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Heuristic methodology for the creation of blueprints in the chemical industry

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Abstract

The European Union (EU) has put the concept of circularity at the heart of its strategy for transitioning towards a low-carbon economy and reducing the use of virgin resources. Concrete measures, such as clarifying rules on co-products or supporting innovative projects, have been taken in order to promote Industrial Symbiosis (IS) - turning one industry's co-product into another industry's raw material. However, one of the main barriers to the democratisation of IS remains the exchange of (confidential) data between industrial partners. Here, the concept of industrial sector blueprints is presented as a solution in order to overcome the challenge of sharing information across industrial sectors. A blueprint is constituted of a series of profiles providing insights on the key inputs and outputs of a given industry in terms of thermal and electrical energy, materials and services. A heuristic and comprehensive methodology is presented detailing a step-by-step approach for building the profiles and the type of data required. It is applied to a typical refinery demonstrating the efficiency of the method and showing how it can be used in an IS context.

Keywords: circular economy, industrial symbiosis, data confidentiality, resource efficiency, pinch analysis, refining

1. Introduction

1.1. Background

In 2015, as part of its continuous effort to make Europe's economy more sustainable, the European Union (EU) has put in place an ambitious Circular Economy Action Plan [1]. This program establishes a set of measures contributing to "closing the loop" of product life-cycles through greater recycling and reuse of co-products. Among these measures is the promotion and stimulation of Industrial Symbiosis (IS). One of the most cited definition of

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IS is given by Chertow [2] who defines IS as the cooperation of separate entities (industries), geographically close to each other, for exchanging materials, energy, water and by-products. This definition was further extended [3, 4, 5] to include all the richness of IS such as the exchange of information, services, knowledge and technologies.

IS is not a new concept. For decades, companies and industries have worked together, joining forces in an effort to operate more effectively and reduce production costs. Chemical clusters provide good examples of such industrial eco-systems, where companies located next to each other and operating different processes are sharing their facilities, utility networks, (co-)products as well as their services such as maintenance and logistics [6]. More generally, one of the typical model for IS is the one where a host company, with by-products and utilities, invites third parties to operate onsite in order to benefit from the economies of scale and scope [4, 7]. IS can also be cross-sectoral or involve municipalities. Because of its long development history, the eco-industrial park located in Kalundborg, Denmark is often cited as the perfect example of such symbiosis, where several industries (refinery, pharmaceutical plant, gypsum board facility, etc.) and the city of Kalundborg are collaborating and are exchanging resources [4].

1.2. Problematic & challenges

Maqbool et al. [8] argue that having access to industrial site's technical and organisational knowledge is key for stimulating IS. However, given the confidential nature of industry, sharing data usually implies non-disclosure agreements and intellectual property rights granting protection to a company's background assets. These constraints are thus limiting the discovery of new potential exchanges between companies [9]. Interactive platforms such as the one developed by the National Industrial Symbiosis Programme (NISP) in the UK [10] or the eSymbiosis project [11] are aiming at facilitating inter-company data exchanges. They use advanced IT-enabled identification techniques, such as the use of ontologies, in order to facilitate the detection of new IS opportunities [12]. However, such tools mostly focus on waste exchanges, require having a secure system to store all information and for the industries to select what they are willing to share. De facto, the detection of new possible symbiosis, that have never been looked at before, becomes limited since it is the user who chooses what he is willing to exchange, disregarding automatically some flows that still might be of high interest for IS. In practice, the platform can only work with a critical number of registered users and a substantial database of resources.

This shows that there is a need for access to qualitative and quantitative data on industries materials, energy and water inputs and outputs [13] but that there is a lack of comprehensive and systematic methodology to generate such information. Golev et al. [14] state that the lack of such databases is clearly one of the main barriers to the development of resource synergies. Publicly available, reliable and comprehensive datasets gathering information on industrial sectors operations could not only provide a base-ground for IS platforms but could also be used for case studies and for testing scientific developments in the field of industrial ecology and beyond.

In order to cope with the incompleteness and inadequate information of industrial systems, Zhao et al. [15] used grey system theory [16]. Although promising, this method

is still standing in the field of emerging disciplines and its mathematical foundations still need further improvements [17]. One could also argue that many studies reporting process industries' specific energy consumption and emissions already exist. For the chemical industry, Best Available Techniques (BAT) reference documents, the so-called BREFs, provide details about applied techniques, emissions and consumption levels of various chemical processes, allowing to create benchmarks for the determination of BAT [18]. PlasticsEurope, the association of European plastics manufacturers, has developed Eco-Profiles that compile average industrial energy and emissions data. They exist for high volume, bulk polymers, some more widely used engineering plastics and some of the standard plastics conversion processes. The profiles provide strong and detailed environmental datasets for polymer production processes and they are acknowledged among life cycle practitioners [19]. Additionally, Bungener created a virtual thermal profile [20], comprising the thermal needs of a typical chemical cluster. The Stratego project [21] is also developing a database gathering information about the heating and cooling requirements of the industry all over Europe. However, in such datasets materials and energy flows are decoupled from one another and overall there are relatively few works discussing the optimisation of both materials and energy networks at the level of industrial parks. Furthermore, most of the time information is only available at a very high level which is not sufficient neither for detecting IS opportunities nor for optimising them, or at a too deep level which makes data exchanges across industrial sectors very difficult, because of confidentiality issues.

1.3. The blueprint concept

In order to facilitate knowledge exchange with the purpose of fostering IS, a compromise should be found between the resolution and the relevance of information as to create a set of data that is representative of a given process sector. To serve this purpose, and in the framework of the EPOS project [22], the concept of industrial sector blueprint is introduced [23]. The blueprints comprise typical processes and include information on the materials inputs and outputs of the processes as well as their thermal and electrical energy profiles. Some understanding of the main services used in a given industrial sector is also embedded. The blueprints are not intended to be exhaustive or to be an accurate description of process units' operations. They are meant to provide an insight on which resources are available and needed in a given process industry. They also help defining a common baseline of understanding between different industrial sectors, thus enhancing the communication and the exchange of knowledge and information between industries.

This article develops the framework for creating a blueprint. The complete methodology is then applied to a typical refinery.

2. Methodology

This section first presents in which context the blueprints will be used (section 2.1). Then a heuristic methodology is detailed, providing a conceptual framework for producing such blueprints. This approach is divided into four major interconnected steps: *data gathering*, *data processing*, *model configuration & sizing* and *profiles visualisation* (see figure 1). Section

2.2 discusses the level of detail required to produce the blueprints and describes the data sets that need to be gathered. In section 2.3, the handling of the collected data is explained. The way blueprints can be configured and sized is detailed in section 2.4. Finally, the different profiles integrated in the blueprints and their characteristics are presented in section 2.5.

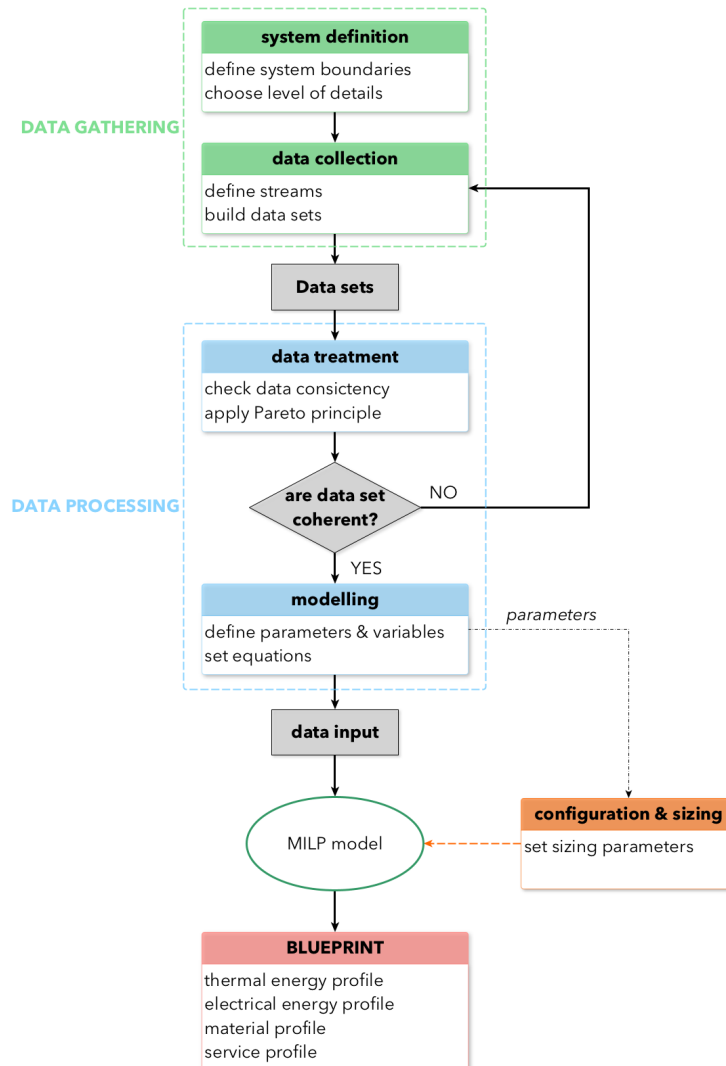


Figure 1: Blueprint creation steps

2.1. Blueprints life-cycle and utilisation

The blueprints' utilisation framework offers the possibility to non-expert users to study the multi-objective optimisation of resources and energy networks inside an IS system. The blueprints are meant to be representative of a given industrial sector, not because of their size but because they have identifiable units, use verifiable data and provide information on the flows of resources available in a typical plant. The chemical blueprints embed information

on the material, thermal and electrical requirements and productions of a given chemical process (energy and material profiles). A fourth profile, providing data on the main onsite services used is also built. Each profile has its specific visualisation as described by figure 2.

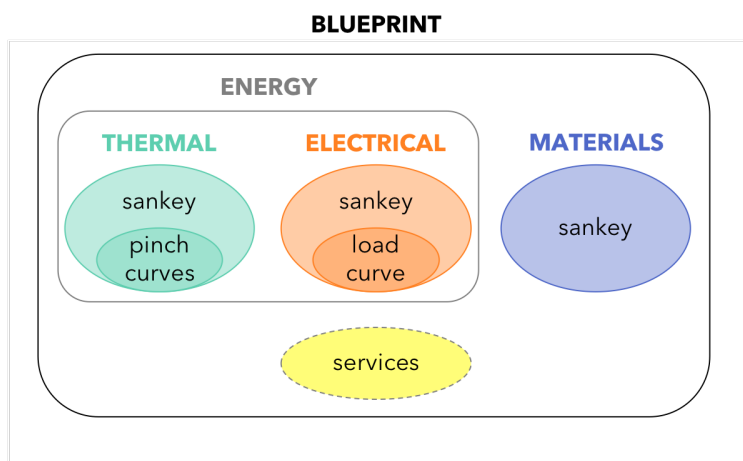


Figure 2: Schematic view of a blueprint

The blueprint concept was first mentioned by Van Eetvelde in 2014 when writing the proposal of the EPOS project and has been developed in the framework of that same project [22, 23, 24]. The blueprints will be available through the use of the EPOS toolbox, an interactive platform, accessible via the EPOS User Club [25]. Figure 3 depicts the blueprints life-cycle and usage. During the *construction phase*, blueprints are created by experts in major industrial sectors and integrated to the EPOS toolbox. During the *utilisation phase*, when screening for IS potential, the user defines a scenario:

- Choose blueprint: the user selects which blueprint will be considered in the scenario.
- Set sizing parameters: the user configures the blueprint(s) he selected according to his needs.
- Define optimisation: the user chooses the objective function (e.g. minimisation of operating costs, environmental impacts) and defines the Key Performance Indicators (KPIs) [26] that will be used to assess the different IS cases detected.

It should be noted that the detection and optimisation of IS opportunities are possible because the blueprints are generated through the use of models compatible with a Mixed-Integer Linear Programming (MILP) framework. MILP is a powerful method for system analysis and optimisation as it is flexible and can solve large and complex problems – typical for IS. The MILP optimisation framework is used to identify the best connections between the blueprints and to achieve the maximum resource efficiency while minimising the costs and the environmental impacts. In a consecutive run, the IS screening can be renewed by modifying the blueprint at two levels (see figure 3):

- Scenario definition: at this stage the user can only modify a restricted set of parameters (see table 1 in section 2.4).

- Blueprints construction: at this level core parameters of the blueprints can be modified. Only expert users are allowed to change them (see table 1 in section 2.4).

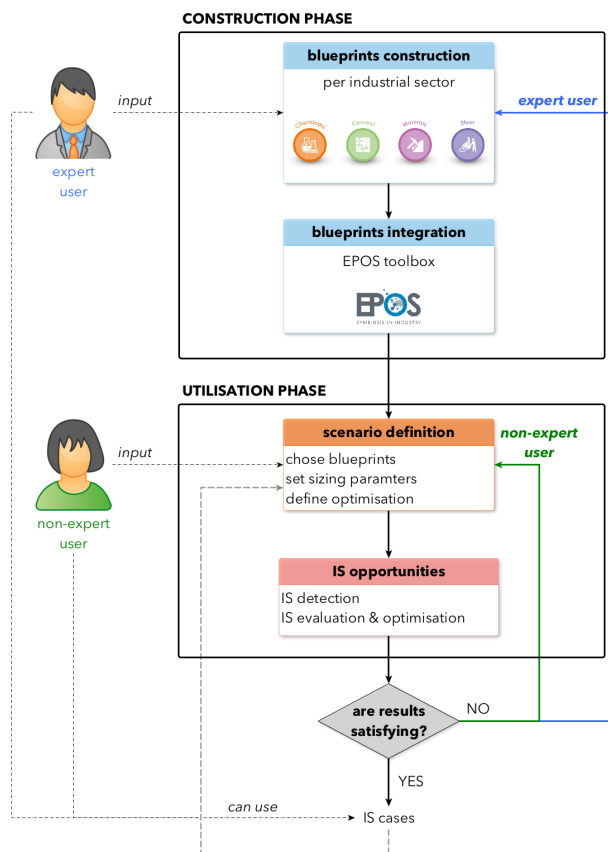


Figure 3: Blueprint life-cycle

2.2. Data gathering

Data gathering is the first and most crucial step during the blueprint creation process. It is typically time-consuming, especially when considering large chemical processes, such as refining or steam cracking. In order to reduce the time for data collection, it is necessary to know what type of data should be gathered and why. A trade-off is to be found between the quality of the information necessary for building the profiles and the complexity of compiling all the required data. This section explains how to choose the right level of detail for data collection and describes which type of data is required for characterising all the flows (thermal, electrical, material and service) enclosed in the blueprints.

2.2.1. Choosing the right level of detail - From black box to process unit

Starting from the approach developed by Hackl et al. [27] for the Total Site Analysis (TSA), who defines three levels of detail for describing process heat and cooling demands (black box, grey box and white box levels), three levels of representation are used to depict

the chemical plant layout: *black box*, *site map* and *process unit* (see figure 4). This generic outline of a chemical site provides the base-ground of each blueprint.

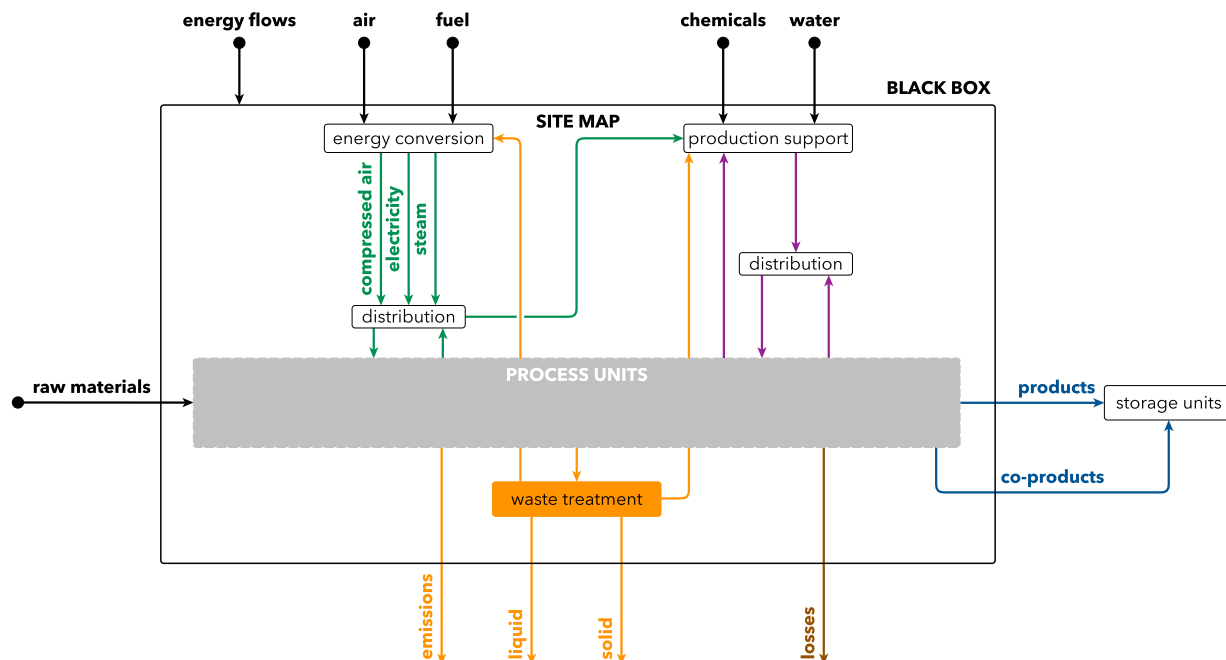


Figure 4: Chemical plant layout - adapted from [23]

Black box. The black box level is the lowest level of detail, it is pictured in figure 4 by the external black rectangle. The horizontal arrows represent the process main material streams whereas the vertical ones symbolise the energy and material flows required to support the production (top). The waste streams, emissions and losses are also included and are represented by vertical arrows exiting the system boundaries (bottom). This view gives an insight on the main input and output flows crossing the system, which also point to potential connections with other sites. However, this level of detail is not sufficient as it does not give any detail on the real needs of the process. Indeed, before looking at IS opportunities it is important to make sure that the process is internally optimised as not to share its inefficiencies, in order to do so a deeper level of detail is required to build the blueprint.

Site map. This level of detail goes a step further in the description of the chemical site. It decomposes the plant into four major sections: production, energy conversion, production support and waste treatment; all interconnected via distribution networks. This view provides additional information on the site operations such as how energy flows and production support chemicals are produced and supplied to the process. For example, if a process is consuming natural gas, at the black box level the stream will be seen as a resource consumption whereas, at site map level the external observer will be able to know if it is a material requirement or if it is burnt to produce steam (energy vector). Based

on this representation, several indications are derived such as the main energy consumers, the cold and hot utility distribution profiles and also the efficiency of the energy conversion units. Still, it does not provide any insight neither on the real process energy requirements (temperature levels, heat loads) nor on the different production steps. One step deeper is therefore required to produce the profiles.

Process units. This level of detail is the one required for creating the actual profiles. It provides information on the process itself and allows the visualisation of all the transformation steps. Even if there exists hundreds of different production pathways, most of them can be broken down into typical processes and operations units involving respectively chemical or physical transformations [28]. For example, in the chemical sector the units are usually classified into three main categories: pre-treatment, reaction and separation/purification. Each chemical production can be generally described using these operation units, as seen in figure 5. The raw materials enter the process, they are pre-treated before going to the reaction unit where co-products and/or products are formed. The reaction products are then sent to the separation and/or purification units that deliver the final products.

Thus the required level of detail for building the blueprints is defined as the *process units* level. The next step is to select the necessary data to build the different profiles constituting the blueprint.

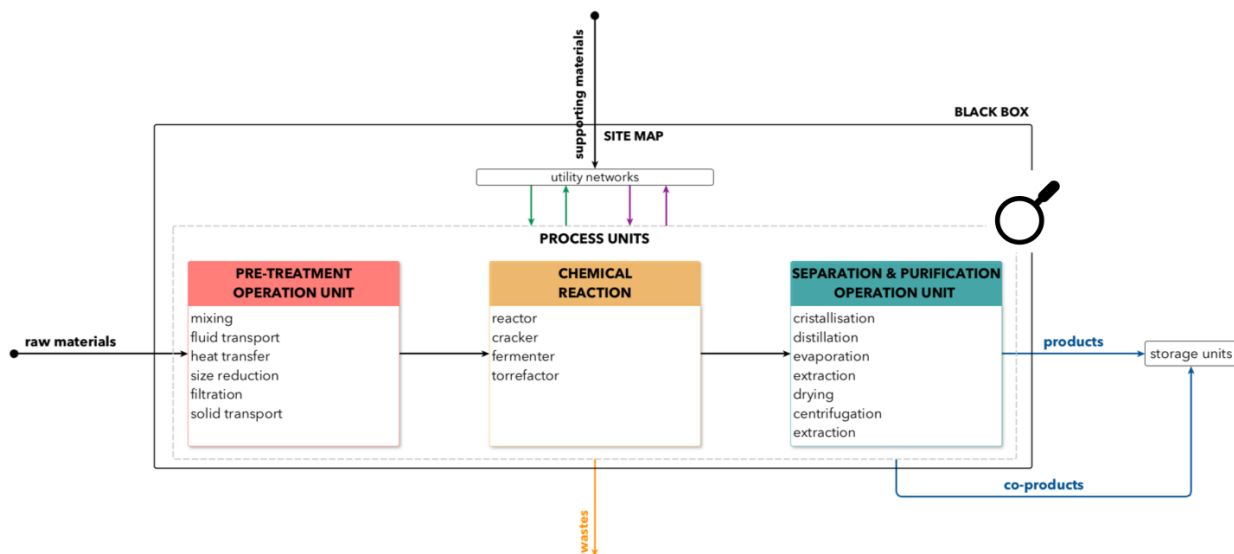


Figure 5: Typical process block flow diagram

2.2.2. Building the dataset

As a first step, it is important to have a clear and general understanding of the process. Documents such as Process Flow Diagrams (PFDs), Piping and Instrumentation Diagrams (P&IDs), information on the pieces of equipment (efficiency for example) and on the process

operation units are primordial to get an overview of the process structure and interconnections between the flows.

The blueprints' profiles are constituted by streams that are classified according to their characteristics into four categories: *thermal*, *electrical*, *material* and *service*. The following paragraphs describe how to create the basic datasets for each stream category.

Thermal stream. The thermal streams represent the heat and cooling requirements of the process. They are divided into two groups: *cold streams* that need to be heated up and *hot streams* that need to be cooled down. The methodology for thermal streams definition for TSA developed by Mechaussie et al. [29] is applied for the creation of the blueprint thermal streams. This method is directly derived from the Pinch methodology [30] in which the streams are characterised by their temperature-enthalpy profile ($T_p \in [T_{p,in}, T_{p,out}]$), heat load (\dot{Q}) and contribution to the minimum temperature difference with respect to the heat exchange ($\Delta T_{min}/2$). As it is usually easier to calculate the heat load from the utility side (when information is available), Mechaussie et al. described the basic data set for defining thermal streams as a combination of process temperatures ($T_{p,in}, T_{p,out}$) and information on utility flows (\dot{m}_u) and thermodynamic properties ($T_{u,in}, T_{u,out}, P_{u,in}, P_{u,out}$). However, when such data are not available, the data set has to be completed with information on the process side such as composition and pressure (P_p). More details about the thermal streams graphical representation and the methodology can be found in [29].

Electrical stream. Electrical streams represent the electrical energy requirements and generation of the process. In order to create the basic data set for building the blueprint electricity profile a load inventory has to be carried out. For each electrical equipment, information is gathered about its average power demand (\mathcal{P}_{avg}). Each device is then assigned a category based on its function (pump, compressors, aero-coolers, steam turbines etc.) and location in the plant (electricity generation, core process or utilities) as detailed by Baetens et al. [31]. This step allows grouping all "similar" loads together, which is then useful for understand how electricity is used within the process. If information is available, complementary data allowing to calculate each equipment capacity factor ($CF = \mathcal{P}_{avg}/\mathcal{P}_{rtd}$) can be collected. This capacity factor gives insight on the equipment utilisation rate and its potential for load shifting or flexibility.

Material stream. The material streams differ greatly from the thermal and electrical streams as they can be used in various ways within the different process operation units. When considering chemical conversion, the possibilities for material streams conversion become even unlimited. In order to distinguish the material flows used to meet the process needs and the ones directly used during the transformation from inputs to outputs, material streams are classified into two categories: *materials integrated in a network* and *materials feeds and products*. In both categories the streams are characterised by their flow (\dot{m}_p), composition, pressure (P_p) and temperature (T_p).

- Material streams flowing in a network can be defined at each point in that network so that the utility system provides these specifications. This is for example the case

for water and hydrogen networks [32, 33] or even fuel gas. In this situation, material streams are treated the same way as heat streams and a methodology analogue to the one used for pinch analysis is applied [34].

- Material feeds and products are used in fewer points throughout the system and undergo several transformations. They also form the basis of the process size in the material profile and are used to scale the utility and production support systems. Usually complementary data such as PFDs, P&IDs and information on process operations are also necessary in order to fully characterised this type of streams.

Service stream. Ancillary services can be defined as services that are necessary to support the production process. This type of flows has a more abstract description than the previous ones as it does not represent physical streams. For example, maintenance is considered as a service stream albeit it obviously does not "flow" through the system. Nevertheless, service streams can be quantified and are characterised by their associated cost. Each service is also assigned to one of the following categories (classification adapted from the one provided by the French Chamber of Commerce [35], which is derived from the European NACE classification [36]):

- Maintenance & Repair: takes into account the repair of goods produced in the manufacturing sector (metal products, machinery, equipment and other products). Maintenance on such products to ensure they work efficiently and to prevent breakdown and unnecessary repairs is also included.
- Transport & Handling: accounts for lifting activities (lift trucks, crane, etc.), working at heights, logistics activities and the transport of goods via trucks, boats and planes.
- Externalised Services: includes all kind of services that can be externalised by companies such as quality control and technical analysis, engineering contracts, periodic inspection of equipment, legal services and cleaning.

2.3. Data processing

The goal of this step is to ensure that the data gathered are valid and typical of a unit operation. Data collected during the previous steps can come from various sources (on-line measurements, documents, assumptions, calculations, etc.). It is therefore imperative to make sure that the data sets created are consistent. In order to do so, several data cleaning techniques can be applied, ranging from simple data auditing when specific constrains are applied, to the use of more advanced statistical methods [37]. If the system redundancy is high enough, data reconciliation can also be used to improve the quality of measures and validate assumptions [20]. More specific checks can also be carried out depending on the stream type and use. For example, Mechaussie et al. [29] developed a specific and systematic methodology using the graphical representation of hot and cold streams for verifying data coherence when carrying a TSA.

Another way to ensure data consistency is the use of flowsheeting software such as Vali [38] or Aspen Plus[®] and Aspen HYSYS[®] that belong to the aspentech[®] suite [39]. They allow to account for the system thermodynamic properties and closing mass and energy balances. They also provide access to wide thermodynamic databases and equations allowing

the good representation of complex chemical compounds and their behaviour. Those tools are specifically customised for the chemical industry and are powerful for performing thermo-economic modelling and analysis of chemical processes.

In case data are missing, an easy way to ensure data reliability is to carry key mass and energy balances. This type of checks can be specifically applied when checking data for the thermal and electrical energy profiles [40].

Finally, data treatment is a key step to ensure data confidentiality. The anonymisation of data is coming from the following aspects:

- Origin of data: the blueprints are created using a mix between public and real site data, which confers them a certain degree of anonymity.
- Pareto approach: only the major mass and energy flows are included, even at the deepest level of detail and sensitive process specificities such as equipment design and operation, catalyst characteristics or process integrations are purposely left out of the profiles' construction process and visualisation. For generalisation purposes, the Pareto principle, a heuristic methodology stating that in general 20% of the causes can explain 80% of the effects [41], is used. Applied to the material and energy flows, it means that data gathering will stop after having identified and characterised at least 80% of the main flows. It should be noted here that applying this principle also allows to save a lot of time during the data collection step.
- Aggregation: part of the data is aggregated such as for the electrical energy profile where electrical pieces of equipment are grouped according to their category, thus not disclosing any confidential detail.
- Anonymisation factor: the datasets are also scaled by a constant factor which allows to confer them a certain degree of anonymity while maintaining their realistic nature.

2.4. Configuration & sizing

The blueprints should be flexible and sizeable so as to provide a good overview of what energy and material flows are available in the right order of magnitude. Two types of users will have access to the blueprint. Expert users will be able to modify the blueprints during its *construction phase* (see figure 3) and thus will be able to change core parameters of the blueprints. Non-expert users will use the blueprints through the EPOS toolbox interface and will only have access to a few selected parameters.

Three configurations levels are defined for the model sizing parameters: *macro*, *meso* and *micro*. Each level will have a different impact on the blueprint model outputs and will require a different level of expertise in order to be modified (see table 1). The highest level of detail is the *macro level*, grouping parameters that must be modified in order to globally size the system such as production rates or site capacities. The values are usually publicly available so that non-expert users can be able to change them, they are thus modifiable during the blueprint's *utilisation phase*. The second level is the *meso level*. It represents the parameters that should be changed if the user wishes to have a more accurate representation of the system. Their influence on the models is still relatively limited but the user should have a good knowledge of the process in order to wisely modify them. They can be for instance

specific energy or material consumptions. The deepest level of detail is the *micro level*. It regroups parameters that have the greatest impact on the model outputs if modified. They are often linked with the system thermodynamic properties. The *meso* and *micro* levels are only modifiable during the blueprint’s *construction phase*.

Table 1: Blueprint configuration levels

Configuration level	Description	User type	Blueprint life-cycle	Examples
<i>Macro level</i>	Sizing parameters that the user will have to define in order to size the entire model according to his needs. Values for these parameters should be easily and/or publicly available.	All	Utilisation phase	- Production rate - Site capacity
<i>Meso level</i>	Parameters that should be adjusted to represent one process more accurately. Their impact on the model is limited compared to the macro level parameters but they should be manipulated with care.	Expert user having a good knowledge of the process.	Construction phase	- Specific energy consumptions - Specific materials consumption - Product yields
<i>Micro level</i>	Parameters that could be adjusted by the user only if required. Those parameters are usually directly linked to the core process or the flows thermodynamic properties. They should be manipulated with great care.	Expert user having a deep insight on the process requirements and thermodynamics.	Construction phase	- Temperature levels - Heat capacities - Compositions - Pressures

2.5. Profile visualisation

The blueprints contain information on the energy, material and service requirements of a given process. Four profiles are created and can be visualised (see figure 2). For the energy and material profiles, the highest level of detail is displayed with the help of Sankey diagrams [42]. In this type of representation, the width of the arrows is proportional to the flow quantity, putting visual emphasis on major flows crossing the system and highlighting the main contributors. The service profile is simply illustrated using a pie chart. For the energy profiles an additional display is available giving access to a deeper level of detail with respect to the process energy consumption. Both additional representations are described in the following paragraphs.

Thermal energy profile - pinch curves. In addition to the Sankey diagram, the blueprint heat profile is also represented by composite curves which are at the heart of Pinch Analysis [30]. In this methodology the process heat and cooling requirements are represented by their temperature-enthalpy profile (hot and cold composite curves). Thanks to this graphical approach, key information can be extracted such as the process Minimum Energy Requirement (MER), the list of penalising heat exchanges or the maximum heat recovery potential. However, the Pinch Analysis method suffers some limitations when applied to large-scale systems as direct integration of process units implies making them interdependent, which in most cases is not possible due to safety reasons, especially in the petrochemical industry. TSA is a methodology that was developed to tackle those limitations [43]. In this method, the utility system is also integrated in the analysis and heat can be exchanged between processes through intermediate utility flows. This dual representation of the system shows integration solutions by interacting with the utility system, which offers more flexibility than directly

integrating multiple process units together and is very interesting when considering IS opportunities. For the blueprint thermal energy profile, the TSA representation is preferred since only process-utility interactions are taken into account, thus limiting the disclosure of confidential information.

Electrical energy profile - load duration curve. The load duration curve (example in figure 7c) is an additional representation of a process electricity profile. It illustrates the evolution of the load with time considering that the ordinates representing the load are plotted in a descending order of magnitude (highest load on the left). The area under the curve represents the total electricity (energy) demand of the system. As the loads are ordered, it is easier to identify peak and minimum loads as well as the total load distribution. It also depicts the relationship between the generated capacity requirements and the capacity utilisation giving a first overview on capacity factor, peak shaving potential and impact of local electricity generation.

3. Results - refinery blueprint

This section applies the methodology previously presented to a typical refinery and illustrates what type of information is made available through the use of a blueprint. First a general overview of the refining process and of the process units constituting the blueprint is given (section 3.1). The data gathering and treatment step is then concisely described, giving a general idea of the origin and validation of the data (section 3.2). Finally, the energy, material and service profiles are presented (section 3.3).

3.1. Typical refinery

The purpose of refineries is to convert crude oil into more valuable products such as transport fuels, combustion fuels, raw materials for the petrochemical and chemical industries, speciality products (oils, waxes, etc.) and even energy as a co-product (steam & electricity) [44]. Several process units are required to transform crude oil in such various products, they can be interconnected in many ways and their configuration depends on several parameters such as market demand, available crude quality or location.

The configuration chosen for the refinery is given in figure 8. It consists of 10 interconnected process units briefly described in Appendix A. The typical refinery configuration is chosen based on existing industrial sites. Its Nelson complexity index [45] is 5.7 which falls into the typical range for European refineries [44] and represents a medium complexity.

3.2. Data gathering and processing

The data used to build the refinery blueprint originate both from the industry and from literature [44, 46, 47, 48]. This allows building a dataset based on reality while ensuring anonymity. First a bottom-up approach is followed meaning that industrial data are used to build thermodynamic models of the different process units. The models help closing the mass and energy balances while ensuring that the system's thermodynamic constraints are respected, they create a second dataset used as input for building the MILP blueprint

models. Since the refining process involves multiple complex process units, the Pareto principle (see section 2.3) has been applied during this first steps, allowing the reduction of the amount of information to be collected. In a second step, a top-down approach is adopted to validate the data. The blueprint outputs are compared with literature in order to check for inconsistencies. For sensitive information such as CO₂ emissions or waste production, the data used are exclusively originating from literature and public databases.

The crude oil processing rate (35'000 t/d) is defined as the *macro* parameter. All the process units are sized with respect to this parameter as its value is often publicly available for any refinery. The *meso* parameters are typically the specific energy and material consumptions/productions while the *micro* parameters are intrinsically linked to the systems thermodynamics, they mainly are the composition, pressure, temperature of each streams (see table 1). The values of the *meso* and *micro* parameters are treated as constant and are set in order to obtain a representative overview of a refinery typical operation. They could of course be modified if one would illustrate another operating mode or describe another site.

For the pinch analysis, ΔT_{min} values are applied to each individual stream according to its physical state. The choice of ΔT_{min} is crucial as it allows the heat transfer difficulty between different streams to be accounted for. This parameter represents the energy savings/capital trade-off and as such should be chosen wisely as it could significantly influence the results in terms of internal heat recovery and utility integration. Dedicated methods such as the one developed by Mechaussie [40] can be applied to determine the ΔT_{min} more accurately. However, since the blueprint purpose is only to give a general overview of a given process it was decided to use typical values for ΔT_{min} (table 2).

Table 2: Typical values for the ΔT_{min}

Stream type	ΔT_{min} (°C)
Gas stream	16
Liquid stream	8
Phase change stream	3

3.3. Profile visualisation

In this part, the four refinery blueprint profiles (thermal and electrical energy, material and service) are detailed.

Thermal energy profile. Figure 6 displays both levels of the refinery blueprint heat profile. The heat Sankey diagram (figure 6a) shows the main energy flows going through the system, clearly indicating that fuel is the main energy vector used within the refinery for heating purposes. The generic term "fuel" can designate many different types of internal or external combustible, ranging from the crude feedstock itself (usually around 3 – 9% of the crude is burnt [44]) to natural gas used to power steam boilers or Combined Heat and Power (CHP) plants.

Here, the fact that the Crude Distillation Unit (CDU) is the refinery’s most energy intensive unit is illustrated as well. The CDU accounts for 40% of the total process energy consumption because high volumes of crude oil need to be heated up to high temperatures ($\sim 350^{\circ}\text{C}$). It is followed by the Vacuum Distillation Unit (VDU), hydro-treatment units (Naphtha Hydrotreater (HDT) and Hydrodesulphurisation Unit (HDS)) and the Catalytic Reforming Unit (CRU). Four pressure levels are available through the steam network (High Pressure (HP), Medium Pressure (MP), Low Pressure (LP) and Very Low Pressure (VLP)). HP steam is produced by boilers while other steam pressure levels are created because of process units’ production or through the use of co-generation turbines and let-downs. The process cooling is done through aero cooling, water cooling or steam production. This first overview already provides useful information on the refinery high-level of integration.

The TSA curves go a step further and constitute the second level of the blueprint heat profile. This level presents the process and utilities temperature-enthalpy profiles (see figure 6b), exhibiting at which temperature level heat and cold is required and provided to the process. The different steam pressure levels are represented by the blue and red plateaus on the utility Composite Curves (CCs). Steam is almost only consumed at the MP, LP and VLP levels. HP steam is only used for co-generation purposes (green rectangle). The MER_h is 286 MW and the MER_c is 290 MW; compared to the utility system currently providing 446 MW of heating and 450 MW of cooling this means that a maximum of 160 MW could be saved. This number is of course theoretical as it does not take into account all the system constraints, but it gives an order of magnitude of the maximum indirect heat recovery potential that could be achieved in a typical refinery. Other techniques can thus be applied on the typical heat profile to estimate the effects of heat losses when exchanging heat over long distances [49, 50], to account for restricted heat exchanges [51] or to calculate the required investments for achieving such a degree of heat recovery.

Electrical energy profile. Figure 7 shows the two levels of the refinery electricity profile. The Sankey diagram (figure 7a) exhibits the main power flows going through the refinery. It highlights that the HDS unit is the one consuming the most electricity with a specific electricity consumption of 20 kWh/t (~ 13 MW). It is followed by CDU and the Hydrocracking Unit (HCK) consuming overall 14 MW. Most of the electricity consumption of the refinery is related to the core process and is due to pumping (50%) and compressing (43%), the other 7% relate to mixing and air cooling (figure 7b).

The second profile (figure 7c) represents the refinery load duration curve. It highlights that the internal electricity production can represent up to 30% of the peak power demand. It is produced via steam turbines that are already integrated into the heat profile (see figure 6b). The total consumption does not show any large variation over time, the refinery electricity demand is 87% of the peak load 80% of the time which confirms that there are few flexibility options when considering the typical refinery consumption. In addition, the capacity factor related to on site electricity production is 79% (table 3) indicating that there is a potential for providing flexibility on the electricity market using the steam turbines.

Table 3: Refinery electrical energy profile - capacity factors

	Capacity factor
Production	79%
Import	83%
Total consumption	90%

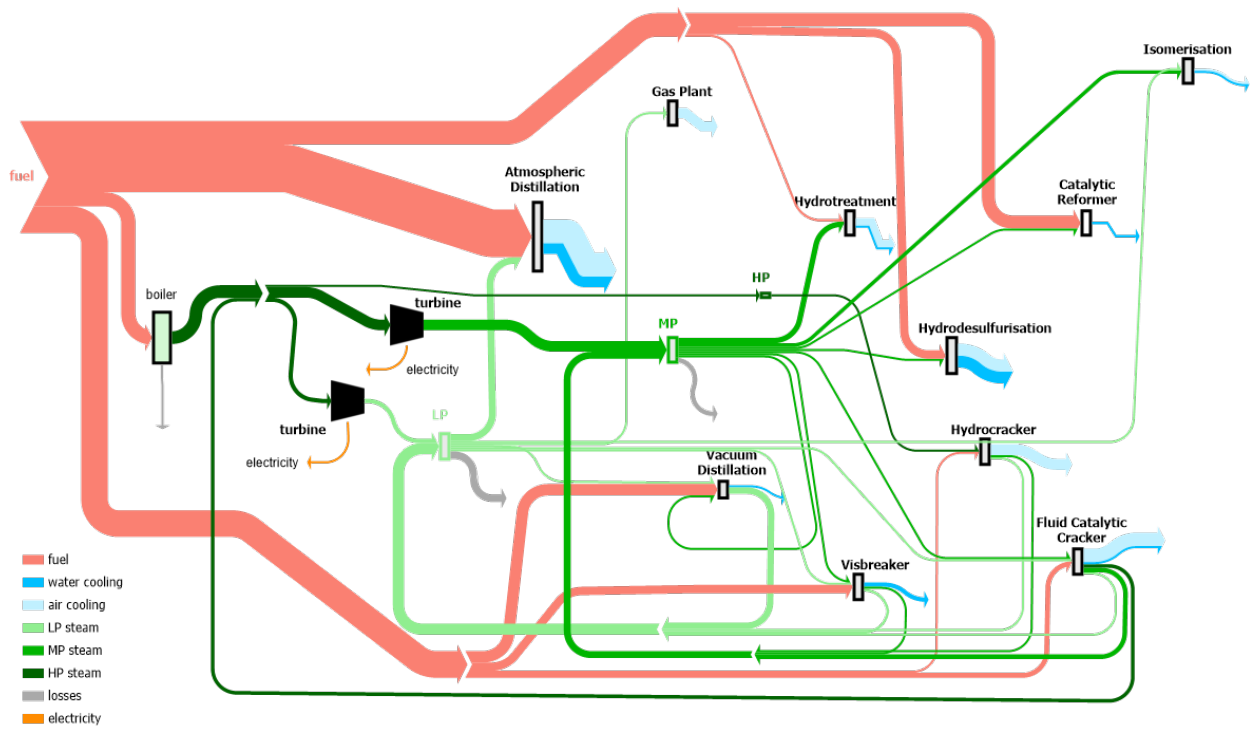
Material profile. Figure 8 shows the main material flows going through the typical refinery. The width of the arrows represents the flows magnitude. The material profile gives access to key information about the refining process, such as the production yields, how the different process units are interconnected or what are the largest flows crossing the system. In addition, estimations about the type and amount of waste generated are also given (table 4) showing that the amount of waste produced is much smaller compared to the main material flows (crude oil). This typically reflects the fact that refineries can have an overall plant efficiency as high as 93% meaning that 7% of the input mass flow of crude oil is either used as fuel for energy production or leaving as a waste [48].

Table 4: Refinery material profile - wastes specific productions [44]

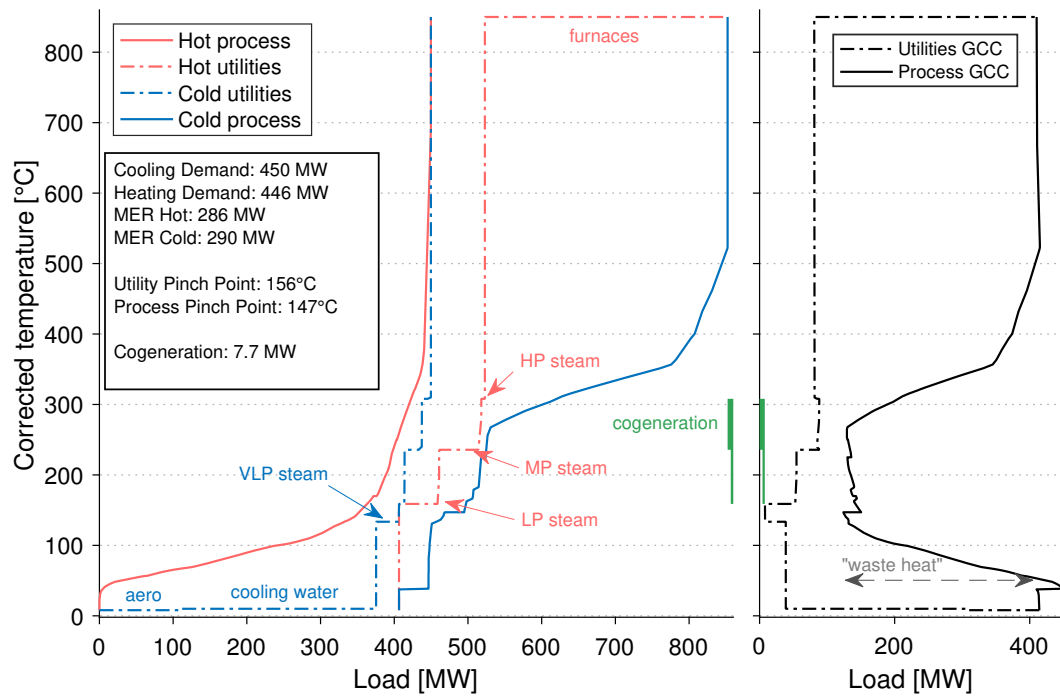
	Waste type	Specific production
Solid wastes	sludges	0.27 – 0.84 kg/t _{crude oil}
	spent catalysts	0.03 – 0.12 kg/t _{crude oil}
Water emissions	COD	9 – 85 g/t _{crude oil}
	BOD	0.5 – 25 g/t _{crude oil}
	suspended solids	1 – 30 g/t _{crude oil}
	total hydrocarbons	0.1 – 3 g/t _{crude oil}
	total nitrogen	1 – 20 g/t _{crude oil}
	heavy metals	0.02 – 2 g/t _{crude oil}
	BTEX	0.001 – 2 g/t _{crude oil}
Air emissions	CO ₂	0.11 – 0.39 t/t _{crude oil}
	NO _x	100 – 450 g/t _{crude oil}
	particulates	4 – 75 g/t _{crude oil}
	SO _x	52 – 1'565 g/t _{crude oil}
	VOC	65 – 1'095 g/t _{crude oil}

Service profile. Figure 9 displays the cost repartition between the main types of services used within the typical refinery. The costs are almost evenly shared among the three items of expenditures. Maintenance & repair accounts for 38% of total expense. This is not unusual for this type of industrial site since it is of crucial importance to make sure that every single piece of equipment is functioning properly as the process unit reliability depends on it. Externalised services are the second almost equally important item of expenditures

(35%). This is mainly due to the fact that a refinery can include thousands of pipes, electric cables and measurement devices that are regularly checked and calibrated by specialised companies (engineering contracts and instrumentation). Finally, the share of transport and handling services accounts for 27% of the costs. It is explained by the high importance of insulation and scaffolding. Indeed, insulation serves an important role in the operation of any chemical facility as it helps to control the process, avoid energy losses and protect people from being seriously injured (burns, etc.). The scaffolding costs are directly linked to the maintenance costs as production units require scaffolding to be erected for preventive and reactive maintenance.



(a)



(b)

Figure 6: Refinery blueprint - thermal energy profile with main thermal flows (a) and TSA curves (b)

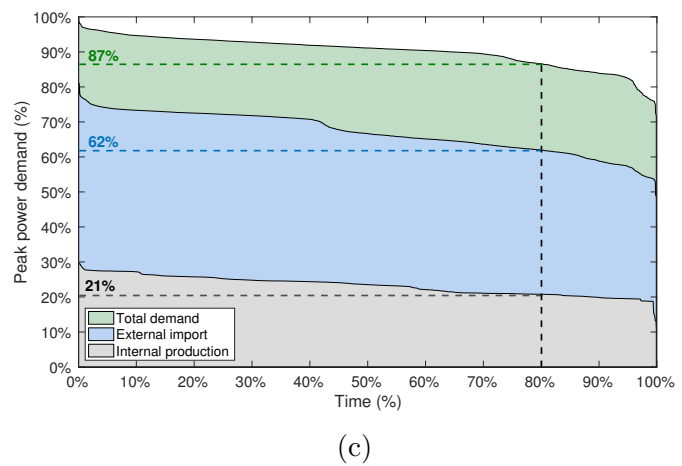
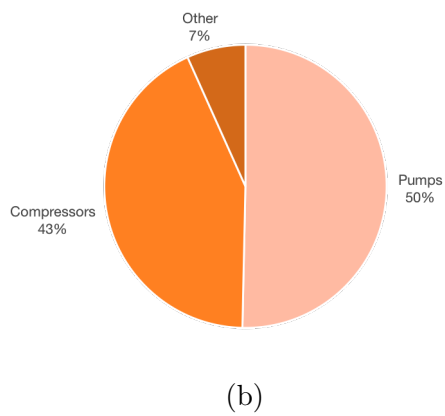
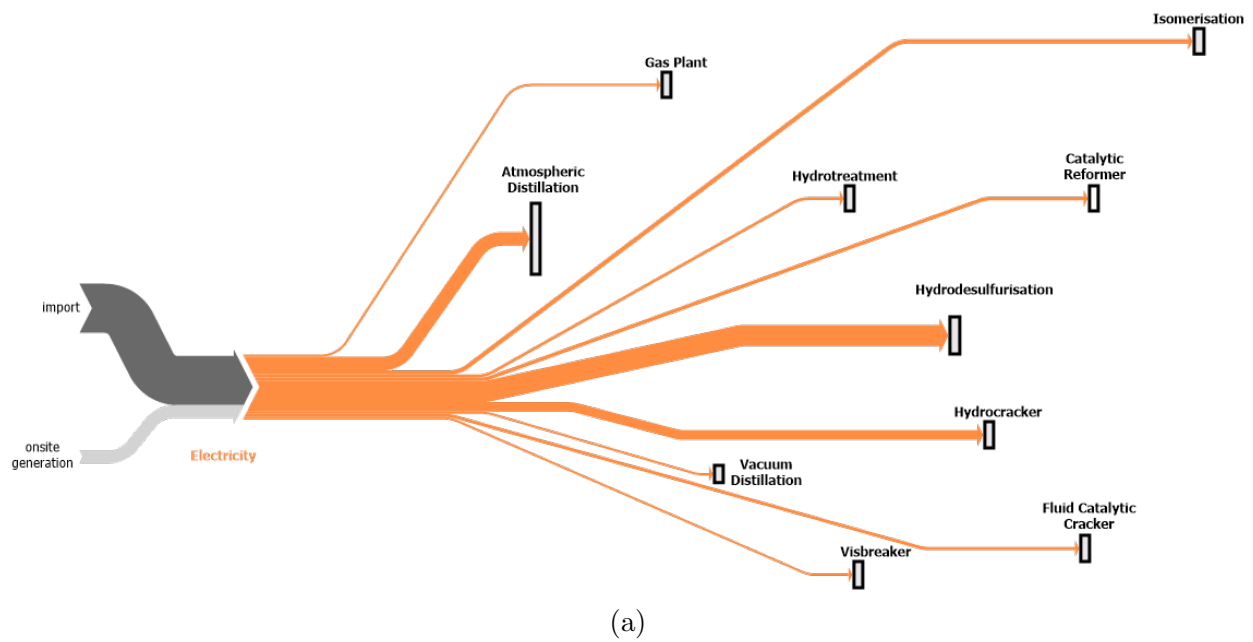


Figure 7: Refinery blueprint - electrical energy profile with main power flows (a), electrical consumptions breakdown (b) and load duration curve (c)

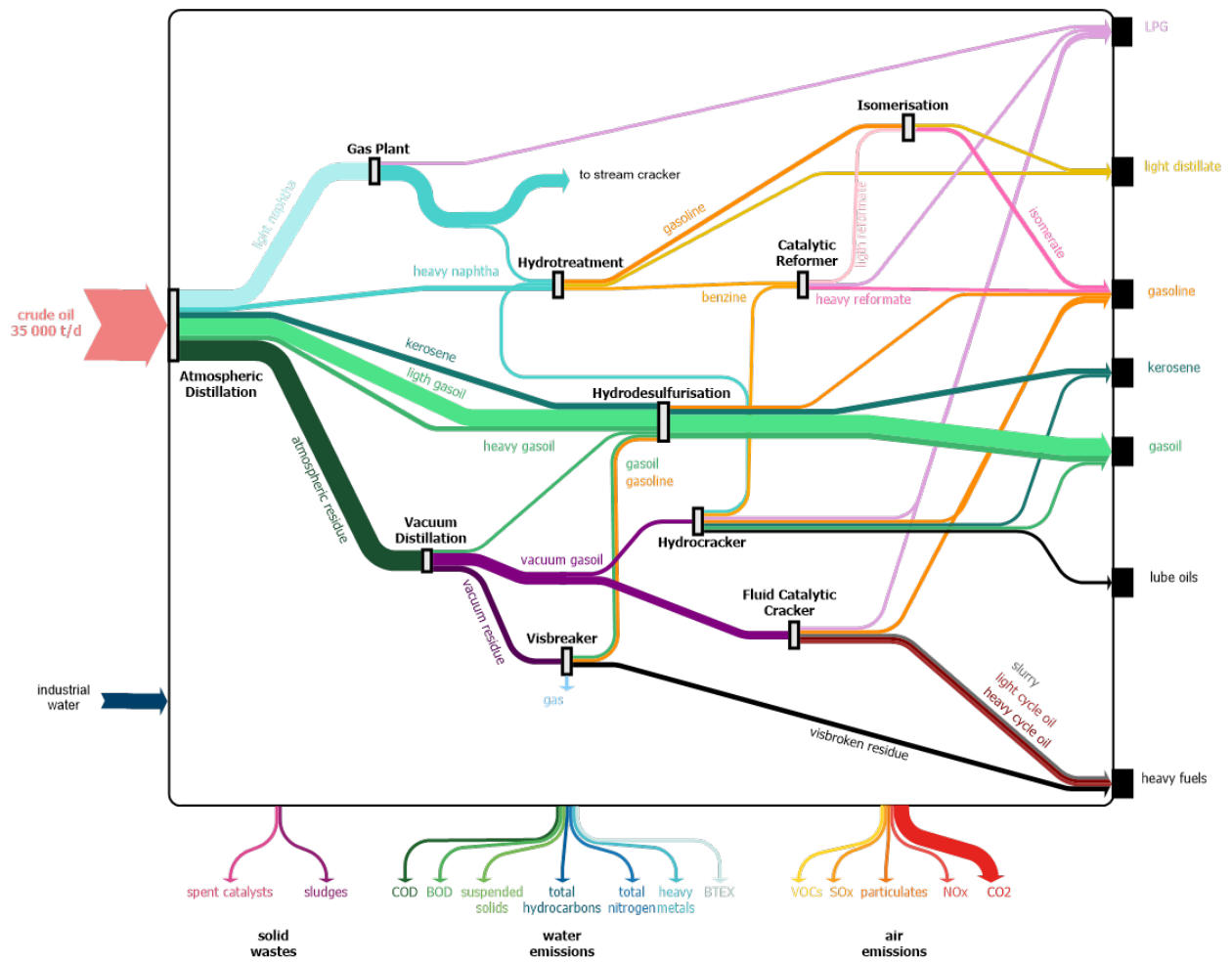


Figure 8: Refinery blueprint - material profile with main material flows and wastes

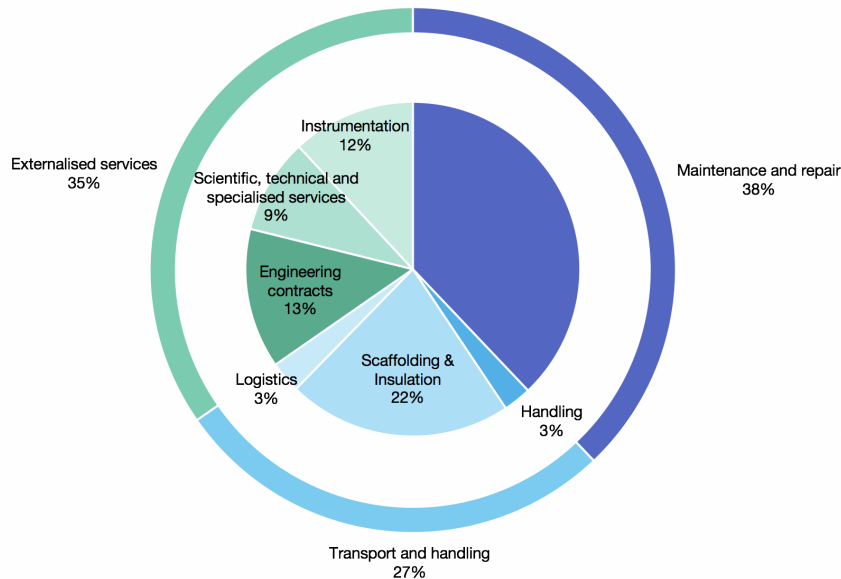


Figure 9: Refinery blueprint - service profile

4. Discussion

4.1. What a blueprint is... and what it is not...

A *blueprint is...* built to give a comprehensive representation of an industrial sector in terms of its main energy, material and service flows typically available, without disclosing any confidential information. It can be used by non-experts. It can as well be modified in order to better represent another plant configuration.

For example and since the refinery blueprint is available, it is drawn for another refinery configuration, with a lower input capacity rate (25'000 t/d) and with no Visbreaking Unit (VISB) (see [Appendix B](#)). With this new set-up, the refinery's global cooling and heating demands are reduced (\sim 299 MW). However, the thermal profile (figure [B.1](#)) shows an increase in HP steam production. This phenomenon is explained by the fact that there is no VISB unit any more. In configuration n°1, this unit produces MP and LP steam that is re-injected in the steam network and used by other units. In configuration n°2, this lack of steam production is compensated by an increase in HP steam generation and thus co-generation. Since the co-generation increases in configuration n°2, the load duration curve is modified (see figure [B.2c](#)). 80% of the time, the internal production represents 30% of the peak power demand, whereas it is only 21% in the first configuration (figure [7c](#)). Additionally, figure [B.2b](#) shows that the pumps share in the overall electricity consumption has increased. It is justified by the removal of the VISB unit that is mainly using electricity to run compressors and not pumps. Finally, the material profile (figure [B.3](#)) illustrates how the flow of vacuum residues is now diverted to other downstream units in the refinery (e.g. the Fluid Catalytic Cracking (FCC)).

The blueprint concept is foreseen as a tool enabling the detection and the optimisation of IS opportunities. In the case of the refinery, the thermal energy profile indicates that there is no internal heat recovery potential between the pinch temperature (147°C) and 53°C (process GCC in figure 6b). A significant amount of waste heat (288 MW) would then be available for IS exchange and could be used as a low temperature energy source in other industrial processes (food industry) or for heating urban areas (district heating network).

The electrical energy profile indicates that part of the electricity consumed is imported from the grid showing that there is a possibility for joint investments in renewable energy sources (e.g. solar panels, wind turbines). In that case, the MILP framework would be very powerful. Indeed, this scenario could be easily simulated and optimised with respect to the system constrains. Depending on the objective function selected, a third party, wishing to sell its renewable electricity to the refinery, could see if the link between its electricity production plant and the refinery is activated and how much electricity it could sell. The capacity factors (table 3) also indicates that some equipment producing electricity on site are not operating at full capacity, implying that they could produce more and thus offer some flexibility to the electrical grid.

The material profile also provides useful insights. For example, spent catalysts are one of the main sources of solid waste. The amount generated ranges within 0.08 – 0.18 $\text{kg}_{\text{spent catalyst}}/\text{t}_{\text{crude oil}}$ representing an average production of 4.5 $\text{t}_{\text{spent catalyst}}/\text{d}$ [44]. They are mainly produced by the hydro-processing units that use catalysts to remove impurities and convert the oil into more useful products. Recent studies have shown that FCC catalysts could possibly substitute up to 15% of the cement content in mortar without sacrificing the quality of concrete [52]. Finally, the service profile proves to be valuable for the identification of mutualisation synergies such as shared services as it highlights in which areas external support is required.

All the above-mentioned examples show that blueprints can trigger new IS exchange possibilities, but also foster internal optimisation of resources and energy efficiency, without the need to gather a significant amount of data. In the refinery thermal energy profile, the TSA curves display the process-utility interactions and can be used to improve the site internal heat integration through indirect heat exchange. Another example is the electrical energy profile indicating that the majority of the electricity consumed is due to pumping. On large industrial site such as a refinery, pumps are key to the process as they are used to carry fluids within the plant, especially cooling water. They are usually oversized and their control is not well optimised. A clear indication is thus given that it would be worth checking pumps operation, especially those belonging to the cooling system, when looking for energy savings opportunities. The refinery blueprint could therefore prove useful for any refinery willing to carry an energy audit as requested by the Energy Efficiency Directive (EED) [53], saving some data gathering time to on-site engineers.

Finally, the blueprint provides a dataset that could be used by researchers for testing new methodologies and publishing.

A blueprint is not.... a detailed model of a process operations. Several aspects of the blueprint construction prevent it to be used for advanced process supervision, optimisation or

control:

- Origin of data: the blueprint is created using a mix of publicly available and real site data. For example, in the refinery blueprint, all facts related to waste generation and emissions are originating from literature. This way, useful insights are still available such as the average amount of CO₂ emitted ($\sim 7'700$ t_{CO2}/d), giving an order of magnitude with respect to the refining process Carbon Capture and Utilisation (CCU) potential. On the other hand, more sensitive information related to where the CO₂ is emitted or in which concentration are not made available. More specific and detailed models, such as the ones developed in the framework of the Elegancy project [54], should therefore be used in order to fully evaluate if any CCU opportunity could be interesting.
- Pareto approach: in the blueprint, only the major flows are included, conferring it a certain degree of anonymity while giving a good overview of the energy and material needs. However, since some flows are discarded, it prevents the blueprint from being used for advanced process optimisation.
- MILP models: the models constituting the blueprint are linear and compatible with a MILP framework. They can thus be used for high level multi-objective optimisation of resources and energy networks. On the other hand, they are not fitted for studying system dynamics. The blueprint validity domain is restricted to nominal operations and stationary regime. The study of specific situations such as start-up and shut-downs therefore requires specific models, most probably non-linear.

4.2. Further developments

The blueprints are useful tools for enhancing the detection of IS opportunities while overcoming the burden of data confidentiality. However, in order to generalise their utilisation, efforts should be put into creating new blueprints representing various industrial processes and sectors. For example, this paper only presents the blueprint of a refinery. One could thus argue that the chemical industry comprises a large variety of chemical processes and that such blueprints should be created for other chemical process units. In the framework of the EPOS project, blueprints of two additional chemical process units (polymers and synthesis), three other industrial sectors (steel, minerals and cement) and one for district heating networks, are built. This database could be enriched by modelling other chemical processes (speciality chemicals, steam crackers, etc.) and industrial sectors (food, ceramic, etc.).

5. Conclusions

A generic and systematic methodology for building blueprints in the chemical industry is developed. It is successfully applied on a petrochemical plant; the blueprint of a refinery is produced and presented. Both bottom-up and top-down approaches are followed during the data collection step, site data are used to build realistic models of typical refinery units adding data from literature. Four profiles summarising the energy (thermal and electrical),

material and service requirements of a typical refinery are produced. The profiles prove useful for identifying IS opportunities with other industrial sectors (waste heat utilisation, re-use of solid wastes, electrical flexibility potential). The methodology uses only a few user defined key parameters to define the state of the system and is flexible as the blueprint is sizeable. It can be applied to a wide variety of chemical processes and should be extended to other industrial sectors in order to generalise the blueprints' utilisation.

The use of blueprints is an elegant way to overcome the burden of industrial data confidentiality. It provides a database representative of a given process industry site that can be used for IS opportunities identification. The dataset is straightforward, transparent and comprehensible allowing non-expert users to have a basic understanding of the main flows crossing the system. The blueprints also open the door to the creation of a common vocabulary framework for the purpose of creating and enabling IS exchanges.

The blueprints can have a broader range of applications than facilitating the exchange of information in an IS context. They can be used for impact studies and enable sector benchmarks. They also provide welcome means to publish and present project results. They enable researchers to challenge scientific methodologies and tools by providing useful information for building case studies. Finally, they provide a common ground for policymakers to try new strategies or, most of all, increase the outreach of innovation projects funded through public grants.

Acknowledgement

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Nomenclature

Acronyms

BAT	Best Available Techniques
BOD	Biological Oxygen Demand
BTEX	Benzene, Toluene, Ethylbenzene, Xylene
CC	Composite Curve
CCR	Continuous Catalytic Regeneration
CCU	Carbon Capture and Utilisation
CDU	Crude Distillation Unit
CHP	Combined Heat and Power
COD	Chemical Oxygen Demand
CRU	Catalytic Reforming Unit
EED	Energy Efficiency Directive
EPOS	Enhanced energy and resource Efficiency and Performance in process industry Operations via onsite and cross-sectorial Symbiosis
EU	European Union
FCC	Fluid Catalytic Cracking
GCC	Grand Composite Curve
GP	Gas Plant
HCK	Hydrocracking Unit
HDS	Hydrodesulphurisation Unit
HDT	Naphtha Hydrotreater
HGO	Heavy Gasoil
HP	High Pressure
IS	Industrial Symbiosis
ISOM	Isomerisation Unit
KPI	Key Performance Indicator
LGO	Light Gasoil
LP	Low Pressure
LPG	Liquified Petroleum Gas
MER	Minimum Energy Requirement
MILP	Mixed-Integer Linear Programming
MP	Medium Pressure
NISP	National Industrial Symbiosis Programme
P&ID	Piping and Instrumentation Diagram
PFD	Process Flow Diagram

TSA	Total Site Analysis
VDU	Vacuum Distillation Unit
VISB	Visbreaking Unit
VLP	Very Low Pressure
VOC	Volatile Organic Compound

Symbols

CF	Capacity Factor	[-]
ΔT	Temperature difference	[°C]
η	Efficiency	[-]
\dot{m}	Mass flow	[kg/s]
\mathcal{P}	Power	[kW]
P	Pressure	[bar]
\dot{Q}	Heat load	[kW]
T	Temperature	[°C]

Indices

<i>avg</i>	average
<i>c</i>	cold
<i>h</i>	hot
<i>in</i>	inlet
<i>min</i>	minimum
<i>out</i>	outlet
<i>p</i>	process
<i>rtd</i>	rated
<i>u</i>	utility

Appendix A. Refinery blueprint process units

The details of the process units are described in this section. The reader can refer to [44] for more details.

Crude Distillation Unit & Gas Plant. The crude oil enters the CDU where it is heated to about 300 – 400°C and distilled under atmospheric pressure separating the different fractions according to their boiling range. The overhead vapours (mixture of gas and naphtha) are sent to the Gas Plant (GP) where they are treated and separated to produce Liquefied Petroleum Gas (LPG) and a naphtha cut. Part of the naphtha is being sent to a steam cracker. The heavy fractions from the bottom of the CDU are further separated by VDU. The CDU are among the most intensive energy-consuming units in a refinery, despite their high-level of heat integration. This is mainly due to the high volume of crude oil that has to be heated up to elevated temperatures.

Naphtha Hydrotreater. In this unit, hydrogen is used to remove impurities such as sulphur or nitrogen and to stabilise the naphtha before sending it to the downstream isomerisation and reformer units. The naphtha feed coming from the CDU, the GP and the HCK is mixed with a hydrogen-rich gas, heated and vaporised before being fed into the reactor. The reactor conditions are usually 30 – 40 bar and 320 – 380°C. The reactor effluents are then cooled down and separated. The gas phase, containing mainly hydrogen, is compressed and recycled back to the reactor whereas the liquid phase is further purified and split into three fractions: gasoline, light distillates and benzene that go respectively to the Isomerisation Unit (ISOM), feedstock and CRU. As the other hydrogen-consuming processes, the HDT consume a significant amount of energy in the form of fuel and steam.

Hydrodesulphurisation Unit. During this process, hydrogen is used to remove the sulphur contained into the three side fractions (kerosene, Light Gasoil (LGO) and Heavy Gasoil (HGO)) leaving the CDU. Similarly to the HDT, the mixture of hydrocarbons is put in contact with a hydrogen rich-gas and heated before entering the reactor. The reaction conditions are slightly more severe than for the HDT (40 – 70 bars, 330 – 390°C). The reactor effluents are also separated between a gas phase that is compressed and send back to the reactor and a liquid phase that will constitute the base of the various refining feedstock.

Isomerisation Unit. The purpose of this unit is to increase the octane index of the light naphtha fraction (gasoline) produced by the HDT. The arrangement of the molecules is altered without adding or removing anything and the low-molecular-weight paraffins (C₄-C₆) are converted to isoparaffins with a much higher octane index. The isomerisation reaction occurs in presence of hydrogen and catalyst. Hydrogen is used to minimise the carbon deposit on the catalyst. For the refinery blueprint, the hydrocarbon recycle isomerisation design, where the unconverted, lower octane paraffins are recycled for further conversion, is modelled. The reaction conditions depend on the type of catalyst (130 – 280°C, 15 – 30 barg). The unit energy requirements will depend on both the design and the catalyst type.

Catalytic Reforming Unit. Similarly to the ISOM, the purpose of this unit is to increase the octane index of the feed entering the CRU. The typical feedstocks to CRU are the hydrotreated heavy naphtha (benzine) from the CDU and the heavy naphtha stream from the HCK. During the process hydrogen is produced along with LPG and reformates (light and heavy). The hydrogen is used in other hydro-processing units. The light reformate can be sent to the ISOM, while the heavy one may be blended to gasoline or further separated into components as chemical feedstocks such as benzene, toluene, xylene and naphtha cracker feed.

There are several catalytic reforming processes in use today. The blueprint is based on the Continuous Catalytic Regeneration (CCR) reforming process in which the catalyst can be regenerated continuously and maintained at a high activity rate. It is the most modern type of process, it gives the highest yields and it has the highest heat integration [44]. The reactor operates at relatively high temperatures (490 – 530°C) and low pressures (3.5 – 10 bar).

Vacuum Distillation Unit. This unit receives the CDU heavier fraction and distilled it under vacuum in order to increase its volatilisation and separation. It allows upgrading atmospheric residues into more valuable fractions such as naphtha, kerosene and mi-distillates and producing feedstocks for the refinery other downstream units. When entering the unit, the atmospheric residues are heated up to 400°C, partially vaporised and flashed into the vacuum column. Steam ejectors, vacuum pumps and condensers are maintaining vacuum inside the fractionator. Heat is required to heat up the feed before it enters the distillation. On the other hand, a significant amount of LP steam is produced thanks to the maximisation of heat recovery from the output streams.

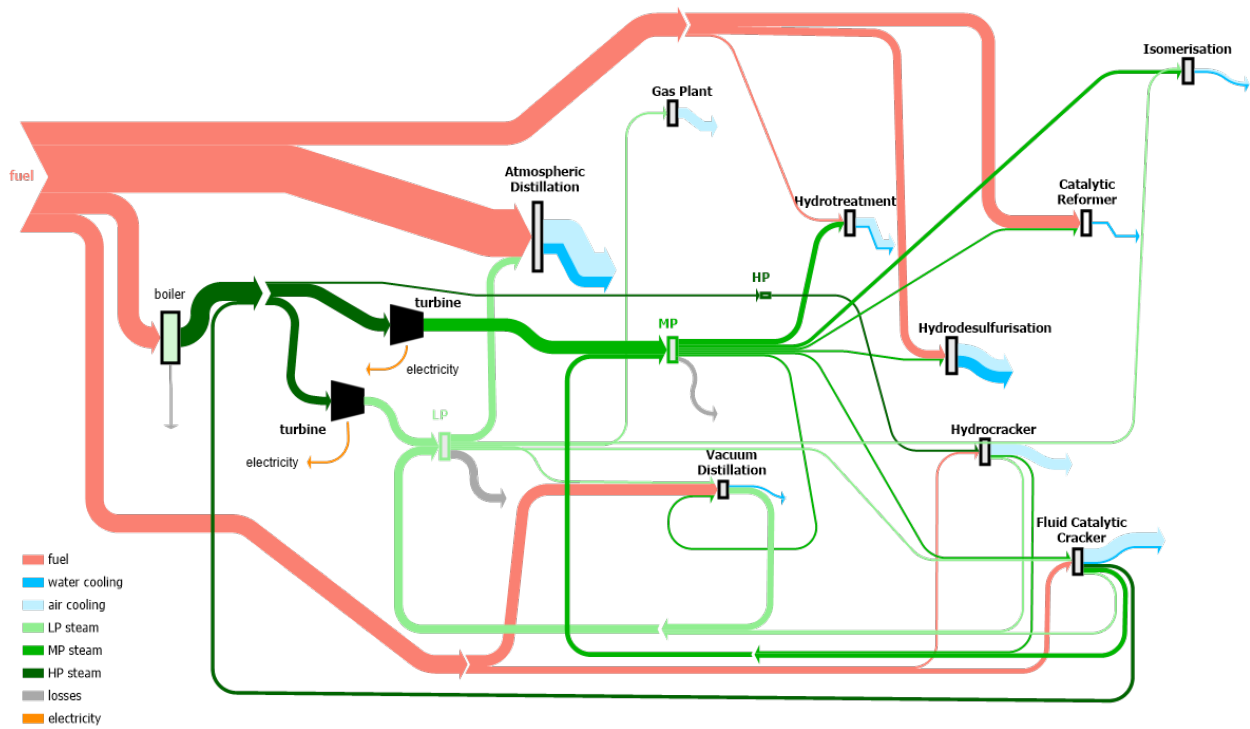
Visbreaking Unit. This non-catalytic thermal process converts the vacuum residues into gas, naphtha, distillates and residues (tar). High temperatures and pressures are used to break large hydrocarbon molecules into smaller ones. The process uses high temperature (430 – 500°C) and high pressures (10 barg) to crack the heavy hydrocarbons. In order to stop the reaction, the process streams are then mixed with cooler recycled streams. The product are then flashed, the light products vaporise and are drawn off. The other products are then further separated into naphtha, gasoil and heavy residues.

Hydrocracking Unit. This process is capable of converting various type of feedstock into lighter products. Hydrogen at temperature between 280°C and 475°C is used in the presence of a catalyst in order to hydrogenate and crack the molecules. Hydrocracking may also be used for the cracking of superior fuels and the production of lubricants. The main feed stream of the HCK is the vacuum gasoil coming from the VDU and the main products are LPG, gasoline, jet fuel and diesel fuel. The process can usually be split into a reaction section where the hydrogen is put in contact with the feed and a separation section in which the various fractions are obtained. Hydrocracking is an exothermic process. The heat generated can be recovered using feed/product heat exchangers. Nevertheless, a significant amount of heat is still required for the products separation.

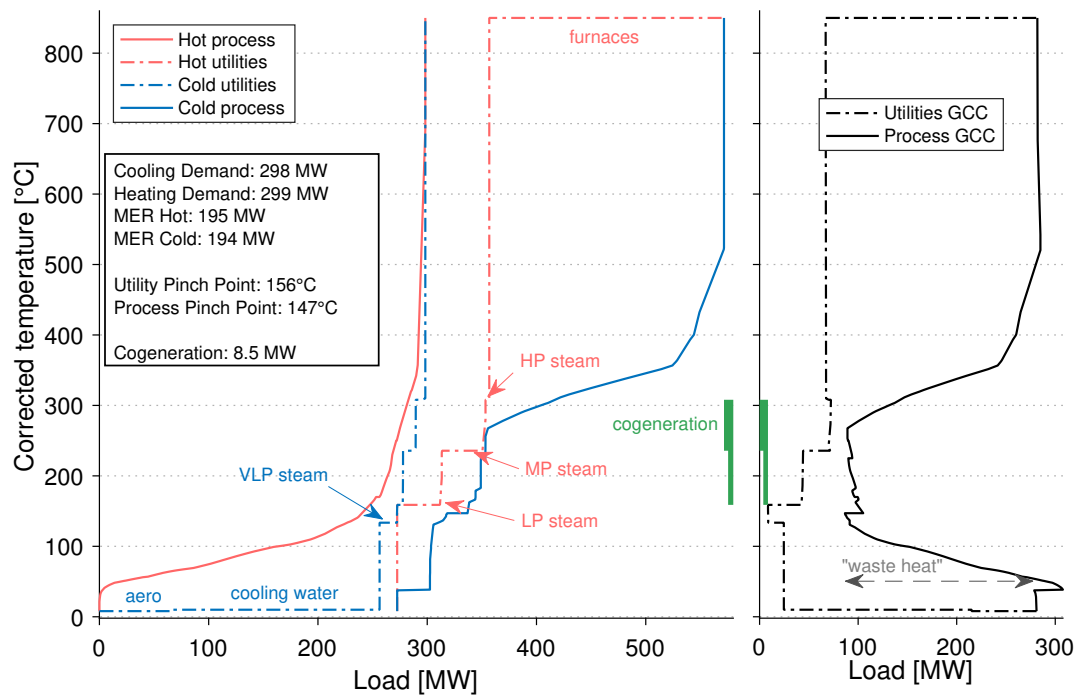
Fluid Catalytic Cracking. This process upgrades heavy hydrocarbons into more valuable low boiling point hydrocarbons in the presence of a hot catalyst (680 – 730°C). Typical feeds are the HGO from the VDU or the bottom streams from the CDU. The FCC unit can be divided into two sections: reaction-regeneration and fractionation. In the reaction-regeneration section, the feed is preheated (250 – 425°C) before being put into contact with the catalyst in the reactor where it is cracked at high temperature (500 – 540°C). In the meantime, the catalyst is continuously regenerated in order to remove the coke produced by the reaction. The cracked hydrocarbons are then sent to the fractionation section where the desired fractions are separated and collected. The flue gases generated by the unit are used to produce HP steam.

Appendix B. Refinery blueprint - configuration n°2

In configuration n°2 of the refinery's blueprint, the input capacity rate is reduced to 25'000 t/d and then VISB is removed. The new refinery has a Nelson Index of 5.48. Figures [B.1](#), [B.2](#) and [B.3](#) illustrate the blueprint profiles with this new set-up.

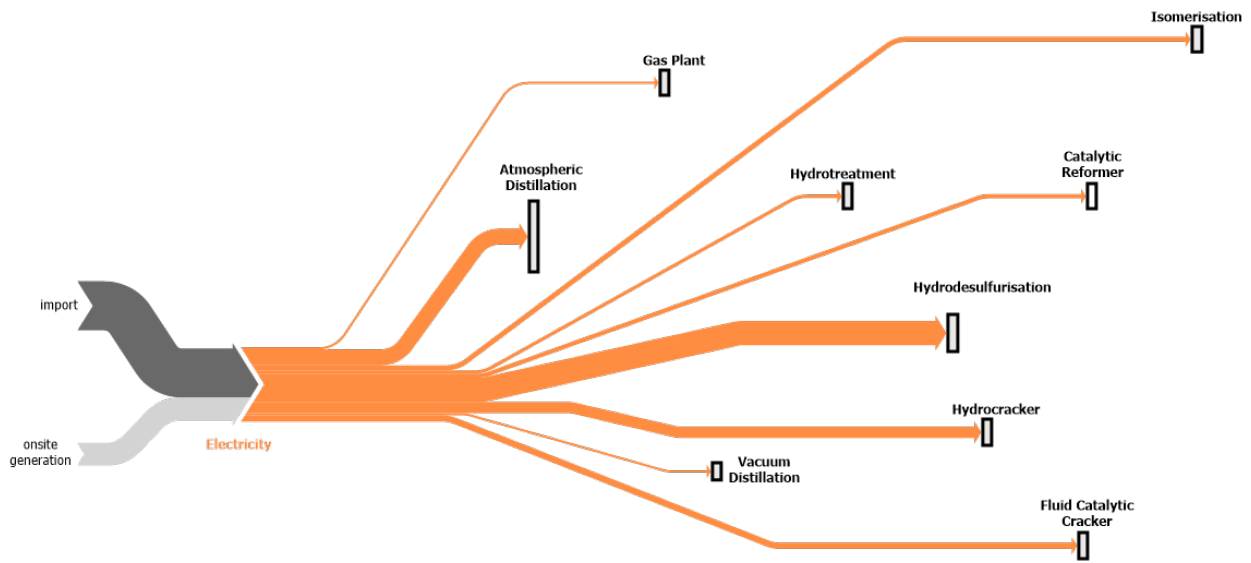


(a)

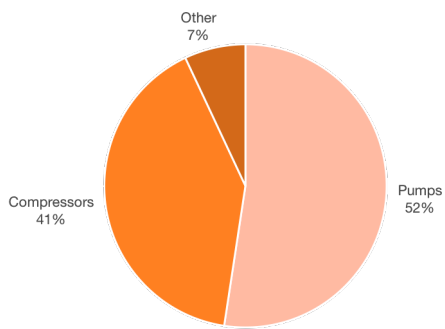


(b)

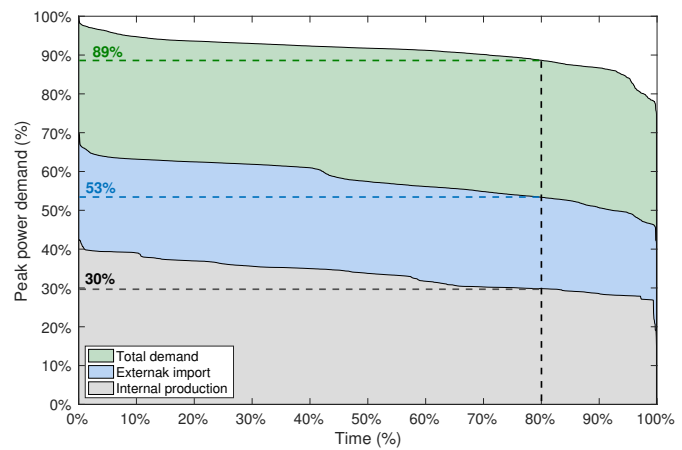
Figure B.1: Refinery blueprint (configuration n°2) - thermal energy profile with main thermal flows (a) and TSA curves (b)



(a)



(b)



(c)

Figure B.2: Refinery blueprint (configuration n^o2) - electrical energy profile with main power flows (a), electrical consumptions breakdown (b) and load duration curve (c)

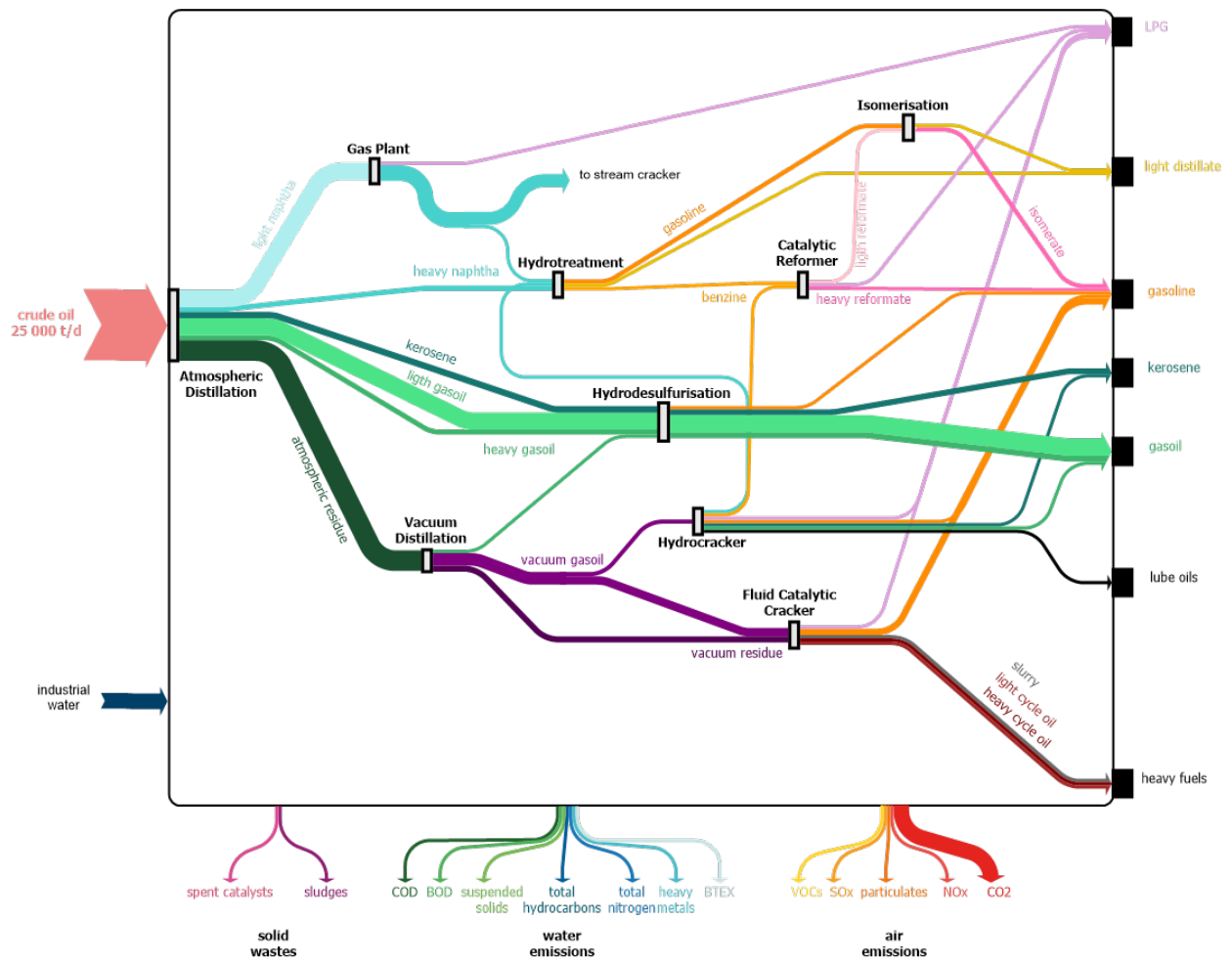


Figure B.3: Refinery blueprint (configuration n°2) - material profile with main material flows and wastes

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