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Electrification in Process Industry – The Role of Process Integration and Future Energy Market Conditions

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Abstract

Electrification of industrial processes is a frequently discussed strategy to reduce greenhouse gas emissions from energy-intensive process industries and is highlighted in many roadmap studies. Electricity is a versatile energy carrier that enables a broad variety of options in which existing process unit operations are replaced with electricity-driven alternatives. However, the implications in terms of greenhouse gas emission reduction potential and cost when integrating such new electrification technologies are not obvious due to often complex interactions between energy flows in existing industrial plants. Understanding these implications and interactions is not only important in order to assess electrification in comparison with current process configurations, but also to allow a comparison with other greenhouse gas emission reduction strategies.

In this thesis, a bottom-up framework to assess opportunities for electrification of energy-intensive industrial processes in terms of greenhouse gas emissions and costs was developed. One particular novelty is that the framework includes heat integration studies with pinch analysis tools to analyse how potential changes in heat surpluses or demands associated with the replacement of a fuel- or heat-driven unit operation by a new electricity-driven process affect the heat recovery potentials and utility demands of the overall site. Furthermore, energy flows between the process site and the background energy system are considered and the use of scenarios is introduced in order to assess the impact of electrification options under different possible future energy market conditions. The framework was tested and validated in three case studies for different industrial processes. In these case studies, different parts of the existing processes-related systems (e.g. the reactor system or utility system) were assumed to be electrified, highlighting different aspects of the proposed assessment framework.

The results emphasise that electrification may significantly change the heat flows through a process site and that detailed heat integration studies are required to capture these effects. Another finding is that the underlying assumptions for future energy market scenarios have a strong impact on greenhouse gas emission reduction potentials and cost. The framework can be used to compare electrification with other process greenhouse gas emission reduction measures and to support policy and industrial decision making.

Keywords: *energy-intensive process industries, electrification, bottom-up assessment, chemical industry, oil refining, oxo synthesis, techno-economic assessment, energy market scenarios*

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List of publications included in the thesis

This thesis is based on the following three appended papers:

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II. Wiertzema, H., Åhman, M., & Harvey, S. (2018). Bottom-up methodology for assessing electrification options for deep decarbonisation of industrial processes. *Proceedings of the ECEEE Industrial Summer Study*, June 11-13 2018, Berlin, Germany. Paper 4-021-18. Proceedings pp 389-397.

III. Wiertzema, H., Svensson, E., & Harvey, S. (2020). Evaluation of hybrid electric/gas steam generation for a chemical plant under future energy market scenarios. *Proceedings of the ECEEE Industrial Summer Study*, September 14-17 2020, Göteborg, Sweden. Paper 4-018-20. Proceedings pp 243-252.

Co-authorship statement

Holger Wiertzema (HW) is the main author of all papers included in the thesis. Elin Svenson (ES), Max Åhman (MA) and Simon Harvey (SH) supervised the work. ES provided critical feedback for papers I and III, MA for paper II, and SH for all papers.

Other publications by the author not included in the thesis

A. Åhman, M., Wiertzema, H., & Arens, M. (2020). *Industrial electrification and access to electricity at competitive prices: Review of climate and energy policy influence on electricity prices for industry and future implications for industrial electrification*. (115 ed.) Lund: Miljö- och energisystem, LTH, Lunds universitet.

B. Rootzén, J., Wiertzema H., Brolin, M., Fahnestock, J. (2020). Electrify everything! Challenges and opportunities associated with increased electrification of industrial processes. *Proceedings of the ECEEE Industrial Summer Study*, September 14-17 2020, Göteborg, Sweden. Paper 6-040-20. Proceedings pp 415-423.

C. Jannasch, A.-K., Pihl, H., Persson, M., Svensson, E., Harvey, S., & Wiertzema, H. (2020). *Opportunities and barriers for implementation of Power-to-X (P2X) technologies in the West Sweden Chemicals and Materials Cluster's process industries*. RISE Research Institutes of Sweden report.

TABLE OF CONTENTS

1 Introduction

In 2018, the industrial sector accounted for 37% (157 EJ) of global final energy use and 24% (8.5 $GtCO_2$) of direct fossil CO_2 emissions. Five energy-intensive sectors, namely chemical and petrochemicals, iron and steel, cement, pulp and paper as well as aluminium dominate with a share of 71% of direct industrial fossil CO_2 emissions (International Energy Agency 2020). A special characteristic of these sectors is that emissions stem from a relatively small number of point sources which is very different compared to other sectors such as households and road transportation.

In the light of the Paris agreement, the pressure on industry to contribute to substantial greenhouse gas emission reduction has increased. Climate policy frameworks to reach net zero emissions are either being discussed or already implemented by many countries. For example, Sweden legislated the target of net zero emissions by 2045 (Swedish Government 2018) while the European Commission strives for net zero emissions by 2050 (European Commission 2020). Several technological options and strategies are available and considered by industrial decision and policy makers (Agora 2019). One strategy, which is also in focus in this thesis, is the direct and indirect use of (renewable) electricity. Another strategy focuses on the carbon cycle and includes technologies to separate carbon dioxide which can then be stored or used in other chemical processes. Furthermore, the replacement of carbon of fossil origin by carbon from biomass is part of this strategy.

Electricity can be used for direct electrification whereby electro-thermal technologies replace natural gas, oil, coke and biomass for industrial heating purposes (EPRI 2009, Åhman et al. 2012) or for indirect electrification whereby fossil feedstocks in (chemical) plants are replaced with electricity-derived hydrogen, methanol and ammonia (Palm et al. 2016, Philibert 2019). The switch from fossil resources to electricity in conjunction with the anticipated increasing amount of electricity from renewable sources can potentially lead to a significant reduction in greenhouse gas emissions from the plant site as well as at the national and global energy systems level. If electricity generation is carbon-free, emissions associated with certain processes could potentially be completely avoided. Depending on the electricity generation mix (especially in terms of carbon-intensity and retail price for industrial users), electrification can already today lead to a reduction of greenhouse gas emissions and energy purchase costs compared to combustion of fossil fuels.

As a consequence, there is a growing interest in expanding the use of electricity in the industrial sector in Europe. A significant number of publications have explored the implications of increased industrial electrification (Berenschot et al. 2017, Brolin et al. 2017, International Energy Agency 2017b, Lechtenböhmer et al. 2016, Umweltbundesamt 2013).

The main driver for this interest in electricity as a future energy carrier in industry is the combined effects of the demand for strong greenhouse gas emission reductions in industry in order to meet ambitious climate targets (80 to 95 % decrease by 2050) together with the concurrent rapid growth of renewable electricity generation. Many recent forecasts indicate falling trends for the cost of renewable electricity generation and electricity from solar and wind power is anticipated to overtake the role as the “primary fuel” from coal, oil and gas in the future (Lechtenböhmer et al. 2016). Carbon capture and storage (CCS), including bio-energy with carbon capture and storage (BECCS) that can potentially achieve negative emissions as a subset, is still an attractive option as a backstop technology for reducing residual CO_2 emissions in the energy-intensive processing industry (see e.g. International Energy Agency 2017a) but several stakeholders have doubts regarding the cost, public acceptability, and the political support for this option (D'Aprile 2016, Lupion and Herzog 2013). However, it should be noted that such doubts can also arise in conjunction with large-scale electrification of industry due to the vast demand for additional electricity generation and transmission capacities. Concerns about increased used of biomass are often related to sustainability and there is currently no consensus about the amount of biomass that can be produced sustainably on a global scale (Wang et al. 2018).

From a company’s perspective, process electrification can enable compliance with national or self-imposed emission limits as well as reducing the costs associated with emitting greenhouse gases (e.g. related to the EU ETS). This will become even more important in the future since the price for EU ETS emission allowances is expected to increase (European Roundtable on Climate Change and Sustainable Transition 2019). The production costs for renewable electricity are expected to decrease in the future at the same time as the combustion of fossil fuels is expected to become significantly more expensive. It is therefore anticipated that process electrification will become increasingly economically feasible (International Energy Agency 2017b). Process electrification can also provide additional (non-energy) benefits such as debottlenecking, higher product quality, as well as better work safety (Wei et al. 2019). In some cases, such benefits can increase the attractiveness of process electrification options greatly (Rightor et al. 2020).

Another driver for electrification of industry is the changing characteristics of power systems in Europe. With rapidly growing shares of intermittent renewable electricity, the power system needs substantial demand-side flexibility (Haas et al. 2013). In such a system, demand response in one of the largest user sectors, industry, could become vital for the system and there is a potential for industrial electricity consumers to engage actively on the balancing market (Brolin et al. 2017, Paulus and Borggrefe 2011). For industrial companies, electrification can enable participation in flexibility markets (e.g. by providing on-demand load-shedding) which can lead to additional revenues. However, it should be noted that this is also connected with costs such as loss of production during periods of load-shedding or costs for installing and operating alternative process energy sources.

In general, electrification options fall into the following categories:

- Power-to-heat in which electricity is used to recover low-grade excess process heat (with heat pumps), to produce steam or hot water (with electric hot water or steam boilers), or in process operations directly (e.g. plasma heating for calcination, electric steam crackers, as well as drying operations)

- Power-to-hydrogen in which water electrolysis is used to produce hydrogen which is used directly (e.g. for direct reduction of iron ore or in hydrogenation processes) or further processed to produce fuels or platform chemicals such as methanol and ammonia
- Electro-catalytic processes other than water electrolysis in which specific chemicals are produced directly
- Power-for-separation in which the pressure to drive membrane separation processes is provided by electricity

Depending on the type of electrification technology, process electrification options can affect different parts of existing processes. Figure 1 shows the design *hierarchy* and the *interactions* of typical process-related systems that can be found at industrial plant sites. For each *hierarchy* level, different electrification options (and combinations of electrification options) are conceivable.

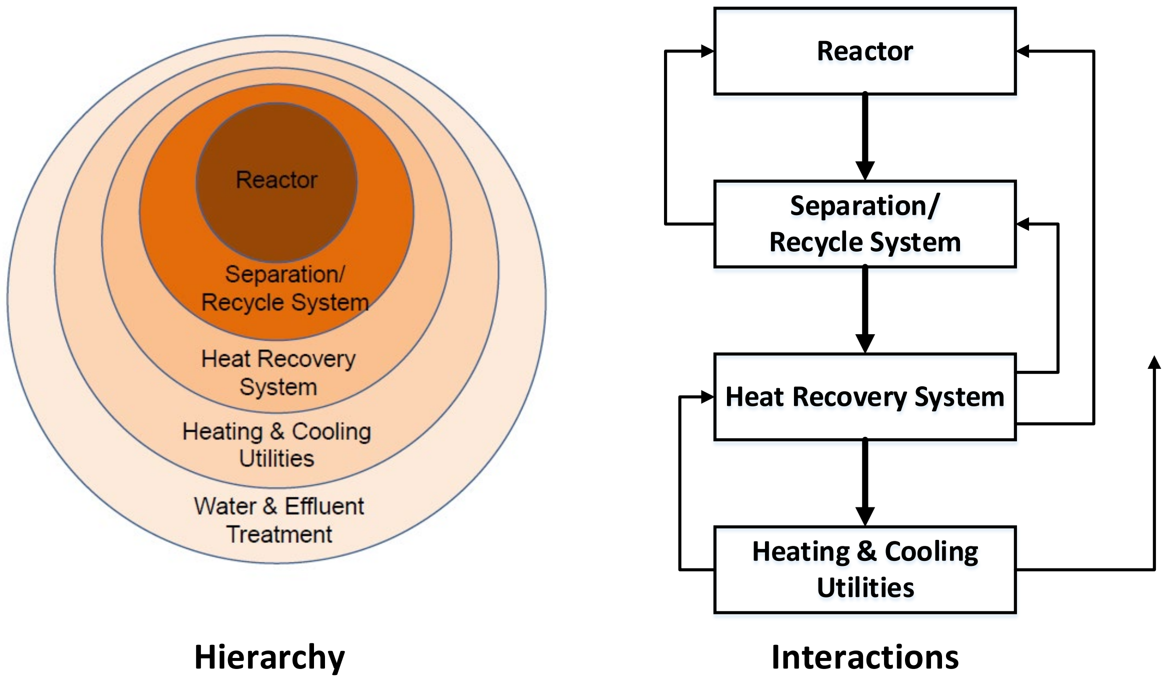

Figure 1: Hierarchy and interactions of industrial process-related systems (based on Gundersen 2002)

Due to the *interactions* between the process-related systems, electrification measures have different effects, depending on how deeply within the process *hierarchy* they are implemented. For example, an electrification measure that is implemented in the utility system (e.g. electric boilers) will not lead to a change in mass and energy flows in the core processes such as the reactor, separation and heat recovery systems. However, before introducing (more) electricity to provide hot and cold utility, it makes sense to investigate possible opportunities for reducing the heating and cooling demand through energy efficiency measures in the heat recovery system. On the next level, technology options that are implemented in the heat recovery system (especially heat pumps) require a more in-depth analysis since possible heat sources in the reactor and separation systems must be identified and the demand for heating and cooling from the utility system will also change. The need for more detailed analysis and design becomes even larger for electrification options implemented in the core processes of the reactor or separation/recycling systems. As a result of such interactions, a systematic approach for the assessment of electrification options should capture the characteristics of electrification technologies with regards to which level of process *hierarchy* is affected, and suggest appropriate analysis tools accordingly.

The number of possible options for industrial electrification is high, and different technologies and combinations of technologies will perform differently in terms of economic feasibility and carbon footprint. Furthermore, such performance indicators are heavily dependent on the characteristics of the power generation technologies and the energy market conditions in the background system, which are highly likely to change over time. For industrial decision-makers, it is thus important to understand the effects of process electrification not only on the process and plant, but also the energy systems level.

A review of literature on process electrification (see Chapter 2) reveals a lack of studies that systematically screen and assess process electrification measures for given industrial sites considering potential future changes in energy market conditions (e.g. share of renewable electricity and electricity prices), but also the integration of the new electrification technology with the existing processes, and the resulting effects on the process heat flows of the industrial site. There is thus a lack of detailed knowledge about how existing processes are affected when electricity is introduced as an energy carrier. Such knowledge is important not only to discard low-performing technologies at an early stage but also to identify conditions under which electrification options are viable, especially in the light of capital-intensive investments and the limited number of investment cycles before 2050.

1.1 Aim

The aim of this thesis is to develop and validate a methodology for screening potential electrification opportunities, assessing their impact on process mass and energy flows, and quantifying the related economic performance and carbon footprint consequences for different possible future energy market conditions. More specifically, this aim can be broken down into the following goals:

- Compilation of an inventory of electrification options for industrial processes and their characteristics that are relevant for performing integration studies.
- Development of a bottom-up assessment framework for the techno-economic and carbon footprint assessment of process electrification options. The framework incorporates energy targeting tools to understand how electrification of certain industrial processes impacts energy flows and heat integration opportunities throughout the industrial site's core processes and utility system (e.g. heat recovery, utility steam demands, generation of internal fuel by-products and high-temperature

excess heat sources, steam cycle power generation, excess heat delivers for external use, fuel use, cooling demands, and emissions). Furthermore, the framework includes scenarios for different future energy market conditions which enables long-term assessments.

- Test and validation of the bottom-up assessment framework through different case studies in which different process electrification options are assessed for different industrial processes, taking short- and long-term options into account.

1.2 Appended papers

Figure 2 highlights the specific contributions of the individual papers that are included in this thesis, also mentioning the case studies that were carried out.

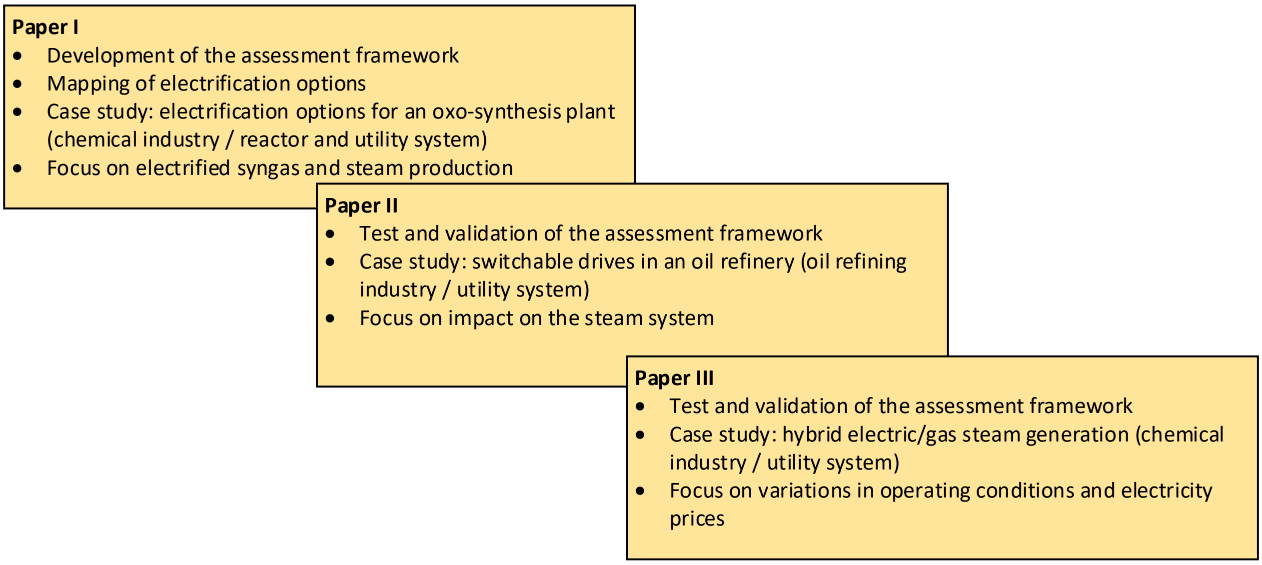

Figure 2: Overview of the appended papers and their main contributions in terms of methodology development and applications in case studies

- **Paper I** proposes a bottom-up assessment framework for the techno-economic and greenhouse gas emission assessment of process electrification options for existing processes in energy-intensive industries. The framework can be used to identify which parts of a process are affected by electrification and how electrification can change the heat recovery potential at the plant level, as well as the fuel demand, co-generation potential and the availability of excess heat. In conjunction with energy market scenarios, the framework can be used to assess medium- and long-term electrification options under different possible future market conditions. The proposed methodology was tested and validated in a case study for an oxo synthesis plant in which a detailed study was performed for the integration of both electrified syngas production and electrified utility steam production. For the electrified syngas production, a reversed water gas shift reaction was coupled with hydrogen production from water electrolysis. Accordingly, the case study investigated both a technology which is available today, affects only the utility system of the plant and is thus easier to implement (electric steam generation) but also a long-term technology that entails more substantial changes to the existing process and that would basically replace the conventional unit operation completely (electrified syngas production). The paper also includes an overview of electrification options for different energy-intensive industries including an indication of the parts of the processes that are affected.

- **Paper II** presents an application of the proposed assessment methodology in a case study focusing on using electricity to replace steam as motive driving force for pumps and compressors equipped with switchable drives in an oil refinery. The purpose was to test and validate the methodology for an electrification option that only affects the utility system and that is available at the plant already today. The paper illustrates the need for an advanced model of the steam system to assess the true impact of making changes to steam flows in a complex steam network. Since a switch between electricity and steam is possible in these switchable drives, this electrification option can be used to provide flexibility. Furthermore, the steam which is released when switching to electricity can be used for other purposes in the future (e.g. to provide heat for CCS).

- **Paper III** investigates hybrid electric/gas steam generation for a chemical plant in terms of cost and greenhouse gas emission reduction potential. A linear optimisation model in conjunction with hourly energy market price data for different future energy markets scenarios was used to study how the fluctuating utility demand in combination with fluctuating conditions on the energy market can be handled. A key contribution of this paper is the illustration of the need to consider variations in operating conditions as well as future energy market conditions when optimizing the design of (partly) electrified industrial heat supply systems. Electric steam generation is an available technology that only affects the utility system. The proposed hybrid system is attractive since it enables the plant operator to adapt to different market conditions assumed to be characterized by relatively stable natural gas prices and very volatile spot market electricity prices. It should also be noted that the steam demand of the chemical plant itself also showed large variations.

2 Literature review

2.1 Role of electrification in selected roadmap studies

As a result of various drivers for industrial electrification, there is an increased activity related to industrial electrification at the company level as well as in research. In the Netherlands, the VoltaChem consortia was established to develop electrification technologies for the chemical industry (VoltaChem 2020). Other ongoing projects focus on specific industries (e.g. the Swedish projects "HYBRIT" (HYBRIT 2020) and "CemZero" (Cementa and Vattenfall 2018) for carbon-neutral steel and cement production, respectively) while others are more related to specific technologies (e.g. flexible use of electrolysers in "ELECTRE" ECN 2016) or materials (e.g. electricity-based plastics Palm et al. 2016, Siemens AG 2016). The ongoing Kopernikus project "Power-To-X" (RWTH Aachen 2016) aims to develop electricity-driven technologies to produce materials, energy carriers and energy-intensive chemical products.

Process electrification is included in many roadmap studies that present pathways to low- or even net zero-emission industrial sectors. A recent comprehensive review of publications related to decarbonisation pathways for the EU includes industrial electrification as an emissions reduction measure (Gerres et al. 2019). Net-zero emissions here refer to a situation in which remaining greenhouse gas emissions that are hard to abate are compensated by removing greenhouse gases from the atmosphere, e.g., through applying carbon capture and storage on biogenic sources. Table 1 presents an overview of electrification options for different industrial sectors based on a number of such roadmaps, which are described in more detail below (for a more detailed list of electrification options, see Table 1 in Paper I).

A recent study (Material Economics 2019) that investigated pathways for net-zero emissions from the EU heavy industry (with focus on steel, plastics, ammonia and cement production) concluded that many industrial strategies and pathways can be combined and that many solutions for net-zero emissions from industry are available and also emerging. Another key finding was that large amounts of electricity and biomass will be needed in addition to increased circularity (with larger material efficiency and increased recycling) to reach net-zero emissions from industry in 2050. Electricity would be used directly or indirectly via hydrogen, eventually leading to a lower dependency on imported fossil fuels. The study also highlighted the importance of a zero-emissions electricity production system in conjunction with affordable electricity prices.

Table 1: Overview of electrification options for different industrial sectors

Sector	**Electrification options**	**References**
Steel	• Hydrogen from water electrolysis for direct reduction of iron ore	Agora 2019
Cement	• Electric (plasma) calcination kilns	Agora 2019
Chemical	• (High-temperature) heat pumps • Electrode boilers (hot water or steam) • Hydrogen for chemical recycling of plastics • Hydrogen for Methanol-to-olefin (MTO) processes • Ammonia and methanol synthesis based on hydrogen from water electrolysis • Electrically heated naphtha or gas steam crackers • Synthetic naphtha production by Fischer-Tropsch synthesis based on syngas produced with hydrogen from water electrolysis and CO_2	Agora 2019, DECHEMA 2019, Material Economics 2019, Wuppertal Institut 2016
Pulp and paper	• Heat pumps for heat recovery • Electric steam generation • Electricity-based drying processes • Production of electro-fuels from biogenic CO_2 and hydrogen from water electrolysis • Electric plasma calcination	Grahn and Jannasch 2018, Rademaker and Marsidi 2019
Aluminium	• Heat pumps for heat recovery	Brough and Jouhara 2020

In a recent study of the German basic materials industry, process electrification is presented as an integral element to reach a climate neutral basic material industry in 2050 (Agora 2019). Electrification options considered include Power-to-heat (e.g. heat pumps and electric steam generation) as well as green hydrogen produced using renewable electricity. The hydrogen is assumed to be used to provide heat (when direct electric heating is not sufficient), especially for direct reduction steel-making using hydrogen. Other large future demands for hydrogen include future production of olefins and aromatics by alternative processes based on methanol, as well as chemical recycling of plastic.

In a roadmap study for the German chemical industry, electrification technologies are mentioned as key options in the pathway towards greenhouse gas neutrality by 2050 (DECHEMA 2019). Technologies mentioned in this context include hydrogen production by water electrolysis, ammonia and methanol synthesis based on hydrogen from electrolysis, as well as electric steam crackers and production of naphtha by electrolysis and Fischer-Tropsch synthesis.

In a study for the port of Rotterdam (an industrial cluster with oil refining, chemical manufacturing and power and steam generation), electrification plays an important role in the "Closed Carbon Cycle" scenario which is one out of four developed future scenarios (Wuppertal Institut 2016). In this scenario, a greenhouse gas emission reduction target of 90% is imposed and CCS and biomass are excluded as options. Accordingly, direct electrification of steam production as well as indirect electrification via water electrolysis to provide hydrogen for methanol synthesis and petrochemical production play a key role in addition to measures to increase recycling rates and thus circularity. An interesting finding for this scenario is that the port of Rotterdam could continue to be a hub for fuels and fuels pre-products while at the same time avoiding on-site emissions almost completely.

2.2 Existing methodological approaches for the assessment of electrification options

Much of the recent research related to electrification of the industrial sector has a strong focus on macro-economic top-down approaches and explorative studies (see previous section) or on technology development. For example, Lechtenböhmer et al. 2016 estimated that full electrification of the basic materials (steel, minerals and chemicals) industry in the EU could lead to an additional electricity demand of 1713 TWh/a in 2050, compared to the level at the time of the study (2780 TWh/a).

Top-down studies usually exclude detailed technological aspects and run the risk of neglecting the many challenges related to implementation in specific plants. Existing industrial process sites, even within the same sector, can be very different. In particular, the degree of integration can vary substantially between plants, i.e. how mass and energy flows between different process units are interconnected. As a result, it is difficult to estimate how the introduction of electrification technologies will affect greenhouse gas emissions and costs without conducting site-specific studies.

The research literature related to process electrification also includes inventories of electrification technology options for different processes as well as information about their technical maturity, often expressed as Technology Readiness Level (TRL). Some of these inventories are rather old (EPRI 1989) and based upon the assumption that electrification is driven by efficient use of electricity rather than greenhouse gas emissions reduction. More recent inventories such as (EPRI 2009) are more extensive and some of them also include comparisons between conventional technologies and electricity-driven equivalents at the unit operation level (DECHEMA 2017). They are not only motivated by identifying opportunities to increase efficiency, but also by finding ways to significantly reduce greenhouse gas emissions from industrial processes.

Studies based on the engineering bottom-up approach consider more detailed descriptions of the technologies and the impact on existing systems. In this work, bottom-up assessment refers to investigating the impact of integrating electrification technologies into existing processes in terms of greenhouse gas emissions and cost, accounting for the specific characteristics of the existing processes. There are many examples of recent studies that adopted a bottom-up approach to access the impact of integrating new technologies and process concepts (not based on electrification) into existing industrial sites.

Ong et al. 2019 developed an iterative procedure based on process simulations tools, pinch analysis and heat exchanger network design tools to maximise energy integration when integrating hydrothermal liquefaction of Radiata Pine with Kraft black liquor in an existing Kraft pulp mill. In the study, heat integration studies for a combined heat and power plant were performed to identify the resulting utility demands. The study also investigated the impact in terms of greenhouse gas emissions but did not include an economic assessment. Magdeldin and Järvinen 2020 assessed the integration of supercritical water gasification of Kraft black liquor into Kraft mills. A process model for the new process was developed and used to establish models on the process unit and system level. Heat integration tools were used to study the integration of the supercritical water reactor. Furthermore, an economic assessment based on a discounted cash flow analysis was performed. However, the future economic performance under different energy market scenarios was not considered. Mongkhonsiri et al. 2020 investigated the integration of black liquor gasification in an existing pulping process. The focus of the study was process design and modelling but also included a techno-economic and greenhouse gas emission assessment. However, heat integration studies were not included at the process conceptual design stage. Cormos et al. 2020 performed a techno-economic and CO_2 emission assessment for the integration of carbon capture technologies into cement and steel plants. Pinch analysis was used to identify options for process-to-process heat exchange in order to minimise the demand for external utility. Sundqvist et al. 2018 investigated the integration of partial carbon capture processes into an existing integrated iron and steel plant. For two alternative CO_2 sources (blast furnace gas and flue gases from a CHP plant), the specific heating demand for CO_2 capture and options to use excess heat at the plant were analysed. Biermann et al. 2019 performed a techno-economic assessment for such partial capture processes driven by excess heat of a steel plant. Nwachukwu et al. 2020 assessed the integration of technologies to produce biomass-based gas into iron and steel plants with a focus on the impact on value chains. Their methodological approach starts with modelling supply chains before performing process and heat integration studies to estimate the heat recovery potential and to target additional heating and cooling demands. Furthermore, the system cost for the production of gas fuel was calculated and sensitivity analyses were performed for biomass and electricity prices, capital recovery factor, CAPEX and transport distance. However, future energy market scenarios were not considered. Andersson et al. 2020 looked into options to integrate the production of algae-based fuels into an oil refinery by using CO_2 and excess heat from the refining process. Different processes were evaluated in terms of energy and carbon footprint. Heat and material integration studies were performed to determine the minimum heating and cooling demands. Ahlström et al. 2020 investigated the economic potential of replacing fossil fuels with liquefied biomethane in the Swedish iron and steel industry. The methodological framework starts from a representation of the integrated liquefied biomethane process based on process modelling and heat integration studies before these insights are used to extrapolate to all iron and steel plants in Sweden which were then combined with supply chain models. Different energy market scenarios were used for the assessment. Berghout et al. 2019 developed a method to identify greenhouse gas emission reduction pathways for industrial plants and applied the method in a case study for a complex oil refinery. The method starts from a bottom-up perspective and includes core processes at the plant level but does not include electrification as primary measure for emission reductions. Furthermore, heat integration is mentioned with respect to increased energy efficiency at the plant but not regarding electrification and how electrification options would change mass and energy balances as well as the heat integration potential.

None of the afore-mentioned studies assessed the integration of electrification options in existing processes. However, the examples of bottom-up assessment methods all include different aspects that are relevant to consider when assessing electrification measures. Nevertheless, while all studies included a case study for a specific industrial plant or cluster, the way that (heat) integration opportunities are considered differs widely, as does the extent to which future changes in energy market conditions are accounted for in economic and greenhouse gas emission assessments.

There are also bottom-up studies that focus on specific electrification technologies or in which electrification plays a subordinate role. Thunman et al. 2019 considered electric heating and hydrogen production by water electrolysis in some of their proposed process schemes to achieve 100% carbon recovery from plastic waste within existing petrochemical clusters. However, the study does not investigate the changes of heat integration potential in any detail. Bühler et al. 2019 conducted an assessment of options for electrification of process heat in milk powder production plants by implementing heat pumps and electric heaters in different configurations. Their study includes an energy, exergy, environmental and economic analysis, as well as different scenarios for future prices and emissions. However, the study focuses on the electrification of heat only. Wallerand et al. 2018 developed a new method for optimal integration of heat pumps based on a superstructure optimisation model. However, the method was not applied to an existing plant and did not consider possible future changes of energy market conditions. Delikonstantis et al. 2019 evaluated a direct plasma-assisted methane-to-ethylene process and a hybrid plasma-catalytic methane-to-ethylene process. The authors state that further adaptions of the existing processes would be needed since the heat flows in the conventional process are highly integrated with the other processes of the plant. This means that heat demand for subsequent separation processes must be provided in another way. Pinch analysis was used to maximise heat integration of the plasma-assisted processes. Oluleye et al. 2016 developed a screening methodology to identify options to upgrade low grade excess heat with heat pumps. However, the focus of their work was to increase the degree of heat recovery and not a fundamental switch to using electricity to provide heat.

2.3 Summary of knowledge gaps in existing literature

The detailed literature review revealed that there is a clear lack of studies with assessment methodologies that systematically screen and assess process electrification measures for given industrial sites for an early-stage bottom-up assessment. More specifically, none of the published studies presents a consistent way of mapping relevant electrification options for a specific process plant, considering how reaction, separation, heat recovery and utility systems are affected (see Figure 1), and how this affects the site's utility demands (e.g. fuel, steam and cooling water) and excess heat availability for other purposes. Furthermore, there is no study that combines the afore-mentioned impacts on process-related systems with a techno-economic and greenhouse gas emissions assessment that takes energy targeting tools and future energy market scenarios (e.g. share of renewable electricity and electricity prices) into account simultaneously. Energy targeting tools are used in some of the studies but not to understand how electrification of specific industrial processes impacts energy flows and heat integration opportunities throughout the industrial site's core processes and utility system (e.g. heat recovery, utility steam demands, generation of internal fuel by-products and high-temperature excess heat sources, steam cycle power generation, excess heat delivered for external use, fuel use, cooling demands, and emissions).

3 Assessment framework and validation in case studies

This chapter describes the proposed bottom-up assessment framework and the selection of case studies for the validation of the methodology. In addition, case study-specific methodological aspects and assumptions are highlighted. The case studies included in this work fulfil a number of important functions. On the one hand, they were necessary to test and validate the proposed methodology. On the other hand, they were selected to highlight the impact of electrification on specific industrial processes. Furthermore, the case studies enabled some general conclusions to be drawn regarding the consequences of electrification in the process industry sector.

3.1 Assessment framework for process electrification options

The steps included in the assessment framework are listed below and the system boundaries for the individual steps are indicated in brackets. It should be noted that the framework can be used to assess individual process electrification options as well as combinations thereof.

1. Definition of the existing process system (reference process) and its unit operations (plant)
2. Identification of electrification options and the affected process-related systems (plant)
3. Establishing process data for the existing plant required to conduct process integration studies, using modelling and simulation if necessary (plant)
4. Establishing process data for the electrified unit operation to conduct process integration studies, using modelling and simulation if necessary (unit operation)
5. Heat integration studies of the reference and the modified process using pinch analysis tools based on flowsheet and process data from steps 3 and 4 (plant)
6. Inventory of all relevant changes in input and output flows of material and energy compared to the reference process (plant)
7. Techno-economic and greenhouse gas emissions assessment (plant plus surrounding energy system)

3.1.1 Definition of the existing process system and its unit operations

All units and process streams in the existing process system are first mapped at the plant level (including process-related systems). This step is important not only as a basis for screening for electrification options that could replace existing unit operations but also to establish a reference case for assessing the impact of electrification options. In this step, information is collected about existing unit operations, their operating conditions, and how they are connected to each other. This also includes the identification of raw materials and intermediates since these could be produced by electricity-based processes as well.

3.1.2 Identification of electrification options and the affected process-related systems

In this step, electricity-driven options are identified for one or several of the existing unit operations. This is an iterative process that starts by identifying candidate electrification technologies (e.g. electric steam generators to provide steam) before ensuring that specific technologies can satisfy the operating condition requirements of the existing system. The process design hierarchy presented in Figure 1 is used here to support the systematic screening for electrification options and to classify them from a process perspective. This allows a first assessment of the electrification options in terms of expected effects (which is important to know for modelling and simulation in the next step), but also in terms if implementation efforts (since options that affect the utility system only tend to be less complex). Results from this first assessment can then be used to identify the electrification options, or combinations of electrification options, to be investigated in the following in-depth studies. Helpful tools for the identification of electrification options are technology inventories (such as EPRI 2009) that list candidate electrification technologies that are suitable for specific industrial processes.

3.1.3 Establishing process data for the existing plant required to conduct process integration studies, using modelling and simulation if necessary

The extensiveness of this step depends on the parts of the existing process that are affected. For cases in which the heat recovery, separation/recycle or reactor systems are affected, the implementation of electrification technologies will change the heat flows and possibly the heat recovery potential as well as the availability of excess heat. To analyse these effects, data for individual process streams is required. Thus, the goal of this step is to establish data for all heat sources and heat sinks that is required for the subsequent heat integration studies. Such data can be derived from process modelling and simulation, but also from access to process data logs or available design data.

If only the water and effluent treatment or the heating and cooling utilities are affected (e.g. electric steam generation instead of natural gas boiler), it might not be necessary to generate data for individual process streams. Instead, information about the heating and cooling demand (and also possible variations) for the utility system or water and effluent treatment system model is sufficient. The model must also deliver information about the fuel demand and related greenhouse gas emissions.

3.1.4 Establishing process data for the electrified unit operation to conduct process integration studies, using modelling and simulation if necessary

In this step, process data for the electrified unit operation(s) needed for the subsequent heat integration studies is established. As in the previous step, the information needed depends on the process parts that are affected. For electrification technologies that have an impact on heat recovery potential and excess heat availability, information at the level of individual streams is required. As mentioned in the previous step, such data can come from modelling and simulation, process data logs or design data. When modelling, it is important to adjust the model parameters to meet the specifications of the existing process, meaning that outlet flows must meet the same specifications as the corresponding flows in the conventional unit. The models must also generate data related to the electricity demand and related on-site greenhouse gas emissions (if any).

3.1.5 Heat integration studies of the reference and the modified process using pinch analysis tools based on flowsheet and process data from steps 3 and 4

If heat recovery, separation/recycle or reactor systems are affected, heat integration studies need to be performed to assess the impact on the heat recovery potential and the excess heat availability in detail. This is done by applying pinch tools to estimate heat recovery as well as heating and cooling utility targets for a given value of the minimum temperature difference ΔT_{min} that is acceptable for heat exchanging. For the reference process, a Grand Composite Curve (GCC) is generated in order to establish the theoretical minimum hot and cold utility demands. Afterwards, process streams that are related to the unit operation(s) to be replaced by the electrified unit operation are removed from the list of process streams included in the analysis (stream table). The remaining streams form the so-called *background* process. The process streams that are related to the electrified unit operation on the other hand form the *foreground* process. The concept of split-GCCs (Kemp 2006) is then used to visualize how well the electrified unit operation (foreground) can be heat integrated with the background process. In the ideal case, heat can be exchanged between the foreground and background processes, resulting in lower utility demands for the combined process. In order to allow a fair comparison, it is assumed that the maximum energy recovery (MER) target, with minimum utility usage, is achieved for both the reference process and the modified process with the electrified unit operation. Using this assumption only for the modified process would be a disadvantage for the reference process which will most likely not reach this target with the current heat exchanger network design.

3.1.6 Inventory of all relevant changes in input and output flows of material and energy compared to the reference process

In this step, a full inventory is compiled for the following parameters for the two cases (reference process and electrified process):

- Minimum heating and cooling demand (assuming maximum heat recovery)
- Electricity demand
- Fuel balances (demand and fuel type)
- Combined heat and power production opportunities
- Excess heat availability
- Direct process greenhouse gas emissions, as well as fuel-related greenhouse gas emissions

3.1.7 Techno-economic and greenhouse gas emission assessment

The final step is to perform a techno-economic and greenhouse gas emission assessment which takes into account energy costs, as well as greenhouse gas emissions and associated costs. It is important to note that the system boundary is expanded in this step to include the surrounding energy system. In this manner, off-site greenhouse gas emissions are included in the assessment. The operating cost and the greenhouse gas emissions for the electrification technologies are highly dependent on process and emission factors for the background energy system. The capital cost on the other hand usually depends on the size of the equipment (economy of scale). The ultimate goal of this step is to calculate the possible reductions in greenhouse gas emissions versus the capital and variable costs compared to the reference case.

The integration of electrification options will normally lead to an increased electricity demand. Consequently, the change in greenhouse gas emissions depends strongly on the carbon-intensity of the electricity grid. However, when modifying existing processes, opportunities for cogeneration of electric power can arise. This can be the case when heat that was previously used by the replaced unit operation is now available to run a steam turbine that is connected to a generator. In this case, the electricity produced on-site can be used to drive the electrified unit operation so that the demand for electricity import is decreased. Since the potential for excess heat delivery (e.g. for district heating) can also be affected, it is important to take the corresponding change in revenues into account. Furthermore, selling new by-products that arise as a result of electrification can lead to additional revenue. For example, when producing hydrogen from water electrolysis, oxygen occurs as a by-product that can potentially be sold. To calculate the corresponding running cost (including revenues from excess heat and by-products) and the greenhouse gas emissions, information about the following parameters is required:

- Fossil fuel prices and emission factors
- Electricity price and grid emission factors
- Costs for greenhouse gas emissions (e.g. EU ETS, national tax systems and other relevant policy instruments)
- Income from export of excess heat and carbon intensity of the heat sink to which excess heat is exported
- Sales prices and emission factors for new by-products

Since electrification is one option for industry to comply with ambitious medium- and long-term national climate targets, the expected development of these parameters is of high interest. This is even more the case for electrification options with a low technical maturity which can only be considered for implementation in the medium- or long-term. This leads to a need for consistent future energy market scenarios in which the values of the aforementioned parameters are internally consistent.

3.2 Selection of relevant case studies for validation of the assessment framework

The bottom-up assessment framework was tested and validated in three different case studies in the three different papers. Figure 3 shows an overview of the case studies together with the affected process parts in the in-depth assessments. The case study in Paper I was selected to illustrate the impacts of an electrification option that affects a core reaction of an existing process, leading to significant changes for the heat recovery potential and the excess heat availability. In addition, it was assumed that the existing boiler was replaced by electric steam generation, i.e. a technology that affects the utility system. In both case studies in Papers II and III, the utility systems of the investigated processes were affected but the industrial processes are different (chemical plant and oil refinery). Furthermore, the case study in Paper II was conducted to illustrate the need for an advanced model of the steam system to assess the true impact of making changes to steam flows in a complex steam network. The case study in Paper III, on the other hand, was selected as an example of a system that is characterized by operating conditions that vary significantly, and thereby illustrates a need to model these variations and optimize the process configuration for a number of different operating conditions. In addition to the in-depth assessments, Papers I and II also map and classify other process electrification options.

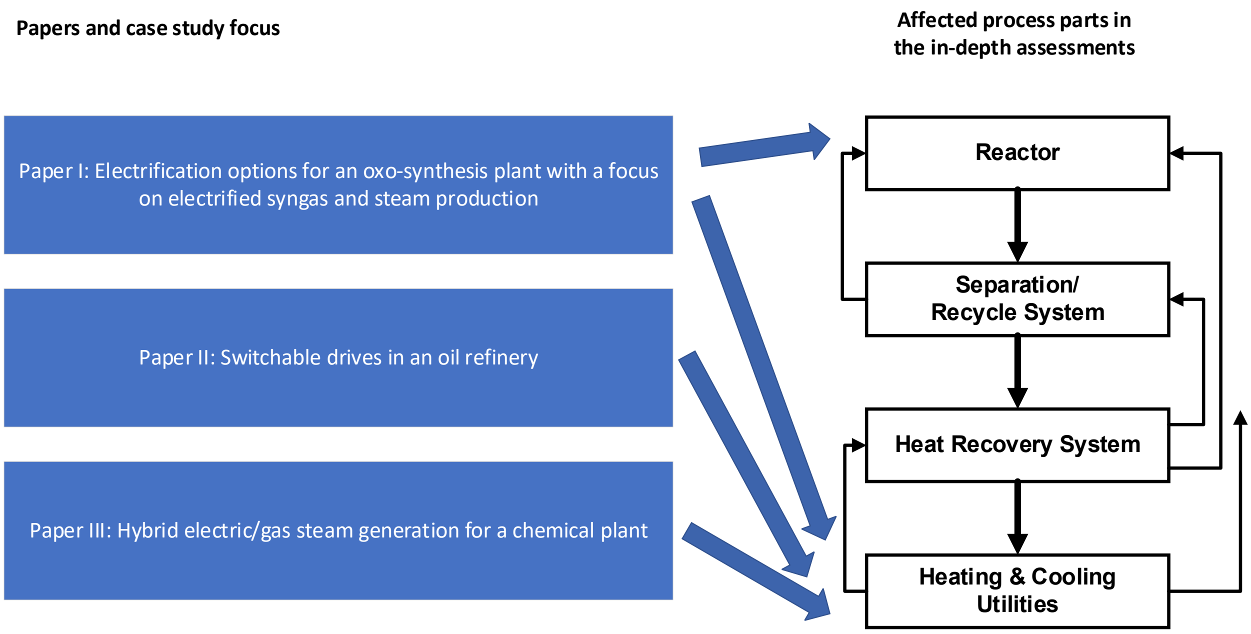

Figure 3: Overview of the case studies together with an indication of the affected process parts for the in-depth assessment.

3.2.1 *Electrification options for an oxo synthesis plant with focus on electrified syngas and steam production (Paper I)*

In this case study, different electrification options for an oxo-synthesis plant and their impacts on the existing process were mapped. Furthermore, a detailed assessment in terms of greenhouse gas emissions and cost was performed for a combination of electrified syngas and steam production. In this approach, the existing non-catalytic partial oxidation (NC-POX) to produce the syngas needed for downstream processing was assumed to be replaced by a reverse water gas shift (RWGS) reaction that was coupled to a water electrolyser. The purpose of the electrolyser is to provide the hydrogen needed for the RWGS reaction (in addition to CO_2). Since process streams from the reference plant could be heat integrated with other parts of the processes at the plant, detailed heat integration studies on the level of individual streams with split-GGCs were performed. For this purpose, an Aspen HYSYS model for the RWGS reaction model was used to establish the required stream data.

Figure 4 show the system boundaries that were used for the greenhouse gas emission assessment. Since the assessment was a well-to-gate assessment, the emissions from the final products during their lifetimes were not considered (since these were assumed to be the same for the reference and the electrified case), and the CO_2 feedstock was accounted as avoided emissions at the plant at which it was assumed to be captured.

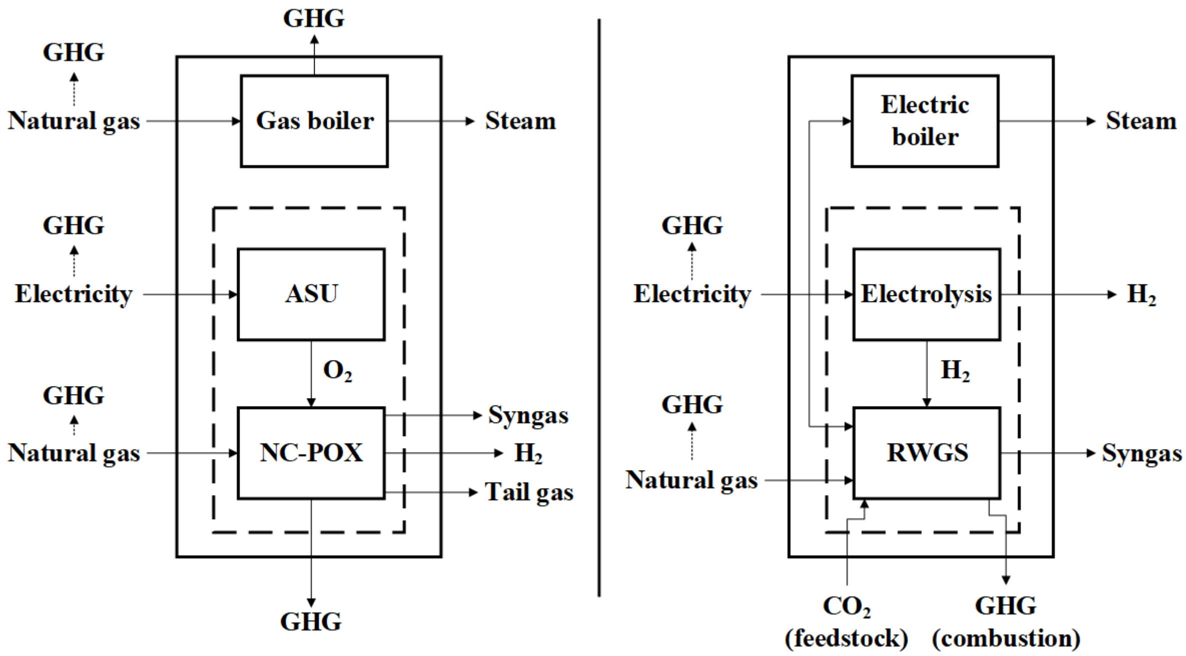

Figure 4: Comparison of the reference with the electrified syngas production concept including on-site and off-site greenhouse gas (GHG) emissions for the conventional syngas production (left) and the electrified syngas production (right). The dashed boxes represent the two syngas production technologies. Emissions crossing the solid lines boxes are on-site emissions while emissions occurring outside of this box are off-site emissions. Abbreviations: NC-POX = non-catalytic partial oxidation, ASU = air separation unit and RWGS = reverse water gas shift.

For the economic assessment, the change of operating cost resulting from switching to electrified syngas and steam production was considered. The assessment was performed following the methodology described in Pettersson et al. (2020), adopting two different future energy market scenarios based primarily on data from IEA's World Energy Outlook 2018 (International Energy Agency 2018) and generated by the ENPAC tool (Axelsson and Harvey 2010, Axelsson and Pettersson 2014).

3.2.2 Switchable drives in an oil refinery (Paper II)

This case study investigated how switchable drives in an oil refinery can be used to increase and decrease the electricity demand for the utility system and to thus estimate the range of flexibility. Switchable drives are a configuration in which either steam turbines or electric motors can be used to drive pumps and compressors in the plant, mainly for the reason of redundancy but also as a way to use excess steam while having electricity as back-up. Figure 5 shows a simplified overview of the refinery steam system that was investigated. Note that a number of steam turbines between the steam headers have been consolidated in the figure. If electric motors are used to run pumps and compressors, steam with a higher enthalpy can be passed on to the next header. The figure also shows that waste heat recovery boilers and additional steam boilers, that can run on liquefied natural gas (LNG) or refinery fuel gas and vaporized liquid products, are used to provide the steam.

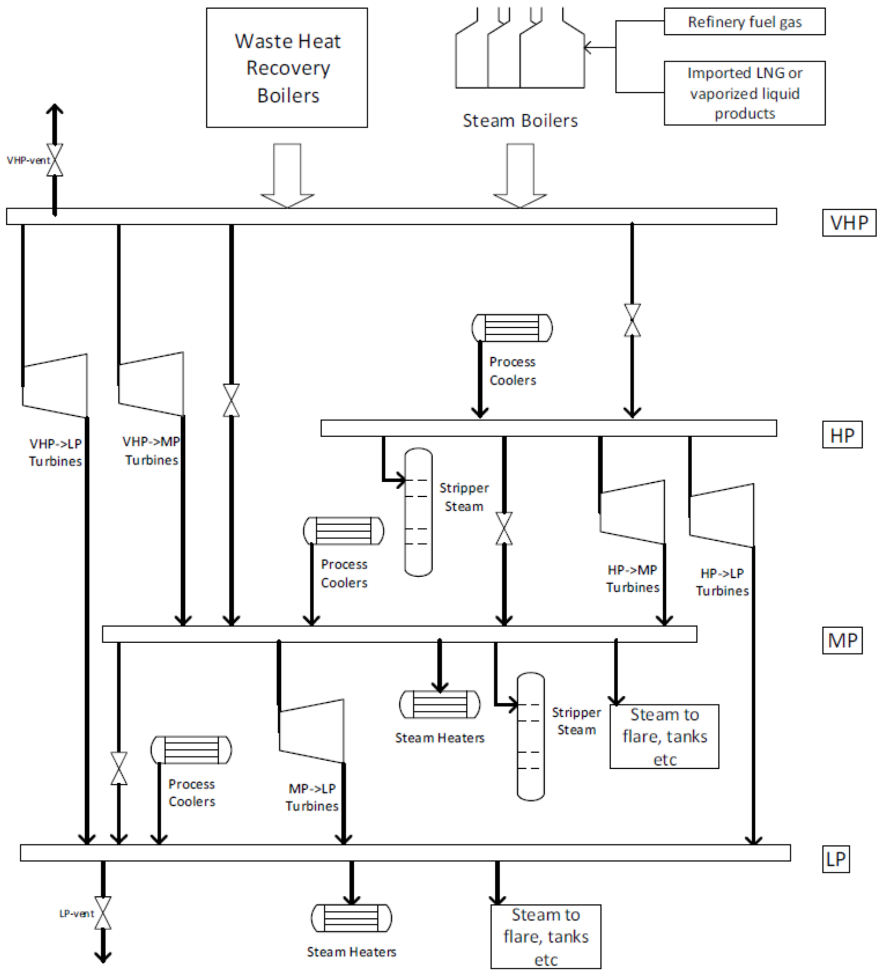

Figure 5: General overview of the refinery's steam system (Marton et al. 2017)

The optimal selection of which, and how many, drives should be in electric motor mode, is a complex problem that involves balancing the steam production and demand at several steam headers, and a very large number of on-off decisions that change steam flows though turbines in discrete steps. To handle this, an Aspen Utilities Planner model for the utility system including the switchable drives was used for the assessment to capture the effects when changing steam flows in this complex steam system. The built-in optimizer function, which uses a mixed-integer linear programming (MILP) solver, was used with the objective function to minimize the total utility cost (i.e. the cost for purchasing electricity and LNG). Decision variables were the on-off decisions for the switchable drives as well as steam flows though valves and turbines. Constraints in the model are related to temperatures and pressures at the steam header and the power demand for pumps and compressors. For typical operating conditions in September, extreme prices for electricity and LNG were used to force maximum and minimum electricity usage. After that, a greenhouse gas emission assessment was performed in which the maximum and minimum electricity usage cases were compared to the reference operation case (i.e. how the plant is operated today).

3.2.3 Hybrid electric/gas steam generation in a chemical plant (Paper III)

In this case study, the impact of using hybrid electric/gas steam generation to satisfy the fluctuating steam demand of a chemical plant was assessed. As can be seen in Figure 6, a hybrid system combines an electric steam generator and a gas boiler that can use either natural gas or biomethane as fuel.

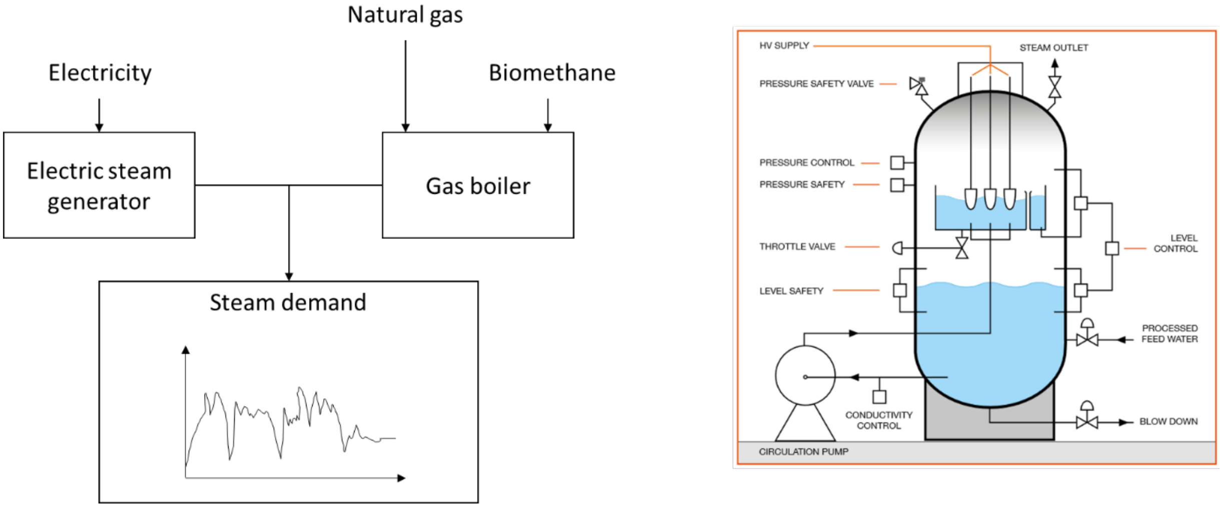

Figure 6: The hybrid steam generation concept considers in this study (left) and an example of a stand-alone electric steam generator (Parat Halvorsen AB 2020) (right).

There are several special aspects in this case study. In contrast to the other case studies, a linear programming model was used to identify the optimal boiler capacities and steam generation (operating) patterns that satisfy the fluctuating steam demand of the chemical plant. The objective function was to minimise the total annual cost for steam production, taking the investment costs, fuel costs (electricity, natural gas and biomethane), as well as costs related to CO_2 emissions into account. The decision variables were the installed capacities of the electric steam generator and the gas boiler, as well as the hourly steam production from the three different fuels. Besides a demand constraint, additional constraints on the electricity grid connection capacity and the annual on-site emissions were implemented. To investigate the interplay with fluctuating conditions on the energy market, reference conditions for 2019 and different scenarios for 2030 and 2040 with hourly resolutions were used. What-if assessments were performed to analyse how the investment in a certain generation mix would perform under different future market conditions.

4 Case study results

4.1 Electrified syngas production in an oxo-synthesis plant (Paper I)

Table 2 presents the results from the mapping of electrification options for the oxo-synthesis plant, together with a classification in terms of affected process-related systems. It was found that electrification options include options that affect only the utility system, options related to feedstock production, as well as options that would replace the existing syngas production at the plant.

Table 2: Detailed description of the process electrification options for the oxo synthesis plant including technical maturity and affected process-related systems (DECHEMA 2017, Foit et al. 2017, Reller et al. 2017). The electrification options selected for the following in-depth assessment are highlighted.

	Electrification option	**Technical maturity**	**Affected process-related systems**
1	Production of electro-methane to replace natural gas for the syngas production unit.	Medium	Electro-feedstock, no changes to the core process
2	Direct electro-catalytic production of ethylene (single-step electro-chemical reduction of CO_2 with a Cu-based catalyst.	Low	
3	Methanol-to-olefins with renewable methanol (methanol can be imported and processed on-site). Hydrogen from water electrolysis is combined with CO_2 in a methanol synthesis reaction to produce methanol. Methanol is then converted to ethylene and propylene.	High	
4	Water electrolysis to produce Hydrogen and oxygen for alcohol and acid synthesis	High	
5a	Syngas production by Reverse Water Gas Shift (RWGS) reaction coupled with CO_2 import and hydrogen production from water electrolysis.	Medium	Syngas production
5b	Syngas production by coupling carbon monoxide production from low-temperature electrolysis of CO_2 with hydrogen production from water electrolysis.	Low	
5c	High-temperature co-electrolysis of water and CO_2 with solid oxide electrolysis cells to produce syngas directly.	Low	
6	Electric steam generation to replace the combustion of fuel gas	High	Steam/utility system

Electrified syngas production as a combination of a RWGS reaction and water electrolysis was coupled with electric steam generation and assessed more in detail. In this configuration, CO_2 is combined with hydrogen from water electrolysis in a RWGS reaction to produce syngas. It was assumed that the required CO_2 feedstock comes from another plant and is available at no cost. A key finding was that replacing the conventional syngas production with electrified syngas production had a strong impact on heat integration potentials, highlighting the importance of detailed energy targeting as part of the developed methodology for the assessment of electrification at an industrial site. This aspect is illustrated in Figure 7 which shows the GCC and split-GCC for the electrified syngas production. It can be seen from the split-GCC that there is essentially no heat integration possible between the foreground and the background GCCs. Accordingly, the minimum heating and cooling demands at maximum energy recovery increased from 4 MW and 89 MW for the existing syngas production to 60 MW and 183 MW (see GCC) for the electrified syngas production, respectively. This strong increase stems from the introduction of a new heating demand for the RWGS reaction but also, notably, from the fact that heat from the conventional syngas production that could have been integrated with the other process streams at the plant was not available anymore (see Figure 6 in Paper I for the GCC and the split-GCC for integration options of the existing syngas production).

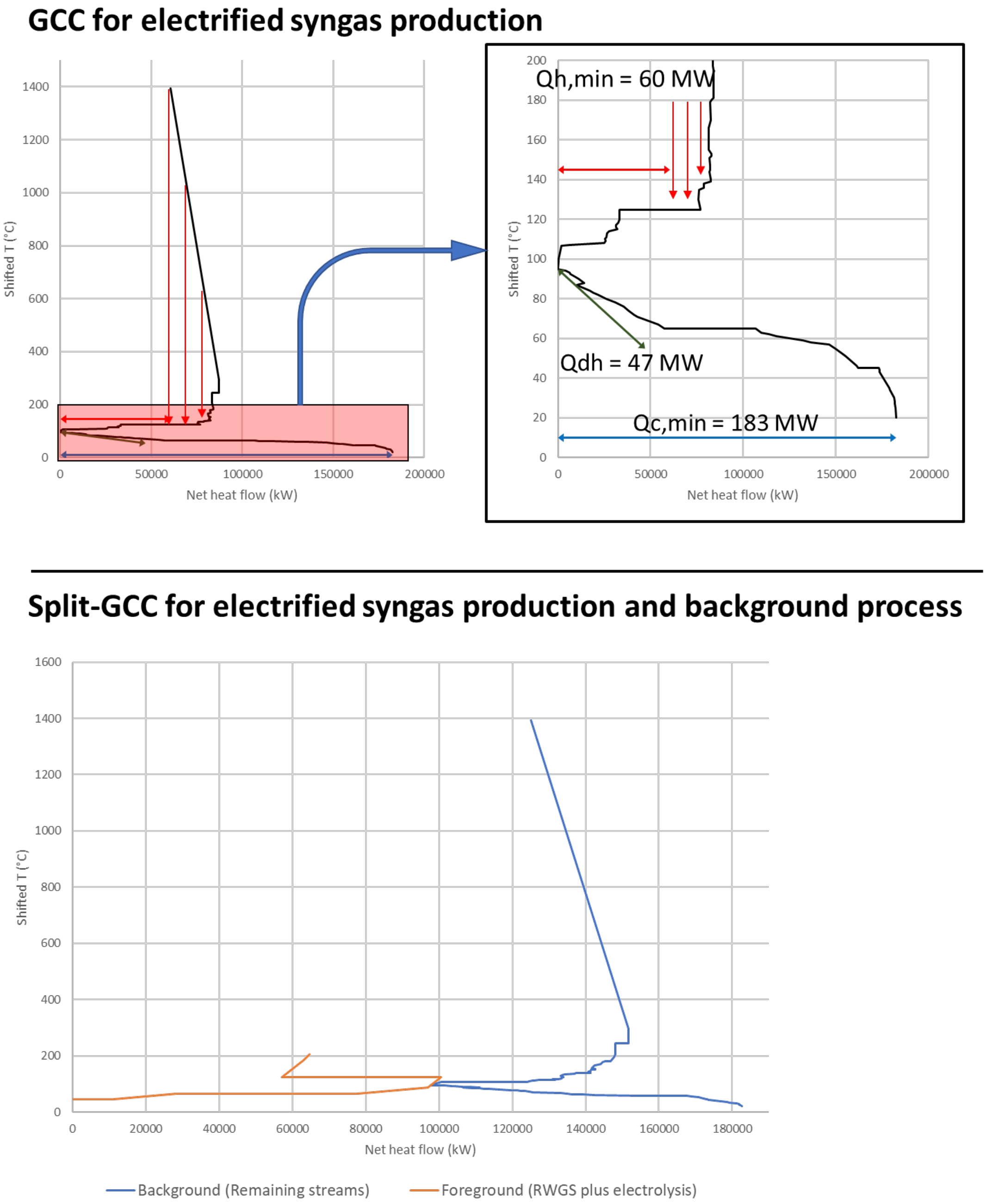

Figure 7: GCC and split-GCC for the electrified syngas case. In the GCC, the minimum heating (Qh,min) and cooling (Qc,min) demands, as well as the district heating delivery potential (Qdh) are indicated. The red vertical arrows indicate the heat pocket.

Another key finding was that there is a strong impact on energy flows related to natural gas feedstock and electricity. The natural gas demand decreased significantly since the conventional syngas production based non-catalytic partial oxidation of natural gas was replaced. The strong increase in electricity demand has two causes. On the one hand, a large electricity demand was introduced for the production of hydrogen by water electrolysis. On the other hand, electricity for electric steam generation was required to satisfy process steam demand that could have been satisfied by heat integration of the conventional syngas production before. The latter finding was the result of the detailed heat integration studies and would have been overlooked in simplified assessment analyses where only natural gas feedstock would be replaced by electricity and CO_2.

For the techno-economic assessment, two energy market scenarios based primarily on data from the "New policies" and the "Sustainable development" scenarios from IEA's World Energy Outlook 2018 (International Energy Agency 2018) were generated, see Pettersson et al. (2020) for further details. The "New Policies" scenario is a predictive scenario that takes the impact of existing policy framework and today's announced policies into account. The "Sustainable Development" scenario on the other hand is a back-casting scenario in which energy-related CO_2 emissions peak in 2020 before they follow a trajectory that is fully aligned with the objectives of the Paris Agreement. In addition, it was assumed that the price for the CO_2 feedstock is zero as best-case scenario. The corresponding cost and carbon factors are shown in Table 3.

Table 3: Cost factors generated with the ENPAC tool based on the two IEA World Energy Outlook 2018 scenarios "New Policies" and "Sustainable Development" (Pettersson et al. 2020).

Parameter	**Unit**	**New Policies 2030**	**Sustainable Development 2040**
CO_2 emission charge (general)	€/tCO_2	29	126
Natural gas price incl. CO_2 charge	€/MWh	41	61
Electricity price incl. grid charge	€/MWh	54	63
Build margin power generation technology	-	Wind power	Nuclear power
Carbon factor	kgCO_2eq/MWh	0	0
Price of CO_2 (feedstock)	€/tCO_2	0	0

Table 4 shows the case study results in terms of avoided greenhouse gas emissions and operating cost for the two energy market scenarios. The avoided emissions are to a large extent caused by the demand for CO_2 as feedstock since it was assumed that these are avoided emissions elsewhere. The other reduction contribution comes from the fuel switch from natural gas to electricity which reduces the on-site CO_2 emissions. A small share of CO_2 emissions is caused by the combustion of natural gas to provide high-temperature heat for the RWGS reaction. It can also be seen that the large emission reduction potential comes at the expense of (much) higher operating costs. However, the large demand for CO_2 which was identified can pose a challenge in terms of infrastructure and is a large uncertainty in the assessment since the future cost of CO_2 as feedstock is uncertain.

Table 4: Avoided GHG emissions and changes in operating cost for the two different scenarios.

Avoided GHG emissions	333 kt/a
• ***Natural gas (NC-POX and gas boiler)***	*77 kt/a*
• ***Natural gas (RWGS)***	*-16 kt/a*
• ***CO_2 feedstock***	*272 kt/a*
Change in operating cost **“New policies 2030”**	+59 M€/a
• ***Natural gas***	*-56 M€/a*
• ***Electricity***	*+115 M€/a*
Change in operating cost **“Sustainable Development 2040”**	+50 M€/a
• ***Natural gas***	*-85 M€/a*
• ***Electricity***	*+135 M€/a*

4.2 Switchable drives in an oil refinery (Paper II)

The main results for this paper are summarised in Table 5. One of the key results of the study was that the electricity demand for the case with very low electricity prices (Max. electricity usage) was lower than the theoretical demand if all available switchable drives would use electricity (9.4 MW). The reason for this lies in the existence of unavoidable residual process gases which are not allowed to be flared. Accordingly, this gas is fired in the utility boilers to produce steam. Since the cost for producing this steam is in practice negligible, it is used for operating a number of switchable drives before the remaining drives switch to electricity, even if the electricity price is very low. The occurrence of side-streams such as fuel gases which do not have a high market value (e.g. due to their changing compositions) or for which there is no available transport infrastructure was clearly identified as one barrier for increased electrification that occurs at other plants as well. It can also be seen from the table that this electrification option has only a rather small CO_2 emission reduction potential compared to the reference operation (which is how the owner operates the plant today). However, the results also show that there is a difference of 5.7 MW in electricity demand between the maximum and minimum electricity usage cases which could be used to provide flexibility rather easily. It can also be seen that the amount of excess LP steam (which is the lowest pressure level in the plant, see Figure 5) which is vented to the atmosphere is much larger for the minimum electricity usage case. The reason for this is that there is an inevitable excess of LP steam when steam is used to drive the turbines at higher pressure levels. In the case of maximum electricity usage, much less fuel is fired within the boilers file its use is optimised before the remaining driving force is provided by electric motor.

Table 5: Results for the reference operation as well as maximum and minimum electricity usage without violating constraints.

Variable	Unit	Reference operation	Max. electricity usage	Min. electricity usage
Electric energy used to operate dual-drive pumps	MWh/h	5.819	7.036	1.332
Total fuel fired within the boilers	t/h	6.684	5.439	13.483
Whereof total site LNG consumption	t/h	0.325	0.264	0.655
On-site boiler fuel emissions	tCO_2/h	23.3	19.0	47.1
Off-site emissions related to electric power purchased from the grid	tCO_2/h	0.3	0.3	0.1
Total emissions	tCO_2/h	23.6	19.3	47.1
Steam production from the boilers	t/h	70.6	57.5	142.4
Number of switchable pumps with “steam turbine driver”	-	15/33	13/33	32/33
Total steam vented to the atmosphere	t/h	16	3	94

Using the advanced steam system model within the proposed assessment framework allowed to capture the effects of switchable drives in the existing complex steam system in detail. In contrast, simple assessments that assume a complete switch to electricity in all switchable drives with fixed ratios between increase in electricity demand and decrease in CO_2 emissions would have overestimated the electricity demand as well as the emission reduction potential. In particular, the availability of unavoidable fuel gases, which occurs also at other plants, limits the effects of using switchable drives to reduce greenhouse gas emissions.

4.3 Hybrid electric/gas steam generation in a chemical plant (Paper III)

Initial runs of the optimisation model led to the optimal generation capacities for hybrid systems with a minimized total annual cost of steam production for each of the scenarios. To simulate investment decisions and analyse the economic performance, two sets of generation capacities were derived from the initial runs. The first set (denoted as “Opt. 1”), is a hybrid system with a 37.9 MW electric boiler and a 29.8 MW gas boiler and represents the average of the optimal values for Swedish conditions in 2030 and 2040 without on-site CO_2 emission and electric grid connection capacity limitations. The second set (denoted as "Opt. 2") consists of a 29.7 MW electric boiler and a 38.0 MW gas boiler and represents the average optimal values when including on-site CO_2 emission and electric grid connection limitations. The underlying market and electricity generation conditions are shown in Table 6 (Scenario data).

Table 6: Reference and scenario-based market and electricity generation conditions for the What-if runs in Figure 8.

	Description	**Value**
Reference conditions (2019)	Electricity price	38 €/MWh on average (hourly resolution)
	Natural gas price	20 €/MWh
	Biomethane price	77 €/MWh
	CO_2 emission charge	25 €/tCO_2
	Grid fee	Electricity grid: 9 €/MWh Gas grid: 15 €/MWh
	Specific on-site fossil CO_2 emissions	NG: 0.202 tCO_2/MWh
		Biomethane: 0 tCO_2/MWh
Scenario data	Electricity price	Time-dependent, 3h resolution for 2 scenarios: 1. SWE NoColl 2030 (average 33 €/MWh) 2. SWE NoColl 2040 (average 44 €/MWh)
	Natural gas price	22 €/MWh
	Biomethane price	77 €/MWh
	CO_2 emission charge	40 €/tCO_2 (2030), 100 €/tCO_2 (2040)
	Grid fee	Electric grid: 9 €/MWh Gas grid: 15 €/MWh
	Specific on-site fossil CO_2 emissions	NG: 0.202 tCO_2/MWh
		Biomethane: 0 tCO_2/MWh

The two sets of hybrid steam generation systems together with a gas boiler only (denoted as "Gas boiler") were used in 15 What-if optimisation runs to investigate how the three configurations would perform in terms of running cost assuming that certain scenarios would come true. Figure 8 shows the corresponding results for these runs.

The results show rather similar running costs for the reference conditions based on historical data for 2019 (denoted as "runs 1-3" below the bars in the figure). However, the running cost is slightly lower for the hybrid systems (Opt. 1 and Opt. 2) which can switch to electricity during periods with low electricity prices. The cost advantage of the hybrid systems becomes much greater for future conditions in 2030 and 2040 due to the increased CO_2 emission charges (runs 4-9). In the hybrid systems, most steam is produced from electricity under such conditions.

To investigate how a constraint on on-site CO_2 emissions would affect the optimal operation, additional What-if runs were analysed. The corresponding limitations for on-site CO_2 emissions in 2030 and 2040 were set in line with a trajectory that follows the Swedish target of net zero emissions by 2045 (assuming a linear decrease from current CO_2 emission levels). For these scenarios (runs 10-15) the optimal steam production as well as the running cost are significantly different from the runs without on-site CO_2 emission constraints. The only option for the gas boiler only to comply with the CO_2 emission limit is to switch to steam production from relatively expensive biomethane, leading to high running costs. The hybrid systems instead can switch to electricity, resulting in running costs similar to the cases without limitations on the on-site CO_2 emissions. As can be seen, the running cost for the two hybrid systems is very similar in all cases.

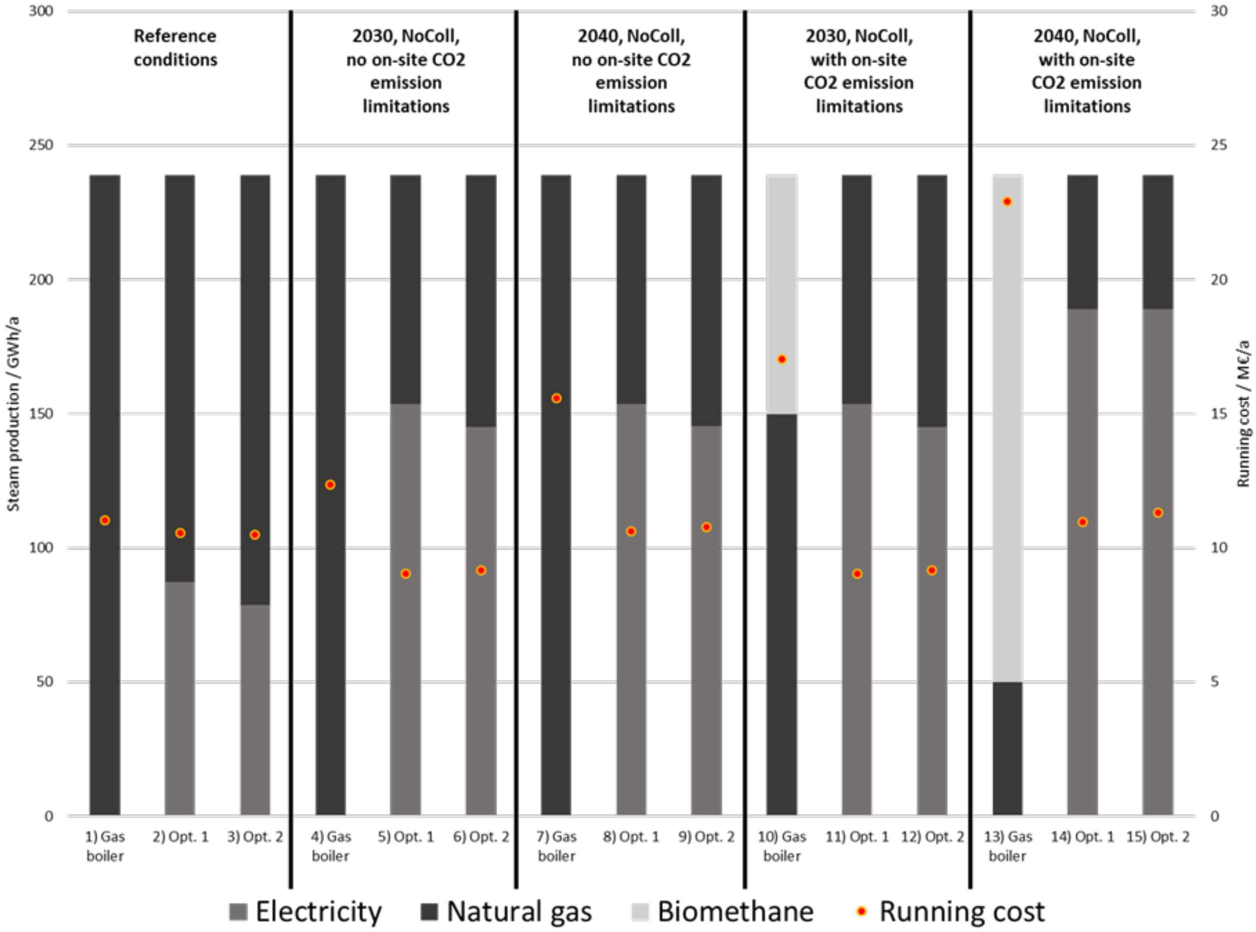

Figure 8: Steam production from different fuels (stacked bars) and running cost (red dots) for the three different investment decisions for current market conditions, 2030 and 2040 and for the cases with and without limitations on on-site CO2 emissions. The numbers below the bars are related to the "runs" described in the text.

This case study about hybrid electric/gas steam generation highlights different aspects of the assessment framework. On the one hand, it indicates that a detailed energy targeting analysis at the process stream level is not required for the assessment of this electrification option in the utility system. On the other hand, the study emphasizes the influence of fluctuating operating conditions and the strong connection to fluctuating fuel and electricity markets. This creates a demand for detailed optimisation of the design (in terms of installed capacities) and operating conditions considering current and future energy market conditions.

5 Discussion

The bottom-up assessment framework proposed in this thesis provides a more comprehensive picture of the greenhouse gas emission reduction potentials and the associated techno-economic performance when integrating electrification technologies into existing plants. In contrast to other methodological approaches, it captures effects down to the level of individual process mass and heat flows that can have a strong impact on the evaluation of process electrification in terms of greenhouse gas emissions and costs. Since different types of process electrification options can be implemented in process-related systems ranging from the core reactor and separation systems to the heat recovery and utility systems (see Figure 1), not all the steps of the framework might be equally important for different options. Nevertheless, this does not affect the key insight that the specific conditions at individual plants must be taken into account and that the assessment of long-lived investments or long-term options needs to consider potential future changes in energy market conditions affecting the performance of the electrification measures.

The applicability and reliability of the bottom-up assessment framework depend strongly on the availability of detailed process data and models for existing unit operations and those that are related to the process electrification technology options. Especially for new technologies, such data and models might not be available. Another integral and significant part of the assessment framework is the selection of system boundaries and energy market scenarios for the background energy system. The system boundaries must be selected carefully to allow a fair comparison with reference cases for existing systems but also with other options for greenhouse gas emission reduction. Furthermore, the choice of energy market scenarios has a strong impact on the estimation of greenhouse gas emission reduction potential and costs. It is important to include sufficiently different scenarios based on possible market developments since specific electrification options might perform well under one scenario but not for others. This is important in the industrial decision making process to find options that perform reasonably well under many scenarios and to reduce the risk of investments in electrification options.

The case studies were selected to perform assessments not only for different industrial plants and processes but also for electrification options that affect the existing process plants at different hierarchy levels (see Figure 1). As can be seen in Figure 3, none of the case studies are related to the separation/recycle and heat recovery systems. Electrification options impacting these parts of existing processes will most likely also affect the heat integration potential with subsequent consequences on overall mass and energy balances, emissions and costs. Thus, corresponding case studies would highlight similar aspects of the assessment framework as the oxo synthesis case study example does. However, electrification within the heat recovery system, e.g. by using heat pumps, would primarily be implemented to reduce the demand for external utility by using comparatively low amounts of electricity.

Electrification within the reactor and separation/recycle systems could potentially introduce much larger electricity demands.

The results from the case studies are to some extent specific for the individual plants that were in focus. However, some of the findings can be generalised. Electrification options that affect the core parts of the process plant, as presented in Figure 1, have an effect on the heat integration potential and thus require more detailed analyses with the help of heat integration tools. As shown by the case study of the oxo synthesis plant (Paper I) it can even be the case that a high degree of heat integration at an existing plant represents a barrier to electrification since certain heat demands that are currently covered by a process heat source, might need be satisfied by a new heat supply if the heat source originates from a process that is replaced by the electrification technology. Options affecting only the utility system are usually easier to implement since they do not require as deep changes in the process plant compared to the options mentioned before. However, the case study for the switchable drives (Paper II) showed that the existence of residual fuel streams that are or could be used to produce steam could be a barrier to electrification of the utility system since these waste streams would have to be combusted anyway. A more general finding from the hybrid steam generation case study (Paper III) is that hybrid systems can be an attractive solution for the transition from a fossil fuel-based technology to a technology that depends on electricity. Such systems also open up the possibility to provide flexibility and to thus participate in different electricity markets, particularly peak-load demand shaving markets. However, the greenhouse gas emission reduction potential of hybrid (fossil fuel and electricity) systems is likely to be lower compared to more far-reaching electrification (also in combination with bio-based fuels) since fossil fuels would still be used. In terms of energy market scenarios, it was shown in all papers that the underlying assumptions have a strong effect on the greenhouse gas emission reduction potential but also the cost. This underlines not only the importance of using such scenarios for risk assessment purposes but also highlights the importance of a co-development of the electricity system towards lower carbon footprint and cost in order to increase the attractivity of process electrification.

6 Conclusions

In this thesis, a bottom-up assessment framework for electrification options in energy-intensive industrial process plants was presented and validated in a series of case studies. The framework accounts for on-site conditions of specific industrial plants and captures effects that are often overlooked in more general top-down studies that assume similar conditions for different industrial sites. One particular novelty is that the framework includes heat integration studies with pinch analysis tools to analyse how the heat surpluses or demands connected to electrification options change heat recovery potentials and utility demands. Furthermore, it includes energy market scenarios to assess the long-term economic performance and the carbon footprint.

The assessment framework was tested and validated in three different case studies for three different industrial plants. In these case studies, electrification options that affect different parts of the existing processes (e.g. the reactor system or utility system) were considered, highlighting different aspects of the proposed assessment framework. Results from the case studies underline the relevance of the proposed bottom-up assessment framework since a number of the consequences of introducing process electrification technologies into existing processes were not easy to predict using simplified methods. This was particularly true for the oxo synthesis plant case study in which the proposed electrification options had a strong influence on the heat recovery potential. This underlined the need to perform heat integration studies to capture effects on a site's overall energy balances and emissions beyond those flows that are directly affected by the electrification measure. The case study that investigated switchable drives in an oil refinery showed the importance of detailed process models (in this case for the steam system) due to the complexity of the steam system in which the effects of changing steam flows were not straightforward. The case study about hybrid electric/gas steam generation in a chemical plant instead highlighted the need to consider variations in operating conditions (of the existing plant) as well as future energy market conditions when optimizing the design of (partly) electrified heat supply systems.

The bottom-up assessment framework can be used to assess different electrification options and to compare them with a reference case or other greenhouse gas emission reduction measures. It can also complement top-down studies to get a more realistic and comprehensive picture of the greenhouse gas emission reduction potential and cost for process electrification. For this purpose, findings from specific bottom-up assessments can be generalised to draw general conclusions and to refine assumptions made in top-down assessments. The mapping of electrification options for different industrial sectors revealed a broad variety of electrification options that would affect the mass and heat flows of the existing processes to different extends depending on how close to the core processes they are implemented. Thus, it is clear that using the proposed assessment framework would be beneficial for the assessment of these electrification options as well.

In terms of process electrification in general, this thesis contributed by presenting an assessment framework that gives a more realistic picture about the effects of process electrification. Future work should focus on comparing electrification to other greenhouse gas emission reduction measures such as biomass and CCS, also from a bottom-up perspective.

7 Future work

Testing and validating the proposed assessment framework in the three case studies included in this thesis revealed certain aspects that can be starting points for further developments. One area of future development involves the assumptions and system boundaries related to feedstock, fuels and products. In the case study for the oxo synthesis plant for example, it was assumed that the CO_2 feedstock is available at no cost and that no additional greenhouse gas emissions are associated with its separation and transportation from the original source to the plant in which it is used. Although similar assumptions are made in many other published studies, they do not reflect reality in many cases, as discussed in Paper I. A further development of the framework would therefore be to refine the choice of system boundaries to include upstream and downstream effects in the general methodology in a more detailed way. Such choices will most likely have a strong impact on the financial feasibility and the greenhouse gas emission reduction potential of many electrification options.

Considering upstream and downstream effects is generally important when electrification involves the introduction of new feedstock to a process plant or leads to new products that will replace other products on the market. In particular, this may be the case for production of chemicals produced by combining a (fossil or bio-based) CO_2 feedstock with hydrogen from water electrolysis (also known as carbon capture and utilisation (CCU) and "Power-to-Chemicals"). In this context, it would be important to consider the spatial distances between hydrogen production, CO_2 capture and conditioning and synthesis of chemicals and fuels (which may require a transportation infrastructure coupled with additional cost and greenhouse gas emissions). It is also important to consider different technologies for CO_2 capture and concentration and electrolyser technologies for producing hydrogen. Regarding the products from CCU and thus the downstream effects, it is significant to consider which fossil or biogenic fuels and chemicals are replaced by electro-fuels and electro-chemicals. For example, there will be a difference in terms of overall greenhouse gas emission reduction potential when comparing the use in industrial processes with the use in the transportation sector. Such issues relate to sector coupling, since electro-fuels produced via CCU can be used in the transport sector while gaseous electro-fuels could also be fed into gas grids and then be used for heating in the residential sector. Consequently, future work should integrate the value chain perspective in the assessment framework.

Another area of development of the framework is to include tools that can support investment and operation decision making processes, as identified in the case study about hybrid electric/gas steam generation. In this context, is important to consider both short-term and long-term developments of energy market conditions, especially the electricity price. By adopting a multi-period optimisation approach, long-term investments could be optimised over the whole technical lifetime of an electrification option. In addition, operating decisions could be optimised for each expected set of operating conditions and prices. The ENPAC tool for example (used in the oxo synthesis case study) provides long-term energy market scenarios relevant for industrial users that include consistent sets of prices and emission factors for a wide range of industrially-relevant energy carriers. Energy systems models on the other hand provide insights into possible future electricity price variations at a higher time resolution than the ENPAC tool. These variations result from e.g. intermittency, as well as different assumptions about interconnections between regional grids or between different types of energy market. Future work could try to combine the insights from such different kind of models, with the aim to include short-term variations as well as long-term development as input to the industrial decision-making process. Future work could also be coupled to a stronger collaboration with experts in the field of energy systems modelling to identify and exchange good input data for the assessments. There could also be a feedback loop back to the energy systems modelling by including models of the electricity demand of individual industrial plants in the overall electricity system model. With this, it would be possible to identify possible bottlenecks in the electricity grid but also the increased demand for renewable electricity generation.

By adopting a multi-period approach the framework could be used to identify optimal investment and operating decisions for specific assumptions about future energy market conditions. However, since possible scenarios related to future energy market conditions vary significantly, it is important to include tools for uncertainty analysis in order to capture and quantify uncertainties related to electricity prices, fuel prices and costs associated with CO_2 emissions. This would allow a better risk assessment of investment decisions. In this respect, hybrid systems (e.g. hybrid electric/gas steam generation) but also storage opportunities (e.g. for heat and hydrogen) that can provide flexibility are attractive concepts to look further into.

Another pathway for future work is to test and validate the assessment framework, extended as discussed above, through additional case studies for other industrial processes and electrification options. In particular, performing a bottom-up assessment for CCU in which biogenic CO_2 from a pulp and paper plant is combined with hydrogen from water electrolysis would be ideal to test and validate a revised version of the assessment framework. Specifically, such a study could investigate heat integration potentials for different technologies to capture and process the CO_2, but also the integration implications of different electrolyser technologies. This would go beyond existing studies that neglect these effects and treat the components related to CCU as isolated unit operations. Furthermore, many current pulp and paper plants are net exporters of electricity that is eventually based on biomass. It can be attractive to use this renewable electricity for the electrification technologies related to CCU concepts since large grid extensions might not be required while being less influenced by electricity price variations. Future case studies could also focus on identifying and quantifying non-energy benefits (improved productivity and quality, environmental compliance and waste reduction) which can be the decisive factor for some electrification options.

In terms of technologies, it would be meaningful to investigate the applicability, greenhouse gas emission reduction potential and cost for heat pumps. It should be noted here that ongoing development of high temperature heat pumps can be expected to lead to a much wider range of applications for heat pumps in industrial processes. In contrast to the case study examples, heat pumps affect the heat recovery systems and utility demand of existing processes. In this regard, opportunities for heat pump integration should be identified before sizing electric or hybrid electric/gas steam generators to provide the remaining process heat demand. Together with heat storage options, such processes could provide larger amounts of flexibility to the electricity grid by shifting steam (and hot water) production heat production to times with low electricity prices. A targeted case study could investigate such combinations and quantify the amount of flexibility that such options could enable which could then be monetised on electricity markets.

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