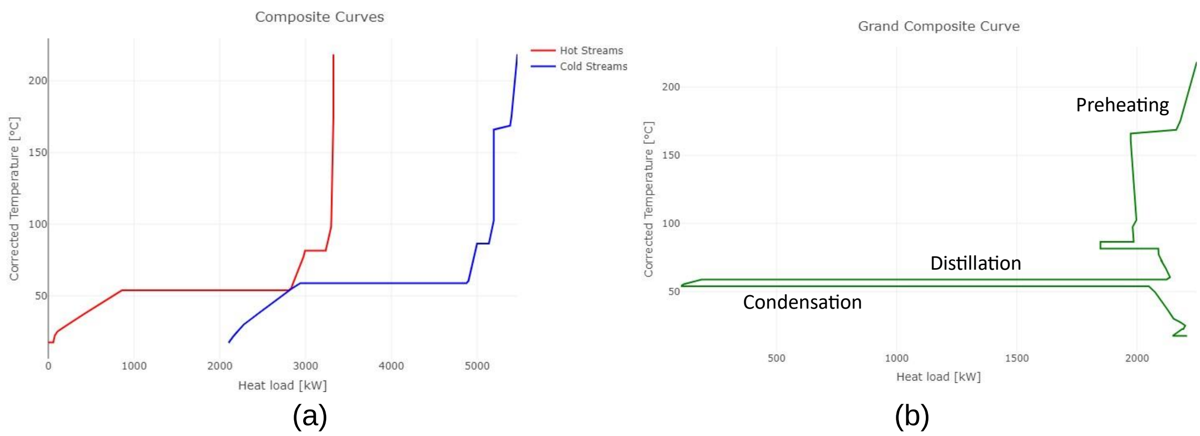


Figure 6 Composite curves (a) and Grand composite curves (b) of the explosives production plant.

3.2.2 Malting plant

The malting process is a key step in the production of alcoholic beverages, such as beer and whisky, in which the barely grains are allowed to germinate in a controlled environment before being dried at a specific rate to obtain the malt grains. The malting process is energy intensive as air needs to be heated for long periods in order to dry germinated barley in a kiln. For this reason, an audit on the actual process conditions was carried out and it can be used for conducting a heat integration analysis of the process. The results allow to identify energy recovery opportunities within the process and propose a setup of technologies to satisfy the process requirements resulting in reduced operational cost and CO_2 emissions.

3.2.2.1 Process Description

The barley grains are firstly steeped in water for several hours to allow for the absorption of water. The grains are then spread out in a vessel to begin the germination process, during which enzymes break down the starches and proteins in the grain, producing sugars and amino acids. The latter components are used in the brewing process during fermentation by the yeast [32]. The grains are transferred to the kiln, where they are dried to the desired moisture content using hot air, usually produced by burning natural gas. Since the kilning process dwarfs the steeping and germination phases in terms of the heating requirements, it was the focus of the energy audit for heat integration analysis of the malting process.

In the kilning process, the germinated barley grains, also called green barley, are dried to a required moisture content for about a day, depending on the type of grain and the desired malt qualities. To determine the energy requirements, the path the grains take throughout the kilning process was analyzed, and the corresponding energy requirements for each step were calculated. Firstly, during the withering phase, barley grains need to be dried from a moisture content (M.C.) of 43% to about 12%. The respective energy of vaporization is calculated by Eq.13. At the curing phase, MC drops to about 4.5%, which also corresponds to an energy of vaporization given by Eq.14.

$$Q_{vap}^{w} = \Delta H_{vap}^{H2O}\,(T_w) * m_{H2O}^{w} \tag{13}$$

$$Q_{vap}^{c} = \Delta H_{vap}^{H2O}\,(T_c) * m_{H2O}^{c} \tag{14}$$

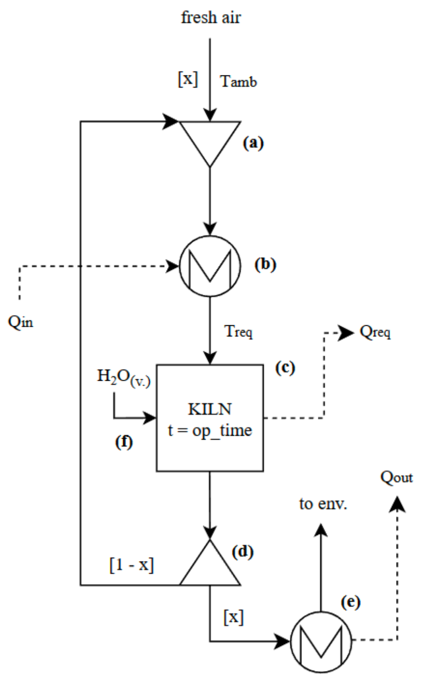
where ΔH_{vap}^{H2O} (kW) is the latent heat of vaporization of water at temperature T, $T_{w,c}$ (°C) is the withering or curing phase temperature, $m_{H2O}^{w,c}\,(kg_w/kg_b)$ is the amount of water to be evaporated per kilogram of barley during the withering and curing phases. The energy needed to heat the barley to the withering and curing temperatures was also taken into account, see Eqs. 15 and 16.

$$Q_{sens}^{w} = (T_w - T_{amb}) * (C_p^b + \xi_w \cdot C_p^{H2O}) \tag{15}$$

$$Q_{sens}^{c} = (T_c - T_w) * (C_p^b + \xi_c \cdot C_p^{H2O}) \tag{16}$$

where $\xi_{w,c}\,(kg_w/kg_b)$ is the grain M.C. right before the withering and curing phases, $T_{amb}\,(°C)$ is the ambient temperature, and $C_p^{b,H2O}\,(kJ/kgK)$ is the specific heat capacity of the barley grains or water. To satisfy these demands, one or more heat transfer interfaces must be utilized. Typically, hot air is used to transfer the required energy through convection. As barley grains are solids, they cannot be processed through typical heat exchangers; therefore, the energy demands of the process must be undertaken from a different perspective considering the energy demands of the air, instead of that of the grains. Other important aspects to consider when modelling the malting process include the solid heat transfer interface between the barley and the heat-transferring fluid, as well as the fact that malting is operated in batch mode, as opposed to a continuous process. This means that a time dimension is present in the process formulation, indicating that certain streams exist at different times, which renders the energy recovery infeasible without the use of energy storage. In the kilning process, the withering phase lasts for about 16 hours, during which hot air enters the kiln at about 55°C. The hot air temperature is continuously raised from 55°C up to 85°C depending on the chosen malt quality.

The continuous equivalent of the batch kilning process is determined following the time average model (TAM). As for the heat transfer interface, a proxy to the barley stream, namely the flux of hot air, needs to be used to reproduce the process demands, since solid grains of barley cannot be passed through conventional heat exchangers. This approach is illustrated in Figure 7. The kilning process is divided into five different periods, each having their own parameters, such as the required temperature, the operating time, and the ratio of fresh air entering the system. Fresh air enters the system and undergoes a non-isothermal mixing (a) with a portion of the exhaust air leaving the kiln (d), as an attempt to recover part of the waste heat and minimize fuel consumption needed to reach the desired temperature. The air is then heated to that temperature (b) and passes through the kiln (c), represented here as a black box. Therein, the temperature of the air drops as sensible heat that the air loses is converted to vaporization heat of the water (f). Finally, in order to close the energy balance, the energy provided to the system leaves (e) in the form of latent heat of the water vapor, which can be condensed and released through the exhaust.



List of Parameters

Period	T_{req} [^oC]	t [h]	x [-]
I	55	16	1
II	60	1	1
III	70	1	0.55
IV	75	1	0.25
V	85	3	0.10

Figure 7. Kilning process model diagram and list of parameters for the five chosen time periods.

3.2.2.2 Energy consumption

The composite and grand curves of the kilning process are shown in Figure 8a-b, which gives information about the potential energy integration, as well as the minimum energy requirements (cooling and heating) in the malting process. It is worth noting that for the typical kilning, there is not a compulsory cooling requirement by the process, as the exhaust stream is normally rejected to the environment. The corresponding gran composite curve of the kilning process shown in Figure 8b gives information the possibility of using heat pumps for upgrading the waste heat at high temperature for supplying the process needs. Furthermore, cogeneration of heat and power to satisfy the curing phase heat requirements and at the same time provide power to a heat pump could be potentially profitable, especially in cases where buying electricity from the grid is more expensive than buying natural gas. In fact, for the typical case of a malt batch producing 16 t, a boiler used as the sole utility to meet the minimum heating demand of the process consumes 402 kW of natural gas. This consumption in turn leads to CO_2 emissions of about 712.3 t/y.

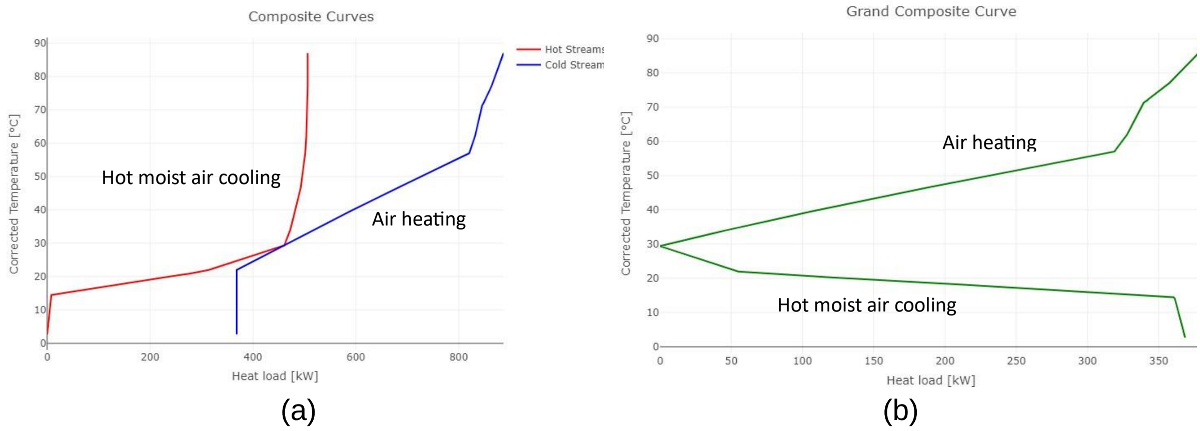


Figure 8 Composite curves (a) and Grand composite curves (b) of the kilning process.

A more detailed look at the graphs reveals a significant scope for improvement, since using a fired furnace may incur high exergy losses if high-quality energy (fuel) is used to provide the heating demands at relatively low temperatures. The electrification or the integration of more sustainable energy technologies, such as heat pumps or biomass integrated digestion and gasification, along with cogeneration units, may be a solution to decarbonize the malting process.

3.2.3 Distillery plant

A distillery produces brandy through distillation of fermented sugars extracted from the pears. Furthermore, the apricot brandy also accounts for a large part of the sales. Based on these two beverages, further products are created through the addition of sugar, water, and fruit compote. A distillery may not only sell alcoholic beverages, but also fruit syrups [33].

3.2.3.1 Process description

Figure 9 shows an overview of the production processes implemented at the distillery. The fruits (pears or apricots) are received in a pre-processing area, where they are sorted out, crushed, peeled and destoned. Next, the fruit undergoes a fermentation process, in which yeast is added to the fermentation tanks in order to convert sugars into alcohol. Lactic and phosphoric acids are also added to decrease the pH and promote yeast activity. In the distillation section, the ethanol content of the fermented fruits is increased through the use of distillation columns operating in batch mode. The hearts of distillation are filtered and combined with water, sugar and fruit compote to create the respective products. The plant also has an independent syrup production section, in which the fruit juice and sugar are combined in a container heated using the hot water produced by an electric boiler. The resulting mixture passes to through the filtration step and is subsequently cooled down using cooling water. The product is bottled as raspberry or blackcurrant syrup, depending on the fruit juice that has been used.

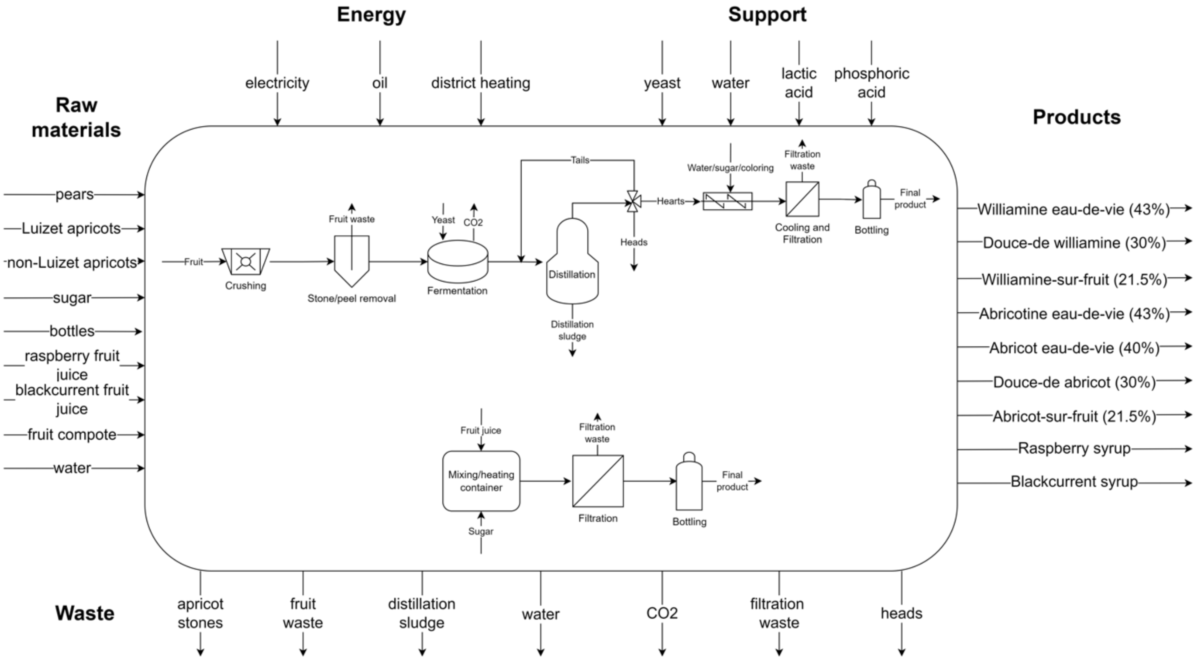


Figure 9. Mass and energy flows of a typical distillery plant based on apricots and pears.

3.2.3.2 Energy consumption

The mass flow rates of all the process streams were determined, so that the total yearly expenditure can be calculated. The plant inputs and outputs include raw materials (e.g., fruit and yeast), electricity and waste streams (e.g., distillation sludge and waste heat). The energy bill is determined based on the costs associated with electricity, oil, district heating, and water for process cooling. The current yearly expenditures were calculated separately for the distillation and syrup processes.

The yearly demand, specific costs, and yearly costs of the distillation process needs are summarized in Table 3. The total yearly cost of the distillation process is around 691 kCHF/y, which amounts to an average of 11.21 CHF/bottle produced. The distribution among the four different types of inputs (i.e. raw materials, energy, waste, and support) is shown in Figure 10. The purchase of raw materials of the process is the most significant cost (86.3%), followed by energy (7.8%), waste removal (3.3%) and chemical support (yeast, 2.7%). Regarding the expenditures in terms of energy consumption (Figure 11), the cost of district heating is the most significant (47.2%), followed by the electricity (39.5%) and the oil (13.3%). Finally, the waste streams (Figure 12) that entail the highest expenditures is distillation sludge (85.0%), followed by apricot stones (8.4%) and fruit waste (6.6%). The capitalization of these waste streams could be a way of simultaneously dealing with two different problems, the amount of wastes released to the environment and the consumption of nonrenewable resources. In fact, the biological digestion of these wastes has been identified as a form of producing sustainable fuel, whereas reducing the effluents to the sewage.

Table 3 Yearly costs of the distillation process at the distillery.

Process needs	Yearly Costs (kCHF/y)
Raw Materials	596
Energy	53.5
Chemical support	18.4
Waste	23.0
Total Cost	691

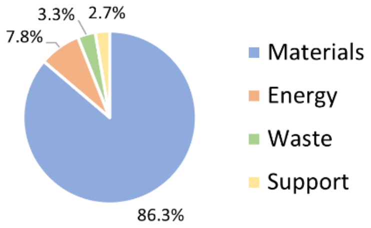


Figure 10 Distribution of total yearly costs of the distillation process.

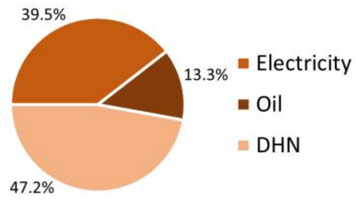


Figure 11 Yearly energy costs by source of the distillation process.

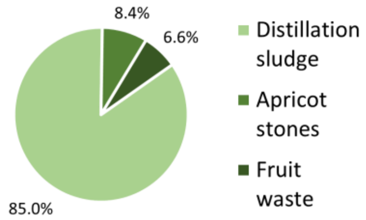


Figure 12 Yearly waste costs by source of the distillation process.

Table 4 summarizes the yearly demand, specific costs and yearly costs of the syrup process. The total yearly expenditures in the syrup section for a production of 83000 l amount to 280 kCHF, which is equivalent to 3.37 CHF/bottle. Figure 13 shows the distribution of the yearly expenditures among the four different sections. The two main cost factors are raw materials (85.1%) and energy (14.2%), since there are no waste streams and the only support process need (water) accounts for 0.7% of total expenditures. The percentage contribution to the total expenditures of the four raw materials are blackcurrant juice (29.2%), raspberry juice (25.7%), sugar (16.5%) and bottles (13.7%). Meanwhile, electricity and district heating account for about 6.2% and 8.0% of the yearly expenditures, respectively. In summary, the total yearly expenditures of the entire plant amount to about 971 kCHF. The distillation and syrup processes account for 71.2 % and 28.8 % of total cost, respectively.

Table 4. Yearly costs of the syrup production process at the distillery.

Process requirement	Yearly Costs (kCHF/y)
Raw Materials	238
Energy	39.7
Support	1.90
Total Cost	280

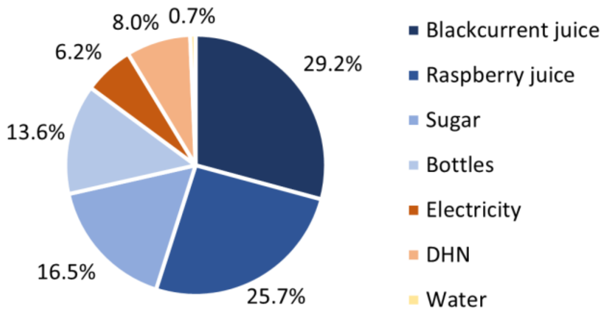
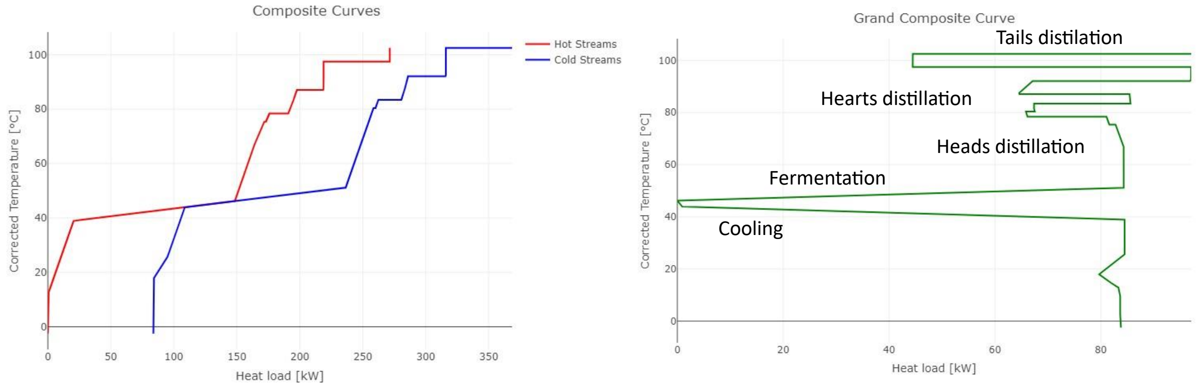


Figure 13 Distribution of the total yearly expenditures of the syrup section at the distillery.

The composite curve and grand composite curve of the base case system are shown in Figures 14a-b respectively. The minimum heating requirement is about 1000 kJ/bottle, typically supplied by a fuel oil furnace. The minimum cooling requirement amounts to 863.6 kJ/bottle, which is normally satisfied by using cooling water (875.0 kJ/bottle) and a refrigeration cycle (42.2 kJ/bottle). The combined cooling energy provided by the cooling water and refrigeration is larger than the minimum energy requirement of the process due to the additional cooling demand required by the refrigerator condenser. A refrigerator that takes heat at a temperature level of -10°C and releases it at 25°C would have a coefficient of performance (COP) of 4.3 and an electrical energy demand of 12.6 kJ_{el}/bottle (assuming an exergy efficiency of 0.5). The pinch point, which is where the overall hot and cold streams touch in the composite curve is at 43.9°C, highlighting the potential to install a heat pump to replace the use of natural gas boilers.



(a) (b)

Figure 14 Composite curves (a) and Grand composite curves (b) of the distillery plant. Note the need for a refrigeration utility.

3.2.4 Leather production plant

Hide tanning is the method used to treat animal skins and hides to create leather. A tannery is the facility where this process occurs. Transforming hide into leather involves altering the protein structure of the skin permanently, enhancing its durability and resistance to decay, while also adding color. Prior to tanning, the skins typically undergo dehairing, followed by the removal of fat, meat, and connective tissue. Subsequently, they are washed and soaked in water containing various compounds, preparing them to receive the tanning agent. The tanning process consumes large amounts of hot water and incur in large inefficiencies due to the thermal bath losses.

3.2.4.1 Process description

The processes of the tannery are fed with water from a river a rate of a 1000 m^3 per day. This amount is distributed into the processes according to Table 5. The water coming from a river is taken at 10°C. To reach the process temperatures, heat exchangers are used and deliver hot water at 45°C and 80°C thanks to the heat supply using steam coming from a gas boiler.

Table 5 General tanning processes in a typical tannery.

Name	T_{out} [°C]	T_{out} [°C]	Water flow $[\frac{m^3}{day}]$	Energy [kW]
Prétrempage	24	20	35	-13.544
Autre bain	24	20	71	-27.476
Enchauceneuse 1	78	27	2	-9.868
Enchauceneuse 2	18	22	4	1.548
Bain (from 1er lavage)	24	23	64	-6.192
1er lavage	24	23	64	-6.192
2ème lavage	24	23	64	-6.192
3ème lavage	24	23	64	-6.192
Bain (from 1er lavage)	24	23	64	-6.192
1er lavage	30	27	64	-18.575
2ème lavage	30	30	64	0
Pré-déchaulage (from 2ème)	32	32	13	0
1er lavage	32	32	16	0
Bain	36	35	13	-1.258
2ème lavage	20	24	13	5.031
Pré-déchaulage	38	32	2	-1.161
Bains	38	32	1.2	-0.696
Lavage	20	24	2	0.774
Togo	23	23	2	0
Négonda	23	23	13	0
Tannage	28	29	3	0.29
Lavage	20	25	4	1.935
1er bain (auto)	20	24	14	5.418
Prétannage (from bain de tannage)	20	20	24	0
Bain de tannage	25	27	14	2.709
Lavage	25	27	24	4.644
Machine essoreuse	30	38	50	38.698
Nettoyage	30	38	20	15.479
Lavage + Neutralisation	38	35	36	-10.448
Bain de teinture	53	43	35	-33.861
Rinçage	23	28	84	40.633
Finissage	20	20	30	0

Figure 15 shows the heat exchangers assembly used in the tanning site. Water storage tanks are required to store the hot water produced by the steam condensation in the industrial heat exchangers. The steam consumed is returned as condensate to the tanks.

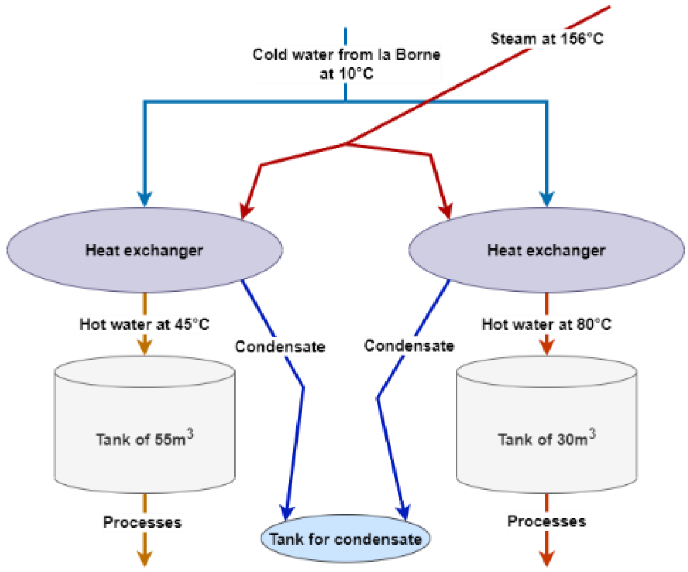


Figure 15 Production of hot water for the tannery processes.

The hides path is graphically represented in Figure 16 [34]. Different processes like soaking, unhairing and liming/deliming, fleshing, degreasing, pickling, tanning, samming, shaving, neutralization, bleaching, retanning, dyeing, drying and mechanical processing (finishing) are responsible for the substantial amount of water and energy input to the plant. Based on the mass flow rates and the temperature changes of the hot water streams (Table 5), the amount of energy delivered or taken by the water can be estimated. This value is shown in the last column of Table 5. To characterize this demand, assumption about the processes functioning are adopted. First, although the specific heat of skin changes with moisture content [35], this change has been neglected, as the amount of moisture is hard to estimate and will change at each step of the processes. Moreover, the specific heat of a calf skin is considered the same as the one of a bovine, since calves are young bovines. The specific heat of the skin is set as $c_{p,leather} = 401.93\ J/kgK$ [36]. A production of 1000 hides per day is considered, and each skin is assumed to weigh approximately 14 kg [9].

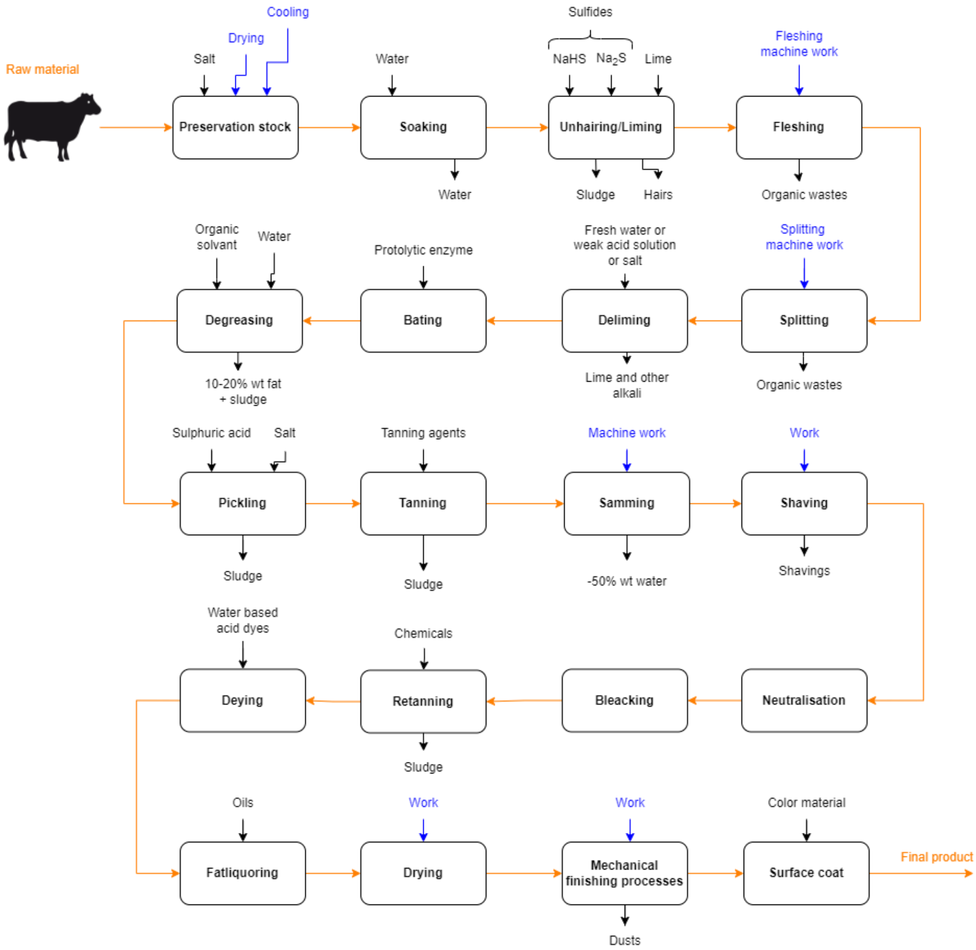


Figure 16. Process flowsheet of a tanning processes.

3.2.4.2 Energy consumption

It is important to mention that the baths are not operating all day long and the process varies from bath to bath and from one type of tanning to another. Indeed, the results shown in Table 5 are a general view of three different types of tanning. Hitherto, the calculations have considered 12 hours of average operations per bath according to the time average method. The electricity consumption of the tannery is approximately 6 GWh/y. Electricity is used to drive the machines, lighting the buildings and operate the cold room where the raw skins are stocked before manufacturing. These operations cannot be removed or modified as those machines are already optimized for specific leather quality. Optimizing the lightning and the cold room does not fall within the scope of this audit.

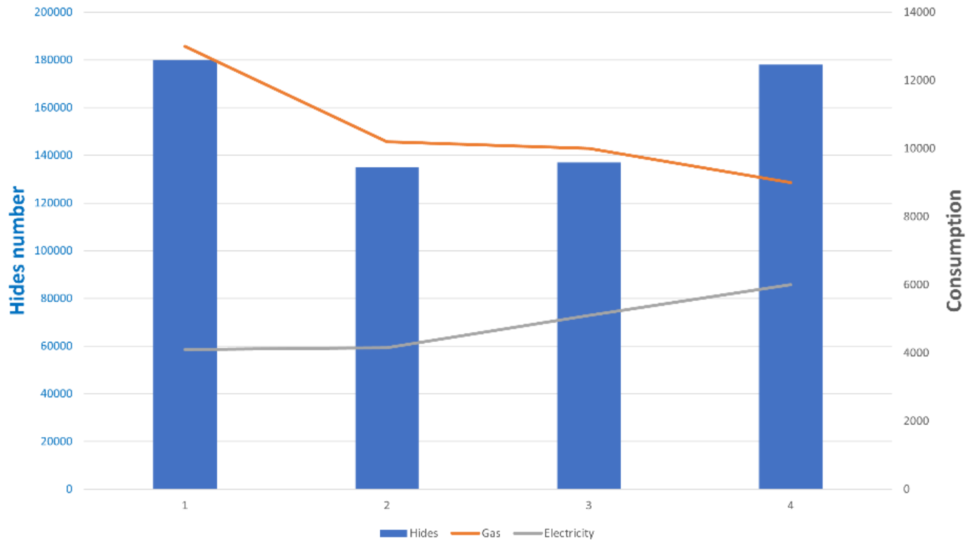


Figure 17 Yearly leather production for each type of hide (bars, left axis) and natural gas and electricity consumptions (solid lines, right axis in MWh/y).

In addition, the gas consumption of the tanning plant is about 9 GWh/y. The gas has two functions in the tannery. First, it directly feeds machines used to manufacture the leather (e.g. the pistoleteuse, the cadreuse, among others). Secondly, it is used to produce steam, which simultaneously feeds some machines and heat up water from 10°C to 45°C and 80°C in the heat exchangers to supply the heating demands of the baths. The condensates are completely recycled into the boilers. The gas grid setup is illustrated in Figure 18. The items enclosed in green are non-modifiable. The ones enclosed in red may be optimized or even replaced by more advances heating technologies, such as heat pumps and cogeneration systems.

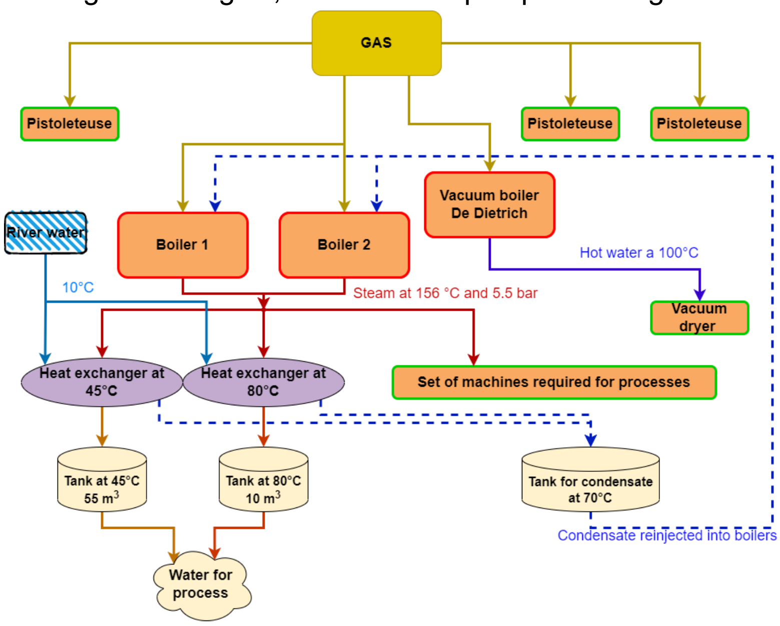
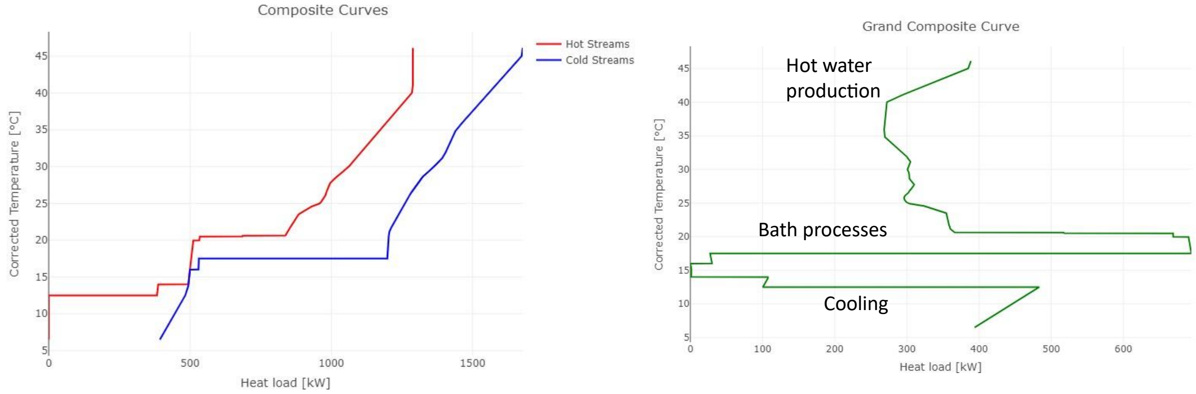


Figure 18 Representation of the gas grid at a tanning plant.

According to Figure 19, the potential step towards the decarbonization of the tannery plant is the replacement of the natural gas boiler by heat pump systems at low temperature. If the gas boiler is unavoidable, still biogas or synthetic natural gas from the waste valorization could be available. Since the tannery produces biomass wastes, it could be interesting to investigate on the potential integration of a biodigestion plant. The advantages are twofold, as the energy consumption and the produced residues are simultaneously reduced. Finally, the boiler hot water coming from the furnace is often mixed with water coming from the river to attain the desired hot water temperatures (45°C and 80°C), it incurs a mixing loss that can be avoided by devising a series of heat pumping systems that match the required hot water production temperatures and that use the heat from the river as heat source in the evaporator.



(a) (b)

Figure 19 Composite curves (a) and Grand composite curves (b) of the tanning plant

3.3 Demonstration of the utilization of the ROSMOSE process integration tool

In this section, the use of ROSMOSE for analyzing the process integration of a dairy and a brewery plant is exemplified.

3.3.1 Case study of a dairy plant

In the dairy process, raw milk is first transformed into concentrated and pasteurised milk, then into final products including cream and cheese. This is mainly achieved through a series of heat exchangers and evaporators. The system includes multiple sections where operating temperatures and flowrates are defined by the process recipes. Fresh milk is received, cooled and stored. In the pasteurization process, milk is heated up to 60°C followed by a separation of the cream in a centrifuge. The milk stream is further heated up to 75°C and quickly cooled back to 4°C to destroy harmful bacteria and assure sufficient shelf-life. The pasteurized milk is sent to the evaporation section, while the cream heated up to 70°C is sent to a mixer where a thickener is added and then gradually cooled down to a storage temperature of 4°C. In the evaporation section (main energy consumer of the dairy process), the milk is preheated then sent to a multiple effect evaporator, where steam is used in the first effect to evaporate part of the water in the milk [37]. The evaporated steam is used for preheating the inlet milk and evaporating more water in the subsequent effects. To allow for such heat recovery, the pressure in each effect is lower than the one preceding it. This approach does not recover all of the latent heat from the evaporated water content of the milk stream, as there is usually more steam from the first effect than what the second effect can really use. The cheese production section starts by preheating the concentrated milk stream up to 56°C, and then the cheese forming cultures are added. After the cheese production, the whey is filtered out. Further cheese processing is necessary, including cooling and addition of water and salt. Other processes, such as the cleaning in place, storage, and wastewater treatment are also important sections of the dairy plant. Notably, the dairy process does not inherently contain any reactions, but rather a series of heating and cooling steps. Some systems irremediably dissipate electrical energy in the form of heat (stirrer, pumps, centrifuge, compressors, etc.). The minimum energy requirements of the conventional dairy process are estimated as 125 $kWh/m^3_{freshmilk}$ of heating utility (i.e. 3485 kW) and 114 $kWh/m^3_{freshmilk}$ of cooling utility (i.e. 3200 kW).

Figure 20 shows a conventional dairy process flowsheet and possible production routes for value-added by-products. These alternatives include valorizing the whey separated in the evaporation and cheese production sections, as well as the sludge produced in the waste-water treatment unit. The first involves the production of brown cheese, known as mesost, which entails evaporating part of the water content in the whey, followed by a mixing with additional cream and cooling down to storage temperature. The second alternative utilizes the whey stream for producing a whey-based soft drink. It implies evaporating a significant portion of the water in the whey stream, followed by cooling the concentrated whey to 50°C, mixing fruit sugar and flavouring ingredients, to finally add water and CO_2 to produce the carbonated soft drink known as Rivella® [38]. The third alternative may capitalize on the energy of both the whey and sludge streams to produce biogas (a mixture of ~ 55% CH_4 and 45% CO_2) through anaerobic digestion under thermophilic conditions [39, 40]. In this option, heat is needed to maintain the reaction temperature in the digester and steam is used to dry the dewatered digestate, which can be sold as a solid fertilizer due to its high nutrient organic load

[41]. Figure 20 also shows the potential utility systems that could be integrated to supply the energy requirements of the dairy plant.

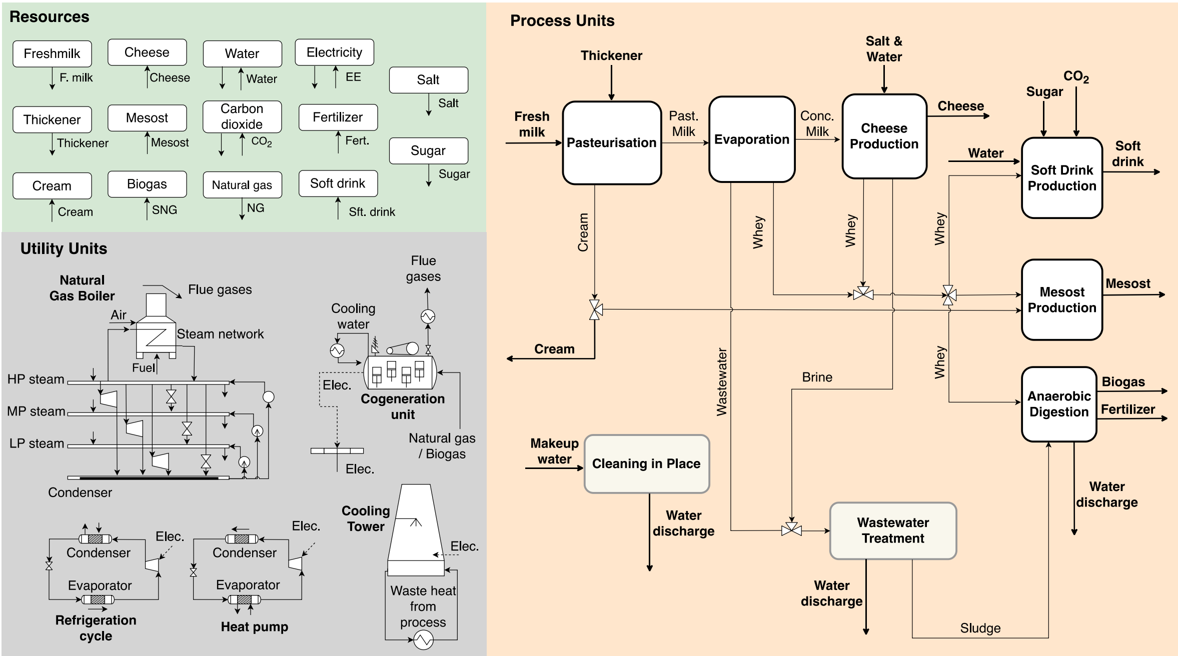


Figure 20. Conventional dairy production process flowsheet integrated to the waste valorization routes: mesost, soft drink or biogas production. Potential utility systems are also depicted.

To systemically evaluate the various integration options, ROSMOSE tool is used to perform the energy integration and total site optimization of the conventional dairy process, and to graphically represent the key performance indicators described in the following sections. Figure 21 shows an example of an ROSMOSE project structure and the typical relationships between ETs, units, and layers. The units belonging to a specific ET can be of two types: *process* or *utility* units. The main difference between them is that, on the one hand, a *process* unit corresponds to an industrial production process, whose requirements must be satisfied and, therefore, its size factor should be fixed during the optimization problem. On the other hand, a *utility* unit represents auxiliary equipment, whose size is optimized to meet the process energy requirements. For instance, a process unit can be defined based on the operating data of a subunit of dairy plant (e.g. the resource flows, the supply and target temperatures, the flows composition, the heating demands, the specific costs, the process constraints and scheduling, etc.). In contrast, the several utility units potentially adopted could be sized to meet these demands, such as heat pumps, steam boilers, cooling systems, refrigeration units, cogeneration units, and markets.

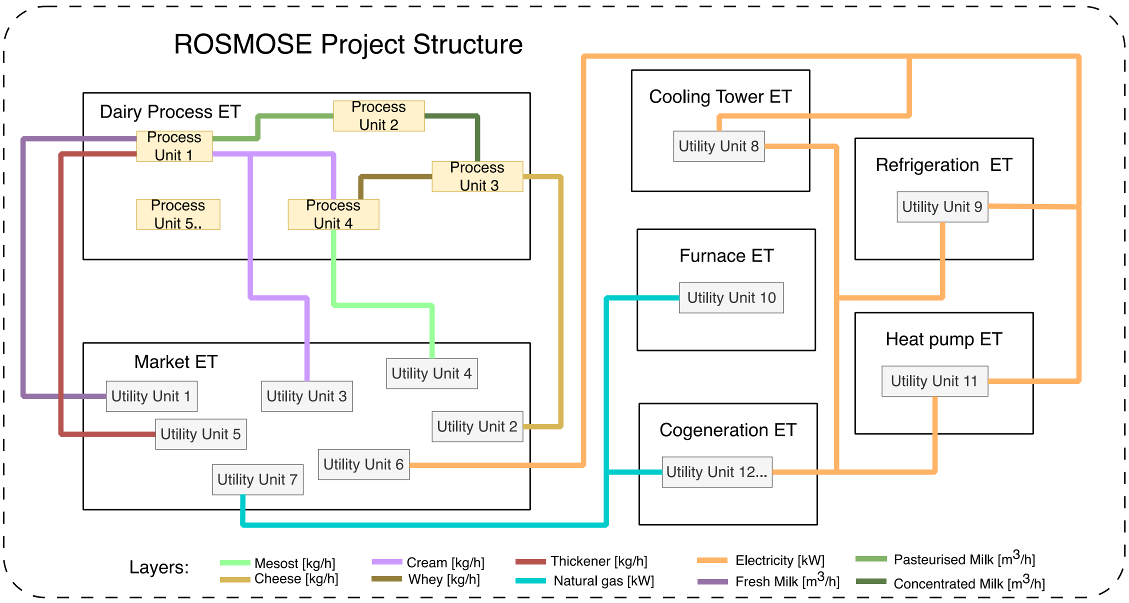
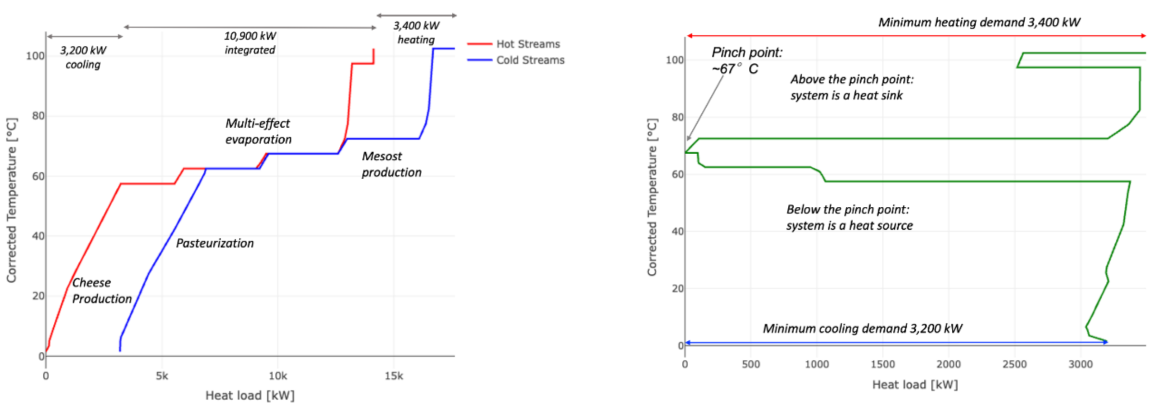


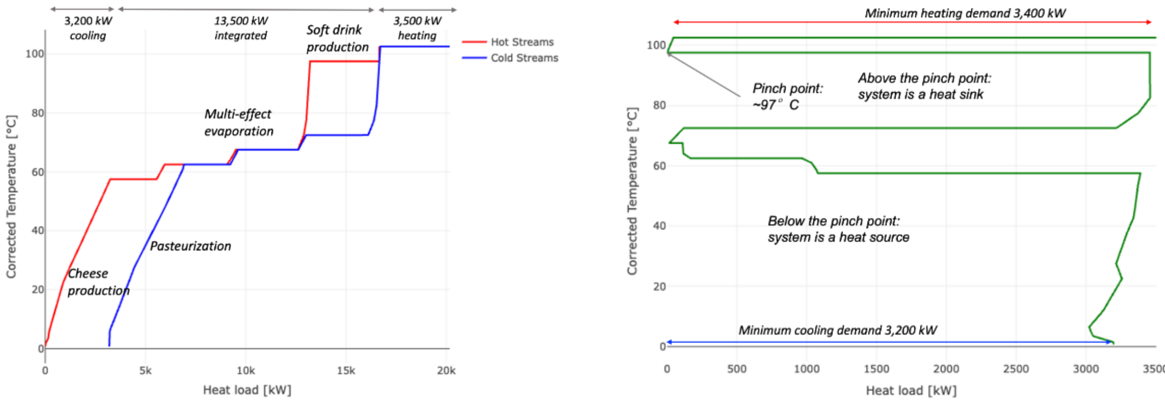
Figure 21 ROSMOSE project structure and the relationship between ETs, units, and layers pertaining to the dairy plant example.

Applying the MILP formulation defined in the Methods section, a graphical representation of the process integration potential in the dairy industry can be devised. Figures 22a-b show composite (a) and grand composite (b) curves of a dairy plant producing mesost. Clearly, there is an opportunity of eliminating the excessive steam generation by integrating the use of a heat pump and valorizing the waste heat. The minimum energy requirements of the dairy plant producing mesost cheese are determined and graphically represented those figures. The total energy integration potential between process-to-process streams is approximately 391 kWh/m$^3_{freshmilk}$ (~10,930 kW), which can be attained by installing a heat exchanging network with an area of approx. 3,000 m^2 and a total annualized cost of roughly 1.38 €/m$^3_{freshmilk}$ (~338,800 €/year). For the mesost production scenario, the minimum energy requirements are estimated as 125 kWh/m$^3_{freshmilk}$ of heating utility (i.e. 3,485 kW) and 114 kWh/m$^3_{freshmilk}$ of cooling utility (i.e. 3,200 kW). Similar trends in heating and cooling utility requirements are found for other process configurations producing soft drinks (Figure 23a-b) or biogas (Figure 24 a-b). Table 6 summarizes the calculated fuel and electricity requirements, and the total product yield of the three processing routes for converting the whey stream (typically considered as waste in the dairy process) into added value products, such as mesost cheese, soft drinks, and biogas.



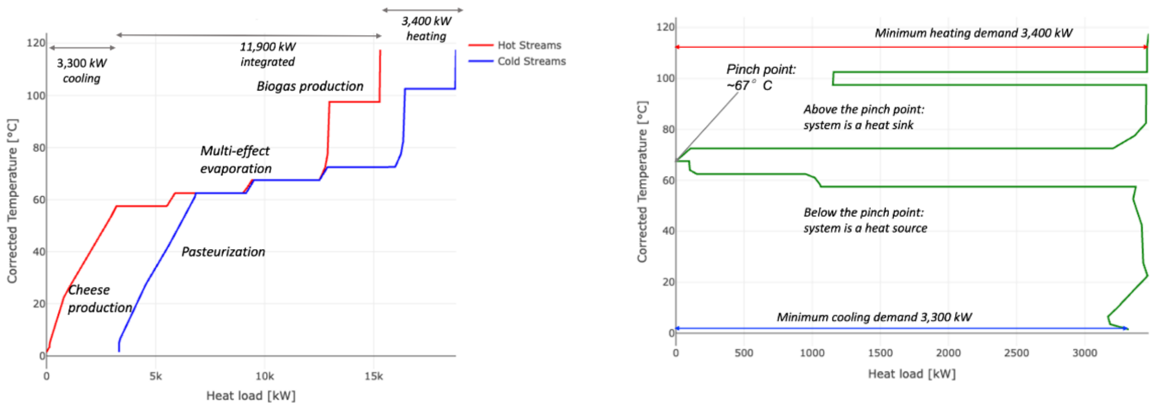
(a) (b)

Figure 22 The composite (a) and grand composite (b) curves of a dairy plant producing mesost. The curves are generated by the ROSMOSE integration and reporting tool.



(a) (b)

Figure 23 The composite (a) and grand composite (b) curves of a dairy plant producing soft drink. The curves are generated by the ROSMOSE integration and reporting tool.



(a) (b)

Figure 24 The composite (a) and grand composite (b) curves of a dairy plant producing biogas. The curves are generated by the ROSMOSE integration and reporting tool.

Table 6 Energy consumption of the dairy plant and other value-added production routes, when integrating biodigestion, heat pumps and cogeneration systems.

	Mesost production (assumed base case)		**Soft drink production**		**Biogas production**	
Process layout	**Conventional**	**Heat pump & Cogeneration**	**Conventional**	**Heat pump & Cogeneration**	**Conventional**	**Heat pump & Cogeneration**
Grid electricity (kWh/m^3_{feed})	5.50	3.50	5.80	15.0	5.50	0.00
Total fuel consumption (kWh/m^3_{feed})	133.90	30.40	134.60	13.80	68.20	- 48.30*
Total electricity consumption (kWh/m^3_{feed})	5.50	15.65	5.80	20.50	5.50	18.20
Cooling tower power	2.47	0.40	2.50	0.30	2.60	0.44

demand (kWh/m^3_{feed})						
Heat pump power demand (kWh/m^3_{feed})	0.00	13.87	0.00	18.60	0.00	16.50
Refrigeration power demand (kWh/m^3_{feed})	3.00	1.38	3.30	1.50	2.90	1.31
Product yield (kg_{prod}/m^3_{feed})	402.10	402.10	359.00	359.00	224.70	224.70

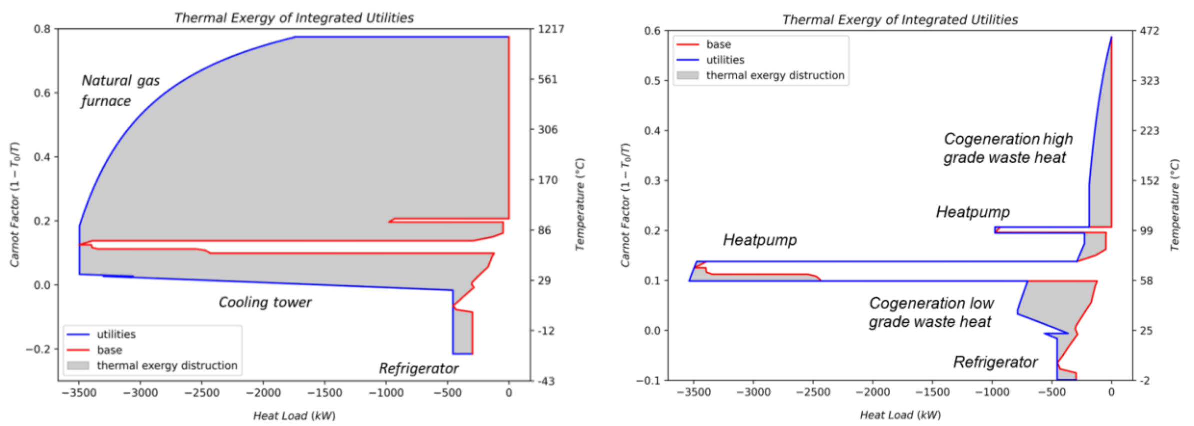
*Note: Negative value indicates net export of biogas in the heat pump and cogeneration case with biogas production.

According to Table 6, a reduction of up to 80% in total fuel consumption is expected for all the value-added production routes, provided that heat pumps and cogeneration systems are used for supplying the heating demands. Interestingly, this improvement comes at the expense of a higher electricity import only for the soft drink production route. Meanwhile, for the mesost and biogas production routes, the grid electricity imported is much less than in the conventional case, in which only boilers are employed. It can be explained by the large share of power supplied (i.e., 30 – 70%) by the cogeneration unit to the heat pump. In this way, the overall site fuel consumption can be reduced from 134 to 30 kWh/m^3 for the mesost production route. The advanced utility schemes evidence an interest in achieving an optimal combination of waste heat recovery to partially meet the heating requirements of the industrial plants. Table 6 also compares the overall product yield of the three routes for converting the whey stream into mesost cheese, soft drinks, or biogas. Due to a better overall yield of the mesost production route per m^3 of whey, this option generates the largest amount of product per unit of volume of processed feedstock.

The so-called integrated Carnot curves (Figures 25-27) show a graphical representation of the impact of the selected utility systems on the process irreversibility in a dairy plant. In this type of diagram, the main y-axis is the Carnot factor ($1-T_0/T$), whereas the secondary y-axis is the corrected temperature. The x-axis is the heat required or available at a certain level of temperature. It is worth noticing a distinction between the base (industrial process, in red) and the utilities (in blue) integrated curves. It indicates the precise superposition of the heat load curves, which entails an overall thermal balance at the industrial site. The area between these two curves corresponds to the exergy destruction in the heat exchanger network (HEN). Thus, smaller area between the curves indicates lower exergy destruction or, equivalently, minimum entropy generation in the dairy production site [42].

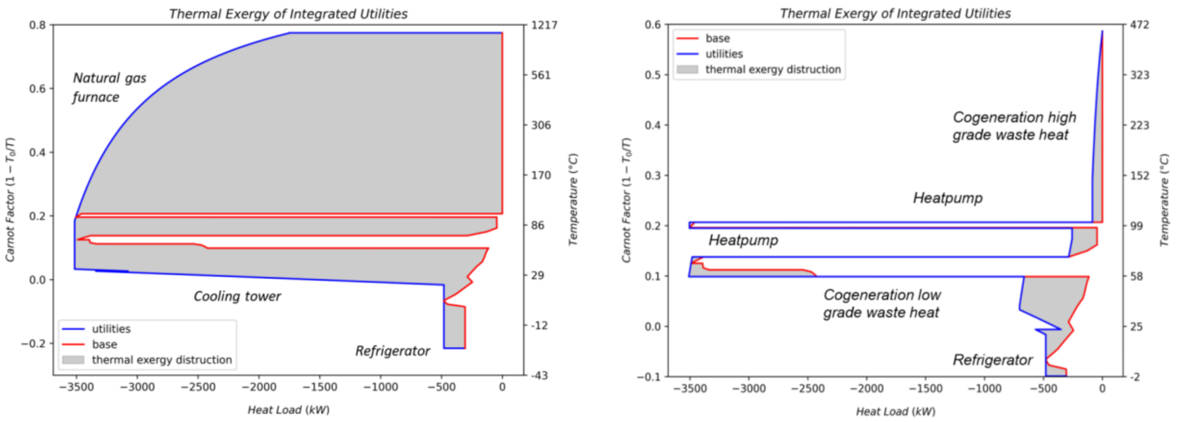
In fact, when comparing Figures 25-27 (a) using conventional utilities (i.e. large grey shaded area) and Figures 25-27 (b) using heat pumps and cogeneration systems, the advantages of the latter configurations become more evident. In the former, larger irreversibility are seen due to the use of a very hot utility profile from a natural gas furnace to satisfy the needs of a process that only requires heat supply mostly around 70°C and at most 120°C. Also, Figures 25-27 (a) exhibit an oversized cooling utility (cooling water plus refrigeration), due to a complete removal of the waste heat from the dairy plant. In contrast, the Figures 25-27 (b) highlight the radical transformation of the integrated Carnot curves when more advanced energy technologies are activated. In those cases, a synergy between the cogeneration and the heat pump system is established, in which the former provides both power and low grade waste heat to a heat pump, thus reducing the losses of the engine cooling system. Moreover, the heat pump also can upgrade the low-grade waste heat available throughout the industrial process, further reducing the natural gas furnace dependency. By eliminating excessive steam generation from natural gas boilers, optimal waste heat recovery below the pinch point temperature is attained. This utility optimization brings about the reduction of the area between the utilities and process integrated curves. Since the process irreversibility is associated to the inappropriate way of the energy resources, the utilization of advanced energy systems redounds to lower environmental impact and more sustainable processes. Similar conclusion can be drawn for all the integrated production routes, namely mesost, soft drink and biogas production routes. Notable, in the latter scenario, the produced biogas is sufficient to supply on site electricity needs and still have a net export if biogas.

Table 7 summarizes some economic and environmental performance indicators, such as income, operating and capital expenses, and net revenue, as well as CO_2 emissions of the various production routes with different utility integration options (e.g. heat pumps and cogeneration units). In addition, carbon taxation was applied to all scenarios. According to these results, thanks to a higher market value of mesost (brown cheese) and a higher yield (compared to soft drink or biogas production), the valorization of the whey stream through mesost production proves to be the most profitable scenario. It is worth mentioning that, although the incremental capital cost of installing heat pumps and a cogeneration unit is considered, it does not significantly increase the annualized investment costs. Hence, the net revenues of all the scenarios integrating advanced utility systems are slightly higher than those using conventional utilities. Finally, CO_2 footprint of the integrated dairy plant is greatly reduced when introducing heat pumps driven by electricity either imported from the grid or produced in an on-site cogeneration unit. Both direct and indirect CO_2 emissions from the overall production processes have been estimated and reductions of up to 90% in fossil fuel CO_2 emissions can be attained by shifting from conventional natural gas furnaces to electricity-powered heat pumps. In practice, the latter ones require much less energy and, therefore, allow optimizing the utilization of waste heat from the process streams. Moreover, if an on-site cogeneration unit is fuelled with biogas from the waste biodigestion, any direct emissions are biogenic, and the integrated dairy plant becomes a carbon neutral solution. The only drawback in this case is a reduced production rate (and thus economic profitability), since a large amount of whey is otherwise transformed to biogas, instead of mesost. These results confirm the potential for decarbonizing many food industries, such as dairy plants, through the integration of optimized utility systems. This comparison and detailed evaluation was possible through the ROSMOSE tool.



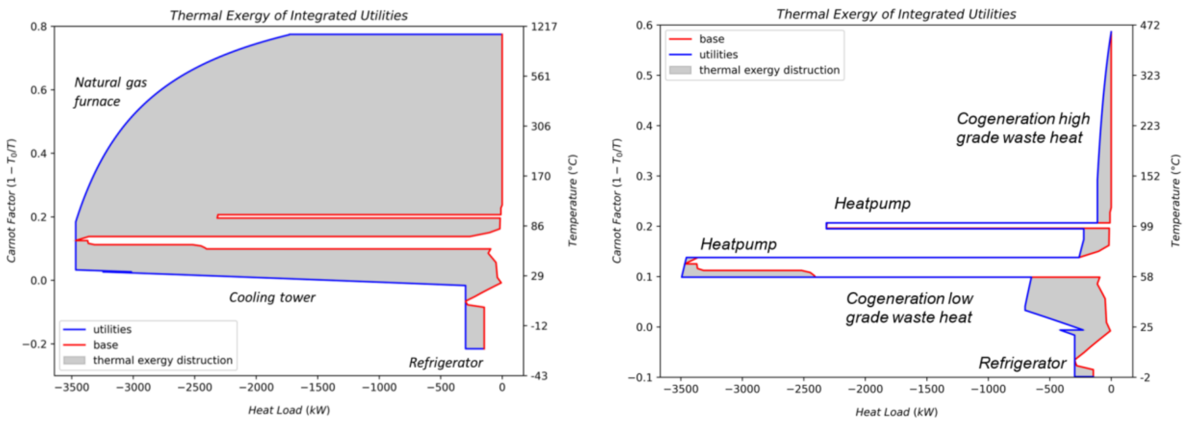
(a) (b)

Figure 25 Integrated Carnot plots for the mesost production scenario (a) using conventional utilities, (b) using optimized utilities (cogeneration unit and heat pumps).



(a) (b)

Figure 26 Integrated Carnot plots for the soft drink production scenario (a) using conventional utilities, (b) using optimized utilities (cogeneration unit and heat pumps).



(a) (b)

Figure 27 Integrated Carnot plots for the biogas production scenario (a) using conventional utilities, (b) using optimized utilities (cogeneration unit and heat pumps).

Table 7 Economic and environmental indicators of the dairy plant and other value-added production routes, when integrating biodigestion, heat pumps and cogeneration systems

	Mesost production Dairy (base case)		Soft drink production (SDP)		Biogas production (BioP)	
Process layout	Conventional	Heat pump & Cogeneration	Conventional	Heat pump & Cogeneration	Conventional	Heat pump & Cogeneration
Income (€/m^3_{feed})	6,108	6,108	1,334	1,334	863	863
Operating cost (€/m^3_{feed})	544	529	587	572	544	529
Capital cost* (€/m^3_{feed})	0.38	0.49	0.38	0.65	0.38	0.57
Net revenue (€/m^3_{feed})	5,564	5,579	747	762	319	334
Direct fossil CO_2 emission ($kgCO_2/m^3_{feed}$)	28.60	6.50	28.70	2.90	14.20	0

Indirect fossil CO_2 emission ($kgCO_2/m^3_{feed}$)	0.63	0.28	0.65	0.97	0.50	0
Net CO_2 emitted ($kgCO_2/m^3_{feed}$)	29.20	6.80	29.40	3.90	14.70	0

*Note: Capital cost is annualized assuming a 40-year investment lifetime and 6% interest rate, and normalized by the processing rate of 28 m^3/h of milk.

Finally, considering the complete electrification of the most economically profitable case, namely, the mesost production route, the resulting integrated Carnot plot is shown in Figure 28. In this highly decarbonized version of the mesost production route, heat pumps can fully satisfy the energy needs of the production system at the expense of an electricity consumption of 19.7 kWh_{EE}/m^3_{feed}. In other words, if the electrical power that drives the heat pumps is generated in a fully renewable and more efficient electricity mix, the installation of a cogeneration system can be spared, resulting in a 34% reduction in capital investment of the utility systems. The net revenue of this scenario remains similar to other mesost production cases at around 5,580 €/$m^3_{freshmilk}$. This approach further contributes to the minimization of the entropy generation throughout the industrial system, the reduction of the environmental impact and the increase of economic attractiveness of energy systems.

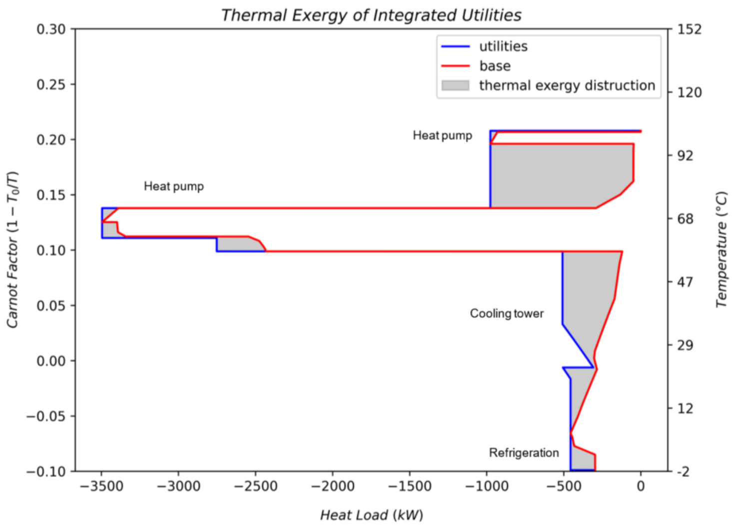


Figure 28 Integrated Carnot plot of the mesost production route with a full electrification approach.

3.3.2 Brewery process

Like the dairy process, the brewery process is a food industry that requires heat supply at low temperature and also produces some wastes that can be upgraded into value-added products. Figure 29 shows the flowsheet of an industrial brewery plant [43]. The milled barley and corn are first mixed with water and heated up to 65°C. A sugar-rich wort is produced due to saccharification of the mash. In the lautering process, the wort is filtered and the husk can be either exported or sent to a biodigestion unit, in which biogas can be produced to replace the fossil fuel consumed in the plant. The filtered wort is boiled slightly above 100°C to achieve 10% wt. of water evaporation and then the hops are added. Next, the mixture is stirred and the trub is removed in a centrifuge. Next, the mixture is cooled down to 10°C and goes through a fermentation process, wherein the sugars are converted into alcohols and a large amount of carbon dioxide by the action of the yeast at anaerobic conditions. The process is slightly exothermic; thus constant cooling is required to maintain the temperature of the fermentation tank. Fermented wort is matured at low temperature (6°C) in a holding tank and then chilled to 1°C before the yeast is eliminated by filtration. Cold water is mixed to the raw beer obtaining the desired alcohol concentration. Next, the pasteurization process occurs by heating the mixture up to 70°C and cooled to 5°C. The beer is finally stored and bottled. The bottle cleaning process is also energy consuming and produces waste water (Figure 30). The bottles are successively pre-rinsed, washed with soda and rinsed in successive baths again before being filled with beer.

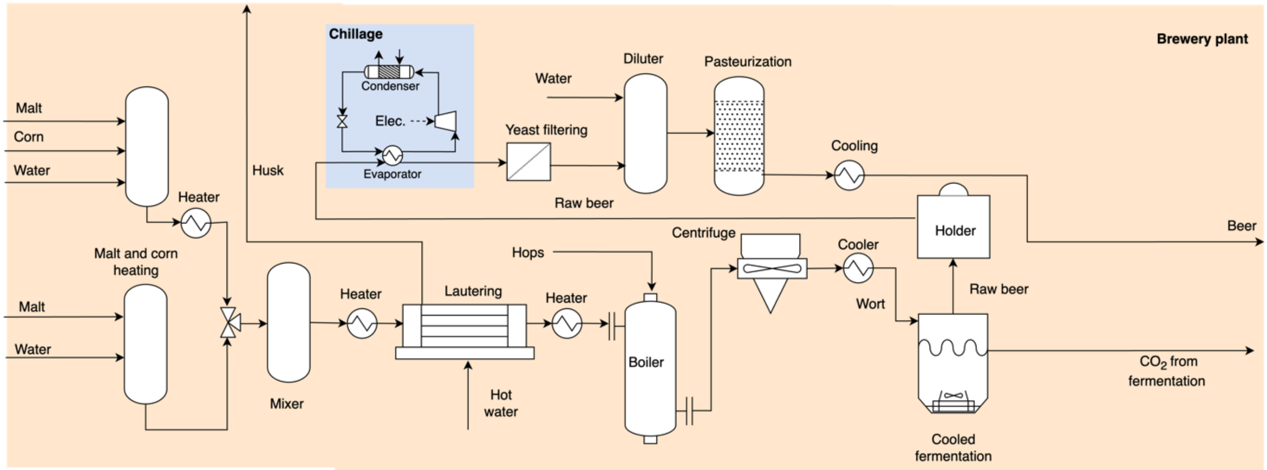


Figure 29. Flowsheet of an industrial brewery process.

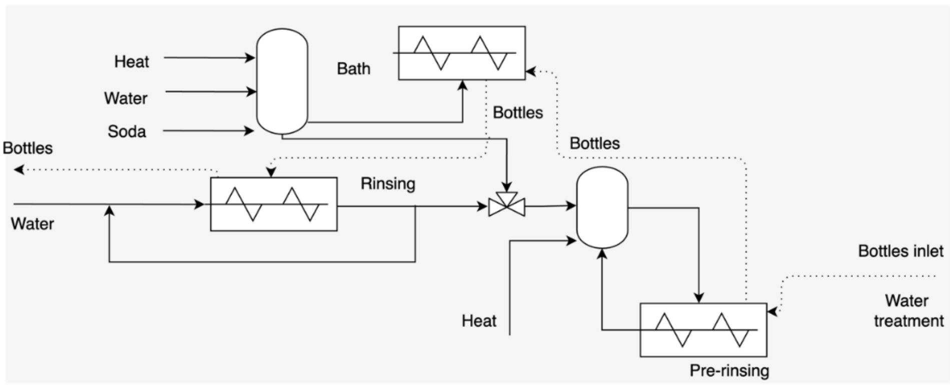


Figure 30. Flowsheet of the cleaning in place process in a typical brewery plant.

The temperature of the baths of the cleaning in place section is set by steam injection. The final rinsing is done with clear water at 15°C. Water of the final bath rinsing is recuperated and sent to the pre rinsing bath, recovering heat form the bottles that are cooled down in the last bath. The total water required at the third rinsing is 20% of the total beer produced and same for the bath rinsing step. The amount of soda is 10% of the water added to the bath rinse.

For a conventional brewery scenario, the total malt, corn, soda and water consumption are 129, 11 and 19 kt/y and 973,263 m^3/y, respectively, for a total production of 892,534 m^3/y of beer and 38 kt/y of husk. The annual direct CO_2 emission from natural gas use (64.95 GWh/y) in the conventional scenario is 13 kt/y, while 24 kt/y of CO_2 are vented from the fermentation process. Other 6 kt/year of CO_2 emissions are related to the indirect emissions of natural gas and electricity supply chains (1.15 kt/y for natural gas, and 5.14 kt/y for electricity), entailing a yearly tax of 4.2 M€. In the conventional brewery scenario, the cooling load reaches 7.56 MW, which is provided by a refrigeration unit that consumes up to 15 GWh/year of electrical energy. In addition, 1.3 MW_e of electricity is required to drive the pump and compressors through all the conventional brewery plant. The typical scenario, based on natural gas combustion, not only has higher associated CO_2 emissions, but also entails large exergy destruction due to the use of high-grade exergy resources, such as natural gas, to only generate steam and hot water. It can be verified in the integrated plot shown in Figure 31.

Accordingly, the use of a steam boiler increases the enclosed area between the base curve (process, red) and the utilities (blue) curve. The refrigerator system is also responsible for a noticeable exergy loss in the system, as it collects and directly rejects the valuable waste heat first into the cooling water and then into the environment, instead of upgrading the waste heat available from the fermentation process for heat pumping purposes. Moreover, the integrated curve suggests potential benefits for installing heat pumping systems also at higher temperatures to capitalize from the waste heat available in self-sufficient zones (i.e. the zones in which process streams can exchange heat with other process streams). A careful scrutiny of the integrated curves also reveals that a temperature-gliding or supercritical heat pump system could be installed to partly deliver the heating demand at temperatures between 50 - 100°C. To this end, the database of ex-ante models of utility systems and decarbonization technologies developed in this project has been activated. Figure 31 shows the flowsheet of the industrial brewery along with the collection of cogeneration and storage technologies to be potentially integrated.

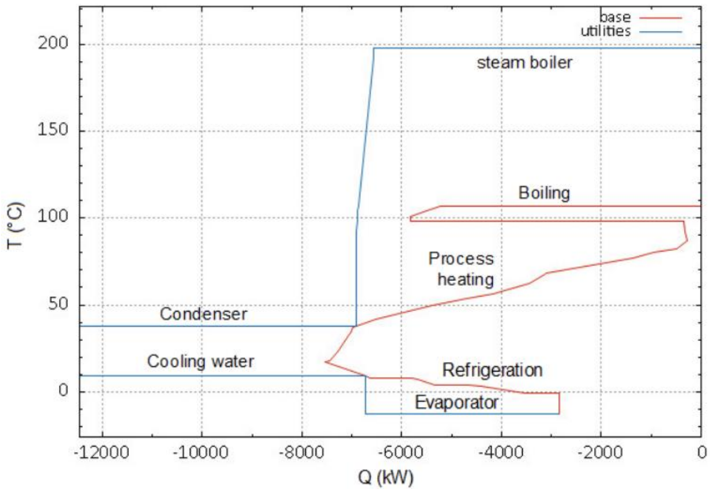


Figure 31 Integrated curve of a typical brewery process.

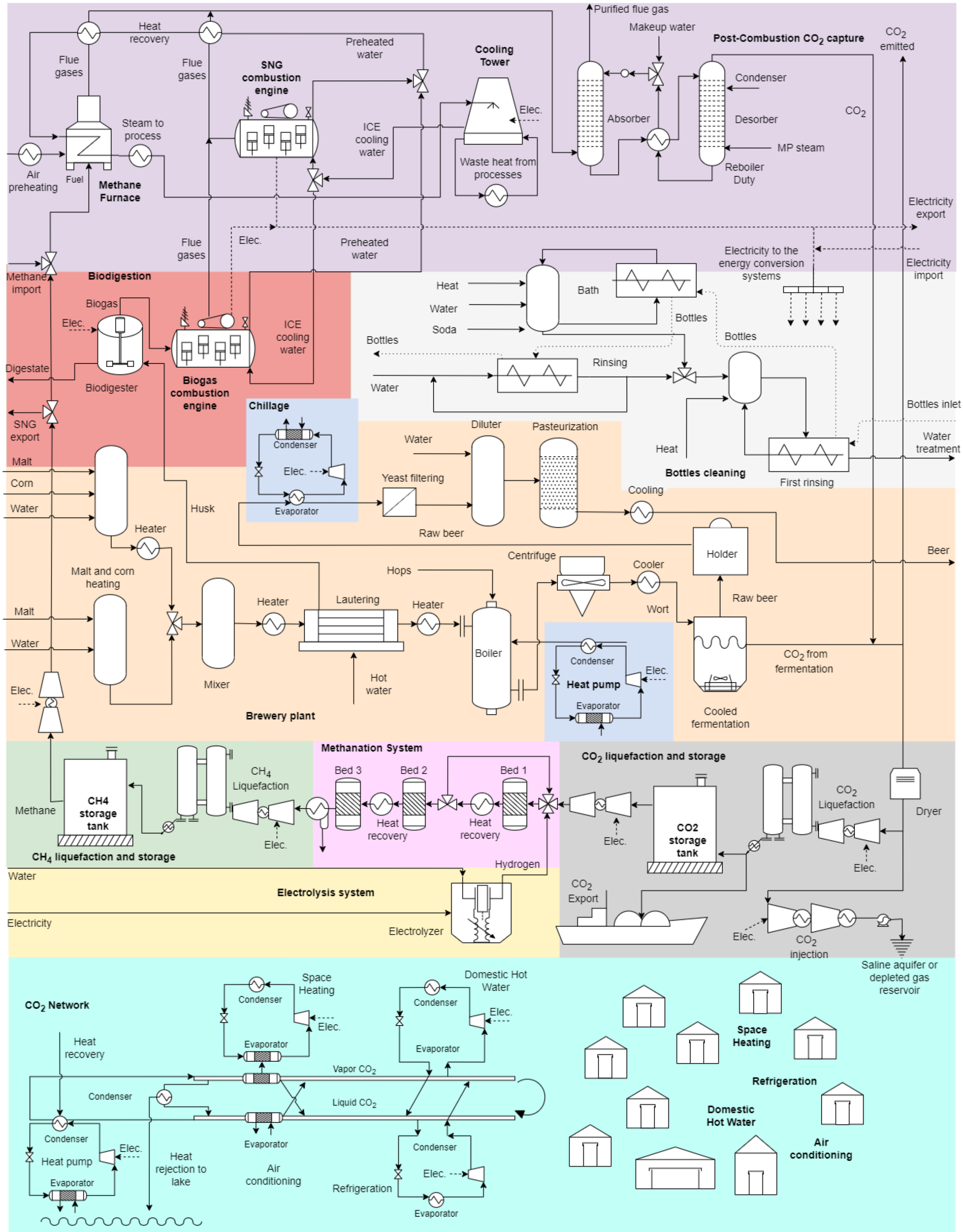


Figure 32 Flowsheet of the brewery plant and potential cogeneration and storage technologies, and the district heating CO_2 network.

The options utility systems and decarbonization technologies still include a gas fired boiler, cogeneration engine with waste heat recovery, sub and supercritical heat pumps, carbon capture units, water cooling and refrigeration, biodigester, electrolysis units, methanator, and gas liquefaction, storage and injection compression units. The synthetic natural gas (SNG) and the CO_2 gas are stored in liquid form at -162°C and -50°C, respectively. The district heating relies on a novel CO_2 network system that supplies the domestic hot water, space heating, air conditioning and refrigeration demands [44]. The waste heat released by the industrial process and the utility systems can be upgraded with the help of heat pump technologies using surplus electricity. Differently from the conventional brewery scenario, which only uses natural gas and electricity from the grid and does not recover the process waste heat for heat pumping applications, a more integrates scenario that make intensive use of the renewable energy conversion and storage systems is devised. This scenario leverages the power-to-gas technologies to capitalize on the excess CO_2 available, and produce and store synthetic natural gas (SNG) using a methanation system. In fact, when the cost of electricity is favorable, SNG can be either produced and directly used in the brewery plant, or exported, together with the purified biomethane produced in the biodigestion system. Despite the fact that an extensive cogeneration system is enabled for self-generation, it is still possible to export electricity from the grid. At the end, the optimal combination of energy technologies and flows has to be determined by using ROSMOSE platform, which handles a MILP that identifies the best energy technologies and operating conditions that minimize the operating costs subject to feasibility and minimum energy requirements constraints.

For both the more advanced, energy integrated brewery plant, the total malt, corn, soda and water consumption remains the same as the conventional brewery plant (i.e. 129, 11 and 19 kt/y and 973,263 m^3/y, respectively). The total production of beer is set as 892,534 m^3/y. The 38 kt/y of produced husk has a biogas potential of 75 Nm^3/t_{husk}. In the typical brewery scenario, the chiller system consumes up to 15 GWh/y of electricity, being the second largest electricity consumer, just after the city (44.6 GWh/y of electricity, and 12.3 GWh/y for space heating heat pumps). Meanwhile, in the advanced scenario, all husk is biodigested to cut down fossil fuel input. However, the biogas derived from the husk digestion falls short to supply the energy demands of the brewery plant, thus requiring to import 133.1 GWh/year of electricity also to drive an electrolysis unit that consumes 76.6 GWh/y or electricity, apart from 12,532 m^3_{water}/y and produces 1,39 kt_{H2}/y. Electricity import is about 41.25% of the total power consumed in the integrated brewery plant, leading to indirect emissions of 8.34 kt/y. Moreover, in the integrated scenario, 16 kt/y of CO_2 from the fermentation unit is injected and only 8 kt/y of CO_2 is emitted. Apart from the biomethane produced in the biodigester, the SNG produced in the methanator (around 39 GWh/y) is also used in the cogeneration systems to supply heat and power required by the whole brewery plant, utility systems and decarbonization technologies.

As expected, one of the major power consumers is the supercritical CO_2 heat pump (11.9 GWh/y), which recovers the heat available at the lowest process temperatures, that otherwise is rejected to the environment in the refrigeration system of the conventional brewery plant. Additionally, the gas liquefaction and storage, along with the recompression and injection compression systems only demand about 3 GWh/y of electricity. It is worthy to notice that the carbon credits (1.6 M€/y) associated to the injection of CO_2 significantly contribute to the increased revenues of the integrated brewery scenario. In contrast, a carbon capture unit becomes prohibitively expensive and is eventually not activated by the optimization routine. For the sake of comparison, Figure 33 shows the integrated curve of the integrated brewery scenario. As with the other integrated curves, the blue curve is the plot of the heat cascade of the utility systems, whereas the red curve corresponds to the process units of the brewery plant. As anticipated, the self-sufficient zones in the industrial process curve indicate a potential to install a temperature-gliding or a supercritical heat pump. The heat pumping of the waste heat available at much lower temperatures to partly deliver the heating demand at temperatures between 50 - 100°C reduces the need of water cooling, while provides the refrigeration duty. This resourceful strategy also poses a trade-off between the use of the combustion gases of the engines and the heat pump setups to deliver waste heat to the brewery process and the district heating network. In any case, the combination of surplus electricity generated in the integrated brewery scenario and the optimal selection of utilities and decarbonization technologies allowed to simultaneously export electricity to drive the heat pumps of a CO_2 network and capitalize on the low-grade waste heat to reduce the environmental footprint of the heat supply of the overall system. The power-to-tank-to-power strategy for renewable energy and CO_2 management proved to be crucial for handling the excess of power generation. It assigns the energy resources in the most convenient way, so that fossil energy consumption is avoided, while reducing the operational cost and offsetting the incremental capital expenditure.

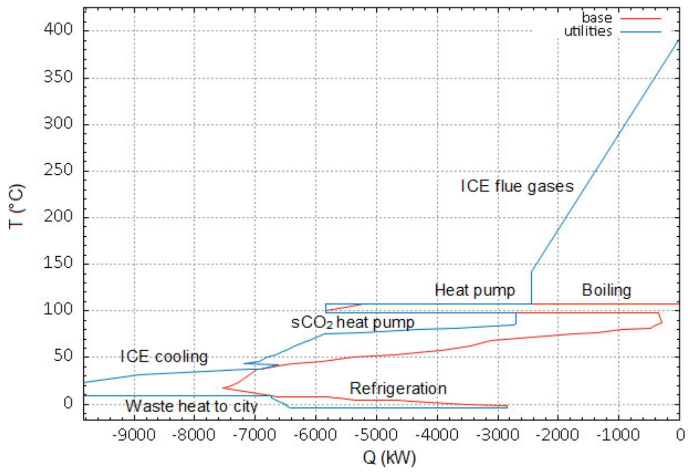


Figure 33 Integrated curves of the typical (left) and the integrated (right) brewery scenarios.

Finally, Figure 34 shows the yearly variation of the storage tanks levels. It is observed that the CO_2 tank level increases gradually starting from October till end of February, which coincides with the emptying of the SNG tanks precisely during the period of in which electricity is more expensive (November to February). Thus, the optimal CO_2 management dictates an intensive monthly power consumption during the months with surplus cheap electricity generation (e.g. excess solar, nuclear or hydro power), which in turn can be stored as fuels.

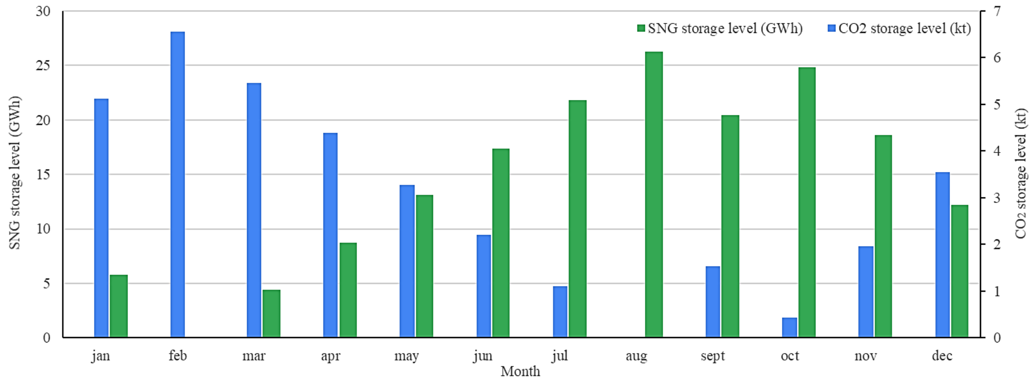


Figure 34. Seasonal variation of the storage tanks levels.

In this way, the upgrading of the industrial residues increases the plant energy security, and contributes to an increase in the revenues of the whole system. Indeed, the annualized incremental capital expenditure between the conventional and the integrated brewery scenarios (5.3 M€/y) is completely offset by a positive incremental operating income (71.7 M€/y) in the latter one, thus leading to an incremental total revenue of about 66.4 M€/y in the integrated scenario. Naturally, the proposed approach represents a riskier investment, as it depends on the commodities prices, the carbon tax, the emissions trading system, the reliability of the newly integrated energy systems and the space budget of the brewery unit. Nonetheless, the proposed setup sheds light on the thermoeconomic and environmental feasibility of integrating advanced energy technologies for tackling the problem of carbon management and intermittency of renewable energy in the food and beverage industry.

As a conclusion, future economic and environmental costs of fossil natural gas calls for more electrification to supply heating in a more efficient way such as using high temperature heat pumps. Meanwhile, the integration of husk biodigestion process, along with the reuse of CO_2 from fermentation (as a source to store intermittent renewable energy in the form of synthetic natural gas), may help to avoid the import of fossil natural gas and still provide an important fraction of the power required by the brewery plant, the utility systems and the decarbonization technologies. The import of electricity is still largely required to balance the capacity of the cogeneration systems, thus, more environmentally friendly and cheaper electricity generation technologies are crucial for the process heat decarbonization in the brewery industry. The carbon trading is an important factor that may boost the deployment of some energy conversion approaches, such as power-to-gas systems, and also promote better CO_2 management approaches. Chemical energy storage systems allowed for a cost-beneficial operating condition, in which the incremental capital expenditure seems to be offset by a substantial gain in plant revenues.

CONCLUSIONS AND PATH FORWARD

The industrial sectors are becoming progressively vocal on the climate action, as investors and governmental pressure increases. This is due to the growing awareness of the impacts of the economic activities on the environmental and social welfare. Many companies are gradually committing to net zero targets, and are willing to use carbon management and energy efficiency-related metrics not only for planning purposes, but also for managing risk. The analysis of the impact of the climate change policies on the assets and the operating revenues is becoming a must-do for enterprises if they want to remain competitive in the coming period of energy transition.

However, as it concerns energy transition, the main bottleneck, after capital allocation, it is training in specialized skills and new methods. Thus, the main goal of this project was to conceive and prepare tools and databases that can be used in a Continuing Education Program at EPFL, with a focus on decarbonization strategies in the Swiss industrial sectors. To this end, energy audits were conducted for processes of representative Swiss economic sectors. In the next steps, the database of ex-ante model was prepared and adapted to the applications of two case studies of dairy and brewery plant presented in this report. The educational material, which includes the utility and decarbonization databases, is fully and adequately documented, and the scheduling of the training course will be adjusted to optimize the knowledge transfer and improve the acceptation of this tool.

ROSMOSE can give researchers and practicing engineers the opportunity to evaluate and compare complex integration systems operating under different scenarios, with the flexibility of designing energy technology models with their own system specifications. It also allows creating impacting reports and draw conclusions from comparative analyses of process integration scenarios. Thus, ROSMOSE certainly will be a key tool to aid decision making for the design and optimization of any industrial or urban energy system.

The launch of the Master of Advanced Studies (MAS) at the EPFL has drawn the attention and motivated the participation of different actors involved in energy planning, efficiency improvement and decarbonization strategies of industrial processes. Discussions and feedback from industrial partners will continue through the development of the MAS course, as industries and practitioners' valuable feedback will be used for improving the description and weighing the suitability of the alternative setups.

The R&I Project Manager of Environmental Performance at Richemont International, Ms. Sara Jardim Cabral (sara.jardim@richemont.com) facilitated the realization of a meeting on-site in Donzé-Baume (Les Breuleux) to kick off the project on industrial decarbonization in this manufacturing industry. Ms. Catherine Houssard (catherine.houssard@polymtl.ca) from Polytechnique de Montréal, who is also part of the CIRAIG consortium, has expressed her interest in the preliminary results of the energy audits in the Donzé-Baume site.

The director of l'Association Recherche Communautaire des Moyens de Production Microtechniques – ARCM), Mme. Catherine Jeanneret (catherine.jeanneret@arcm.ch) has also visited the EPFL facilities to discuss potential synergies on the decarbonization routes evaluated in this project. The ARCM association is developing a project called ECOPROD (Optimization of energy consumption in production).

Lastly, the president of the Patronal Association of Industries (AIP) in Neuchatel, Mr. Philippe Lebet (phlebet@vtx.ch) expressed its interest in facilitate the interaction between the academia and the industry. Meeting at Chaux-de-Fonds and email communications was held to select representative industries to participate in the project, including Breitling, Singer, Detech, Lauener SA and IMA Medtech. Although some industries are still reticent to apply the developed tools and methodologies, the advantage of the proposed approach is expected to become more clear as soon as the MAS programme starts to be imparted.

Many other important firms, representative of the Swiss industrial sectors, including the Swiss Society of Explosives, CIMO, Novelis, Cremo, Elsa, Morand, Hermes, Buhler, Richemont, OIKEN, Gustav Spiess, Terega, Technip Energies, GazoTech, Louis Dreyfus, VITO, among others have partnered with the Industrial Processes and Energy Systems Engineering (IPESE) group looking for the implementation of the cost-benefit analyses on process integration and decarbonization strategies using the ROSMOSE and OSMOSE framework. In addition, various universities, such as KU Leuven, University of Liege, Ghent University, HES-SO Sion, University of Applied Sciences of Eastern Switzerland, Haute École d'Ingénierie et Gestion du Canton de Vaud and University Clermont Auvergne have benefited from the knowledge transferred by the interaction with researchers and experts that developed the ROSMOSE tool [58-73].

APPENDIX A0. PUBLICATIONS IN INTERNATIONAL CONFERENCES AND JOURNALS

The following publications in journals and conferences have been written during the time of the development of this report:

1) Girardan L., Correa-Laguna, J.D., Valee, J., Sharma S., Florez-Orrego D., Ribeiro-Domingos, M., Castro-Amoedo, R., Zhao, Y., Granacher, J., Jones, M., Mendez-Alva, F., Clymans, W., Kantor, I., Meinke-Hubeny, F., Marechal, F., AIDRES: A database for the decarbonization of the heavy industry in Europe. 36th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2023, June 25th – 30th, Las Palmas de Gran Canaria, Spain.

2) Florez-Orrego, D., Ribeiro Domingos, M., Maréchal, F., Heat pumping and renewable energy integration for decarbonizing brewery industry and district heating. 33rd European Symposium on Computer Aided Process Engineering – ESCAPE 2023, June 18th – 21 th, Athens, Greece.

3) Dardor, D., Florez-Orrego, D., Terrier, C., Ribeiro Domingos, M., Maréchal, F., ROSMOSE: A web-based optimization tool to aid decision-making for the design and operation of industrial and urban energy systems. 36th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2023, June 25th – 30th, Las Palmas de Gran Canaria, Spain.

4) Florez-Orrego, D., Dardor, D., Ribeiro Domingos, M., Germanier, R., Maréchal, F., Renewable energy integration and waste heat recovery for the production of sustainable jet fuel and decarbonization of industrial heating applications, AIChE 2023 Annual Meeting, November 5-10, 2023. Orlando (FL), United States.

5) Ribeiro Domingos, M., Florez-Orrego, S., Teles, M., Maréchal, F., Alternative energy supply approach for industrial complexes and district heating networks based on biomass integrated gasification. 36th Int'l Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2023, June 25th – 30th, Las Palmas de Gran Canaria, Spain.

6) Florez-Orrego, D., Ribeiro Domingos, M., Maréchal, F., Techno-economic and environmental analysis of high temperature heat pumps integration into industrial processes. Sustainable Energy Technologies and Assessments, v. 60, 2023, 103560.

7) Florez-Orrego, D., Aimone, L., Dardor, D., Germanier, R., Maréchal, F., Comparative analysis of biomass utilization routes in industrial and district heating systems: integration of an aluminium industry and an urban agglomeration. 37th Int'l Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2024, June 30th – July 5th, Rhodes, Greece.

8) Florez-Orrego, D., Dardor, D., Ribeiro Domingos, M., Germanier, R., Maréchal, F., Renewable Energy Integration and Waste Heat Valorization in Aluminium Remelting Mills for the Co-Production of Kerosene and Methanol. 34th European Symposium on Computer Aided Process Engineering / 15th Int'l Symposium on Process Systems Engineering (ESCAPE34/PSE24), June 2-6, 2024, Florence, Italy.

9) Ribeiro Domingos, M., Florez-Orrego, D., Dardor, D., Marechal F., Sustainable Methanol Production Using a Multi-Time Energy Integration and CO2 Management Approach As an Energy Carrier for Synthetic Natural Gas Synthesis, AIChE 2023 Annual Meeting, November 5-10, 2023. Orlando (FL), United States

10) Domingos, M. E. G., Flórez-Orrego, D., Maréchal, F. Decarbonizing the fertilizers sector: an alternative pathway for urea and nitric acid production. International Journal of Energy Resources Technology ASME Transactions, 2024, 146(3): 030907 (13 pages)

11) Domingos, M. E. G., Flórez-Orrego, D., Teles Dos Santos, M., Oliveira Junior, S., MARÉCHAL, F. (2023). " Multi-time integration approach for combined pulp and ammonia production and seasonal CO2 management " Computers & Chemical Engineering: v.176, 108305

12) Lander, Florez-Orrego, D., Maréchal, F., Bongartz, D., Data-driven systematic methodology for the prediction of optimal heat pump temperature levels and refrigerants in process integration. 38th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2024, 30 June - 5 July, 2024, Rhodes, Greece.

13) Salman, M. Florez-Orrego, D., Maréchal, F., Leonard, G. Superstructure-based approach to assess the heat pumping and renewable energy integration potential in the sugar industry. 38th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2024, 30 June - 5 July, 2024, Rhodes, Greece

14) Ribeiro Domingos, M., Florez-Orrego, D., Sfeir, S., Maréchal, F., Integration of biodigestion, gasification, renewable energy, reversible solid oxide cell and CO2 management strategies for sustainable natural gas production. 38th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2024, 30 June - 5 July, 2024, Rhodes, Greece

15) Dardor, D., Florez-Orrego, D., Aimone, L., Germanier, R., Margni, M., Maréchal F., Modelling The Effect of Future Uncertainty in Energy Prices on Decarbonization Pathways for Secondary Aluminium Production. 38th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2024, 30 June - 5 July, 2024, Rhodes, Greece

16) Florez-Orrego, D., Aimone, L., Dardor, D., Germanier, R., Maréchal F., Comparative analysis of biomass utilization routes in industrial and district heating systems: integration of an aluminium industry and an urban agglomeration 38th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2024, 30 June - 5 July, 2024, Rhodes, Greece

17) Corre, S., Ribeiro Domingos, M., Florez-Orrego, D., Amoedo, R., Dimitrova, Z., Maréchal, F., On exergetic efficiency and reference environment of the analysis of cement production with and without CO2 carbonatation, 38th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems - ECOS 2024, 30 June - 5 July, 2024, Rhodes, Greece

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APPENDIX 1 MODELS DEVELOPED FOR THE DATABASE OF THE UTILITY SYSTEMS

This appendix describes the models developed for the database of the utility systems used in the Continuing Education Program. These models can be downloaded from the project repository:

https://gitlab.epfl.ch/ipese/mas/masbook

A.1.1 Biogas production, purification and cogeneration models

Biogas has diverse applications, including electricity generation and heating. Biogas can be generated by the biodigestion of the organic waste material from industrial facilities, such as industrial waste water, agricultural residues, animal manure and sewage sludge. In the anaerobic biodigestion, organic matter is broken down by microorganisms, producing biogas primarily composed of methane (CH_4) and carbon dioxide (CO_2). This process not only helps in reducing the environmental impact by treating wastes and reducing methane emissions, but also produces a valuable renewable energy resource [43].

The production of biogas depends on various factors, such as the dry matter content (DM), volatile solids (VS), and substrate composition. Higher DM and VS contents in feedstock generally result in increased potential of biomethane production per unit of mass of waste treated. Additionally, low energy consumption membrane purification systems of biogas have improved the quality of biogas by removing impurities like CO_2 and hydrogen sulfide, enhancing its energy content and marketability. Biogas marketing and export have gained momentum as countries seek to diversify their energy sources and meet renewable energy targets. Exporting biogas and biogas-derived products can generate revenue while also promoting sustainable waste management practices globally, thus contributing to the transition towards a circular economy and reducing reliance on fossil fuels.

Also, combined heat and power production (CHP) systems based on internal combustion engines (ICEs) can be used in many industrial processes to meet both electrical and thermal energy demands. ICEs can run on various fuels, including gasoline, diesel, natural gas, and also on biogas. The high power-to-weight ratio makes ICEs suitable for applications where compact power sources are needed, such as in industrial machinery and decentralized power generation. They can be quickly started and stopped, allowing for rapid response to changes in power demand or grid instability [45]. ICEs are known for their robustness and reliability, which is essential for continuous operation in industrial settings where downtime can be costly. They can be also easily rated down to meet different power requirements at very low partial loads, without a substantial drop in generation efficiency. Moreover, internal combustion engines often have lower initial costs compared to other power generation technologies, making them economically viable for a wide range of industrial applications.

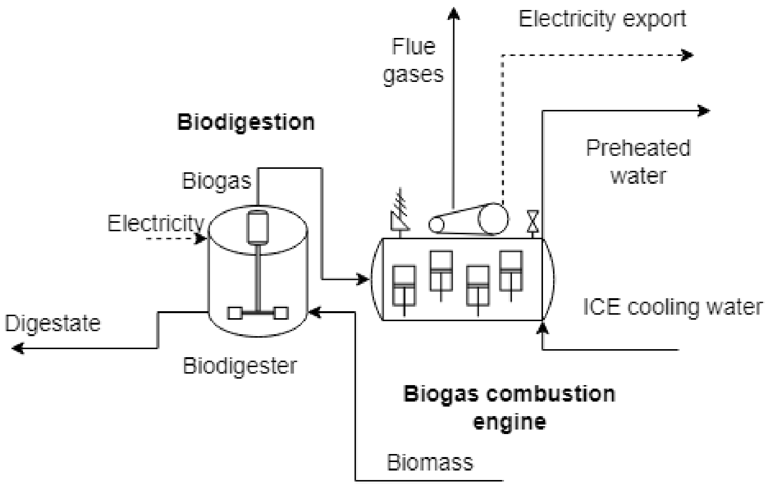


Figure A1.1. Model of biogas production and purification and internal combustion engine.

The reciprocating engine, also known as piston–cylinder engine, is a device that uses one or more reciprocating pistons to convert fuel energy into a rotating motion. They can be classified either as spark-ignition (SI) engines or compression-ignition (CI) engines. In SI engines, the combustion of the air–fuel mixture is initiated by a spark plug; whereas in CI engines, the air–fuel mixture is ignited as a result of compressing the mixture above its self-ignition temperature. Otto and Diesel thermodynamic cycles are the ideal representatives for the SI and CI reciprocating engines, respectively. During the compression stroke, the piston moves upward, compressing the air–fuel mixture. Before the piston reaches its highest position, the spark plug fires and the mixture ignites, increasing the pressure and temperature in the cylinder. The high-pressure gases force the piston down, which in turn forces a crankshaft to rotate, producing useful power during the expansion stroke. At the end of the stroke, the piston is at its lowest position and the cylinder is filled with combustion products. Next, the piston moves upward in order to purge the exhaust gases through the exhaust valve. Finally, the piston goes down again drawing in the fresh air–fuel mixture through the intake valve and the cycle is repeated. Components cooling is required to remove excessive heat, as overheating can cause engine failure, usually from wear, cracking or warping. The rejected heat can be used for industrial heating purposes. In fact, roughly half of the waste heat removed from the engine jacket, oil cooler and after-cooler circuits can be recovered around 90 °C [43], whereas the remainder can be recovered at a higher exhaust temperature, which makes it suitable to generate pressurized hot water or steam in a waste heat recovery steam generator.

A.1.2 Gas turbine

Gas turbines have played a key role for electricity generation, propulsion, and cogeneration in modern industrial processes. They can start up quickly, making them ideal for meeting sudden spikes in electricity demand or providing emergency backup power. Gas turbines drive various industrial processes, such as compressors, pumps, and generators, in sectors like oil and gas, manufacturing, and petrochemicals. They can operate independently or in conjunction with steam turbines in combined cycle power plants for enhanced efficiency. In the latter case, the exhaust of the gas turbine is used as heat source for steam generation.

These technologies can run on a variety of fuels, including natural gas, diesel, and even biofuels. For instance, biomass can be used in integrated gasification combined cycles to generate syngas that is consumed in a gas turbine, instead of burning biomass in a boiler to generate steam and drive a low efficiency steam turbine. On the other hand, gas turbines also have significant initial capital costs, primarily due to their sophisticated design and construction. They may also experience reduced efficiency when operated at part load, leading to higher fuel consumption per unit of power generated. If using fossil resources, gas turbines can be less environmentally friendly than more advanced types of electricity generation systems, such as fuel cells.

A gas turbine system consists of compressor, a combustion chamber, and an expander. An electrical generator coupled to the shaft of the gas turbine also allows generating electricity. A recuperator can recover heat from the turbine outlet temperature gases and use it for preheating the air at the compressor discharge up to a certain temperature level, thus increasing the efficiency of the overall system. The pressure ratio is thus a key parameter for the gas turbine modeling. In the turbine, gases expand to the atmospheric pressure while producing power. The air in the gas turbine system has two important functions: it supplies the necessary oxidant for the combustion of the fuel, and it also serves as a coolant to keep the temperature of various components within the safety limits. In fact, a large amount of excess air is needed and air to fuel mass ratios can go above 50 [46].

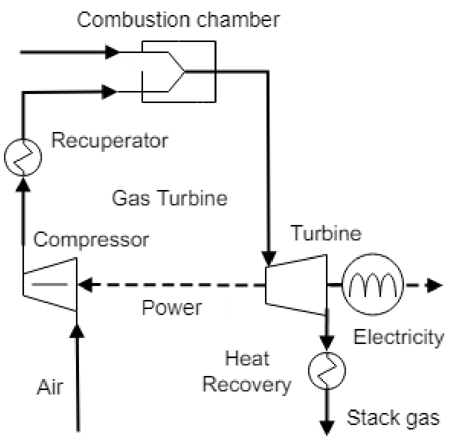


Figure A1.2. Gas turbine model.

A.1.3 Refrigerator

Some industrial processes, such as liquefaction, solidification, conservation and separation, require cooling below ambient temperatures. Since conventional water and air cooling cannot achieve the desired operating conditions, other cooling cycles, based on specialized working fluids called refrigerants, become necessary. The thermodynamic properties of those fluids confer them suitable characteristics to absorb heat from process streams by evaporating in a heat exchanger at a temperature below that of the environment. When the evaporated fluids are recompressed, the temperature significantly increases above the ambient temperature, facilitating the heat rejection in a condensation heat exchanger using air or water cooling. The capacity of these fluids to achieve much lower temperatures is due to Joule-Thomson effect, by which certain fluids exhibit rapid cooling accompanied by partial vaporization if throttled or expanded through a valve, a capillary tube or a hydraulic expander. The main electricity input is the compressor power consumption, which depends on the isentropic efficiency and other compressor design details. Since a refrigerator is a thermal cycle, the actual coefficient of performance (COP) is limited by the theoretical Carnot COP ($T_{evap}/(T_{cond}-T_{evap})$), which is only a function of the temperatures, and not of the substance. Although the ideal COP is virtually impossible to achieve, it can be approached by reducing the technology inefficiencies. Commercially, the ratio between COP_{actual} and COP_{Carnot} is around 0.45-0.55 [47], which can be used as a heuristic correction factor to estimate the actual performance. Based on the previous parameters, it is possible to calculate the total power demand and the corresponding condenser heat rejection.

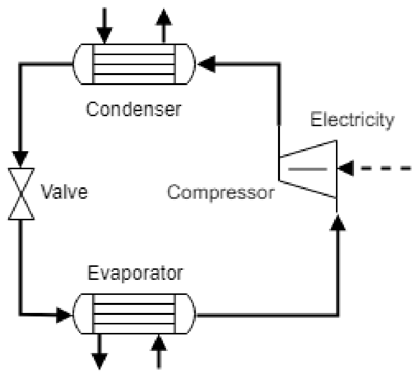


Figure A1.3. Refrigeration system model

Although some transcritical refrigeration cycles can be implemented, minimum evaporator and maximum condenser temperatures are typically limited by the freezing and critical temperatures of the fluid employed. Moreover, since for pure substances in the subcritical two-phase region, both temperature and pressure properties are not independent, the selection of the temperature also fixes the operating pressure. In order to avoid air leakage into the evaporator, the lowest cycle pressure is preferably set slightly above the ambient pressure. On the other hand, the maximum pressure (and temperature) is chosen to enable the heat rejection at temperatures compatible with common cooling methods (e.g. air or water cooling). In practice, other structural constraints and fluid properties influence the selection of the refrigerants, as well as the operating conditions and the materials used in the refrigerator components.

A.1.4 Heat Pump and mechanical vapor recompression

Low-grade residual heat is produced in practically any industrial process that converts high quality energy into value-added products. Industry has traditionally regarded this thermal waste as an undesirable side-product of the main production activity and devised means to collect and reject it to the environment, as long as internal heat recovery is not further applicable. This approach entails larger process inefficiencies and worsened environmental impact. To tackle these issues, waste heat can be upgraded using a specialized equipment called heat pump, whose working principle is similar to that of a refrigeration cycle.

Heat pumps also use working fluids called refrigerants that can absorb heat by evaporating in a heat exchanger at low temperature in order to supply that heat at a higher temperature. When the evaporated fluids are recompressed, the temperature significantly increases, which facilitates the heat exchange with other process streams in a condensation heat exchanger. The main electricity input is the compressor power consumption, which in turn depends on the isentropic efficiency and other compressor design details. Although the selection of the evaporator and condenser temperatures is similar than for refrigerators, the heat exchange in the heat pump condenser is aimed for useful heating applications at high temperatures [47].

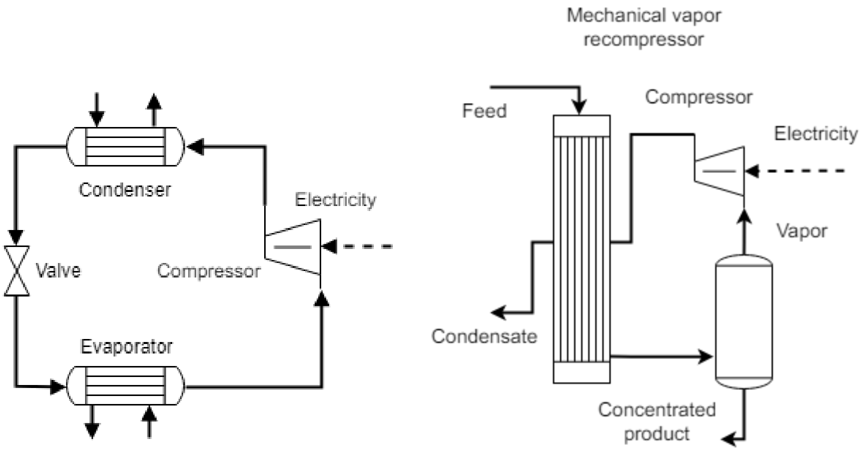


Figure A1.4. Heat pump model (left) and MVR model (right).

Mechanical vapor recompressor (MVR) is another type of heat pump system, particularly useful in industries where the concentration of a solution or the recovery of a solvent is needed. MVR also found applications in concentrating brine or for extracting fresh water from seawater; and drying and treating sludge or organics wastes. The process begins with the evaporation of a volatile component from a solution, usually water. The vapor produced is then recompressed using an MVR which increases the temperature. The compressed vapor releases heat to the incoming feed solution, which vaporizes more water. In this way, the vapor condenses back into a liquid state and is either discarded or recycled to the process, depending on the MVR cycle (open or closed).

Thus, while both MVR and heat pumps involve the compression and expansion of a vapor to transfer heat, there are key differences between them. MVRs typically operate at much higher temperatures and pressures compared to heat pumps. In addition, heat pumps commonly use specialized fluids called refrigerants, whereas MVR systems may use water or other solvents depending on the application. It is important to mention that, in both cases, to avoid a misplacement of heat pump or MVR, low-grade waste heat must be only shifted from below to above the pinch. If placed below the pinch, it increases the cooling requirement; and if placed above, it behaves as a simple electricity dissipation device (i.e. no heat pumping benefit). Heat pumps and MVRs are also thermal cycles, thus the actual coefficient of performance (COP) is limited by the theoretical Carnot COP ($T_{cond}/(T_{cond}-T_{evap})$). Commercially, MVR have higher COPs (> 10) than heat pumps (< 5), as the former operate normally under much smaller temperature lift.

A.1.5 Organic Rankine cycle

An organic Rankine cycle (ORC) is a variation of a conventional Rankine cycle that uses organic working fluids in lieu of steam [48]. These fluids have lower vaporization temperature than pure water, which allows for waste heat recovery from low-temperature sources, such as industrial waste heat, geothermal heat, and bottoming cycles of cogeneration systems. The low-temperature heat is converted into useful power, that can be later converted into electricity or any other forms of energy. The working principle of the organic Rankine cycle is the same as that of the conventional Rankine cycle. First, the working fluid is pumped in a centrifugal pump up to the pressure of the waste heat recovery boiler (WHRB). Next, the fluid is evaporated and is fed to an expansion device (e.g. a turbine, a screw, a scroll, etc.) in order to generate electricity. The outlet stream of the expander goes through a condensing heat exchanger, so that it can be pumped back to the WHRB and restart the cycle. In real applications, the presence of irreversibility lowers the efficiency of the ORC and only a part of the fluid expansion in the turbine is transformed into useful work, whereas the other part is dissipated in the form of heat to the environment. The selection of the working fluid is important as the performance of the cycle depends on the thermo-physical properties of the fluid. Refrigerants and hydrocarbons are among the most commonly used fluids. This model is another example of the use of Aspen HYSYS software to characterize the thermal and electrical streams.

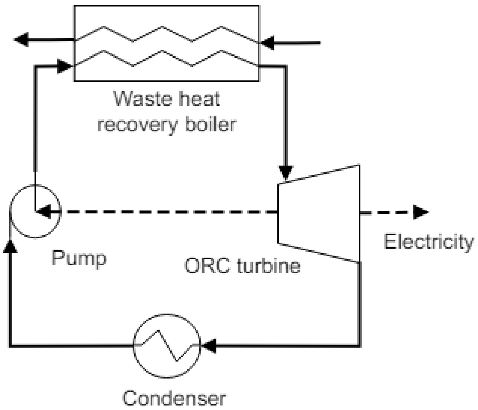


Figure A1.5. Organic Rankine cycle model.

A.1.6 Electrical heater

The electrical heater is a utility unit that can supply heat at various temperature levels (up to 700°C) to different industrial applications. The electrical heater model converts the electrical energy into the thermal energy of hot gases (i.e. convective heating) or radiant energy (as in radiant elements or tubes) using a dissipative resistance (Joule effect). An electrical heater model can be represented by a collection of electricity and heat streams that simulates the cooling process of hot gases or radiative elements (e.g. tubes, plates, rods, wires) delivering heat to a load and, due to imperfect isolation (e.g. wall and leakages), also to the environment. Electrical heaters do not release directly CO_2 emissions since they spare stack.

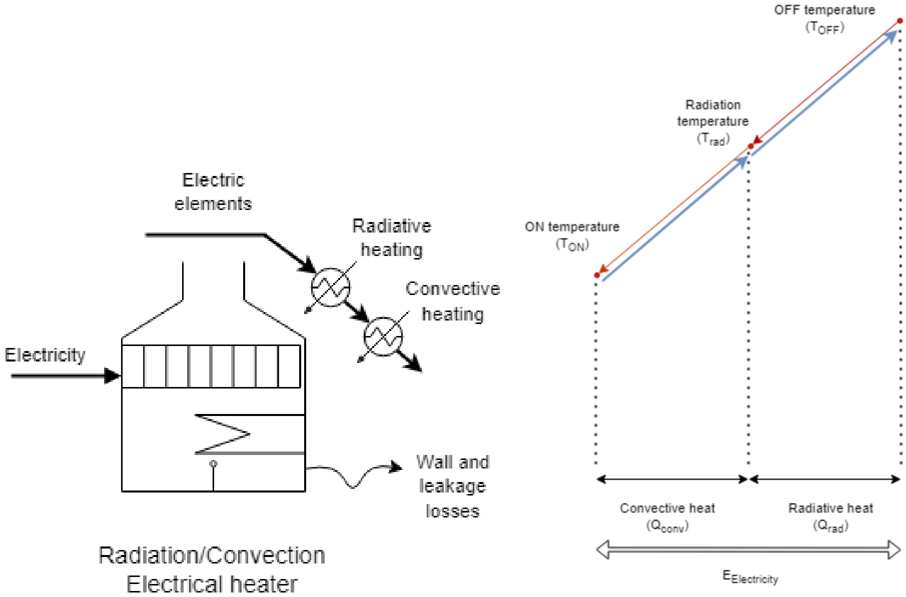


Figure A1.6. Model of the electrical heater

A.1.7 Conventional furnace model using biomass, hydrogen, syngas and natural gas and synthetic natural gas (SNG)

The furnace is a utility unit that can supply heat at very high temperatures (> 500°C) to industrial processes, like sintering, curing, metallurgical and thermal treatments, among other applications. A furnace converts the chemical energy of a fuel into the thermal energy of hot flue gases by burning the fuel with air. A furnace model can be represented by a collection of mass and heat streams that simulates the cooling process of hot flue gases delivering heat to a load and, due to imperfect isolation (e.g. wall losses and leakages), also to the environment [46].

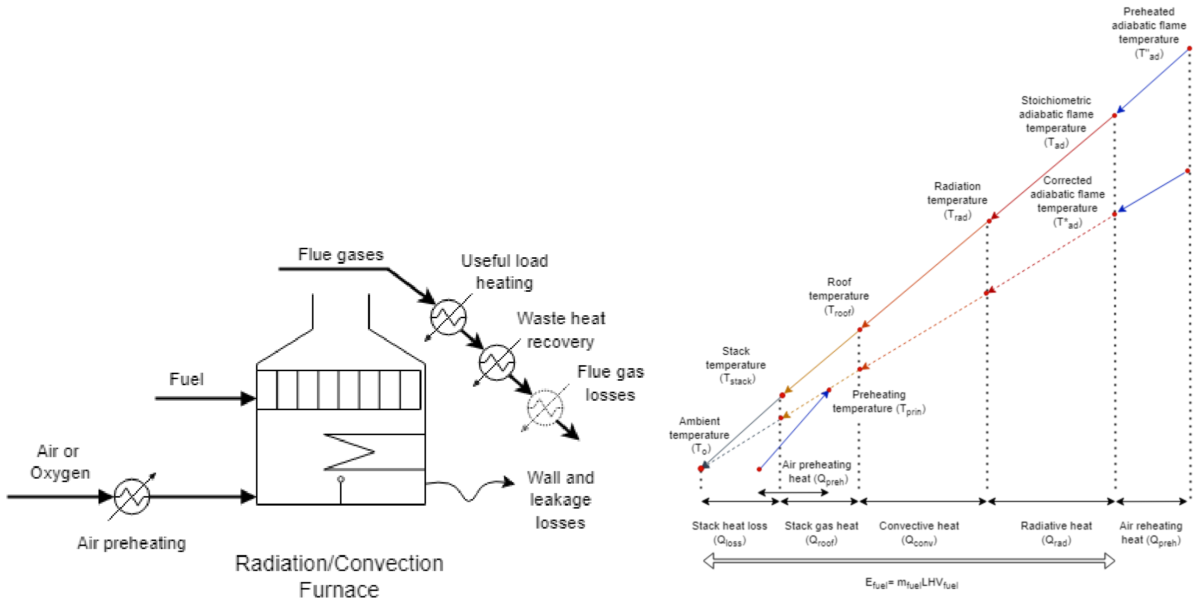


Figure A1.7. Model of the conventional combustion furnace.

In addition, the furnace model includes the heat streams related to the preheating of the cold combustion air. Aside from the heat streams, mass streams, such as CO_2 emissions released with the hot gases dissipated to the environment must be also considered. Emissions leaving via the furnace stack may still be conducted to a purification unit to partially remove the CO_2 in the flue gases. Finally, the mass flow rate of the fuel consumed is computed based on both the useful heating capacity of the furnace and the additional energy required to offset the aforesaid losses. Some modeling parameters need to be adapted for different operating conditions, e.g. air or oxy combustion; roof, stack, wall and air preheating temperatures; excess air; heat losses and other costing parameters. It is worth noticing that the waste heat available at the stack outlet can still be utilized for heating purposes, depending on whether the hot stream could be safely cooled below its dew point temperature without triggering excessive corrosion. Preheating temperature should be selected depending on the nature of the energy integration problem and the localization of the pinch temperatures. The energy input during the preheating process can be also interpreted as the amount of fuel that can be saved while supplying the same heat load.

A.1.8 Natural gas oxycombustion furnace with CO_2 recycle

The oxycombustion furnace is similar to the conventional furnace technology, except for the fact that the hot flue gases are mainly composed of carbon dioxide and water due to the use of very enriched air or even pure oxygen for burning the fuel. For this reason, the CO_2 gas leaving through the stack of the oxycombustion furnace can be easily separated from water by condensation, which facilitates its capture and the subsequent treatment, utilization or sequestration. The CO_2 produced can be even partially recirculated to control the high temperatures attained during the combustion with pure oxygen. It is worth mentioning that, although CO_2 recirculation may be helpful for controlling the adiabatic flame temperature, very high recirculation rates may lead to a reduced amount of energy available at high temperature levels inside the combustion chamber. This fact translates into a higher amount of energy available at the furnace stack. For this reason, recirculation rates should be selected as a tradeoff between the maximum affordable temperature and the minimum stack losses.

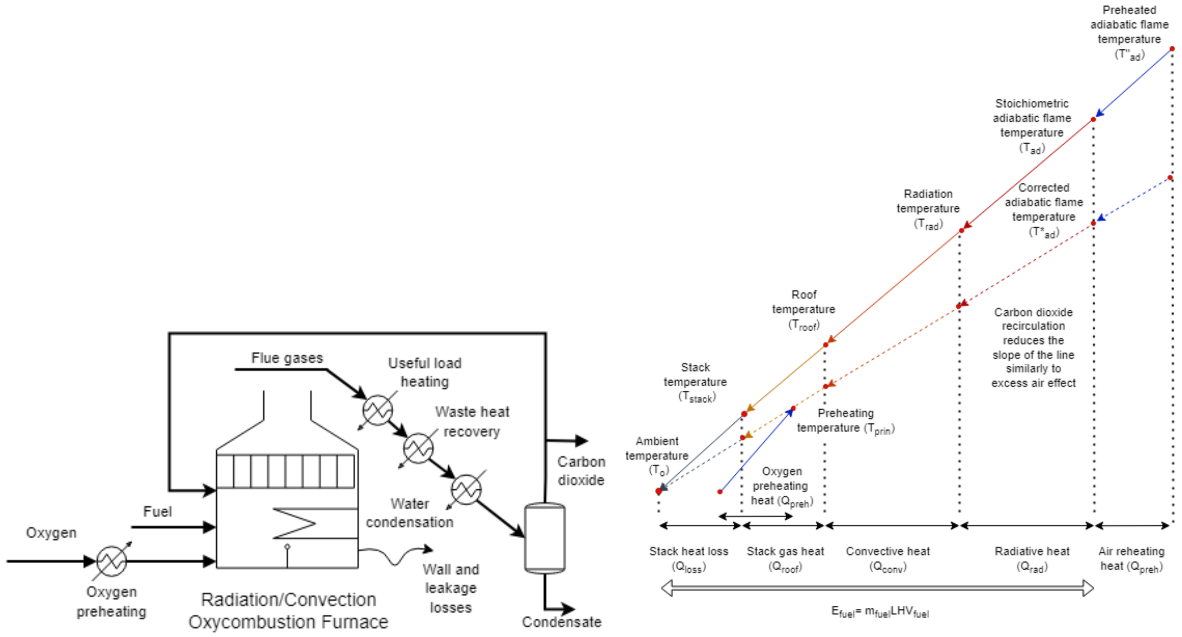


Figure A1.8. Model of the oxycombustion furnace.

A.1.9 Plasma Furnace

Plasma is an ionized gas consisting of positive ions and free electrons in a share resulting in almost no overall electric charge. Plasma is generated when an electric current is applied across a dielectric gas (i.e. an electrically non-conducting gas), such as e.g. N_2, CO_2, or Ar. As the voltage increases, the current stresses the fluid beyond its dielectric limit into a stage of electrical breakdown, marked by an electric spark, where the material transforms from an insulator into a conductor. The potential difference and subsequent electric field pull the bound electrons (negative) toward the anode (positive electrode), while the cathode (negative electrode) pulls the nucleus. It causes collisions between electrons and neutral molecules that split into atoms and eventually into more electrons, thus forming ions in a process called Townsend avalanche. Thermal plasma can be produced using either direct or alternating current, radio frequency or microwave sources and can achieve temperatures around 2,000 - 20,000 °C. Because of their sizable temperature and density ranges, plasmas find applications in many fields of industry, for example thermal spraying, etching, glass melting, and metal cutting and welding. Plasma torches can be used in waste treatment, since the high temperatures allow for instantaneous gasification, becoming an alternative technology for syngas production.

In heating applications, transferred arcs and non-transferred plasmas differ from each other by the generation and heating principles. In the former, the target material is part of the circuit; whereas, in the latter, the generation and acceleration of the plasma is limited to the torch. The positioning and relative speed of the plasma-generating elements are important design factors. Auxiliary systems are also required for the adequate operation (e.g. electrical converters, gas compressor and cooling systems). For a specific plasma torch application based on nitrogen as ionizing gas, a continuous flow of nitrogen must be also guaranteed, which entails the installation of a nearby dedicated air separation unit. A plasma furnace model can be represented by a collection of mass and heat streams that simulates the cooling process of plasma gas delivering heat to a load and, due to imperfect isolation (e.g. wall and leakages), also to the environment. The plasma furnace model may also include the heat stream related to the preheating of the plasma-forming gas and the cooling water needed for maintaining the plasma torch operating at suitable temperatures. No direct CO_2 emissions from the plasma furnace are expected, although the presence of oxygen in the furnace atmosphere may pose challenges in terms of undesirable NO_x production.

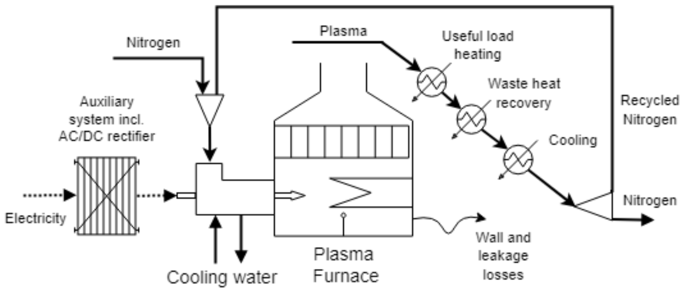


Figure A1.9. Plasma-torch furnace model.

A.1.10 Photovoltaic panels

Photovoltaic panels (PV) are essential components of renewable energy infrastructure that convert sunlight into electricity. Their performance is subject to various design and external factors. The global horizontal irradiance (GHI) is the amount of terrestrial irradiance falling on a surface horizontal to the surface of the earth [W/m^2] and dictates the potential energy yield of PV systems. Irradiation values can be obtained from an insolation map or from insolation tables that reflect historical data over various years. The output of a photovoltaic panel also depends on the angle of the sun relative to the panel, but it can be controlled by using actuators.

Moreover, part of the solar radiation reaching an object is absorbed and the remainder is reflected. The fraction of solar irradiation that passes through a PV glass determines the absorbed energy. Usually, the absorbed radiation is converted to thermal energy, increasing the object temperature, which also affects the PV panel efficiency. Elevated temperatures lead to decreased power output due to the PV material sensitivity. In this regard, the thermal transmission coefficient of a PV panel affects the heat dissipation capacity and the overall performance. Thus, the temperature coefficient of efficiency quantifies performance changes with temperature.

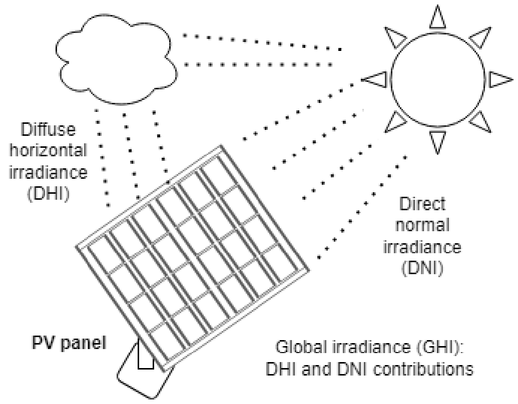


Figure A1.10. Photovoltaic panel model.

The electric power output of the PV panel is calculated considering the effective area, the temperature dependent efficiency factor, and the total solar radiation incident on the PV surface. The efficiency of the PV panel is also affected by the module temperature. The thermal transmission coefficient and the temperature coefficient of efficiency depend on the type of PV panel and are provided by the manufacturers. The fraction of solar incidence passing through the PV panel glass is determined by an empirical factor. The maximum installation size can be limited by the area of a roof, calculated as the product of the length and the width of a building, considering the constraints for PV panel installations.

A.1.11 Hot water production unit

In industrial settings, hot water is required for several purposes, including bathing, cleaning, sterilization, three-phase separation or for general heating needs. The choice between pressurized and ambient pressure hot water systems depends on the specific requirements of the industrial application, including temperature needs, control demands, and energy efficiency considerations. Hot water can be produced in water boilers fueled using various sources, such as natural gas, oil or biomass. Electrical heaters can be also used to generate hot water, offering precise temperature control and rapid heating capabilities.

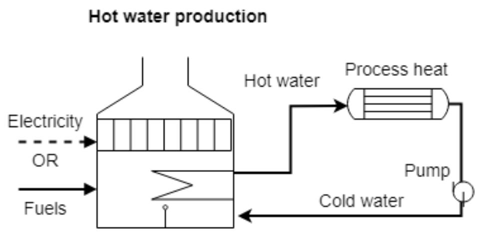


Figure A1.11. Hot water unit model.

Hot water systems often operate in closed-loop configurations to minimize energy losses and water treatment requirements. Proper water quality is essential in these systems to prevent corrosion and scale buildup, maintaining operational reliability and extending equipment lifespan. The maximum temperature of the hot water loop and the return water temperature, as well as other properties, like the water heat capacity and density can help determining the specific amount of energy delivered during the water heating process and the water pumping power consumption.

A.1.12 Steam generation and steam networks

In industrial settings, steam is required for several purposes, including cleaning, separation or general heating needs. The choice between high and low-pressure steam systems will depend on the specific requirements of the industrial application. Low pressure steam can be produced in steam generators fueled by natural gas, oil or biomass. Electrical heaters and heat pumps can be also used to generate steam, even though the latter are less widely used due to limitation in terms of temperature.

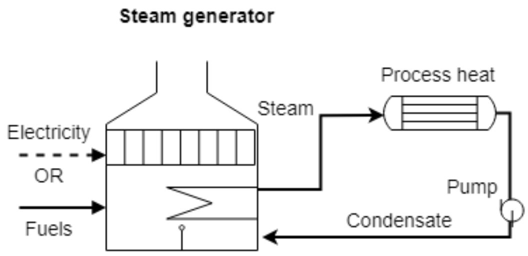


Figure A1.12. Steam generator model.

Like hot water systems, steam generators also often operate in closed-loop configurations to guarantee water quality, prevent corrosion and scale buildup, and maintain operational reliability and extending equipment lifespan. The temperature of the saturated steam and the return saturated liquid (actually, slightly subcooled) can be assumed to be constant over the condensation process, so that subcooling process are avoided and condensates are handled at by temperature by industrial pumps.

Meanwhile, steam networks and Rankine cycles have a very important role in the industrial processes integration. Steam networks serve as robust transportation systems for heat, facilitating the transfer of thermal energy across various industrial operations. Meanwhile, the Rankine cycle partially converts the waste heat recovered into mechanical or electrical power in steam turbines. By integrating these technologies, industries can harness waste heat from chemical and industrial processes and utilize it in cogeneration systems, which significantly enhances the energy efficiency and sustainability of the overall plant.

In a Rankine cycle, the working fluid is pumped to the heat recovery boiler (HRB), where it is superheated. The superheated steam passes through an expansion device (a turbine) in order to generate mechanical power that can be converted into electricity in an electrical generator. The turbine outlet stream goes through a condensing heat exchanger in which releases heat and condenses, so that it can be pumped back to the HRB. When there is an extraction of steam from a turbine, the approach is known as backpressure or extraction-condensing steam turbines. In the latter case, other part of the steam is expanded up to a pressure and a saturation temperature corresponding to the vacuum in the condenser. The model was developed in the Coolprop open source library based on Equation Oriented Modeling approach [49].

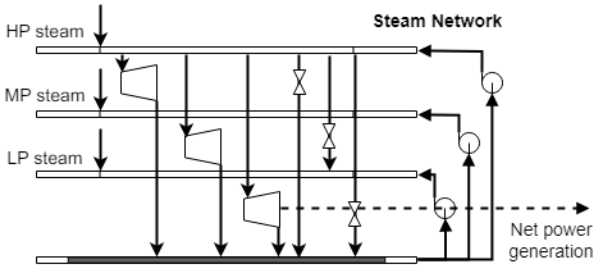


Figure A1.13. Steam network model.

A.1.13 Cooling tower

The industrial processes usually need to reject a large amount of waste heat as byproduct. The source of this residual heat can be the exothermic chemical reactions occurring in reactors or combustion chambers, as well as other dissipative components that partially degrade electricity into heat, e.g. intercooled compression systems or stirrers. The resulting hot streams need to be cooled down, but in some situations, those streams might not be further able to exchange heat with other processes streams for internal heat recovery. Therefore, the excess heat removal must be achieved using auxiliary fluids, such as air or water. The choice between air or water cooling depends on factors like the temperature requirements, cost, and availability of resources.

In the case of air coolers, the air can be put in direct contact or used in a heat exchanger to remove heat from the process streams. Forced convection is maintained by the circulation of cold air using fans. On the other hand, in a water-based cooling system, circulating water collects the waste heat from industrial processes and is then treated in a cooling tower. The cooling tower is a specialized heat and mass exchange equipment in which the hot circulating water is sprayed and brought into contact with fresh air in order to reduce the water temperature. As this occurs, a small volume of water is evaporated, reducing the temperature of the water being passed through the tower. The cooled water is pumped back to the process equipment, where it absorbs heat, then it is pumped back to the cooling tower to be cooled once again.

In the cooling tower, return water can enter around 30°C and reduce the temperature by evaporative cooling below 20°C. The temperature difference is important to determine the flow of the circulating water, considering the enthalpy change of water at the specified pressure and temperature. The cooling tower can achieve lower temperatures than the intake air thanks to the water evaporation effect, which drops the system temperature from the dry to the web bulb temperature. The latter is a function of the former temperature and the relative humidity, and can be found using psychometric charts. Considering the cooling tower supply and return temperatures, and the heat removal capacity, a cold stream can be associated to the cooling tower unit. In addition, both recirculation pumps and forced draft fans consume electricity at a ratio of around 0.021 kW_{ee} per kW_{th}.

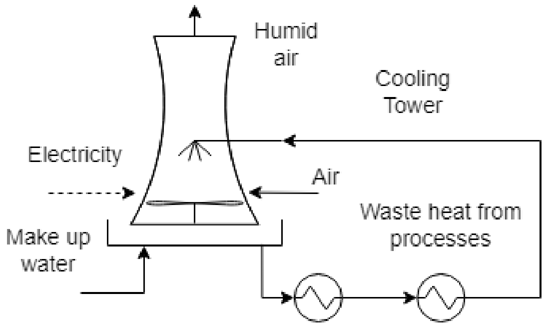


Figure A1.14. Model of cooling water system.

A.1.14 Cryogenic air separation unit

Many industrial processes require the continuous supply of pure oxygen or nitrogen for its adequate operation. Examples of these applications are autothermal reformers for syngas conditioning, and oxygen-blown entrained and fluidized bed gasifiers. Moreover, heating applications employing pure oxygen as oxidant instead of air, also known as oxycombustion processes, aim to achieve higher temperatures by avoiding dilution of flue gases with the nitrogen in the air. Pure nitrogen production is also an important industrial activity, since nitrogen has innumerable applications, such as in nitrogen fertilizers production, plasma torch gases and unreactive atmospheres [50].

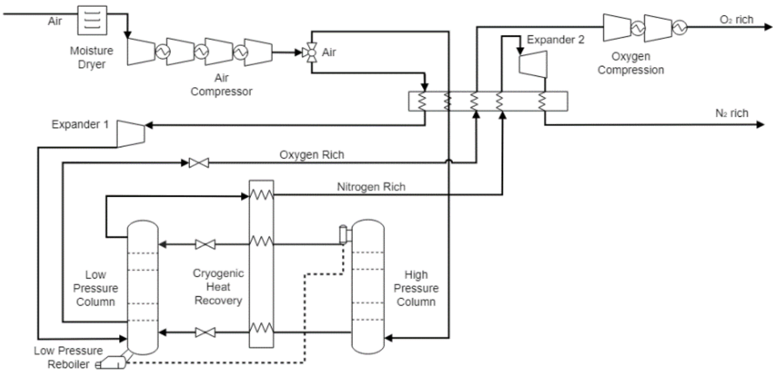


Figure A1.15. Model of the cryogenic air separation unit

Atmospheric air is the most obvious source of nitrogen, whereas oxygen could be produced either from air splitting or from the electrolysis of water. Different technologies are available to separate the nitrogen and oxygen present in the air, including membrane, adsorption, and cryogenic air separation units (ASU). The cryogenic ASU is the most adequate when large oxygen production yields at high purity are necessary. In this type of air separation unit, the components of the mixture can be separated by distillation in a double column arrangement thanks to their different cryogenic boiling points.

In this unit, first normal air at 25°C and 1 bar is compressed to around 7 bar and 40°C. About 95% of the compressed air is cooled down in the main recovery heat exchanger and then it is fed into a high pressure separation column (HPC). The remaining 5% of the compressed air is expanded to around 3 bar before entering the low-pressure separation column (LPC). Next, both the liquid bottoms and vapor overheads exiting the HPC are cooled down by using the nitrogen-rich stream coming from LPC overhead, and then expanded and sent to the LPC, wherein further air separation occurs. Both columns are thermally integrated, as the HPC condenser provides the duty required by the LPC reboiler. A last expansion step (1 bar) of the nitrogen rich stream produced in the LPC allows for an increased cooling effect in the main heat exchanger. The main products of the cryogenic ASU are an oxygen-rich stream (99.5% molar, 1 bar) and a nitrogen-rich stream.

Depending on the pressure levels at which the industrial applications demand oxygen and/or nitrogen, either of them could be used directly at low pressure (e.g. at 1-7 bar in oxycombustion or plasma furnaces), or further compressed to medium (e.g. 30 bar, for autothermal reformers and entrained flow gasifiers) or high pressures (200 bar, to export). If some of those gases is not used or commercialized, it can be vented to the environment, entailing a reduction of efficiency. The cryogenic air separation unit (ASU) is one example of model that has been simulated in detail using thermo-physical properties of substances, costing parameters, empirically determined values reported in literature and others values calculated using flowsheeting tools (e.g. Aspen® Hysys).

APPENDIX 2 MODELS DEVELOPED FOR THE DATABASE OF THE DECARBONIZATION TECHNOLOGIES

This appendix describes the models developed for the database of the decarbonization technologies used in the Continuing Education Program. These models can be downloaded from the project repository:

https://gitlab.epfl.ch/ipese/mas/masbook

A.2.1 Biodigestion of the organic fraction of metropolitan solid waste

Anaerobic digestion is a biological process in which organic matter decomposes and transforms into biogas in an anaerobic (i.e. oxygen-free) environment through the action of microorganisms [39]. The process takes place within a reactor called biodigester, which can break down organic matter from agriculture, metropolitan waste or sewage to produce a mixture rich in methane and carbon dioxide. The non-gaseous product of the process is referred to as digestate, and can be used as a fertilizer after dried. Anaerobic digesters can be classified into thermophilic or mesophilic. Mesophilic setups operate at a temperature around 35–37 °C and thermophilic ones usually work between 55–60 °C [51]. A thermophilic digester has a higher biogas yield for shorter retention times, and improves pathogen destruction and substrate degradation; while a mesophilic one is much easier to maintain and is more stable due to the fact that a wider diversity of bacteria grows at mesophilic temperatures. Thermophilic systems are usually more expensive to operate as they require additional energy to maintain the higher operating temperatures. Thermophilic systems are preferred for high solid content in feedstock. The heating demand of both the inflowing feed and the digestion vessel is usually fulfilled on-site from the conversion of part of the biogas to heat directly or via the recovered heat in a combined heat and power production (CHP) unit.

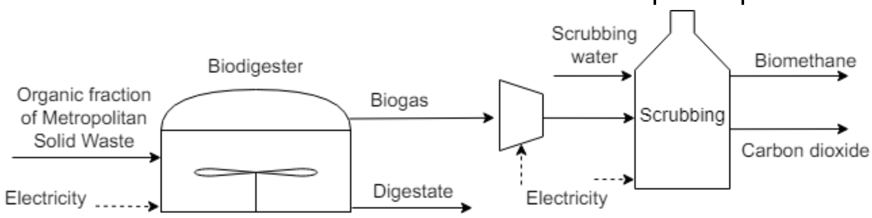


Figure A2.1. Biogas production and purification

During the loading process, the organic matter (e.g. grains, molasses, animal fat, cattle and chicken manure, household waste and sewage sludge) is crushed to obtain a homogenized substrate, which is fed via a hopper to the digester. The biomass is continuously heated up to 55°C and stirred in a thermophilic anaerobic reactor. Digestion vessels are insulated as changes in ambient temperature can affect digestion performance. Retention times of around 30 days can be necessary to address the induced biochemical transformations that convert the waste organic matter into biogas. The gas contains around 55% mol of methane and 50% mol of carbon dioxide, and usually small amounts of sulfur. It may be used on-site in a cogeneration engine for producing combined heat and power, or it can be purified with a scrubber to separate the methane and inject it into a natural gas network. The digestate, or material leftover following the conversion of the substrate, is typically used as fertilizer for crops. The carbon dioxide produced can be also purified and sold as a byproduct.

A.2.2 Mineralization

CO_2 mineralization involves the conversion of CO2 into stable carbonate minerals, which can be stored safely for long periods [52]. This process can occur naturally over geological timescales or be accelerated through industrial processes such as direct carbonation. Ex-situ mineralization requires the provision of several reactants including serpentine, NaCl, and $NaHCO_3$. Several products result from this process, the main one being magnesium carbonate or magnesite $MgCO_3$, which can be used as cement additive, in addition to other marketable byproducts, such as magnetite and SiO_2. Serpentine pretreatment for CO_2 carbonation consists of activation, cooling, preheating, and pumping steps. First, mineral ores are mined and transported to the plant location, where magnetic separation, grinding, and a chemical treatment based on the utilization of additives are required. The grinding process reduces the particle size to μm, increasing the surface area and carbonation rate. In the direct carbonation pathway, grinding has proved to increase the reaction conversion from 10 to 90%. After the magnetic separation of Fe_2O_3, a heat treatment at 600 °C partially dehydroxylates the serpentine to ensure faster reaction kinetics and more reactive material.

In the direct carbonation, activated minerals are fed into a fluidized bed reactor, in which they are mixed with water and a solvent mixture of 0.6 M NaHCO3 and 1 M NaCl. The captured CO_2 is compressed up to 115 bar and fed to a reactor where the activation of the serpentine is done at 155°C and 140 bar. Under these reactor conditions, a CO_2 conversion of 74% can be achieved. CO_2 undergoes exothermic reactions with minerals rich in Ca and Mg to form carbonates, such as calcite ($CaCO_3$), magnesite ($MgCO_3$), dolomite ($CaMg(CO_3)_2$), and often silica (SiO_2). In the case of serpentine, the chemical that takes place is exothermic (-64 kJ/mol CO_2): $Mg_3Si_2O_5(OH)_4 + 3CO_2 \rightarrow 2MgCO_3 + 2H_2O$ [52]. The importance of CO_2 sequestration, particularly via direct carbonation and mineralization, lies in the possibility of capturing and storing permanently CO_2, thus enabling hard-to-decarbonize industries to transition to more sustainable practices, while reducing the carbon footprint.

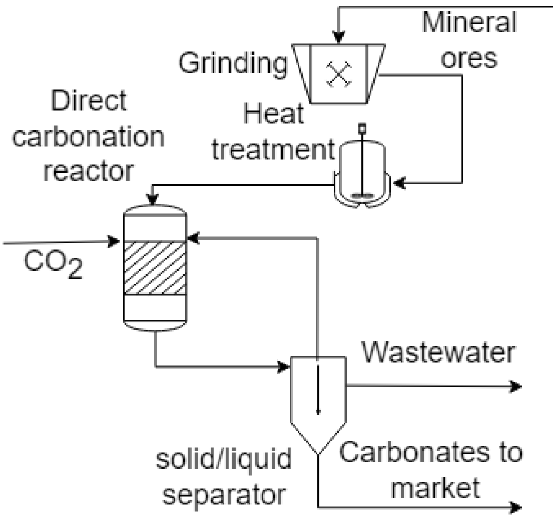


Figure A2.2. CO_2 mineralization model.

A.2.3 CO_2 capture using amines

Post-combustion carbon capture with amines is a widely used method to reduce CO_2 emissions from power plants and industrial processes. The operating principle involves passing the flue gas through an absorber where CO_2 is captured by contacting it with a chemical solvent, typically a lean amine solution at 40°C. The CO_2-rich solvent, also known as rich amine, leaving the absorber is pumped to a desorber column. In the desorber, heat is supplied to the rich amine solution typically via low pressure steam in the reboiler (120°C, 3.6 MJ/kgCO_2), which helps stripping CO_2 out from the solution. The CO_2 is compressed, whereas the regenerated solution (lean amine) is recycled back to the absorber to capture more CO_2 from the flue gas. The lean amine solution concentration should be less than 45% wt. and the CO_2 loading must not be higher than 0.3 kmol CO_2 per kmol of amine to avoid corrosion problems. Carbon capture with amines is considered a mature technology and plays an important role in the energy transition by enabling the reduction of CO_2 emissions from large-scale fixed sources, such as power plants and industrial facilities. As the world shifts towards cleaner energy sources, CCS technologies will be essential for mitigating climate [53].

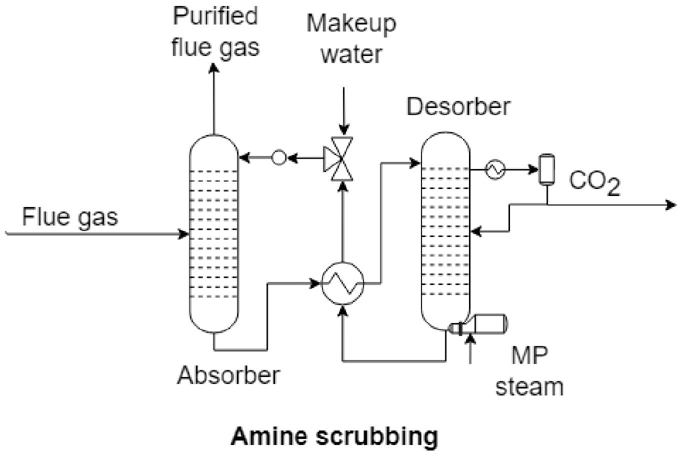


Figure A2.3 CO_2 capture using amines model.

A.2.4 CO_2 capture using adsorption systems

An adsorption unit captures carbon dioxide emissions from industrial processes or power plants by adsorbing them onto solid materials. A key difference between adsorption and absorption lies in the capture mechanism: the first one involves the adherence of the gas molecules to the surface of a solid, while absorption entails the dissolution of gas molecules into a liquid. Solid adsorbents, such as zeolites, possess a high surface area and specific pore structures, making them effective for capturing CO_2. Pressure swing adsorption (PSA) and temperature swing adsorption (TSA) are two common methods for carbon capture that differ in how the captured CO_2 is released by regenerating the capturing material. In PSA, the adsorbent material is exposed to high pressure to capture CO_2 and then depressurized to release it. Conversely, TSA count on temperature variations to desorb CO_2 from the adsorbent. Typically, this method of carbon capture employs multiple beds or rotary beds to ensure continuous operation.

Power consumption is a critical factor in the efficiency of carbon capture systems using adsorption. The energy required for compression, heating, and cooling during regeneration can be significant and must be minimized to make the process economically viable. The choice of filled material, such as zeolites or activated carbon, can also impact the power consumption and the overall performance. Other materials, such as the metal organic frameworks (MOFs) in the SVANTE's VeloxoTherm RC-TSA process, can be used in rotary adsorption machines that capture the carbon dioxide contained in a flue gas by using the temperature swing adsorption (TSA) principle. By capturing CO_2 from industrial sources, these technologies mitigate the transitional use of fossil fuels. Yet, as efforts to decarbonize the industries intensify, more advancements in adsorption carbon capture systems will be essential for biogenic carbon management systems.

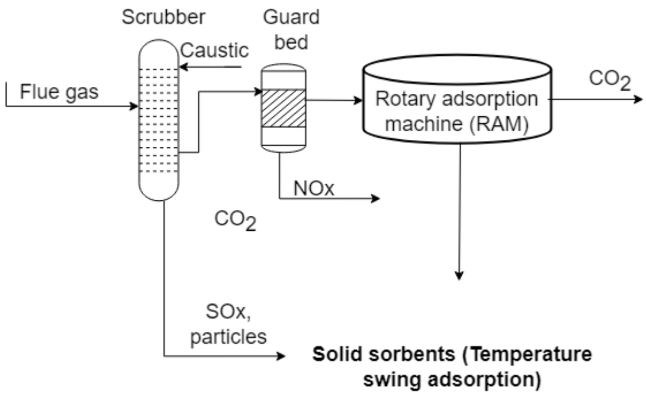


Figure A2.4. CO_2 capture using adsorption systems model.

A.2.5 CO_2 capture using membranes

Membrane-based carbon capture leverages the properties of semi-permeable membranes to selectively separate CO_2 from gas streams. The membrane separation principle is based on differential permeability of gases through membranes material. Typically, membranes are designed to allow CO_2 molecules to pass through, while blocking other gases such as nitrogen or methane, thanks to specific pore sizes and surface chemistries optimized for CO_2 permeation. By adjusting the pressure and the composition of the feed gas, as well as the properties of the membrane material, the CO_2 gas can be enriched on one side of the membrane (permeate), while the undesired components are retained on the other side (retentate). Polymer-based membranes are commonly used due to their tunable properties and cost-effectiveness. In addition to polymers, advanced materials like mixed matrix membranes incorporating inorganic fillers into a polymer matrix offer enhanced selectivity and durability under harsh operating conditions.

Pressure operating conditions influence the separation efficiency and energy consumption. Relatively high pressure differences between retentate and permeate enhances the driving force for CO_2 permeation and improves the capture efficiency. Yet, high pressures also need robust membrane materials and structural integrity to withstand mechanical stresses. The power consumption in compressors also increases with higher operating pressures. One disadvantage of membranes is the relationship between selectivity and permeability, as simultaneously achieving higher recovery rates and high-purity CO_2 streams may require additional purification steps. Membrane fouling or degradation can also impact long-term performance and necessitate maintenance or replacement.

Post-combustion carbon capture unit using membranes is based on Aqualung technology, which incorporates amine compounds embedded in hollow-fiber membranes. These amines facilitate the absorption and diffusion of CO_2 through the membrane selective layer under the presence of water in flue gas. In a broader context of the energy transition, the integration of carbon capture systems is fundamental for reducing the environmental impact from industrial processes and power generation. By capturing CO_2 emissions at the source, these technologies can help not only to mitigate climate change, but also facilitate the transition to a low-carbon economy, in which biogenic carbon capturing and utilization enable the pathways towards decarbonizing the industrial sectors.

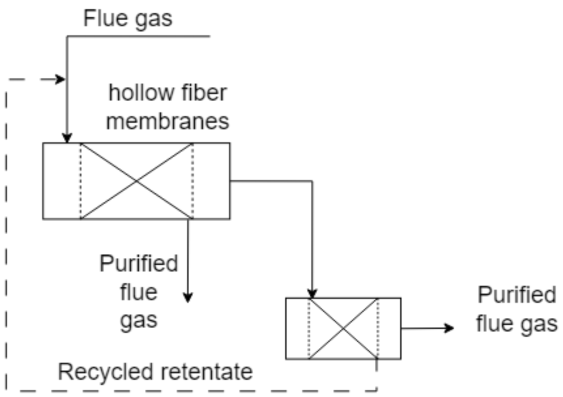


Figure A2.5. CO_2 capture using membranes model.

A.2.6 Biomass dual bed gasifier for syngas production

Biomass gasification is a thermochemical conversion that decomposes biomass at elevated temperatures (>700°C) in presence of a gasification agent such as air, O_2, steam, CO_2 or combination thereof. The gasification process consists of interrelated processes of drying, pyrolysis, reduction and combustion. The actual yield of volatiles, condensables and solids in the pyrolysis step, and the fractions of hydrogen, carbon monoxide, carbon dioxide, and methane produced in the reduction step strongly depend on the parameters of the gasifier operating, such as temperature, pressure, feed moisture, gasification agent, chemical composition, energy supply, among other hydraulic and structural characteristics [13].

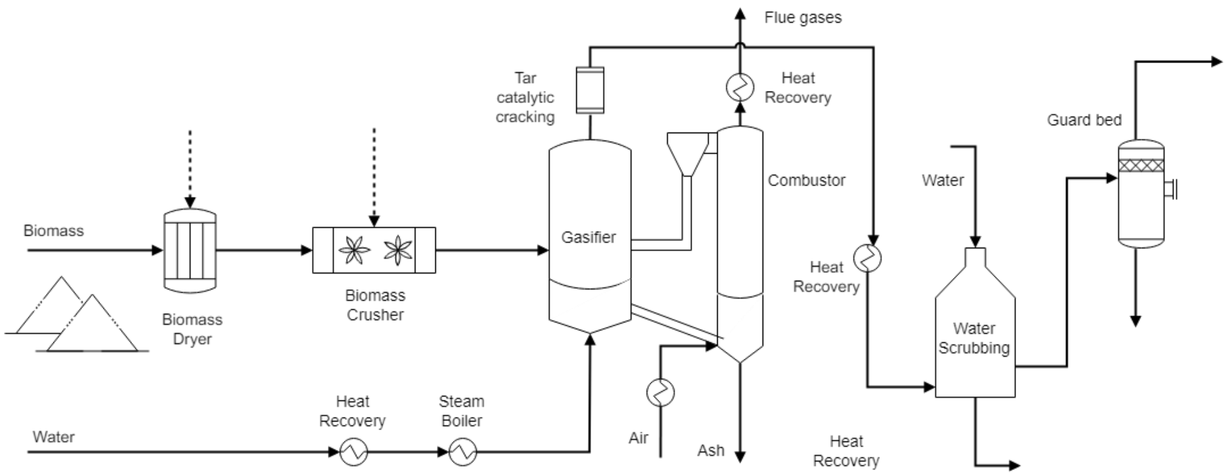


Figure A2.6. Biomass gasification for syngas production model.

In particular, a dual bed gasifier consists of two interconnected fluidized beds. The first bed is a bubbling fluidized bed, in which biomass is converted into syngas. The second bed is a fast fluidized combustion bed, which oxidizes the residual char with air or oxygen, providing the heating requirements of the highly endothermic gasification reactions occurring in the first bed. The biomass or other gasifying material is supplied to the first gasifier bed with the help of a screw conveyor. The two fluidized beds are controlled separately, but they are interconnected to ensure the circulation of the heat-carrying particles (sand with olivine). A cyclone separator is employed to separate the heat-carrying material and the flue gases in the top of the combustion bed. The heat-carrying material is returned to the first gasifier, while the flue gases are sent to the heat recovery system. The product gas obtained from the gasifier is primarily composed of H_2, CO, CO_2, CH_4, and small amounts of tar and other undesired components. The syngas mixture continues to the purification units (e.g. water scrubber and ZnO guard bed) in order to remove the impurities and to upgrade the syngas quality.

A.2.7 Dual Bed Gasifier for Fischer Tropsch liquids production

For FT liquids production, the syngas from the gasification process is compressed at 35 bar and purified by removing the excess of carbon dioxide using a physical absorption solvent in the absorber. The dominant driving force is the difference in partial pressures between CO_2 in the syngas and CO_2 in the solvent, thus CO_2 selectively dissolves into the solvent, leaving behind a purified gas stream. Next, the CO_2-rich solvent is expanded through valves or expanders, desorbing the CO_2. The solvent is recycled for further use in the absorption tower, whereas the CO_2 is compressed and purified [54].

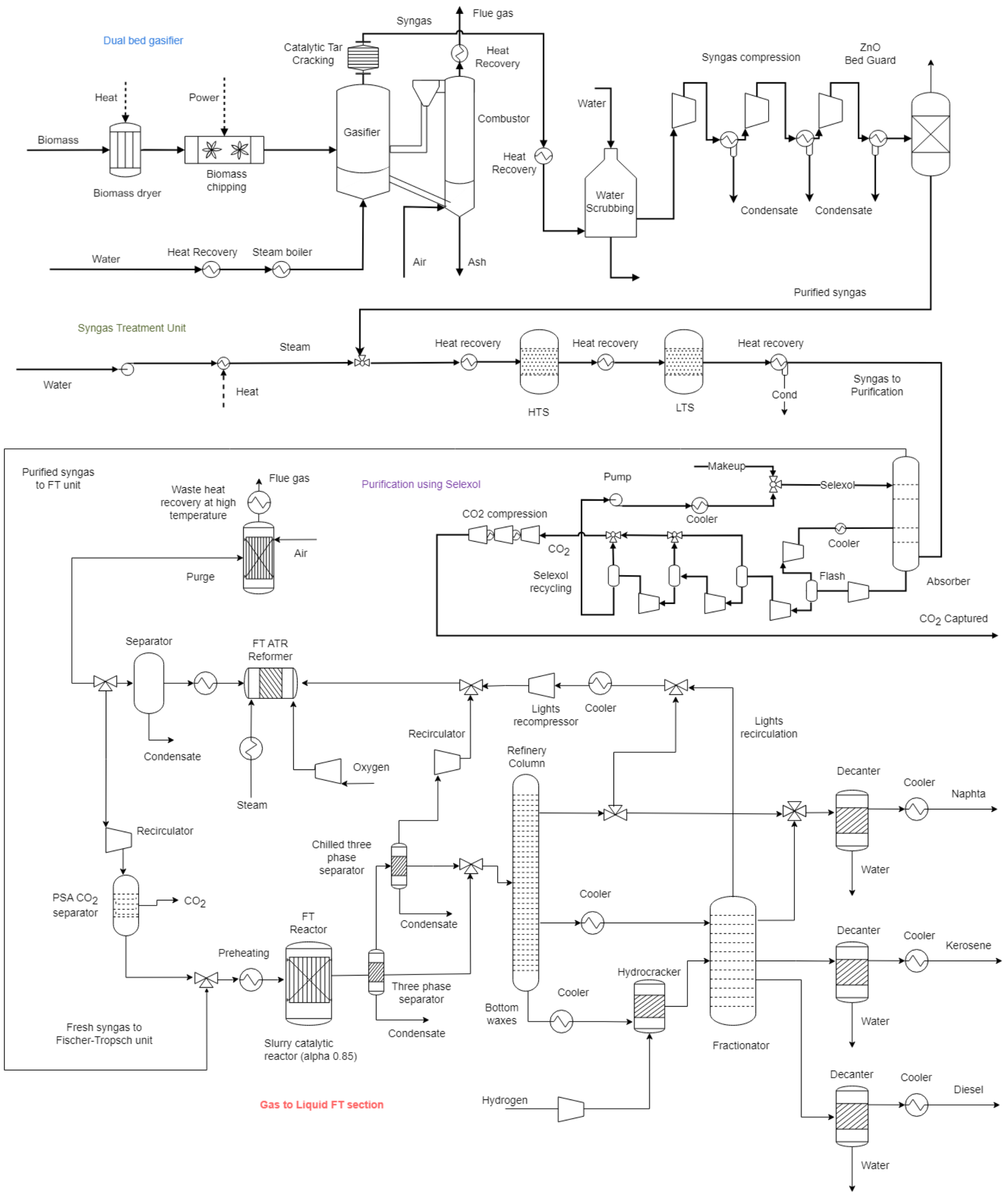


Figure A2.7. Biomass gasification for FT liquids production model.

The conditioned syngas (2:1 CO:H_2 ratio) is further compressed up to 41 bar, and fed to the Fischer-Tropsch synthesis loop, in which hydrocarbons like kerosene, but also gasoline and diesel are produced, according to the reaction: $CO + 2H_2 \rightarrow -CH_2- + H_2O$, where $-CH_2-$ represents a product consisting mainly of paraffinic hydrocarbons of variable chain length. FT reactions occur in the presence of metal catalysts, typically at temperatures of 150–300 °C and pressures around 40 bar. A series of separation, distillation, lights recirculation and hydro-treating steps are performed in order to achieve better distribution of hydrocarbon in each cutoff range (i.e. naphtha or gasoline C_{5-10}, kerosene C_{11-16}, diesel C_{17-20}). The ASF (Anderson–Schulz–Flory) distribution is used to determine the composition of the products as a function of the catalyst and operating conditions at the reactor. Some advantages of FT hydrocarbons, compared to crude oil-derivatives, are the absence of sulfur, nitrogen or heavy metal contaminants, and the low aromatic content.

A.2.8 Dual Bed Gasifier for hydrogen production

To produce hydrogen via the biomass gasification route, the syngas is purified in a similar way than for producing FT liquids. However, in order to increase the hydrogen yield, water is reacted with the CO-rich syngas in a medium temperature water gas shift reactor, which produces further CO_2. The gaseous mixture is partially purified using a physical absorption method and it passes through a bed of adsorbent material at high pressure. It selectively adsorbs the hydrogen molecules until the bed becomes saturated with hydrogen and the feed is interrupted. Next, the bed pressure is reduced, which causes the adsorbed hydrogen to desorb and be released as a high purity product. The purified hydrogen is compressed (200 bar) for its commercialization [55].

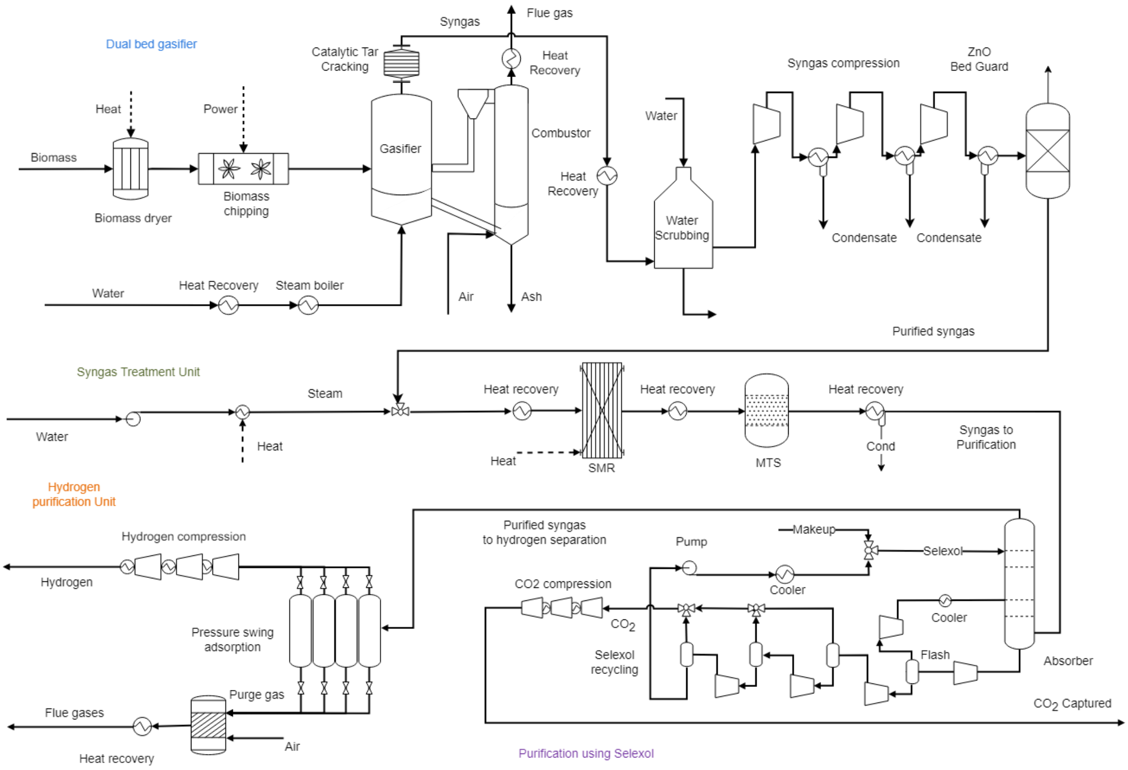


Figure A2.8. Biomass gasification for hydrogen production model.

A.2.9 Dual Bed Gasifier for SNG production

Unlike the hydrogen production, the synthetic natural gas (SNG) production via gasification of biomass considers both high and low temperature water gas shift reactors to fine tune the ratio of H_2, CO and CO_2 in the syngas. A physical absorption-based carbon capture unit is also used. Next, synthetic natural gas occurs in a methanation reactor composed of three sequential catalytic beds with intercooling. In the so-called Sabatier reaction, hydrogen, CO and CO_2 are converted into methane and water at temperatures between 250 - 700 ◦C and pressures about 30 bar [55]. Since the methanation reaction is exothermic, an efficient heat recovery is essential for controlling the reactor temperature. To this end, bed intercooling and flow recycling are required to avoid catalyst deterioration. The gaseous mixture produced in the methanator has a high methane (>97%) and moisture content, thus, an additional dehydration process is required in order to achieve commercial standards.

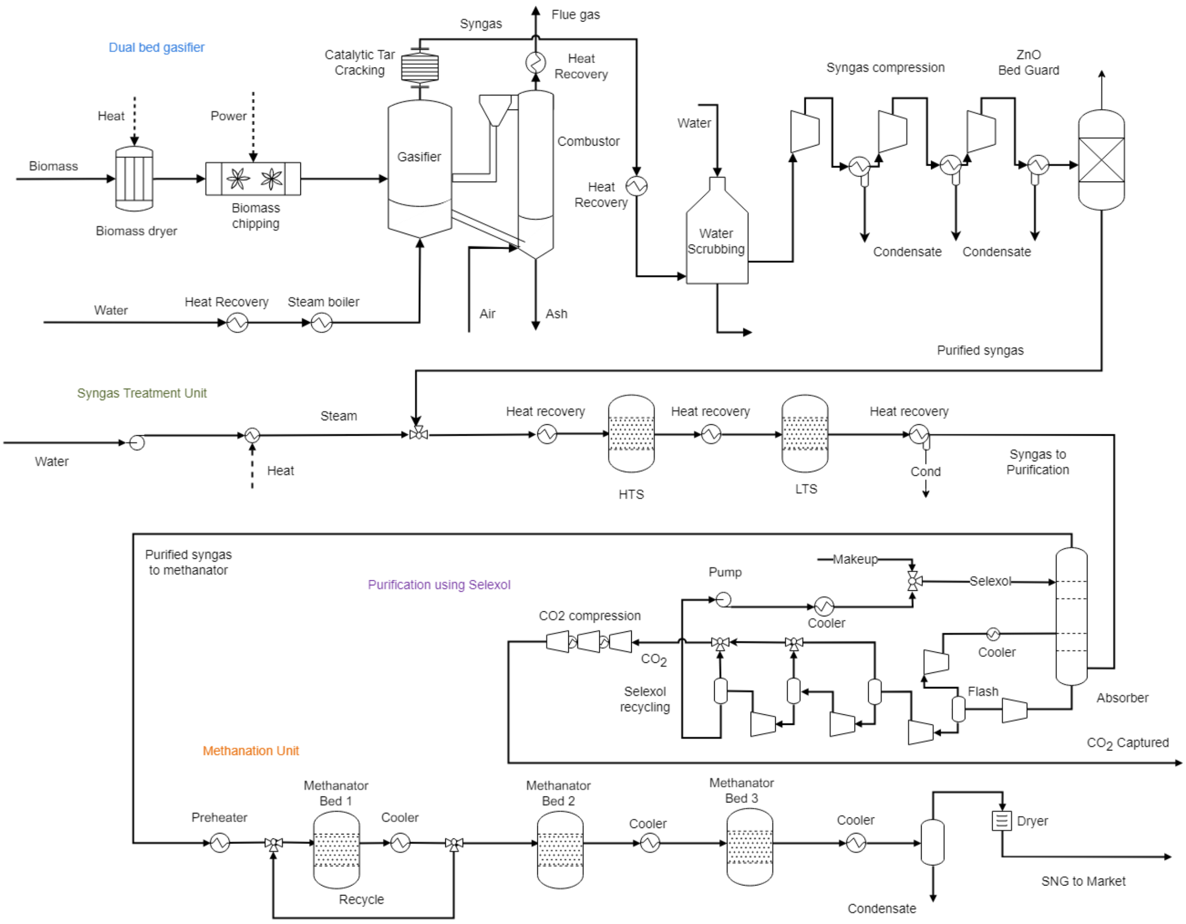


Figure A2.9. Biomass gasification for SNG production model.

A.2.10 Low temperature electrolysis

Hydrogen is used in chemical and industrial applications, such as fuel cells, hydrogenation reactions, protective atmospheres, transportation, among others uses. The most mature technologies for industrial hydrogen production are low temperature electrolyzers, which consume liquid water to produce hydrogen. Alkaline water electrolysis is a type of electrolyzer with two electrodes operating in a liquid alkaline electrolyte, such as potassium or sodium hydroxide (25-40 wt%). Typical operating temperatures are between 80-90°C. As voltage and current increase, irreversibility appear in the electrolyzer, and the total power consumption increases compared to the ideal power consumption (endergonic process). This fact limits the maximum applicable current density, and thus the hydrogen yield and the production efficiency, apart from increasing the electricity losses in the form of waste heat. Also, since the theoretical ideal energy consumption for water electrolysis reduces while the temperature increases, low temperature electrolyzers are more energy-intensive than their high temperature counterparts. The low temperature electrolysis systems are typically operated at higher voltages than the thermoneutral voltage (~1.8 V) since a higher cell potential is needed to compensate for ohmic losses. Consequently, the stack electricity consumption in steam electrolysis technology is lower (33-38 kWh/kg H_2), compared to the low temperature water electrolysis system (above 50 kWh/kg H_2) [56].

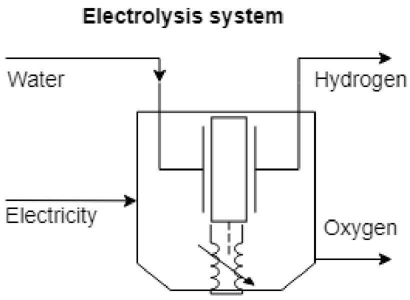


Figure A2.10. Low temperature electrolyzer cell model.

A high temperature solid oxide electrolysis cell (SOEC) is an electrochemical cell capable of converting steam and optionally carbon dioxide (co-electrolysis) into hydrogen and carbon monoxide. An oxygen-rich stream is also produced. SOEC consists of a ceramic oxygen ionic conducting electrolyte, surrounded by two porous electrodes. Steam is converted at the porous cathode into hydrogen and oxygen ions due to the absorption of electrons. When the voltage increases, the oxygen ions are transported through the dense ceramic oxygen ion-conducting electrolyte to the porous anode, in which oxygen is formed with the release of electrons.

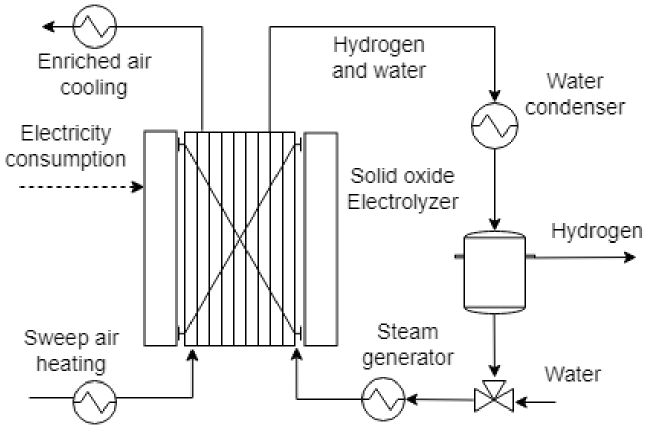


Figure A2.11 Solid oxide electrolyzer model.

The SOEC technology operates at higher temperatures than other electrolysis technologies, typically between 600-850ºC, which is required to have sufficient oxygen ion conductivity in the ceramic electrolyte. Also, the theoretical energy consumption for splitting water and carbon dioxide decreases with increasing temperature. Since the alkaline (AWE) and PEM electrolyzers technologies operate at lower temperatures, SOEC has higher efficiency and faster kinetics.

Electrolyzers will play a key role in harvesting and transforming renewable electricity into storable chemicals and fuels. Their ability to efficiently convert surplus electricity from renewable sources, such as solar and wind, into storable hydrogen will be key for balancing the intermittency of these energy systems. In fact, electrolyzers will play a dual role: as a way to store excess electricity in the form of gas (power-to-gas) and for the direct production of hydrogen or other energy carriers (e.g. SNG, methanol, etc.), providing grid stability, backup power, and fuel for industrial applications.

A.2.11 Proton exchange membrane fuel cell

Hydrogen can be converted into electricity in a fuel cell in a more efficient way than burning it in a cogeneration system. Currently, low temperature proton exchange membrane (PEM) fuel cells are among the most mature technologies. Typical operating temperatures in this type of fuel cells range between 60°C to 80°C. PEMFC are made of a polymer electrolyte membrane that conducts protons and separates the anode and cathode compartments. As the current increases, irreversibility emerge, leading to a decrease in the total power generation compared to the ideal potential (hydrogen oxidation is an exergonic process). This phenomenon limits the maximum applicable current density and, consequently, the power generation efficiency, while increasing fuel energy losses in the form of waste heat.

In the context of sustainable energy solutions, fuel cells also play an important role in transforming the fuels that have been used to store renewable energy back into electricity in a more rational way. Their ability to efficiently convert stored chemical energy in the form of hydrogen or synthetic natural gas will be key for balancing the intermittency of these energy systems. In fact, fuel cells will play a complementary role in the so-called power-to-gas systems, using the stored hydrogen previously produced by an electrolyzer, providing grid stability and backup power for industrial applications.

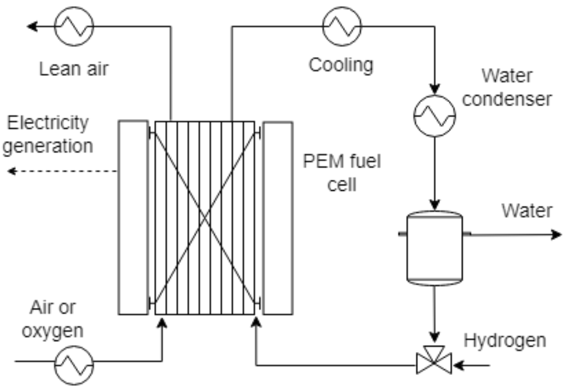


Figure A2.12. PEM fuel cell model.

A.2.12 Methanator

The methanation reaction, also known as the Sabatier reaction, is the conversion of carbon dioxide to methane through hydrogenation. Although it has been proposed as a way of producing synthetic natural gas since the 1970s, it has gained renewed interest due to its potential use in renewable energy management, particularly in the implementation of power-to-gas technology. This approach involves converting surplus renewable electricity from solar or wind power into hydrogen via water electrolysis, followed by a methanation process to further convert hydrogen into synthetic natural gas, which is a more convenient form of energy for storage and transportation. SNG can be integrated into existing natural gas infrastructure, serving as a clean and versatile fuel source across various sectors like transportation, chemical and heating.

Optimal operating pressures and temperatures are critical for enhancing the efficiency of the methanator, which typically operates at pressures between 20-30 bar and temperatures from 300 to 600°C [57]. The process is characterized by a highly exothermic reaction, releasing heat during the conversion of hydrogen and carbon dioxide into methane, which can be readily integrated in the industrial facilities to supply high grade process heat. Carbon dioxide sources for this process vary, encompassing pre-combustion carbon capture units, biogas and fermentation facilities, or post-combustion carbon capture in power generation systems. Meanwhile, hydrogen primarily originates from water electrolysis, powered by renewable electricity, but can be also provided by gasification of biomass resources. This technology offers a solution for energy storage and grid stabilization, enabling the storage of excess renewable energy during periods of low demand and its redistribution during peak demand. In this way, its integration with power-to-gas-to-tank technologies and existing infrastructure allows advancing the transition towards an enhanced scenario of renewable energy utilization.

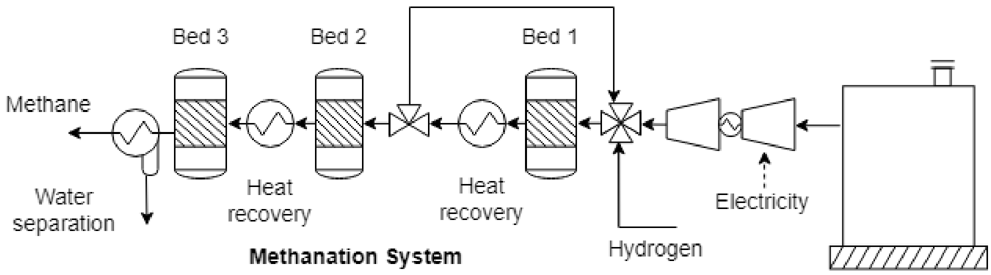


Figure A2.13 Methanator model.

A.2.13 Reverse water gas shift unit

Reverse water gas shift (RWGS) is a reaction that can be tailored for production of different mixtures of syngas. In this process, carbon dioxide and hydrogen react to generate a syngas with a particular composition ratio, for instance 2:1 H2:CO, ideal for subsequent methanol or Fischer-Tropsch syntheses. A notable byproduct of this reaction is water. The unreacted gas is typically recycled to increase the carbon conversion in the process. The reaction typically occurs at 5 bar and 750 °C, being moderately endothermic. Part of the heat rejected during the cooling of the reactor effluent can be recovered to preheat the fresh incoming H_2 and CO_2 mixture, but an external hot utility is necessary to maintain the reactor temperature. Although catalytic RWGS reaction can be addressed in specific reactor beds, it also occurs in applications that operate at high temperature under an atmosphere rich in H_2 and CO_2. It explains the fact that RWGS is one of the most representative mechanisms for the CO production in the co-electrolysis systems.

In the context of energy transition, the RWGS reaction plays a crucial role in the production CO and H_2-rich syngas necessary for various downstream chemical processes, enabling the production of the so-called e-Fuels and e-Chemicals. In fact, the integration of a RWGS unit with a water electrolysis system offers an alternative pathway to the co-electrolysis process, becoming an important technology in the power-to-gas energy managing approaches.

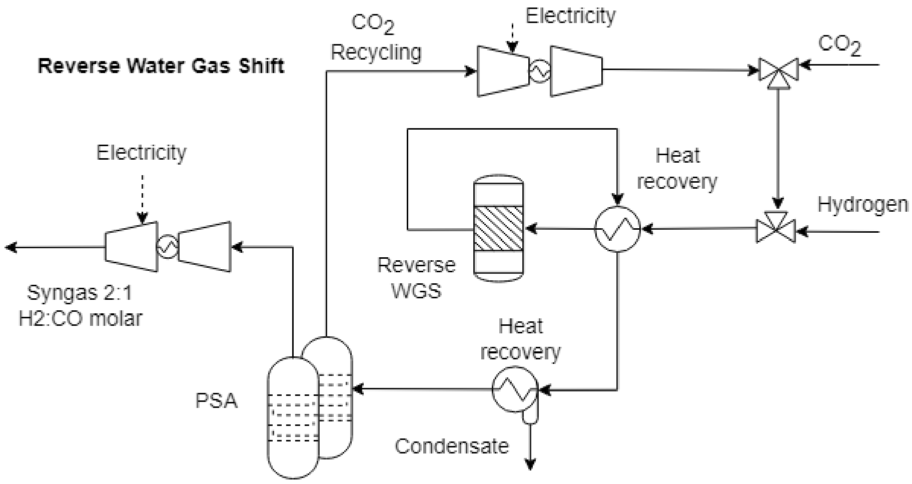


Figure A2.14 Reverse water gas shift model.

A.2.14 Methanol production

Methanol is a versatile chemical compound that serves as a fundamental feedstock in various industrial processes. It is also a promising energy storage and carrier, particularly in the context of renewable energy technology integration. It can be produced from a number of feedstock, including syngas derived from biomass or via power-to-gas technologies, such as water and carbon dioxide co-electrolysis.

In the methanol production process, the syngas undergoes a series of transformations to yield high-purity methanol. The syngas in a molar proportion of (H_2-CO_2)/(CO+CO_2) ~ 2 is compressed up to 90 bar and fed to the methanol synthesis loop, where it is preheated in a heat-exchanger to achieve the operating conditions of an isothermal catalytic reactor (90 bar and 210 °C) [56]. Since the reactor temperature is kept constant, a large amount of waste heat is available to be integrated to other industrial processes. The outlet stream of the methanol reactor is a gaseous mixture of methanol, water and unconverted reactants. The mixture is cooled and flashed first to 45 bar, and then to 3.5 bar, in order to separate the condensable products (i.e. water and methanol) from the non-condensable substances. The condensed stream continues to a distillation column at atmospheric pressure, in which methanol is distilled with a purity over 99% wt. A fraction of the non-condensable stream is purged to avoid the built up of inerts, while the remainder is recycled back to the methanol synthesis loop. This model has been rigorously simulated using a Langmuir - Hinshelwood Hougen - Watson (LHHW) kinetics model. The synergy between renewable energy sources and methanol production not only enhances energy security, but also fosters sustainability by promoting carbon-neutral or even carbon-negative feedstock.

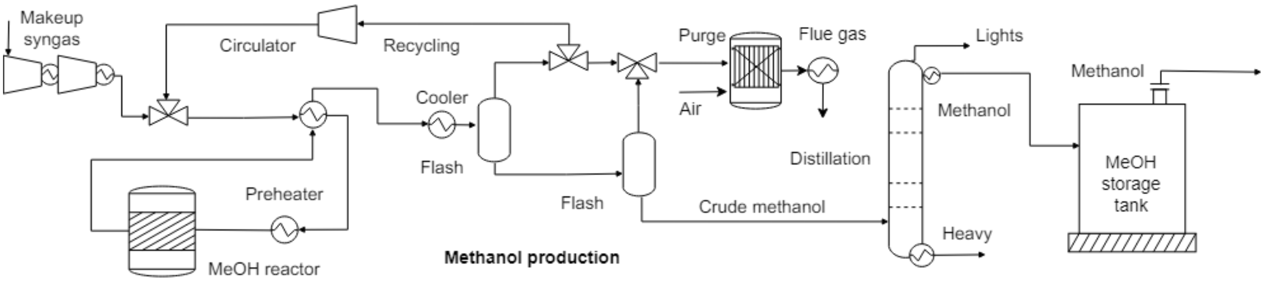


Figure A2.15 Methanol production model.

A.2.15 Methanol to synthetic natural gas unit

Methanol is liquid at room temperature, which makes it more compact and convenient to store energy, compared to SNG. Thus, it offers a promising pathway for renewable energy management and storage. The autothermal reforming (ATR) of methanol allows producing syngas that can undergo methanation to produce a methane-rich gas, suitable for injection into existing natural gas pipelines. In this way, the compatibility of the methanol supply chain with existing infrastructure facilitates the integration into current energy networks. This fact enables the utilization of methanol as a flexible energy carrier that can be stored and transported easily, offering greater energy security and stability to the gas networks. Methanol can be readily marketed or converted into value-added products, but the use of methanol as an energy carrier has drawn recent interest due to the diversification of the syngas production technologies and energy resources, including biomass gasification, reverse water gas shift reaction and co-electrolysis of water and carbon dioxide.

In the reforming process, the liquid methanol and the water are pumped at high pressure (35 bar) and preheated up to the reactor temperature of 350 °C using heat exchangers [56]. The methanol reforming process is highly endothermic, thus a given amount of oxygen is fed to the reformer, so that it can partially burn the produced syngas to maintain the reaction rates and temperatures inside the autothermal reactor. The stoichiometric ratio for SNG production from syngas is (H2-CO2)/(CO+CO2) ~ 3, which is achieved by the utilization of water gas shift reactors and pressure swing adsorption membrane purification systems. In the methanation process, carbon dioxide is converted to methane through hydrogenation. Optimal operating pressures and temperatures are critical for enhancing the efficiency of the methanator, which typically operates at pressures between 20-30 bar and temperatures from 300 to 600°C. The process is characterized by a highly exothermic reaction, releasing heat during the conversion of hydrogen and carbon oxides into methane, which can be readily integrated in the industrial facilities to supply high grade process heat. Produced SNG can be compressed for distribution via pipelines, or consumed in industrial facilities.

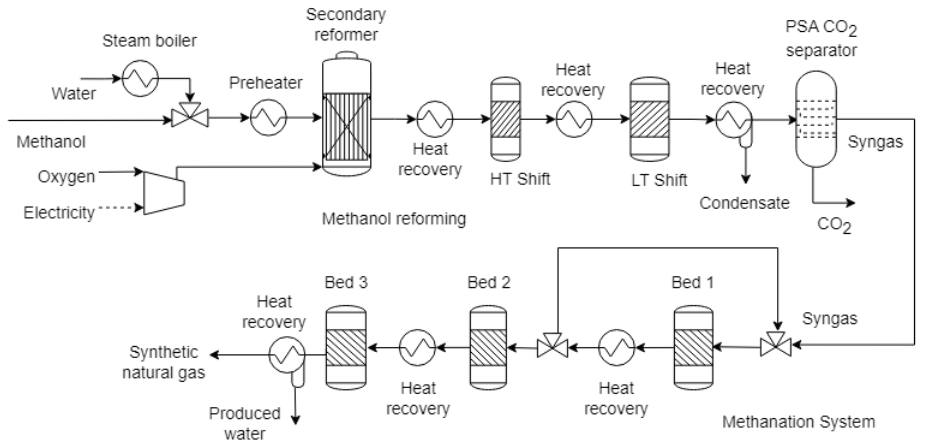


Figure A2.16 Methanol to synthetic natural gas model.

APPENDIX 3 ACCESS, INSTALLATION, AND EXECUTION OF THE TOOL

A3.0 Access and setup procedure

In the time being, the tool can be accessed after registration into EPFL IT ecosystem. In this way, the students of the Continuing Education Program are granted the right to have a VM (Virtual Machine) hosted by EPFL that can be easily accessed even from outside the campus using a VPN (Virtual private network) and the respective user account credentials.

In anticipation to a wide deployment of the open-source tool developed and the utilization by various interested partners, EPFL is devising a strategy for managing the unattended installation of ROSMOSE along with the open source programming languages (R, python, etc.), libraries (cool-prop, Scipy, Matplotlib, Rmarkdown), IDEs (Visual Studio Code), software (AMPL, Solvers) and engines (Quarto, OSMOSE, etc.) required for the correct functioning of the modeling, documentation and reporting tool.

The following steps must be followed to ensure that all the dependencies are installed in the VM and that the MAS Book can be rendered:

1. Open the terminal in VS code.
2. Install Quarto. More information about Quarto can be found here.
3. Verify that a connection to EPFL network, either directly or via the VPN, is active.
4. Verify the installation of R and Python in the computer, e.g. executing the command python --version
5. Run the script provided with the MAS Book that defines the CRAN repository and also installs some important packages:

   For mac:
   - Run ./installation/install_R_mac.sh in the terminal in order to install R, set environment variables and install important packages.

   For windows:
   - Verify the installation of R in C:\Program Files\R\<version installed>\bin (copy it).
   - In the environment variables, under System Variables, open the variable PATH and add the new path previously copied.
   - Test R by running R --version in the command line
   - Run installation/install_R_win.bat as administrator to set environment variables and installs important packages.

6. Run in the terminal quarto render to build the book or quarto preview to open it directly on your browser.

To install ROSMOSE, executing the following chunk of R is sufficient to source external R scripts:

````
```{r}
source("https://ipese-internal.epfl.ch/rscripts/rosmose-setup.R", local = knitr::knit_global())
```
````

A.3.1 Structure of directories and files of the ROSMOSE project

The frontend is the main script that contains all the information about which processes and utilities are to be included in the optimization problem and it is the first file to run. Further details about the content and configuration of the frontend.Rmd file will be discussed later on this section. When running the frontend, some folders are generated automatically, such the images and the result folders, listed in Figure A3.1.

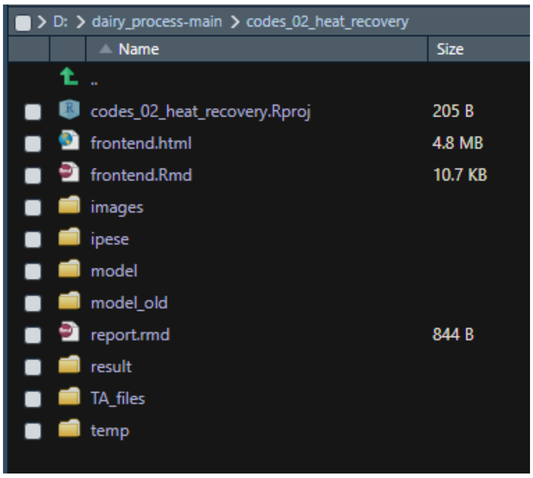


Figure A3.1. Folders are generated automatically and other folders manually modified (e.g. models) in ROSMOSE.

Those folders contain the images for the optimization report and the results in. JSON format that are generated automatically by ROSMOSE. The Report.rmd file contains instructions on how to convert the separate Rmd files into a .html report, and does not need to be modified by the end-user.

The building blocks of any ROSMOSE project are the energy technology (ET) models. Each ET can be defined by several input and output tags, have multiple units, and be connected through layers to other ETs and their associated units. The layer concept in ROSMOSE can be interpreted as the pipe through which similar streams flow and it is characterized by a name, a quality and a physical unit. In addition, each unit of an ET can be classified as either process or utility. The main difference is that the sizing factor of the former is fixed in the optimization problem, as it represents the specified energy requirements that must be satisfied by the variable utility systems

To call the energy technologies available in the 'model' folder, the frontend file must be executed. According to Figure A3.1, the frontend file is a combination of text and code chunks, and it is the core file that contains all the elements that will be included in the report. In fact, the frontend.Rmd file can be regarded as a canvas, in which all the results retrieved by the execution of ROSMOSE can be summarized and documented, to be eventually rendered when building the .html book

The process and utility models can be tailor-made, combined or adapted from existing ones to create more complex energy technologies (ETs). Thus, the model folder is virtually the only one that needs to be modified by the end-user. Figure A3.2 shows the content of the 'model' folder, in which a dairy plant was chosen as sample process to apply the pinch analysis method, whereas considering the potential installation of the following utility systems:

- a hot utility system (e.g. furnace)
- a cogeneration system (e.g. an engine with waste heat recovery),

- a cool utility system above (e.g. water cooling) or below (refrigeration) ambient temperature,
- a set of heat pumping systems (from low to high temperature levels),
- and a market for commodities and products transaction.

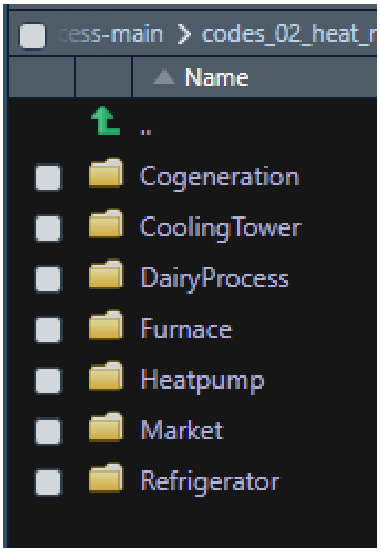


Figure A3.2. Content of the 'model' folder in the ROSMOSE environment.

It is important to highlight the "child" functionality shown in the frontend, which is used to insert .Rmd code available in other .Rmd files in the specified position of the frontend. For instance, both DairyProcess and a CoolingTower .Rmd files, which contain the respective models of those energy systems, can be enabled from the frontend in order to be included in the integration process (Figure A3.3). Moreover, any text (preceded or not by #) corresponds to plain text that will be rendered together with the code enclosed by the triple inverted quotation marks ```{r}```, thus producing a rich report with meaningful descriptions of the optimization results. In the frontend, it can also be found the command SOLVE followed by a given objective function, such as TotalCost or MER, which calls OSMOSE in the backend. The project must have a codename (e.g. "dairy") provided after the command SOLVE, followed by the list of the models or ETs previously enabled in the frontend. The number of operating hours needs to be also defined (Figure A3.4).

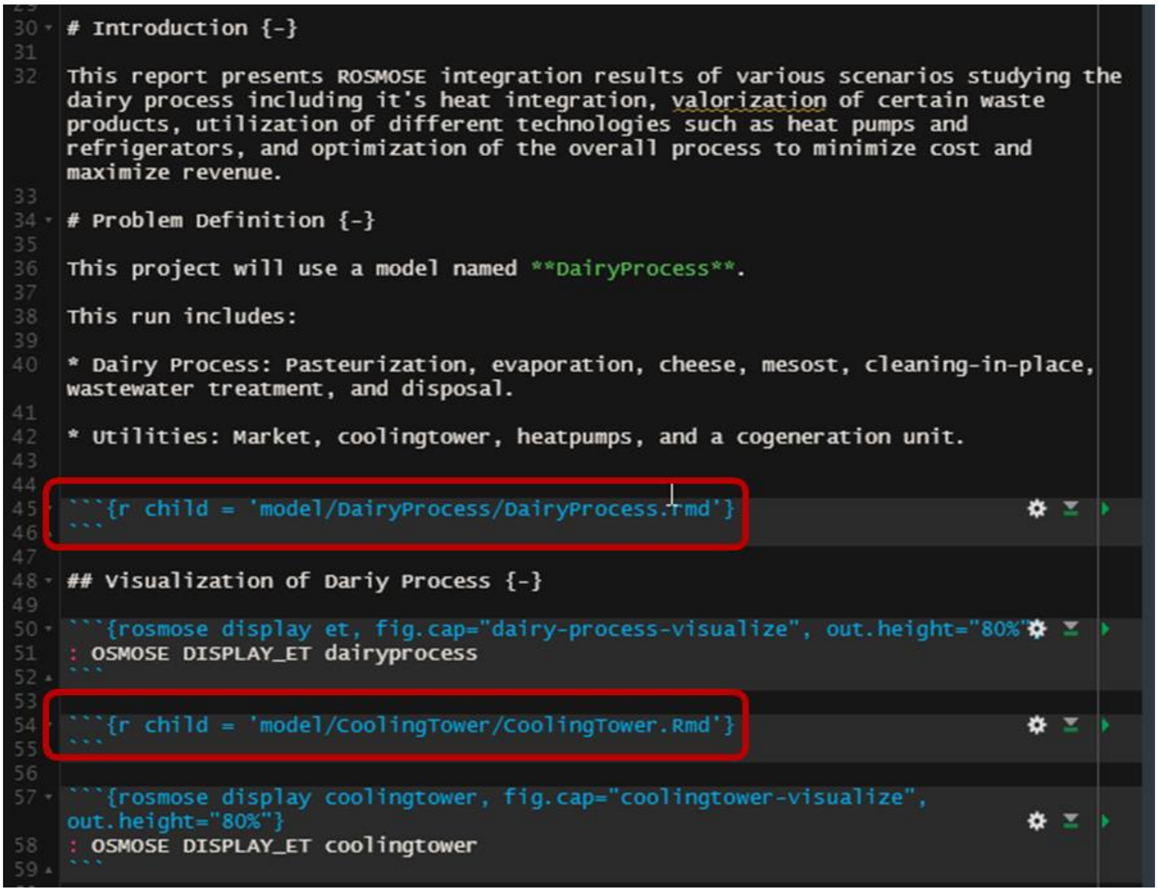


Figure A3.3. Structure of the frontend file: calling the models of the energy systems.

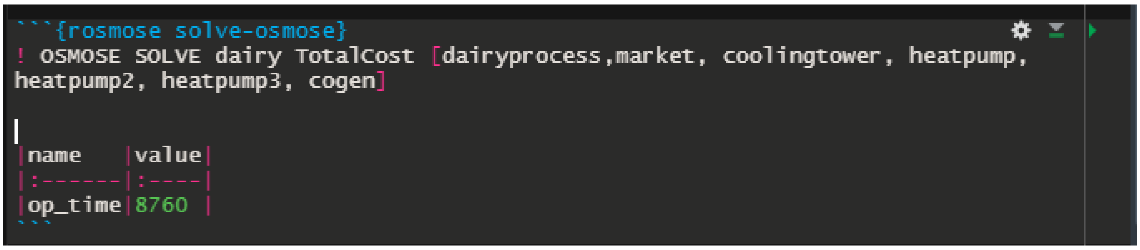


Figure A3.4. Structure of the frontend file: solving the optimization process using the models.

In ROSMOSE, there is a functionality called Serialization that helps experienced developers to debug more complex convergence issues. Serialization allows verifying that OSMOSE is receiving correctly the information that the end-users are willing to transfer, and it is not mandatory to be enabled to use ROSMOSE. An example of serialization command is shown in Figure A3.5.

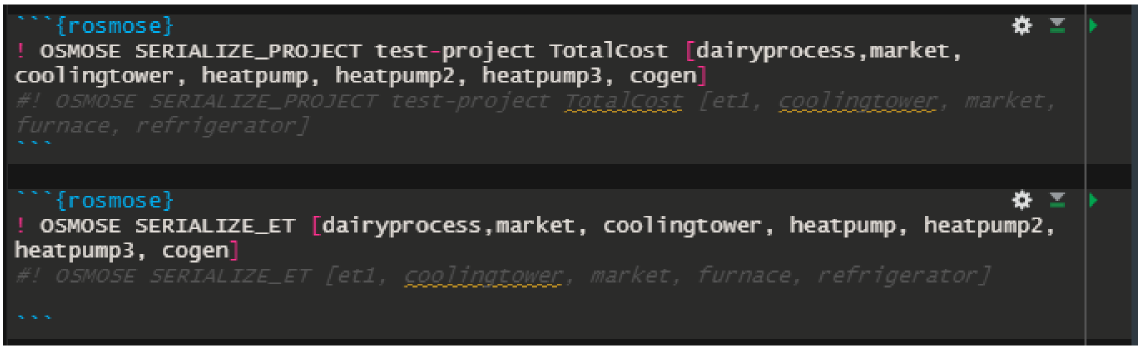


Figure A3.5. Example of serialization command to generate .lua files.

A.3.2 Description of the files in the ‘model’ folder of the ROSMOSE implementation

In this section, the schema of the .Rmd files that represent the energy technologies is described in more detail. Firstly, each ET needs to have a name, which is defined in the beginning of the .Rmd file using a triple inverted quotation marks notation (```{ }```) to create an ROSMOSE chunk. Note also the “# Cooling Tower” text at the beginning, which only inserts a title header in the .Rmd file, but is not related to any ROSMOSE chunk of code.

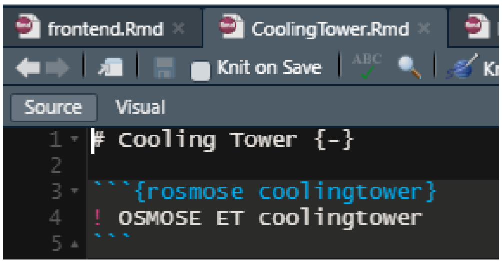


Figure A3.6. Naming of a coolingtower ET in a CoolingTower.Rmd file.

After creating the ROSMOSE ET, a series of variables can be defined as tags in order to declare the user defined or the calculated parameters, representative of the operating conditions, design parameters, and other characteristic of the energy technologies. Thus, in ROSMOSE, a tag is an object containing (Figure A3.7):

- a name,
- a value,
- a physical unit, and
- a description.

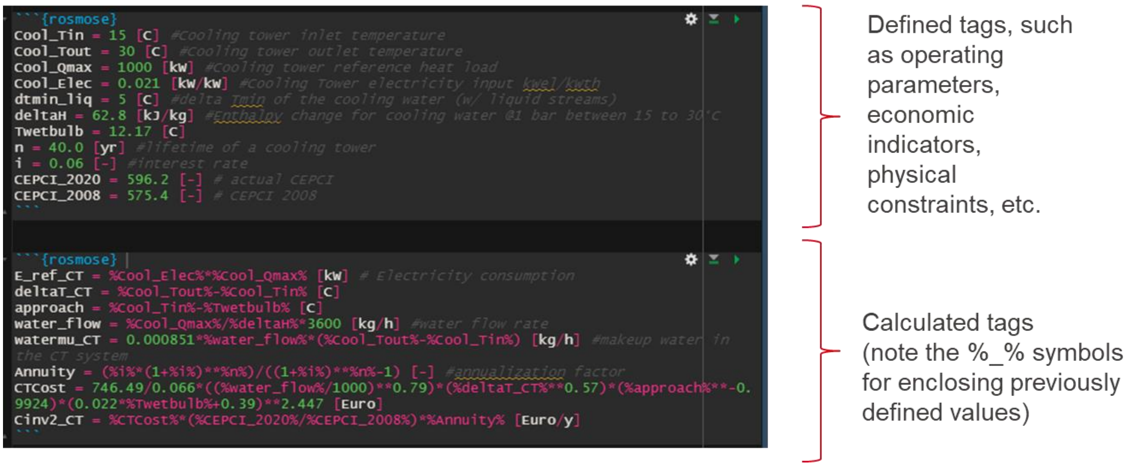


Figure A3.7. User defined or calculated parameters in ROSMOSE.

Each ET may enclose one or more units, which are linked to each other and to other units of other ETs by mass and energy balances, using a concept previously defined as layer. In addition, each unit in an ET can be classified either as a process or as a utility. Process units are characterized by fixed operating data of industrial processes (e.g. flows, supply and target temperatures, composition, energy demands etc.). In contrast, utility units can be enabled or disabled, and sized to meet the energy demands of the process unit(s). To this end, each utility unit gas the minimum and maximum sizing factors, as well as the variable and fixed investment and operating costs. All these objects, namely, layers, units, and unit parameters can be defined in ROMOSE as shown in Figure A3.8:

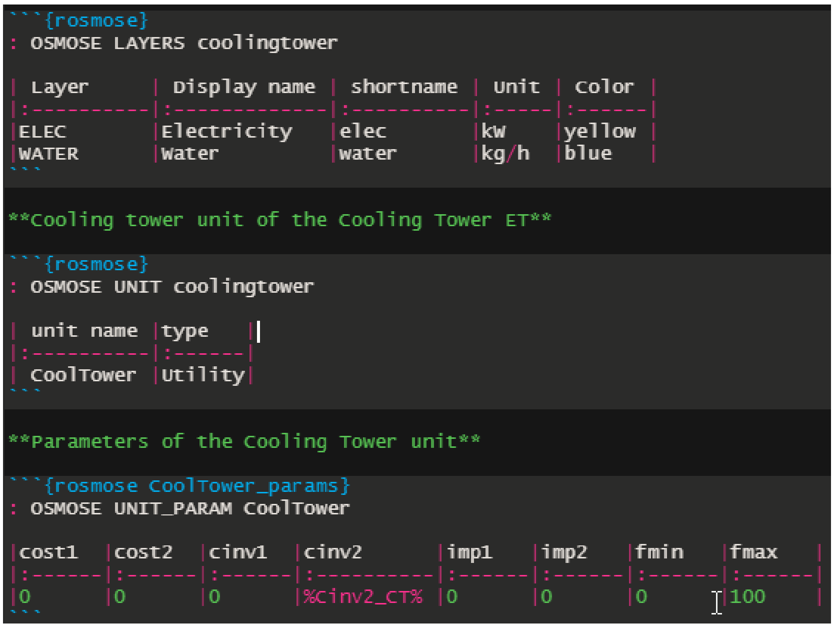


Figure A3.8. Definition of layers, units, and unit parameters in ROMOSE.

Two types of streams may be assigned to any process or utility units, namely:

- *Resource streams*, which are linked to only one of the defined layers and require an indication of their direction with regard to the unit, for instance, in (for consumption) or out (for production) (see Figure A3.9),

- *Heat streams*, which correspond to thermal energy flows and require the definition of tags such as supply and target temperatures, inlet and outlet enthalpies (or heat capacities), a minimum temperature approach contribution and a heat transfer coefficient (see Figure A3.10).

```
*Resource Streams*

```{rosmose CoolTower_rs}
: OSMOSE RESOURCE_STREAMS CoolTower

|layer      |direction|value                |
|:----------|:--------|:--------------------|
|ELEC       |in       |%E_ref_CT%           |
|WATER      |in       |%watermu_CT%         |
```
```

Figure A3.9. Definition of the Resource streams in ROSMOSE.

```
*Heat Streams*

```{rosmose CoolTower_hs}
: OSMOSE HEAT_STREAMS CoolTower

|name           |Tin        |Tout       |Hin |Hout          |DT min/2       |alpha |
|:--------------|:----------|:----------|:---|:-------------|:--------------|:-----|
|cooltowerheat  |%Cool_Tin% |%Cool_Tout%| 0  | %Cool_Qmax%  | %dtmin_liq%   |1     |
```
```

Figure A3.10. Definition of the Heat streams in ROSMOSE.

In summary, by defining the input and calculated parameters, the layers, the units and their cost and bounding parameters, as well as the resources (mass or electricity) and heat streams, the ROSMOSE ET can be completely defined. All the other ETs are programmed in a similar way and can be called in the frontend.Rmd to determine the best combination of energy technologies that satisfy the constraints and minimize the objective functions.

A.3.3 Predefined functions for retrieving the data and displaying the relevant plots

After executing the optimization routine, ROSMOSE generates a. json file with all the pre-defined key performance indicators and plots. This .json file can be loaded into a data object in the R environment (Figure A3.11):

```
```{r, eval=T}
library(jsonlite)
pfilename<-"result/dairy-6.json"
data <- fromJSON(pfilename, flatten=FALSE)
x<-data$results$KPIs$opex
y<- data$results$delta_hot[[1]]$Clu$DefaultHeatCascade
```
```

Figure A3.11. Retrieving the ROSMOSE results available in the .JSON file.

By using this object is possible to display KPIs, composite curves, integrated composite curves, Carnot curves, heat exchanger information, etc., as it is exemplified in Figure A3.12:

````
# Optimization Results {-}

## Capital and Operational Expenditures {-}

```{r print economic results}
cat("CAPEX:", data$results$KPIs$capex)
cat("OPEX:", data$results$KPIs$opex)
```
````

Figure A3.12 Retrieving the capital and operational expenditures in .JSON file.

Pre-defined functions for plotting characteristic curves are already programmed and only need to be executed, as in Figure A3.13, to plot the Carnot grand integrated composite curve.

````
```{r carnot}
display_carnot <- function(time=1){
  graphs <- data$results$graph[[1]]
  graph <- graphs[[time]]
  graph <- graph[graph$plot_type == "carnot.utilities",]$data[[1]]
  base <- graph[graph$title == "base",]$curve[[1]]
  utilities <- graph[graph$title == "utilities",]$curve[[1]]

  if (!is_empty(base) && !is_empty(utilities)){
    plot_ly() %>%
            add_trace(x=base$Q, y=base$T, mode = 'lines', line=list(color='red'),
name='base') %>%
            add_trace(x=utilities$Q, y=utilities$T, mode = 'lines',
line=list(color='blue'),  name='utilities') %>%
            layout(xaxis= list(title = "Heat load [kW]"),
                   yaxis= list(title = "Carnot factor 1-To/T [-]"),
                   margin= list(l=50, r=20, b=40, t=40),
                   title = "Thermal Exergy of Integrated Utilities"
            )

  } else {
    print(paste("There is no Carnot for timestep", time))
  }
}

display_carnot(1)
```
````

Figure A3.13. Pre-programmed function to plot the Carnot grand integrated composite curve.

Other relevant data, such as that related to the minimum number of heat exchangers, estimated heat exchanger area and HEN cost can be also reported (Figure A3.14):

````
## Heat Exchanger Network {-}

The heat exchanger network area required to attain the minimum energy requirement
is extracted from OSMOSE optimization results.
The minimum number of heat exchangers for the network and average area per heat
exchanger can also be calculated from the simulation outputs.
Next the cost of this heat exchanger network can be computed based on the equations
published in Turton 1998 and corrected by the chemical engineering plant cost index
(CEPCI) for 2023.

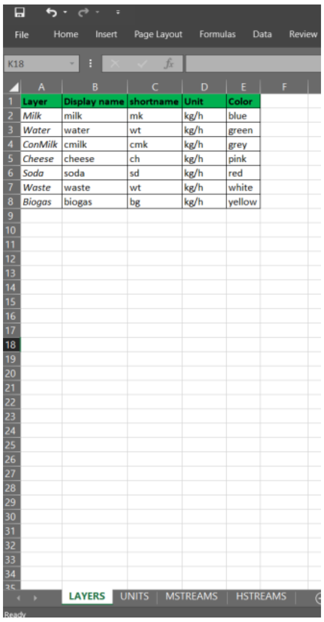
```{r}
get_HEN <- function () {
  spag_area <- data$results$spaghetti[[1]]$Clu$DefaultHeatCascade$area_total
  min_number_HEX <- data$results$spaghetti[[1]]$Clu$DefaultHeatCascade$HEs
  hex_area <- spag_area / min_number_HEX
  n <- 15 # years, lifetime of a heat exchanger
  i <- 0.05 # fractional interest rate per year
  an_factor <- (i*(1+i)^n/((1+i)^n-1))
  k1 <- 3.2138
  k2 <- 0.2685
  k3 <- 0.07961
  Fp <- (10^(k1+ k2*log10(hex_area)+ k3*(log10(hex_area))^2))
  Fm <- 3 #stainless steel shell and tube
  B1 <- 1.8
  B2 <- 1.5
  F_BM <- (B1+(B2*Fm*Fp))
  CEPCI_1998 <- 382
  CEPCI_2023 <- 600
  c_hen <- (F_BM*(CEPCI_2023/CEPCI_1998)*an_factor*min_number_HEX)
  return(list("hen_area" = spag_area,"min_number_HEX" = min_number_HEX ,"hex_area"
= hex_area, "an_factor" = an_factor, "c_hen"= c_hen))
}

hen <- get_HEN()
```
````

Figure A3.14. Pre-programmed function to calculate the minimum number of heat exchangers, estimated heat exchanger area and HEN cost

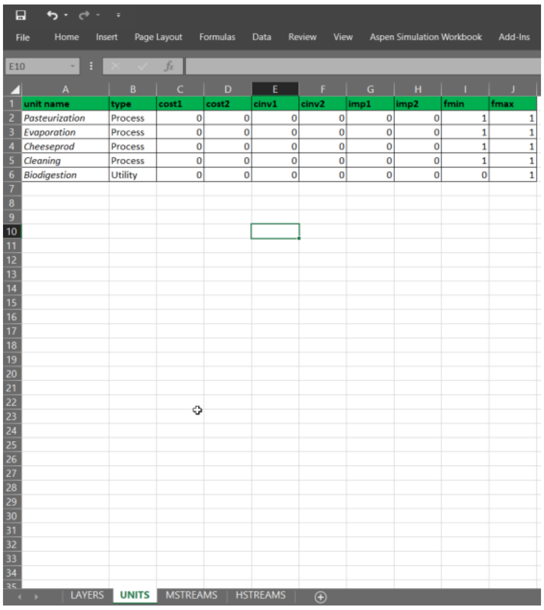
A.3.4 Template for data input using Excel software

Considering that Excel is one of the most widespread office suites and that a lot of data generated in industries is stored in this format, the web-based tool incorporates a function to read the content of an Excel file and automatically build the ET in the ROSMOSE syntax. The name of the Excel file is the same name of the ET, which contains four tabs for inputting the layers (LAYERS), the units (UNITS), the resource streams (MSTREAMS) and the heat streams (HSTREAMS) (Figures A3.15-A3.16):



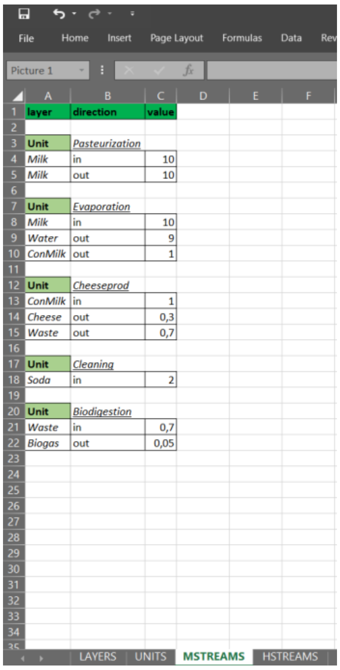
Layer	Display name	shortname	Unit	Color
Milk	milk	mk	kg/h	blue
Water	water	wt	kg/h	green
ConMilk	cmilk	cmk	kg/h	grey
Cheese	cheese	ch	kg/h	pink
Soda	soda	sd	kg/h	red
Waste	waste	wt	kg/h	white
Biogas	biogas	bg	kg/h	yellow

Figure A3.15. Schema of the LAYERS tab



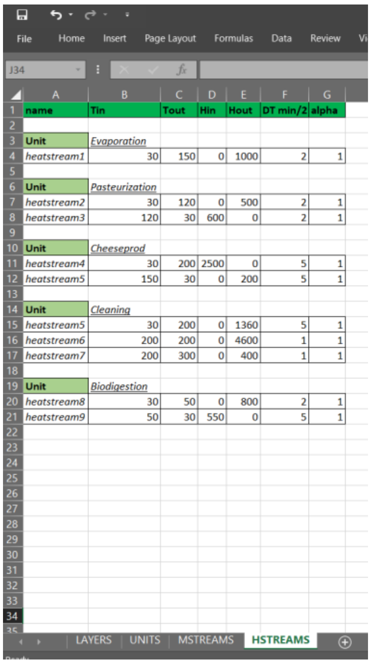
unit name	type	cost1	cost2	cinv1	cinv2	imp1	imp2	fmin	fmax
Pasteurization	Process	0	0	0	0	0	0	1	1
Evaporation	Process	0	0	0	0	0	0	1	1
Cheeseprod	Process	0	0	0	0	0	0	1	1
Cleaning	Process	0	0	0	0	0	0	1	1
Biodigestion	Utility	0	0	0	0	0	0	0	1

Figure A3.16. Schema of the UNITS tab.



layer	direction	value
Unit	Pasteurization	
Milk	in	10
Milk	out	10
Unit	Evaporation	
Milk	in	10
Water	out	9
ConMilk	out	1
Unit	Cheeseprod	
ConMilk	in	1
Cheese	out	0,3
Waste	out	0,7
Unit	Cleaning	
Soda	in	2
Unit	Biodigestion	
Waste	in	0,7
Biogas	out	0,05

Figure A3.17 Schema of the MSTREAMS tab



name	Tin	Tout	Hin	Hout	DT min/2	alpha
Unit	Evaporation					
heatstream1	30	150	0	1000	2	1
Unit	Pasteurization					
heatstream2	30	120	0	500	2	1
heatstream3	120	30	600	0	2	1
Unit	Cheeseprod					
heatstream4	30	200	2500	0	5	1
heatstream5	150	30	0	200	5	1
Unit	Cleaning					
heatstream5	30	200	0	1360	5	1
heatstream6	200	200	0	4600	1	1
heatstream7	200	300	0	400	1	1
Unit	Biodigestion					
heatstream8	30	50	0	800	2	1
heatstream9	50	30	550	0	5	1

Figure A3.18. Schema of the HSTREAMS tab.

Figure A3.19 shows the first lines of the code used for parsing the Excel data into an .Rmd file. Then, the latter can be readily added to the other files in the ‘model’ folder.

```python
import openpyxl

et_name = 'MyET'

# Load the Excel file
wb = openpyxl.load_workbook(et_name+'.xlsx')

# Generate the Rmd content
rmd_content = f"# {et_name}\n```{{rosmose}}\n! OSMOSE ET {et_name}\n```\n\n"



################################################## Process LAYERS tab #####################################
layers_sheet = wb['LAYERS']
layers_data = layers_sheet.values
layers_columns = next(layers_data)
rmd_content += f"**Layers of {et_name}**\n```{{rosmose}}\n: OSMOSE LAYERS {et_name}\n"
rmd_content += "\n"
rmd_content += "|" + "|".join(layers_columns) + "|\n"
rmd_content += "|:-----|:-----|:-----|:-----|:-----|\n"
for row in layers_data:
    rmd_content += "|" + "|".join(str(cell) for cell in row) + "|\n"
rmd_content += "```\n\n"
#print(rmd_content)
```

Figure A3.19. Example of function in Python language that parses the Excel data provided by the industrial partners in order to generate the .Rmd file of the ET model.

A.3.5 Process statement of the sample brewery process and layouts of selected outputs

Figure A3.20 shows the layout of the problem definition in ROSMOSE for a brewery sample process and illustrates the style of the output report that can be used simultaneously for calculation and documentation of the process parameters and the optimization solution:

Brewery Process Optimization

AUTHOR
EPFL IPESE

PUBLISHED

```
source("../rosmose-setup.R", local = knitr::knit_global())
```

Introduction

This report presents energy integration results for a brewery process including pinch analysis, valorization of waste products, utilization of different technologies such as heat pumps and refrigerators, and optimization of the overall process to minimize cost and maximize revenues.

Problem Definition

This project will use a model named **BreweryProcess**.

A brewery process is composed of a high temperature section, low temperature section, cleaning in place section, biodigestion section, and it can also be equipped with a (co)electrolysis and utilities section (market, coolingtower, heatpumps, supercritical CO2 cycles and a cogeneration unit).

Brewery Process

The calculated parameters are defined as follows:

Brewery Process ET Layers

OSMOSE LAYERS breweryprocess

Layer	Display name	shortname	Unit	Color
ELEC	Electricity	elec	kW	yellow
NATGAS	Gas	ng	kW	green
BEER	Beer	beer	m3/h	white
HUSK	Husk	husk	kg/h	black

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Figure A3.20. Layout of the problem statement in ROSMOSE.

Figure A3.21 exemplifies the layout of the Market Unit definition in ROSMOSE tool and the energy flows pertaining to this unit. Figure A3.22 shows the embedded hideable code for plotting Carnot integrated curves of a brewery process and the utility systems in ROSMOSE.

Market

Layers of the Market ET

OSMOSE LAYERS market

Layer	Display name	shortname	Unit	Color
NATGAS	Gas	ng	kW	green
ELEC	Electricity	elec	kW	yellow
WATER	Water	water	kg/h	blue
SALT	Salt	salt	kg/h	grey
SUGAR	Sugar	sugar	kg/h	grey
FRESHMILK	Fresh milk	f_milk	kg/h	white
THICKENER	Thickener	thick	kg/h	orange
CREAM	Cream	cream	kg/h	white
CHEESE	Cheese	cheese	kg/h	white
MESOST	Mesost	mesost	kg/h	white
CO2	CO2	co2	kg/h	red
EnvCO2Em	EnvCO2Em	envco2	kg/h	red
RIVELLA	Rivella	rivella	kg/h	white
BIOGAS	Biogas	biogas	kg/h	green
FERTZ	Fertilizer	fertlizr	kg/h	green

Units of the Market ET

OSMOSE UNIT market

unit name	type
ElecSell	Utility
ElecBuy	Utility
NatgasSell	Utility
EnvCO2tax	Utility

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Figure A3.21. Layout of the layers definition in ROSMOSE tool.

Thermal Exergy of Integrated Utilities

```
display_carnot <- function(time=1){
  graphs <- data$results$graph[[1]]
  graph <- graphs[[time]]
  graph <- graph[graph$plot_type == "carnot.utilities",]$data[[1]]
  base <- graph[graph$title == "base",]$curve[[1]]
  utilities <- graph[graph$title == "utilities",]$curve[[1]]

  if (!is_empty(base) && !is_empty(utilities)){
    plot_ly() %>%
            add_trace(x=base$Q, y=base$T, mode = 'lines', line=list(color='red'), name='base') %
            add_trace(x=utilities$Q, y=utilities$T, mode = 'lines', line=list(color='blue'),  na
            layout(xaxis= list(title = "Heat load [kW]"),
                   yaxis= list(title = "Carnot factor 1-To/T [-]"),
                   margin= list(l=50, r=20, b=40, t=40),
                   title = "Thermal Exergy of Integrated Utilities"
            )

  } else {
    print(paste("There is no Carnot for timestep", time))
  }
}

display_carnot(1)
```

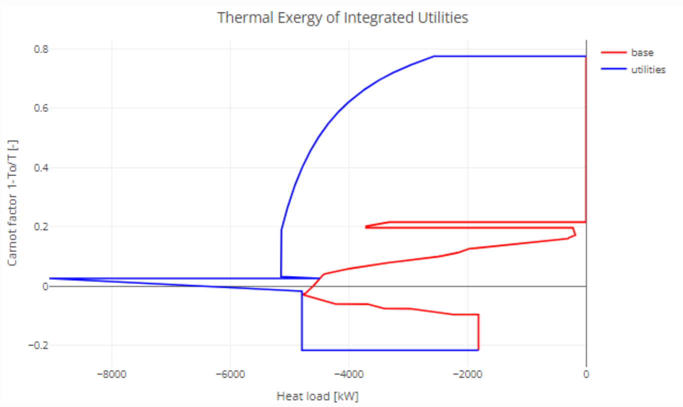
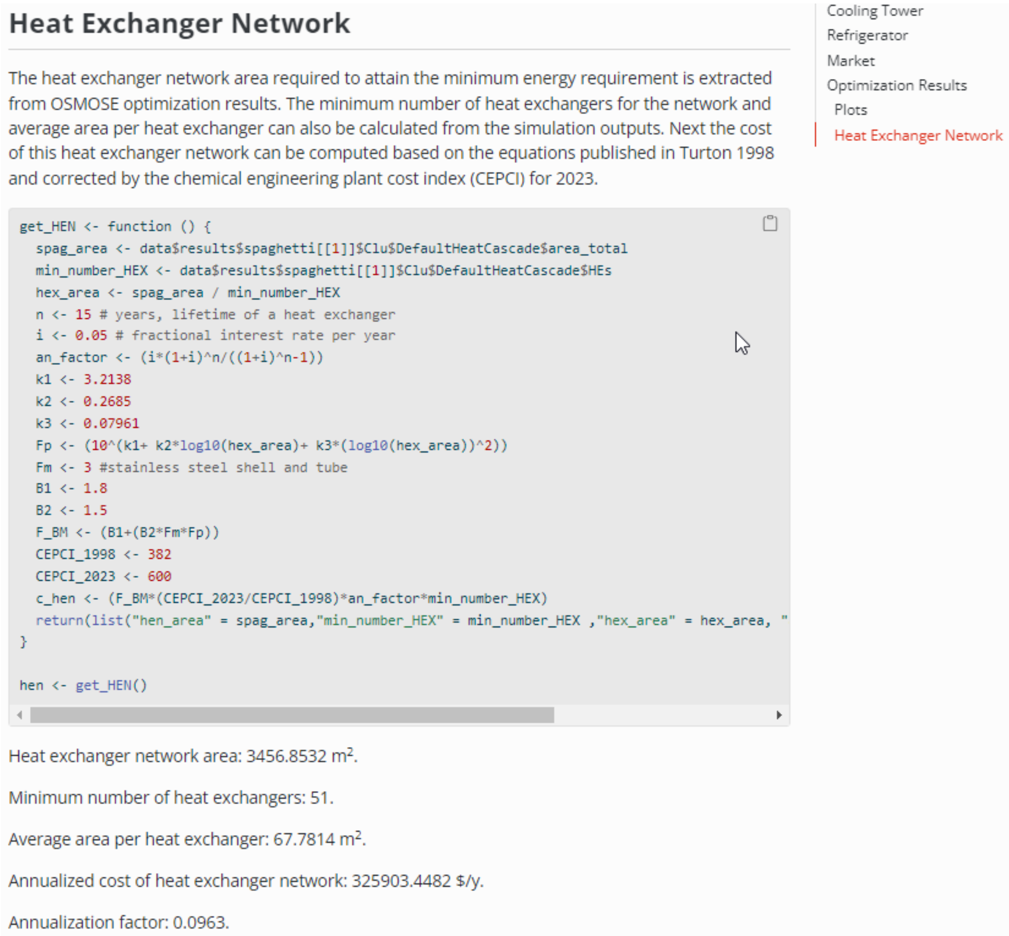


Figure A3.22. Embedded hideable code for plotting the Carnot integrated curves of the brewery process and the utility systems in ROSMOSE tool.

Other results, such as the heat exchanger network area, the minimum number of heat exchangers, the average area per exchanger, as well as the annualized cost of HEN (heat exchanger network) can be calculated based on tailor-made code chunks in R language that retrieve the JSON output file generated by ROSMOSE tool.



Heat Exchanger Network

The heat exchanger network area required to attain the minimum energy requirement is extracted from OSMOSE optimization results. The minimum number of heat exchangers for the network and average area per heat exchanger can also be calculated from the simulation outputs. Next the cost of this heat exchanger network can be computed based on the equations published in Turton 1998 and corrected by the chemical engineering plant cost index (CEPCI) for 2023.

```r
get_HEN <- function () {
  spag_area <- data$results$spaghetti[[1]]$Clu$DefaultHeatCascade$area_total
  min_number_HEX <- data$results$spaghetti[[1]]$Clu$DefaultHeatCascade$HEs
  hex_area <- spag_area / min_number_HEX
  n <- 15 # years, lifetime of a heat exchanger
  i <- 0.05 # fractional interest rate per year
  an_factor <- (i*(1+i)^n/((1+i)^n-1))
  k1 <- 3.2138
  k2 <- 0.2685
  k3 <- 0.07961
  Fp <- (10^(k1+ k2*log10(hex_area)+ k3*(log10(hex_area))^2))
  Fm <- 3 #stainless steel shell and tube
  B1 <- 1.8
  B2 <- 1.5
  F_BM <- (B1+(B2*Fm*Fp))
  CEPCI_1998 <- 382
  CEPCI_2023 <- 600
  c_hen <- (F_BM*(CEPCI_2023/CEPCI_1998)*an_factor*min_number_HEX)
  return(list("hen_area" = spag_area,"min_number_HEX" = min_number_HEX ,"hex_area" = hex_area, "
}

hen <- get_HEN()
```

Heat exchanger network area: 3456.8532 m^2.

Minimum number of heat exchangers: 51.

Average area per heat exchanger: 67.7814 m^2.

Annualized cost of heat exchanger network: 325903.4482 $/y.

Annualization factor: 0.0963.

Figure A3.23. Other calculations based on tailor-made code chunks in R language that retrieve the JSON output file generated by ROSMOSE tool.

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