Wired for Change

Handling Intermittency in a Renewable-Energy-Driven Chemical Industry

Svenja Bielefeld

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Contents

Summary

Almost 50 % of global CO_2 emissions are caused by power and heat generation and industrial processes [1]. If emissions allocated to energy generation for the industry are included in the industry's share, the industry is the biggest contributor to global emissions [2]. Almost one-fifth of industrial CO_2 emissions are attributed to the chemical industry [3]. Therefore, net emissions from the chemical industry need to be reduced if international CO_2 emission reduction goals are to be met.

About one third of the chemical industry's CO_2 emissions stem from using fossil fuels, such as natural gas, for heat and power generation for chemical plants [4]. Often, energy is generated onsite, in the plant's utility system. To reduce CO_2 emissions, the processes' power and heat demand could be supplied by electricity from low-carbon, renewable sources such as wind or solar power, instead of using fossil fuels. However, the availability of power from renewable sources is variable. This is expected to be a challenge for the chemical industry, since most existing processes require a continuous and constant supply of heat and power. Therefore, flexibility, i.e., the ability to adapt the electricity demand to external signals such as the availability or price of low-carbon energy, will be required.

However, the potential benefits and limitations of exploiting flexibility in the chemical industry are unclear, and knowledge about the requirements for implementation is lacking. Moreover, the potential for electrifying existing utility systems of chemical plants with intermittent sources is unknown. More specifically, it is unknown how electrified systems would compare to fossil fuel-based ones in terms of costs and CO_2 emissions, and it has not been explored which technologies would enable a cost-optimal electrification under which conditions.

This thesis aims to explore the conditions for mitigating the impact of intermittency on the chemical industry, specifically by electrifying existing utility systems. To this end, the following research questions are answered.

[1] European Commission and Joint Research Center. "GHG emissions of all world countries". In: Luxembourg: Publications Office of the European Union, 2024. ISBN: 978-92-68-20572-3. DOI: 10.2760/0115360

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1. *What requirements and limitations should be considered to implement flexibility in the chemical industry?*

This question was answered by a literature review, complemented with a series of stakeholder interviews, which contributed several requirements and limitations that had not been mentioned in the literature. Technical, economic, organisational, and regulatory requirements and limitations were identified.
Examples of technical requirements are a sufficiently big connection capacity to the local power grid, the need to vary the electrical load of the process or site within the specified time, and the availability of excess capacity for a potential ramp-up of production in times of excess power. Technical limitations of a flexible process operation include potential safety risks, long start-up times of processes. Moreover, implementing flexibility is complex in general.
There has to be a business case for flexibility, and yet, there are a number of economic limitations. Typical limitations are potentially high investment costs, economic losses due to relinquished production, potential damage to the equipment, and a potential decrease in product quality. Moreover, the financial compensation is low, and the uncertainty inherent to energy markets requires knowledge on how to cope with market uncertainty.
Organisational requirements are diverse, and include the requirement for chemical industries to acquire knowledge about the power sector and vice versa, and the capability to refine the planning of the plant's operation. In addition, the planning horizons of the chemical plant and the grid operators must align. Markets for flexibility have to be accessible for chemical companies, and tariff structures must be attractive for the chemical industry to participate in grid-balancing services. Examples of organisational limitations include strict delivery obligations of chemical plants, confidentiality of process operation data when considering a collaboration between the two sectors, and the chemical industry's concerns about the security of the IT connection to the grid operator. Moreover, the awareness of the opportunities of Demand Response within the chemical industry is low. Regulatory limitations highlighted by stakeholders are the relatively high minimum power bid size and the requirement for installing qualified metering equipment to offer grid-stability services.

2. *To what extent, and under which circumstances, can flexible utility systems enhance the electrification of chemical plants?*

To answer this question, cost-optimally electrified utility systems were modelled for a range of processes, energy prices, technology costs, grid connection capacities, and the flexibility of fossil-fuel-based technologies[5]. The technology portfolios and performances of the utility systems were obtained using three versions of a utility system model. This model provides the option to install and operate different power-to-heat technologies next to an existing CHP or natural gas boiler, and can choose to install energy storage units. The mode is equation-based and simulates hourly energy (heat and power) flows between the existing fossil fuel-based and newly installed generation and storage units, and the grid, and optimises the units' capacity and operation to achieve the lowest possible total

[5] represented by their minimal load

annual cost. The total annual costs include the required (annualised) investment, the cost of electricity and natural gas, and costs for Scope 1 CO_2 emission allowances.

The results showed that for historical energy price data and plants with a constant utility demand, partial electrification, and hence, an increase in the flexibility to choose between electricity and natural gas, can be cost-optimal under two conditions. First, the electricity-to-gas price ratio is approximately 2, and second, the number of hours during which it is cheaper to use electricity than natural gas[6] (referred to as 'hsE<NG' in the remainder of this summary) is greater than 500 hours for plants with existing CHPs. For plants with an existing natural gas boiler, the hsE<NG has to be greater than 600 hours. This is found to be independent of the utility demand of the plant, as the cases studied exhibit a wide range of absolute utility demand and ratios of power to heat demand. These findings also do not change for the explored values of grid connection capacity, technology costs, and minimal load of the CHP or natural gas boiler.
Additional flexibility in the form of energy storage is added to the utility system when the hsE<NG doubles compared to the hsE<NG in years for which no energy storage is installed[7].
When a heat pump is added to the technology options the model can choose from, and the explored energy price scenarios have a lower electricity-to-gas price ratio compared to the historical price data, installing a heat pump leads to cost savings even in an energy price scenario with only 100 hsE<NG. Under these conditions, the explored technology cost scenarios have little impact on the potential for cost-optimal electrification.

The research results show that the conditions for electrification cannot be described as a set of fixed values for, e.g., the electricity-to-gas-price ratio. Instead, they are a combination of the following parameters.

- The hsE<NG (number of hours during which using electricity is cheaper than natural gas),
- the conversion efficiency of the PtH technology,
- the conversion efficiency of the existing fossil fuel-based technologies,
- average energy and CO_2 emission allowance prices, and
- the yearly average electricity-to-gas-price ratio.

For historical energy price data, the extent of electrification, measured as the achieved reduction in natural gas consumption, does not exceed 24%. When the flexibility of the existing CHP and natural gas boiler is increased in the model by increasing the minimum load at which the technology has to operate, CO_2 emissions are reduced by up to 31%. Cost and emission savings are much higher when the minimal load constraint of the fossil fuel-based technologies is removed from the model.

[6] including the costs of the required CO_2 emission allowances
[7] while the electricity-to-gas price ratio remains similar

3. *How do changing conditions affect cost-optimal technology portfolios of electrified utility systems for chemical plants?*

Comparing the technology portfolios of the cost-optimal systems presented in this thesis allowed to identify the impact of changing energy prices, technology costs, and conversion efficiencies on the technology portfolios.

The model installs electric boilers as soon as the hsE<NG allows for cost-optimal electrification. When, due to a higher price variance, the hsE<NG doubles compared to the hsE<NG that leads to utility systems with only electric boilers, thermal energy storage is added. When mean prices increase about 2.5-fold, the model installs batteries. Note that the model did not include the option to install a heat pump.
If heat pumps are included in the utility system model, technology portfolios change. Then, the model prefers to install heat pumps over electric boilers when average energy prices are high. However, electric boilers combined with large thermal energy storage capacities are the preferred technology choice when energy prices are low and variable. Batteries are no longer installed.
The results in this thesis show that only low and medium levels of heat pump integration are worth the additional investment due to increased installation costs. Price mean and variance have little impact on this conclusion. Whether existing fossil fuel-based technologies can be used for heat generation in the model does not change this finding.

The technology cost has an impact on the installed capacities, but it barely impacts the technology choices the model makes. The electricity-to-gas-price ratio is important to determine whether electrification is cost-optimal, but it has a limited impact on the technology portfolio. If installed, the electric boiler and thermal energy storage capacities increase in proportion to the grid connection capacity, while the battery capacity remains constant. Heat pumps are sized according to the process's average heat demand. Thermal energy storage is installed when heat demand and/or energy prices are fluctuating.
Hydrogen as an energy carrier is never part of the cost-optimal technology portfolio, unless the technology cost of the electrolyser decreases by at least one order of magnitude

In conclusion, this thesis shows that (partial) electrification of utility systems can lead to cost savings for industrial plants under the following conditions.

Industries need to have sufficient grid connection capacity. This implies that they need to assess the extent to which their existing connection to the grid allows electrification. Note that, in this thesis, it was assumed that fossil-fuel-based technologies were already installed and could continue to be used in most cases.

Energy prices determine the potential for cost-optimal electrification and the required technology portfolios. However, there is no single indicator that determines the potential and cost-optimal portfolio. Which PtH technology is ultimately the best choice for a company is uncertain and depends on the development of energy prices. The development of energy prices is less critical for thermal energy storage when heat demand is variable. When it is constant, however, thermal energy storage is only required when price fluctuations are high.

The extent to which electrification reduces direct CO_2 emissions depends on the energy prices, the conversion efficiency of the installed PtH technology, and the flexibility of the fossil fuel-based legacy technology. If energy prices were to be similar to the historical data, additional incentives or natural gas reduction regulations are needed to achieve an emission reduction of more than 30%.

While important insights for electrification with intermittent energy sources have been gained in this thesis, recommendations for future research include exploring the robustness of the proposed utility systems to a wider range of uncertain conditions, to, for example, find potential 'low-regret' technology portfolios. Adding CO_2 emission reduction as a second optimisation objective would increase the understanding of potential trade-offs between cost and emission reduction, and could help companies in their decision-making and policymakers in designing potential subsidies. In addition, the uncertainty of the business case for flexibility should be addressed by investigating potential collaboration schemes (e.g., special tariffs or grid balancing services) between the power sector and the chemical industry.

Samenvatting

Bijna 50 % van de wereldwijde CO_2-emissies wordt veroorzaakt door de opwekking van elektriciteit en warmte en industriële processen [1]. Als emissies die worden toegeschreven aan energieopwekking voor de industrie worden meegerekend in het aandeel van de industrie, is de industrie de grootste bijdrager aan de wereldwijde emissies [2]. Bijna een vijfde van de industriële CO_2-emissies wordt toegeschreven aan de chemische industrie [3]. Daarom moeten de netto-emissies van de chemische industrie worden verminderd om internationale CO_2-reductiedoelstellingen te halen.

Ongeveer een derde van de CO_2-emissies van de chemische industrie komt voort uit het gebruik van fossiele brandstoffen, zoals aardgas, voor warmte- en elektriciteitsopwekking in chemische fabrieken [4]. Vaak wordt energie ter plaatse opgewekt, in het nutsvoorzieningssysteem van de fabriek. Om CO_2-emissies te verminderen, zou de vraag naar elektriciteit en warmte van processen kunnen worden gedekt door elektriciteit uit koolstofarme, hernieuwbare bronnen zoals wind- of zonne-energie, in plaats van fossiele brandstoffen. De beschikbaarheid van elektriciteit uit hernieuwbare bronnen is echter variabel. Aangezien de meeste chemische processen continue opereren, en een constante toevoer van warmte en elektriciteit vereisen, wordt dit verwacht een uitdaging te zijn. Daarom zal flexibiliteit, d.w.z. het vermogen om de elektriciteitsvraag aan te passen aan externe signalen zoals de beschikbaarheid of prijs van koolstofarme energie, noodzakelijk zijn.

De potentiële voordelen en beperkingen van het benutten van flexibiliteit in de chemische industrie zijn echter onduidelijk, en kennis over de vereisten voor implementatie ontbreekt. Bovendien is het potentieel voor elektrificatie van bestaande nutsvoorzieningssystemen van chemische fabrieken met intermitterende bronnen onbekend. Meer specifiek is het onbekend hoe geëlektrificeerde systemen zich zouden verhouden tot op fossiele brandstoffen gebaseerde systemen in termen van kosten en CO_2-emissies, ook is niet onderzocht welke technologieën onder welke omstandigheden tot de minimale kosten leiden.

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Dit proefschrift heeft al doel de voorwaarden te onderzoeken voor het beperken van de impact van variabiliteit op de chemische industrie, specifiek door het elektrificeren van bestaande nutsvoorzieningssystemen. Daartoe worden de volgende onderzoeksvragen beantwoord.

1. *Welke vereisten en beperkingen moeten in aanmerking worden genomen om flexibiliteit in de chemische industrie te implementeren?*

Deze vraag is beantwoord door middel van een literatuuronderzoek, aangevuld met een reeks interviews met belanghebbenden, die verschillende vereisten en beperkingen opleverden die niet in de literatuur waren genoemd. Technische, economische, organisatorische en regelgevende vereisten en beperkingen zijn geïdentificeerd.
Voorbeelden van technische vereisten zijn een voldoende grote aansluitcapaciteit op het lokale elektriciteitsnet, de noodzaak om de elektrische belasting van het proces of de locatie binnen de gespecificeerde tijd te variëren, en de beschikbaarheid van extra capaciteit voor een mogelijke productieverhoging in tijden van overcapaciteit. Technische beperkingen van een flexibele procesvoering omvatten mogelijke veiligheidsrisico's en lange opstarttijden van processen. Bovendien is het implementeren van flexibiliteit in het algemeen complex.
Er moet een businesscase voor flexibiliteit zijn, maar er zijn een aantal economische beperkingen. Typische beperkingen zijn mogelijk hoge investeringskosten, economische verliezen door opgegeven productie, mogelijke schade aan apparatuur en een mogelijke afname van de productkwaliteit. Bovendien is de financiële compensatie laag, en de onzekerheid die inherent is aan energiemarkten vereist kennis over hoe om te gaan met markt-onzekerheid.
Organisatorische vereisten zijn divers en omvatten de noodzaak voor chemische bedrijven om kennis op te doen over de energiesector en vice versa, evenals het vermogen om de planning van de bedrijfsvoering van de fabriek te verfijnen. Daarnaast moeten de planningshorizonten van de chemische fabriek en de netbeheerders op elkaar aansluiten. Markten voor flexibiliteit moeten toegankelijk zijn voor chemische bedrijven, en tariefstructuren moeten aantrekkelijk zijn voor de chemische industrie om deel te nemen aan netbalanceringsdiensten. Voorbeelden van organisatorische beperkingen zijn strikte leveringsverplichtingen van chemische fabrieken, vertrouwelijkheid van procesdata bij samenwerking tussen de twee sectoren, en zorgen van de chemische industrie over de beveiliging van de IT-verbinding met de netbeheerder. Bovendien is het bewustzijn van de mogelijkheden van Demand Response binnen de chemische industrie laag. Regelgevende beperkingen die door belanghebbenden zijn benadrukt, zijn onder andere de relatief hoge minimale biedgrootte voor vermogen en de vereiste installatie van gekwalificeerde meetapparatuur om netstabiliteitsdiensten aan te bieden.

2. *In welke mate, en onder welke omstandigheden, kunnen flexibele nutsvoorzieningssystemen de elektrificatie van chemische fabrieken verbeteren?*

Om deze vraag te beantwoorden, zijn kostoptimale geëlektrificeerde nutsvoorzieningssystemen gemodelleerd voor een reeks processen, energieprijzen, technologieprijzen, netaansluitcapaciteiten en de flexibiliteit van fossiele technologieën[5]. De technologieportefeuilles en prestaties van de nutsvoorzieningssystemen zijn verkregen met behulp van drie versies van een nutsvoorzieningsmodel. Dit model biedt de mogelijkheid om verschillende power-to-heat-technologieën te installeren en te exploiteren naast een bestaande WKK of aardgasboiler, en kan ervoor kiezen om energieopslagunits te installeren. Het model, bestaande uit een reeks vergelijkingen, simuleert uurlijkse energiestromen (warmte en elektriciteit) tussen de bestaande fossiele en nieuw geïnstalleerde opwek- en opslagunits, en het net, en optimaliseert de capaciteit en werking van de units om de laagst mogelijke totale jaarlijkse kosten te bereiken. De totale jaarlijkse kosten omvatten de vereiste (geannualiseerde) investering, de kosten van elektriciteit en aardgas, en kosten voor Scope 1 CO_2-emissierechten.

De resultaten toonden aan dat voor historische energieprijsgegevens en fabrieken met een constante nutsvraag, gedeeltelijke elektrificatie, en dus een toename van de flexibiliteit om te kiezen tussen elektriciteit en aardgas, kostoptimaal kan zijn onder twee voorwaarden. Ten eerste is de elektriciteit-tot-gas-prijsverhouding ongeveer 2, en ten tweede is het aantal uren waarin het goedkoper is om elektriciteit te gebruiken dan aardgas[6] (in de rest van deze samenvatting aangeduid als 'hsE<NG') groter dan 500 uur voor fabrieken met bestaande WKK's. Voor fabrieken met een bestaande aardgasboiler moet de hsE<NG groter zijn dan 600 uur. Dit blijkt onafhankelijk te zijn van de nutsvraag van de fabriek, aangezien de onderzochte gevallen een breed scala aan absolute nutsvraag en verhoudingen van elektriciteits- tot warmtevraag vertonen. Deze bevindingen veranderen ook niet voor de onderzochte waarden van netaansluitcapaciteit, technologieprijzen en minimale belasting van de WKK of aardgasboiler.
Extra flexibiliteit in de vorm van energieopslag wordt toegevoegd aan het nutsvoorzieningssysteem wanneer de hsE<NG verdubbelt ten opzichte van de hsE<NG in jaren waarin geen energieopslag is geïnstalleerd[7].
Wanneer een warmtepomp wordt toegevoegd aan de technologieopties waaruit het model kan kiezen, en de onderzochte energieprijsscenario's een lagere elektriciteit-tot-gas-prijsverhouding hebben vergeleken met de historische prijsgegevens, leidt het installeren van een warmtepomp tot kostenbesparingen, zelfs in een energieprijsscenario met slechts 100 hsE<NG. Onder deze omstandigheden hebben de onderzochte technologieprijsscenario's weinig invloed op het potentieel voor kostoptimale elektrificatie.

De onderzoeksresultaten tonen aan dat de voorwaarden voor elektrificatie niet kunnen worden beschreven als een set vaste waarden voor bijvoorbeeld de elektriciteit-tot-gas-prijsverhouding. In plaats daarvan zijn ze een combinatie van de volgende parameters:

- De hsE<NG (aantal uren waarin elektriciteit goedkoper is dan aardgas),
- de conversie-efficiëntie van de PtH-technologie,
- de conversie-efficiëntie van de bestaande fossiele technologieën,

[5] weergegeven door hun minimale belasting
[6] inclusief de kosten van de vereiste CO_2-emissierechten
[7] terwijl de elektriciteit-tot-gas-prijsverhouding vergelijkbaar blijft

- gemiddelde energie- en CO_2-emissierechtenprijzen, en
- de jaarlijkse gemiddelde elektriciteit-tot-gas-prijsverhouding.

Voor historische energieprijsgegevens is de mate van elektrificatie, gemeten als de gerealiseerde reductie in aardgasverbruik, beperkt tot 24%. Wanneer de flexibiliteit van de bestaande WKK en aardgasboiler in het model wordt vergroot door de minimale belasting waarbij de technologie moet werken te verhogen, worden CO_2-emissies tot 31% verminderd. Kosten- en emissiebesparingen zijn veel hoger wanneer de minimale belastingbeperking van de fossiele technologieën uit het model wordt verwijderd.

3. *Hoe beïnvloeden veranderende omstandigheden de kostoptimale technologieportfolio's van geëlektrificeerde nutsvoorzieningssystemen voor chemische fabrieken?*

Het vergelijken van de technologieportefeuilles van de kostoptimale systemen die in dit proefschrift worden gepresenteerd, maakte het mogelijk om de impact van veranderende energieprijzen, technologieprijzen en conversie-efficiënties op de technologieportefeuilles te identificeren.

Het model installeert elektrische boilers zodra de hsE<NG kostoptimale elektrificatie mogelijk maakt. Wanneer, door een hogere prijsvariatie, de hsE<NG verdubbelt ten opzichte van de hsE<NG die leidt tot nutsvoorzieningssystemen met alleen elektrische boilers, wordt thermische energieopslag toegevoegd. Wanneer de gemiddelde prijzen ongeveer 2,5 keer stijgen, installeert het model batterijen. Merk op dat het model niet de optie bevatte om een warmtepomp te installeren.
Als warmtepompen worden opgenomen in het nutsvoorzieningsmodel, veranderen de technologieportefeuilles. Dan geeft het model de voorkeur aan het installeren van warmtepompen boven elektrische boilers wanneer de gemiddelde energieprijzen hoog zijn. Elektrische boilers gecombineerd met grote thermische energieopslagcapaciteiten zijn echter de voorkeurskeuze wanneer energieprijzen laag en variabel zijn. Batterijen worden niet langer geïnstalleerd.
De resultaten in dit proefschrift tonen aan dat alleen lage en middelhoge niveaus van warmtepompintegratie de extra investering waard zijn vanwege verhoogde installatiekosten. Prijsniveau en variatie hebben weinig invloed op deze conclusie. Of bestaande fossiele technologieën kunnen worden gebruikt voor warmteopwekking in het model verandert deze bevinding niet.

De technologieprijs heeft invloed op de geïnstalleerde capaciteiten, maar nauwelijks op de technologiekeuzes die het model maakt. De elektriciteit-tot-gas-prijsverhouding is belangrijk om te bepalen of elektrificatie kostoptimaal is, maar heeft een beperkte invloed op de technologieportefeuille. Indien geïnstalleerd, nemen de elektrische boiler- en thermische energieopslagcapaciteiten toe in verhouding tot de netaansluitcapaciteit, terwijl de batterijcapaciteit constant blijft. Warmtepompen worden gedimensioneerd op basis van de gemiddelde warmtevraag van het proces. Thermische energieopslag wordt geïnstalleerd wanneer warmtevraag en/of energieprijzen fluctueren.
Waterstof als energiedrager maakt nooit deel uit van de kostoptimale technologieportefeuille, tenzij de technologieprijs van de elektrolyser met minstens één ordegrootte daalt.

Concluderend toont dit proefschrift aan dat (gedeeltelijke) elektrificatie van nutsvoorzieningssystemen kan leiden tot kostenbesparingen voor industriële fabrieken onder de volgende voorwaarden.

Industrieën moeten voldoende netaansluitcapaciteit hebben. Dit impliceert dat zij moeten beoordelen in hoeverre hun bestaande aansluiting op het net elektrificatie mogelijk maakt. Merk op dat in dit proefschrift werd aangenomen dat fossiele technologieën al waren geïnstalleerd en in de meeste gevallen konden blijven worden gebruikt.

Energieprijzen bepalen het potentieel voor kostoptimale elektrificatie en de vereiste technologieportefeuilles. Er is echter geen enkele indicator die het potentieel en de kostoptimale portefeuille bepaalt. Welke PtH-technologie uiteindelijk de beste keuze is voor een bedrijf, is onzeker en hangt af van de ontwikkeling van energieprijzen. De ontwikkeling van energieprijzen is minder kritisch voor thermische energieopslag wanneer de warmtevraag variabel is. Wanneer deze constant is, is thermische energieopslag echter alleen vereist wanneer prijsfluctuaties hoog zijn.

De mate waarin elektrificatie directe CO_2-emissies vermindert, hangt af van de energieprijzen, de conversie-efficiëntie van de geïnstalleerde PtH-technologie en de flexibiliteit van de fossiele bestaande technologie. Als energieprijzen vergelijkbaar zouden zijn met de historische gegevens, zijn aanvullende prikkels of aardgasreductieregels nodig om een emissiereductie van meer dan 30% te bereiken.

Hoewel belangrijke inzichten voor elektrificatie met intermitterende energiebronnen zijn verkregen in dit proefschrift, omvatten aanbevelingen voor toekomstig onderzoek het verkennen van de robuustheid van de voorgestelde nutsvoorzieningssystemen voor een breder scala aan onzekere omstandigheden, om bijvoorbeeld potentiële 'low-regret'-technologieportefeuilles te vinden. Het toevoegen van CO_2-emissiereductie als een tweede optimalisatiedoel zou het begrip van potentiële afwegingen tussen kosten en emissiereductie vergroten, en zou bedrijven kunnen helpen bij hun besluitvorming en beleidsmakers bij het ontwerpen van mogelijke subsidies. Bovendien moet de onzekerheid van de businesscase voor flexibiliteit worden aangepakt door het onderzoeken van potentiële samenwerkingsregelingen (bijv. speciale tarieven of netbalanceringsdiensten) tussen de energiesector en de chemische industrie.

1

Introduction

1

1.1. Background

Almost 50 % of global CO_2 emissions are caused by power and heat generation and industrial processes [1]. Figure 1.1 shows that, if emissions allocated to energy generation for the industry are included in the industry's share, it is the biggest contributor to global emissions. Figure 1.1 also shows that almost one-fifth of industrial CO_2 emissions are attributed to the chemical industry. Therefore, net emissions from the chemical industry need to be reduced if international CO_2 emission reduction goals are to be met.
The large amount of CO_2 emissions generated by the chemical industry is a result of the sector using fossil fuels as feedstock and for energy generation. Chemical building blocks like methanol, ethylene, propylene, and benzene are currently produced from fossil fuels such as naphtha or natural gas [2], and their production is energy-intensive [3]. Therefore, the path towards emission reduction for the chemical industry must include the substitution of fossil feedstocks, alternative ways to generate the required heat and electricity or the capture and storage of CO_2 emissions. In this thesis, the focus is on the electrification of the industry's heat and power supply.

The remainder of this introduction elaborates on electrification and the need for flexibility (Section 1.2), before introducing the knowledge gaps and the research questions that steered the work (Section 1.3). Section 1.4 describes the research approach and the outline of the remainder of the thesis.

1.2. Electrification and the need for flexibility

About one third of the chemical industry's CO_2 emissions can be attributed to using fossil fuels such as natural gas, oil and coal for heat and power generation for chemical plants [3]. Often, energy is generated onsite, in the plant's utility system, as depicted in Figure 1.2a. A typical utility system consists of a combined heat and power plant (CHP) and/or natural gas boilers, and a connection to the local power grid [4]. Instead of using fossil fuels, the processes' power and heat demand could be supplied purely by electricity from the power grid and low-carbon, renewable sources such as wind or solar power directly, as depicted in Figure 1.2b. As shown in the utility system in Figure 1.2b, power-to-heat (PtH) technologies are necessary to convert electricity into heat.

PtH technologies can be divided into three groups. The first group converts power directly to heat and includes electric boilers and electric heaters. Electric boilers can produce steam up to 500 °C and are established in industry [5]. The second group, which includes heat pumps and mechanical vapour recompression units (MVRs), uses electricity to lift heat to higher temperatures. Heat pumps are technologically mature for delivering temperatures below 100 °C, and are expected to be able to deliver heat of up to 400 °C in the near future [6]. The third group of PtH technologies uses electricity to produce an intermediate energy carrier, for example, hydrogen, which can be used and converted directly, or stored and combusted later. Hydrogen boilers are not common in industry yet, but work similarly to natural gas boilers [7].

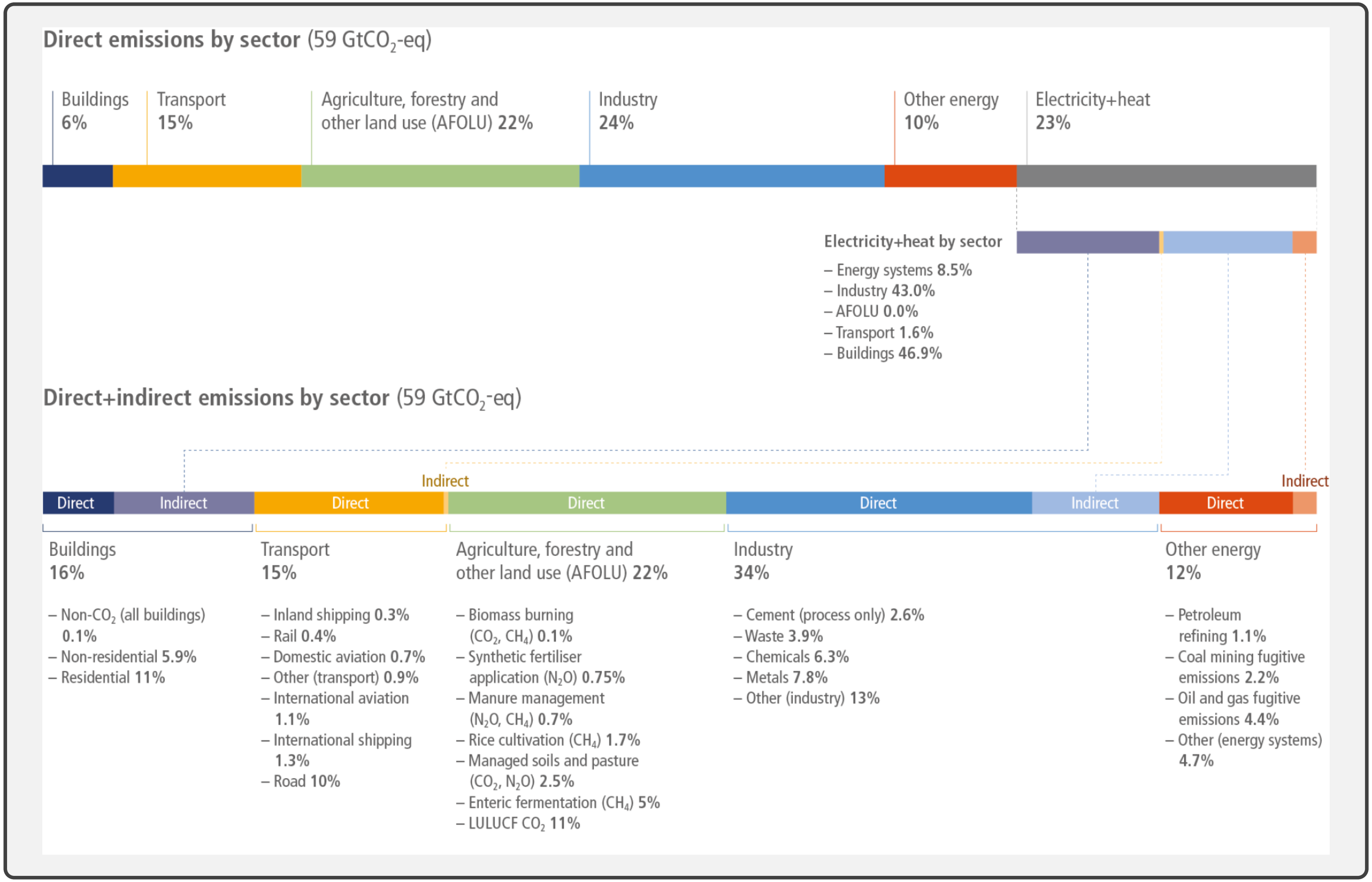
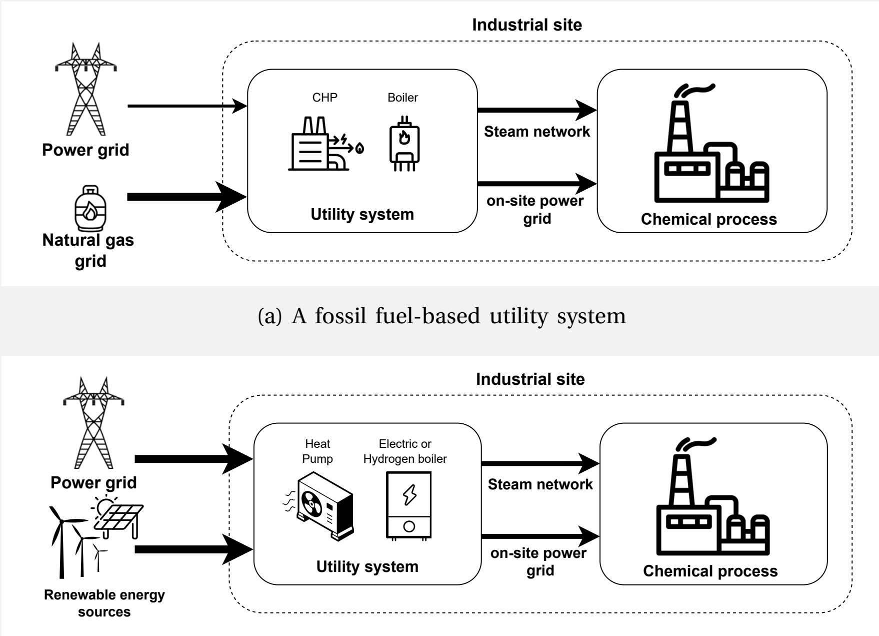


Figure 1.1.: Total anthropogenic direct and indirect GHG emissions for the year 2019 (in $GtCO_2$-eq) by sector and subsector. Figure taken from [8].



(a) A fossil fuel-based utility system

(b) An electricity-based utility system

Figure 1.2.: The utility system located within the industrial site. Currently, energy generation is mostly fossil fuel-based. To reduce CO_2 emissions, electricity from renewable sources could be used instead. The icons in the figure are obtained from thenounproject.com
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PtH technologies have different benefits and limitations. Electric and hydrogen boilers, for example, are currently less capital-intensive than heat pumps [7, 9, 10] but require more electricity input since their efficiency is lower than that of heat pumps [6]. Therefore, it is important to understand which PtH technology suits which conditions best to support industries in their decision-making process.
The assessment of the tradeoffs of different PtH technologies for the chemical industry has not received much attention yet. Studies on utility systems for the chemical industry have focused on increasing either efficiency (see [11] and [12]), heat integration ([13]), or on using power from renewable energy sources directly (see the studies in [14–17]). The application of PtH technologies is studied, for example, in the work by Bauer et al. [4]. Although the authors explored using an electric boiler next to a baseload CHP, they discussed using the electric boiler as baseload technology only qualitatively. A second example is the work by Hoffman et al. [18]. They developed an approach to optimise heat integration in combination with an electric boiler for load shifting when batch processes require flexible utility systems, but did not consider

alternative PtH technologies. To the author's knowledge, only two studies have assessed the use of several PtH technologies for the electrification of utility systems for chemical production. One is the work by Baumgaertner et al. [19], which included a wide range of technological options, such as electric boilers, heat pumps, compression chillers, batteries and TES, for a pharmaceutical facility. However, options from the third group of PtH technologies, i.e., the production of intermediate energy carriers which can be stored, such as hydrogen, were not included in their utility system model. The second study is the work presented in [20]. This study considered using electric furnaces, heaters, boilers, and heat pumps for a complete electrification of industrial utility systems, but did not consider the presence of existing fossil fuel-based technologies. Like in Baumgaertner et al., PtH technologies from the third group were not included in the assessment. Moreover, the study assumed a steady-state operation of the utility system. Why considering only steady-state operation is a limitation for electrified utility systems will be discussed in the following.

For a substantial reduction of CO_2 emissions via electrification, resulting emissions could either be captured with carbon capture and storage technologies or avoided by using low-emission energy sources. This thesis explores using low-emission sources such as wind power or solar energy. The availability of power from these sources is variable. This is expected to be a challenge for the chemical industry, since most existing processes require a continuous and constant supply of heat and power. Therefore, it will be necessary to shift the availability or the demand for electricity or heat over time.
Adapting the industry's energy demand to the availability of power has been identified as an important measure for ensuring power grid stability in literature [21–23], and is referred to as industrial Demand Side Management (DSM) or Demand Response (DR). Using DR in chemical processes for short- and long-term grid balancing has received increasing attention in literature [24, 25]. A requirement for DR is flexibility. Here, the term 'flexibility' is used as the ability to adapt the electricity demand to external signals, such as availability or price, following Zhang and Grossmann definition of flexibility in [26], where flexibility is the "load profile adjustment in response to electricity market signals".

Two options for achieving flexibility in chemical plants can be considered. They are depicted in Figure 1.3. The first one is via a flexible chemical process operation. The second option is to operate the plant's utility system flexibly. Literature on flexible process operation has mostly focused on electrified processes such as chlor-alkali production [27–32], while some studies have explored the production of 'green' ammonia [33–37] and hydrogen [34, 38–40]. The potential for flexible process operation has thus been explored for electrolytic processes. The flexibility of other processes present in the chemical industry has gained less attention. Furthermore, those studies considered process modifications or proposed new process designs, but did not consider using the existing utility system of chemical plants as a source of flexibility.
Research on flexible (electrified) industrial utility systems has been carried out in two

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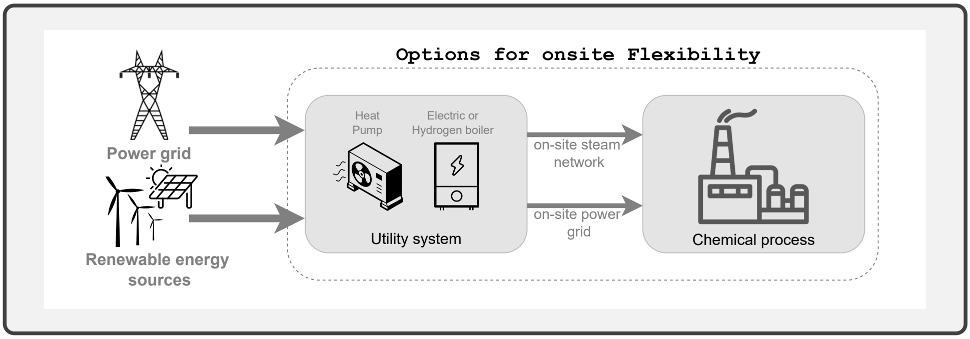

Figure 1.3.: Two options for flexibility on industrial sites are considered in this work. The first is to operate the utility system flexibly, and the second is to operate the chemical process flexibly. The icons in the figure are obtained from thenounproject.com.

studies. Klasing et al. focused on the use of thermal energy storage and electric boilers to replace the CHP in times of low electricity prices [41]. Integration concepts and operation strategies were, however, only qualitatively discussed. The second study is the work by Fleschutz et al. [42]. The authors modelled the use of different PtH and storage technologies next to a fossil fuel-based CHP and boiler and showed that achieving cost-competitiveness with the reference system was challenging. However, varying prices for purchasing natural gas and CO_2 emission allowances were not considered, which could lead to different results. The work was carried out for a manufacturing company with a much lower heat demand than the average demand of chemical processes. It is thus uncertain whether the findings of the study are applicable to the chemical industry.

1.3. Knowledge gaps and research questions

Based on the literature discussed previously, two knowledge gaps about flexibility in the chemical industry motivated the research plan.
Firstly, the potential benefits and limitations of exploiting flexibility in the chemical industry were not clear. Moreover, knowledge about the requirements for implementation was missing. Secondly, the potential for electrifying existing utility systems of chemical plants with intermittent sources was unknown. More specifically, it was unknown how electrified systems would compare to fossil fuel-based ones in terms of costs and CO_2 emissions, and it has not been explored which technologies would enable a cost-optimal electrification under which conditions.

This thesis aims to address these knowledge gaps and, more specifically, explore the conditions for electrifying existing utility systems for chemical plants with intermittent energy sources. The following research questions guided the work.

1. What requirements and limitations should be considered to implement flexibility

in the chemical industry?

2. To what extent, and under which circumstances, can flexible utility systems enhance the electrification of chemical plants?

3. How do changing conditions affect cost-optimal technology portfolios of electrified utility systems for chemical plants?

1.4. Thesis outline and research approach

The research questions listed above are addressed in four chapters.

Chapter 2 addresses the first research question by identifying the potential benefits, limitations, and requirements for flexible process operation identified in peer-reviewed and grey literature, and compares them to findings from stakeholder interviews. The chapter provides an overview of how the potential of flexible process operation for demand response is viewed by stakeholders from the chemical industry and the power sector, and highlights similarities and differences between the expectations of the two groups. These findings are valuable for a successful coupling of both sectors, which is likely to become more important with the increasing electrification of the chemical industry.

Chapters 3 to 5 address the conditions for flexible utility systems in existing industrial plants. To allow for assessments with a high level of detail regarding the industry's requirements, a case study-based approach is chosen. A possible alternative would be to work with a general but abstract model. However, choosing a demand profile representative of the industry as a whole is challenging because of the industry's heterogeneity in terms of utility requirements. The case studies are selected to capture a wide range of utility demand profiles and conditions to allow drawing conclusions for the industry as a whole. Among these plants, energy demand (electric and thermal combined) ranges from 3 MW in the case of the biodiesel plant in Chapter 4 to 360 MW in the case of the Olefins plant in Chapter 3. The energy demand of the biodiesel plant is in the range of other small-scale plants, e.g., formaldehyde production in the Port of Rotterdam [43], while Olefins production is one of the most energy-intensive processes in the chemical industry [44].

Chapter 3 presents a study that explores the deployment of PtH and storage technologies for the electrification of utility systems. A model of an existing utility system provides the option to install and operate electric boilers and hydrogen boilers (combusting hydrogen generated on site from water electrolysis) next to an existing CHP or natural gas boiler. In addition, the model can choose to install energy storage units in the form of batteries, thermal energy storage (TES), and hydrogen tanks. The equation-based model simulates hourly energy (heat and power) flows between the existing fossil fuel-based and newly installed generation and storage units, and optimises the units' capacity and operation to achieve the lowest possible annual cost. The annual costs include the required (annualised) investment, the cost of electricity

and natural gas, and costs for Scope 1 CO_2 emission allowances.
The model is used to explore the potential for cost-optimal utility system electrification for five chemical plants and six historical energy price years. The cases and energy prices studied are used to assess the impact of energy prices and utility demand (absolute demand and ratio of power to steam demand) on the cost-optimal technology portfolio of the utility system. Sensitivity analyses are carried out for the capacity of the connection to the power grid, the type and flexibility of the fossil fuel-based generation technology, and for potential technology cost developments. The study examines the extent to which utility system electrification can be cost-optimal and presents the required technology portfolios.

Chapter 4 focuses on using heat pumps for utility system electrification, since the ongoing development of high-temperature heat pumps makes them an increasingly interesting PtH technology for the chemical industry. The advantage of heat pumps compared to (gas, electric or hydrogen) boilers is a higher conversion efficiency [6], indicated by its coefficient of performance (COP). Since the COP is a function of the temperature lift that the heat pump has to realise, it is a function of the heat pump's placement within the process. An integration of the HP that leads to a lower temperature lift increases its conversion efficiency. However, this often increases the installation costs, which add to the investment required for the heat pump, which is already higher than that for boilers.
The study presented in Chapter 4 investigates the extent to which it pays off to invest in increasing the heat pump's COP to save energy costs when energy prices decrease in average and increase in variance. To this end, the model presented in Chapter 3 is extended by adding a heat pump to the technology portfolio that the model can install, integrated into a biodiesel plant in four ways with increasing COP and installation cost. By analysing which HP integration option leads to the utility system with the lowest total annual cost, and how the costs differ between the utility systems, insights into the tradeoff between investment cost and efficiency are provided.
To assess how energy prices affect the extent to which increasing the COP of the heat pump is worth the additional investment, the effect of decreasing mean prices and increasing price volatility is assessed. In addition, it is tested whether the findings are different if utility systems were to be fully electrified and their operational costs fully determined by the electricity price. The study adds insights about the technologies required for cost-optimal electrification of utility systems, specifically about the tradeoff between investment and operational costs inherent to heat pumps.

As it became apparent that energy prices significantly affect the choice and sizing of the technology portfolio required for cost-optimal electrification, Chapter 5 presents an assessment of the impact of three uncertainties in energy price developments. The mean price, the price variance, and the ratio between electricity and natural gas prices. To this end, a model similar to the one presented in Chapter 4 is run for a total of eight energy price scenarios. To account for uncertainties in technology cost developments of the heat pump and their impact on the technology portfolio, two technology cost scenarios are added to each energy price scenario. One

that would be favourable for heat pump installation and one that would not.
Since all processes studied in the previous chapters have a constant energy demand, but chemical production includes processes with a varying energy demand, the plant that serves as a case study in Chapter 5 is a paper drying facility with highly fluctuating energy demand. The case study is considered representative of chemical plants with fluctuating energy demand because the paper industry is an energy-intensive industry like the chemical industry, heat is required at temperatures similar to those required by chemical processes (250 °C) and energy demand fluctuations are considered similar to those of batch processes from the chemical industry. Therefore, the findings presented in Chapter 5 contribute further knowledge about the technology portfolio required for cost-optimal utility system electrification in the chemical industry and show how energy prices can affect the technology portfolio.

Finally, Chapter 6 discusses the findings of the previous chapters and presents the conclusions and limitations of this thesis.

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Should we exploit flexibility of chemical processes for demand response? Differing perspectives on potential benefits and limitations

Electrification of processes and utilities is considered a promising option towards the reduction of greenhouse gas emissions from the chemical industry. Since the sources of future low-carbon electricity are variable in nature, there is a need for strategies to match availability and demand. Literature identified the flexibility of chemical processes as one promising strategy to address intermittency. This chapter aims to provide insights into how stakeholders from the power sector and the chemical industry consider flexibility in chemical processes and to identify key benefits and limitations. For this chapter, we combined a review of peer-reviewed and grey literature with stakeholder interviews to map and describe the state of the art of flexible chemicals production, and to identify requirements for further research. The main drivers to investigate the flexibility potential are first, the contribution to energy system reliability, and second, potential cost savings for the industry. Main limitations are considered to be first, the uncertain economic performance of flexible processes due to investment costs, reduced production and uncertain revenues from flexible operation, and second, the complexity of the implementation of flexibility.

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2.1. Introduction

To limit the impact of climate change on ecosystems and on life on Earth, joint efforts are needed to cap the concentration of greenhouse gases (GHG) in the atmosphere. Consequently, all sectors of the world's economic system must stop emitting GHG like carbon dioxide (CO_2) as soon as possible. The urge to speed up the decrease of GHG emissions has been stated in several reports at international level, such as the latest IPCC report [1], the IEA's roadmap towards net zero by 2050 [2] or in the pledges made during COP27 in Egypt [3].
In 2019, 44% of global CO_2 emissions were caused for the generation of electricity and heat [4]. To reach the net zero CO_2 emission goal, a key pathway is the deployment of renewable energy sources (RES) like solar power and wind energy.
However, these energy sources are inherently variable. Hence, scheduling or influencing how much electricity is produced at a given moment is difficult. To guarantee a stable electricity supply, intake and outtake from the power grid must be balanced. Grid balancing is required in the short and long term (to address seasonal imbalances), so with increasing RES deployment, there is an increased requirement for options that can supply balancing services at all timescales [5].
Looking at the global CO_2 emissions resulting from fuel combustion, the industrial sector accounts for 39% [4], and after cement and iron and steel production, the chemical industry is the third largest industrial emitter [6]. Therefore, it is necessary to defossilise the chemical industry to reach emission reduction goals. Industry's GHG emissions are caused by the fossil-fueled generation of heat and electricity required in the process(es) and by the use of fossil carbon as a feedstock. Typical examples are the use of naphtha in the production of olefins, natural gas to produce ammonia, limestone to produce cement or the use of coal in steel production. Therefore, solutions must be found to decrease the energetic and non-energetic use of fossil carbon.
Direct electrification of processes and utilities such as heat is considered a promising alternative to replace fossil-based sources of process energy [7] and hydrogen from water electrolysis (indirect electrification) is foreseen to play a crucial role, as a carbon emission-free energy carrier and as a feedstock [8, 9]. In scenarios where electrification and low-carbon hydrogen are implemented in the European production of ammonia, methanol, ethylene, propylene, chlorine, benzene, toluene and xylene to achieve a CO2 emission reduction of 84% by 2050, 16.6 EJ of low-carbon electricity are required, i.e., 135% of the expected European electricity production in 2050 [8]. Another estimation is that the decarbonization of global ammonia, methanol, olefins and aromatics production in 2050 with an assumed growth of demand of 50% would require 65 EJ of low-carbon electricity, and 14 EJ of fossil fuels (resulting in 0.2 billion tons of CO2), which is a 6.6-fold increase of the current energy demand (12EJ) [10].
The foreseen increase in electricity consumption of the chemical industry, and the intermittency of low-carbon electricity consolidate the need for options to address problems in matching source and demand. One option that has been identified in literature, to offer flexibility on the demand side, is to adjust the production schedule of chemical plants according to the available electricity generation [11]. Flexible production of chemicals has therefore gained attention in literature as an option for

both short-term grid balancing via demand side management (DSM) [12] and mid- or long-term balancing as a form of energy storage in chemical bonds [13, 14], often referred to as *Power-to-Chemicals*.

Industrial demand side management has been discussed in literature [15–22], but little attention has been paid to the chemical industry (the authors know of one study by [11] available in German). It is not clear which impact flexible production of chemicals could have on the industry and on the power sector, and if both sectors have a common perspective on flexibility. Regarding the expected steep increase in electricity demand in the chemical industry and the importance of flexibility for the stability of the future electricity grid, it is crucial to address this knowledge gap.

In this chapter, we map and describe the state of the art of flexible chemicals production as a measure to cope with variable electricity supply. We present the potential benefits, limitations and requirements and identify where further research is needed. We combine a review of peer-reviewed and grey literature with stakeholder interviews to provide an overview of expectations and requirements from different perspectives, to detect options for synergies or bottlenecks. The chapter shows that the discussions about flexibility in peer-reviewed literature and within the power sector are, to a large extent, not mirrored in industrial publications from the chemical industry. The analysis of industry publications and stakeholder interviews added several requirements and limitations for actual deployment as seen by industrial stakeholders that were not considered in previous scientific studies. This chapter, therefore, provides valuable insights for future sector-coupling between the power sector and the chemical industry.

The remainder of this chapter is organised as follows. Section 2 describes the methodology that was chosen for this study. Section 3 presents the state of the art in literature and the perspective of industrial stakeholders. Finally, section 4 provides the conclusions and recommendations for further research.

2.2. Methods

For this chapter, we reviewed peer-reviewed and grey literature (i.e., reports of knowledge institutes, industrial associations and consulting firms) to analyse if and how flexibility in chemical processes has been studied and whether there are differences in the way it is discussed in the chemical industry and the energy sector. We complemented the literature review with stakeholder interviews.

In the literature review, we included publications that discuss flexibility in the context of the energy transition and did not consider studies that address industrial demand response in general, unless one or more chemical processes were included in the study. Using a keyword search as well as the snowball method, we found 44 peer-reviewed publications that matched the scope.

For the analysis of industry publications and for the interviews, stakeholders from the Dutch industry were selected. In the Netherlands, the chemical sector has the highest energy demand in the industrial sector, both in terms of energy use (43%) and in terms of feedstock (97%) [7], and it accounted for 11% of total electricity demand in 2018 [23]. As a result, the chemical industry was responsible for 44% of the Dutch industrial GHG emissions [24]. The Dutch industry comprises five large petrochemical clusters, including the Port of Rotterdam (PoR) where the entire value chain is covered from chemical building blocks (for instance, propylene, ethylene, benzene) to high-value chemicals (for instance, PVC, polyols, acetic acid). The PoR has five oil refineries (85 million tonnes total distillation capacity), one olefins plant (annual ethylene production of 900 kt/year) and seven sub-clusters, including an ethylene cluster, a propylene cluster, an aromatics cluster and a chlorine cluster. In 2021, the chemical industry at the PoR accounted for 4% of the Dutch GHG emissions [25, 26]. The Dutch clusters are similar (in terms of the type of processes, capacities and feedstocks) to other petrochemical clusters inside Europe (like Antwerp, Tarragona, Lyon or Hoechst) and outside Europe (e.g., in Texas, and Shanghai), where both, building blocks and intermediates are produced. The Dutch chemical industry is representative of the global chemical sector and key insights gained in this study can also apply in different geographical contexts. It is also important to note that, as the Dutch power and chemical sectors are subject to European climate targets, the use of flexibility as a potential demand response option is relevant beyond the Dutch boundaries.

The interview series consisted of six interviews with a total of eight participants (see Table 2.1) and were conducted in October/November 2021. The interviews were aimed to verify and complement information from literature and are not a representative survey of the Dutch industry.

The interviews with stakeholders from the petrochemical industry aimed to 1) identify whether electrification and hydrogen use play a role in their current GHG emission mitigation strategies, 2) understand whether they have considered flexible production as a viable option to handle intermittent electricity supply, and 3) to find out whether they have considered the possibility of generating revenues from providing grid balancing services to the grid as an interesting business opportunity. The main objectives for the interview with stakeholders from the power sector were to 1) understand which role grid operators assign to the chemical industry as a provider for demand response (DR) or other grid stabilising services, and 2) find out whether they have identified specific barriers for collaborating with the chemical sector. The interviews were semi-structured, the questions and notes can be found in the supplementary material. Relevant information for this study was extracted from the notes after the interviews took place.

Literature and interviews were analysed and compared regarding identified potential benefits (Table 2.3), requirements (Table 2.4), and expected limitations and trade-offs (Table 2.5). Based on the literature study and the interviews, knowledge gaps were identified.

2.3. State of the art in literature and perspectives from stakeholders

Literature studied flexibility of chemical processes in the context of the energy transition from different perspectives, namely from the energy system perspective [15, 19, 27–32] and from the industry perspective (remaining studies in Table 2.2).

Table 2.1.: Overview of interview participants

Interview reference	Company domain	Offices in	Job description participant
a	Chemical industry	Netherlands/ worldwide	Manager public affairs
b	Energy sector	Netherlands/EU	Innovation lead
c	Chemical industry	Netherlands/EU	Innovation technologist
d	Chemical industry	Netherlands/ worldwide	Innovation manager/Academic liaison Academic partnership manager Principal systems engineer
e	Energy sector	Netherlands/EU	Senior electricity market developer
f	Energy sector	Netherlands/ worldwide	Innovation manager

The studies had different objectives, such as the identification of requirements and challenges [33, 34], the quantification of aggregated flexibility potential [11] and the analysis of the potential of a single plant or process (Table 2.2). The majority of publications analyse the flexibility potential of a single industry or process, partly including the application for demand response. Despite the number of publications, the range of production processes that have been studied is limited to mainly electrochemical processes, with most of these studies focusing on chlorine production. Chlorine production is a process based on electrochemical conversion, with electricity costs having a high share in overall production costs (50-70% [35]), which may explain the attention given to the process. Furthermore, the process does not require continuous operation and has a high installed capacity, which means that flexible capacity is likely to influence grid reliability [11, 15, 27]. Next to the production of chlorine, publications cover the production of hydrogen, ammonia, methane, methanol, synthetic natural gas, ethylene oxide and formic acid. The studies considered either the process designed as implemented in the industry today [12, 19, 27, 36–40], modifications to the design aiming to increase flexibility [41–50] or they propose a completely new design [30, 31, 45, 51–55]. All authors used modelling for simulation or optimisation to study the flexibility potential, capturing the complexity of the processes with varying levels of detail, ranging from a simplified representation as a battery to dynamic process modelling. Only one study [41] compared options to increase the flexibility capacity of an existing process by using auxiliary units, namely a water electrolyser, a fuel cell and a redox flow battery. Optimisation has often been used to find the least cost solutions with regard to the cost of production or electricity costs, using historical data for electricity prices and market prices from different balancing markets. Not all studies considered investment costs in their models.

An analysis of companies' sustainability roadmaps [58–83] depicted in Figure 2.1 shows that the possibility of operating processes flexibly is not only being discussed in literature, but it is also on the agenda of industrial stakeholders from the energy sector domain. Especially grid operators have been highlighting potential benefits

Table 2.2.: List of publications that analyse the flexibility potential of individual processes, showing the product(s) they were focusing on and if they considered a design based on existing process technology or a new process design

		Process design based on		
Publication	Industry	Industrial standard	Standard with modifications	New design
[12]	Chlorine	•		
[31]	Ammonia			•
[42]	Chlorine		•	
[19]	Polyvinylchloride (Chlorine)	•		
[37]	Chlorine	•		
[41]	Chlorine		•	
[51]	Methane			•
[56]	Hydrogen, Ammonia, Methanol	•		
[28]	Hydrogen	•		
[29]	Hydrogen	•		
[38]	Chlorine	•		
[52]	Chlorine			•
[57]	Hydrogen peroxide, Adiponitrile, Chlorine	•		•
[40]	Ethylene oxide (Oxygen)	•		
[30]	Ammonia			•
[44]	Polyvinylchloride (Chlorine, Ethylene dichloride)		•	
[39]	Ammonia	•		
[53]	Formic acid			•
[43]	Ethylene oxide (Oxygen)		•	
[46]	Chlorine, (Copper, Aluminium)		•	
[47]	Epichlorohydrin		•	
[45]	Methanol			•
[48]	Ethylene oxide (oxygen)		•	
[54]	Synthetic natural gas			•
[49]	Ammonia		•	
[55]	Zeolite			•
[50]	Polyvinylchloride (Chlorine)		•	

already for some years, and are interested in further developing the implementation [23, 84–86]. However, how the topic is being discussed among stakeholders from the power sector is different from what studies in literature are focusing on. In literature, studies assess the flexibility of individual processes (Table 2.2), whereas reports from the power sector focus on the estimation of the flexibility potential of the entire industrial sector. However, the *Power to Products* project [84] is an example project where several companies across industry and power sector assessed a

possible implementation route and the business case of flexibility. They concluded that there is no general answer for the business case, as the assessment differs per case. Two out of five cases were positive, the remaining three were depending on future developments, e.g., market developments.
In the selected company roadmaps from the chemical domain (for a list of companies see Table A.1 in Appendix A), flexibility is barely discussed, as shown in Figure 2.1. The roadmaps predominantly address GHG emission reduction measures, where electrification is considered a potential solution (among others), but the intermittency of the electricity supply is not mentioned, and neither are potential measures to cope with it, like flexibility. The lack of discussion around flexibility might point out that the awareness of the topic in the chemical industry is low.

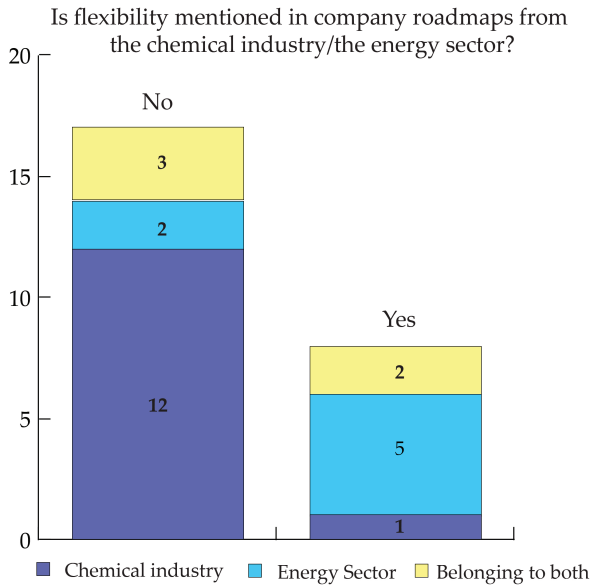

Figure 2.1.: Consideration of flexibility in companies' sustainability roadmaps, and company domains. A list of selected companies is shown in Table A.1 in Appendix A.

To identify which assumptions exist about flexibility, we present potential benefits of flexibility, requirements and its limitations and trade-offs in the rest of this section. We compare what is being stated in peer-reviewed and grey literature to what is stated in industrial roadmaps, complemented with insights from the stakeholder interviews. Findings from stakeholder interviews are referenced with letters *a* to *f* that refer to Table 2.1 in Section 2.2.

2.3.1. Potential benefits

Three potential benefits were identified (see Table 2.3). The first addresses *power grid reliability*. Power grid reliability as a reason for flexibility was mentioned by both

Table 2.3.: Potential benefits of flexibility according to peer-reviewed/grey literature and industry publications/interviews. Bold text indicates an agreement between the two

	Literature	Industry perspective
Power grid reliability at increased deployment of RES	•	•
Decrease of costs in system	•	•
Cost reduction for individual industries	•	•

stakeholders from the power sector and the chemical industry [*b, d, e, f*], [59]. Studies looking at the consequences of fluctuations in electricity supply generally argue that flexibility in chemical processes can make an important contribution to the reliability of the grid since the chemical industry is among the largest industrial electricity consumers and therefore, the potential capacity available for grid balancing is high [11, 33, 40]. [11] found that there was a significant DR potential in Germany for processes such as chlorine production. Results were based on a potentially flexible share of the nominal capacity multiplied by the installed capacity, and the results did not account for time-dependent conditions influencing the availability of a plant for DR, such as maintenance or production targets settled with customers. [27] quantified the contribution of industrial flexibility for grid congestion reduction on regional level in Germany until 2030 but included only one chemical process in her study, chlorine production. Each process was represented by its available flexible capacity, defined as the difference between installed capacity and nominal capacity. Unlike in [11], the study accounted for ramping times, duration of the change of operational mode and resulting changes in efficiencies, the frequency of shifting and times of non-availability due to maintenance, the time of the day and the season. The resulting potential is therefore lower than the potential found by [11]. In addition to the potential flexibility of the processes, the potential flexibility of components like motors, pumps, ventilation systems, and heat or cooling storage has also been quantified. Taking hydrogen production from water electrolysis as another example, two studies [28, 29] looked at the impact of a large-scale PEM electrolyser on system reliability: In [28], a 1 MW electrolyser was found to have a positive effect on frequency stability (on a time scale of milliseconds to seconds), since it was able to respond faster to deviations than conventional generators. [29] showed that flexible operation could be used for grid balancing (on a time scale of 5-15 minutes) and that it had little impact on the lifetime of the electrolyser. The rising interest in hydrogen use from across all sectors indicates that the hydrogen production volume will increase in the future. Hence, it is important to assess the flexibility of the process. However, findings for water electrolysis can only give insights about (the parts of) the chemical processes that are based on electricity. The applicability to processes that are based on heat, such as the majority of current processes in petrochemistry, is limited.
Studies looking at the consequences of fluctuations in electricity supply from the perspective of the (chemical) industry point out that flexibility could also help industries to cope with fluctuations in electricity generation [87, 88] and enable a

disconnection from the power grid by consuming electricity generated from RES that industries generate themselves. This would reduce the load on the electricity grid. As a beneficial side effect, it would also enable a decrease in industrial CO_2 emissions, as shown in the case of ammonia production. For instance, by using an electrolyser and a storage tank for hydrogen [31], or with a reversible solid oxide fuel cell stack integrated with the Haber Bosch process [30]. The ability to cope with fluctuating electricity supply was also the motivation for [51] to investigate the methanation of CO_2 from renewable electricity as a form of chemical energy storage. The reactor was able to operate with a fluctuating hydrogen inflow between 50% and 100% of the maximum inflow. How this range relates to the intermittency of renewable electricity generation was not specified further.

The second benefit assigned to flexibility is the potential to *decrease overall system costs*. In the case of the power system, flexibility can increase the reliability of the grid in a more cost-effective way than installing backup power generation plants [23, 89]. Reduction of system costs was also shown in [56] where the production of fuels and chemicals was studied as an integrated system (including feedstock production and process energy generation) from solely air, water and electricity from renewable sources. They found that the intermittency of electricity generation led to additional costs (up to two-thirds of the total cost) compared to continuously available electricity because storage capacity was necessary to operate the system throughout the year. Assuming it was possible to vary the operation of one of the possible production routes by 50% to shift production between seasons, the flexible production route became the most cost-efficient option.

Reduced system costs were also found by [90], where the potential contribution of flexible production and consumption of hydrogen in an industrial cluster was quantified. The authors found that adapting hydrogen production and consumption to the availability of locally generated electricity decreased the operational costs of the energy system of the cluster by approximately 50%.

The third benefit is the *reduction of production costs for individual industries*, compared to continuous production. Two options to reduce production costs have been identified. First, by avoiding production during periods of high electricity prices via an active adaption of operation [12, 38, 39, 41–43], and second by process operation for power grid frequency regulation [37, 53, 57], for which the electricity grid operator pays the plant operator. The first option is also seen as a possibility to overcome the electricity cost barrier that is attributed to electrification [87]. Note that the resulting economic performance strongly depends on the required investment and on assumptions about future electricity prices, like shown in the case of chlorine production with process modifications to increase process flexibility [41, 42]. Not only existing technology has been studied, but also novel production processes such as a fully electrified methanol production [52]. Assuming a fully renewable electricity generation, the authors found that a flexible operation process decreased the levelised cost of methanol by 21% and 34% for the two electricity generation profiles chosen. Flexibility was achieved with flexible equipment (electrolyser and methanol synthesis unit) and buffer facilities for energy and material flows. As discussed before, flexibility could enable a disconnection from the power grid by consuming electricity generated from RES that industries generate themselves. This could be financially beneficial for industries in three ways. First, it might lead to electricity cost savings if the electricity generated onsite is cheaper than the electricity purchased from the grid. Second, costs related to the grid connection of industries can be avoided [91], and last, independence from electricity market prices would increase [21], which reduces the risk induced by the uncertainty of the development of electricity prices.

2.3.2. Requirements

Flexible operation of chemical industries itself comes with requirements, deploying it for grid stabilising services requires additional conditions. An overview is presented in Table 2.4.

Technical requirements

A fundamental requirement for flexible process operation is that the process, including all technical components, can be operated safely in a range of operating conditions while maintaining the quality of the product within a range that is acceptable for the company that owns the plant, and with an efficiency that is high over varying loads. There are several types of flexibility in chemical engineering, as described and analysed by [92] and [93]. Key technical requirements for the kind of flexibility relevant to the application in the context of this chapter are the ability to, first, *vary the electrical load* of the process; second, to meet *required ramping rates* [86] (the rate determines the qualification for grid stabilizing services); and third, the ability to react to requested changes in operation within a *specific response time*. The duration for which the flexibility can be offered is an important parameter, as well [15]. If the change in electrical load is aimed to be a service that can be provided to an electricity grid operator, the specific values of the requirements described above are defined by the grid operator. Additionally, a *data exchange infrastructure* needs to be in place [15], and *sufficient grid capacity* is a prerequisite [*e*].
Offering demand response capacity can be achieved in two ways, by increasing electricity intake, or by decreasing electricity demand. In case of the latter, if it is technically possible to increase production at a later point in time to make up for the production reduction, this is referred to as load shifting. Otherwise, if the production cannot be recovered, it is referred to as load relinquishment. If load shifting is considered, there needs to be a strategy that allows for it, such as installing *excess capacity* units for the process [19]. However, [19] indicated that the financial benefit for larger overcapacities decreases with increasing size of overcapacity since the most expensive electricity hours are avoided first. Hence, the amount of additional capacity that can be installed in a financially viable manner is limited. Another strategy to maintain the production volume that has been proposed is to use *storage facilities*, such as product buffers [*a*], [94]. Hence, *products need to be storable* [*c*]. Buffers come with additional investment, spatial requirements, and possible safety risks that need to be taken into account when this flexibility strategy is assessed.

Table 2.4.: Requirements according to peer-reviewed/grey literature and industry publications/interviews. Bold text indicates an agreement between the two

	Literature	Industry perspective
	technical	
Variation of electrical load	•	•
Required ramping rates	•	•
Specific response time	•	
Data exchange infrastructure	•	
Sufficient grid capacity		•
Excess capacity and/or storage facilities	•	•
Storable products		•
	economic	
Business case	•	•
Economically feasible bridging technologies	•	
	organisational	
Cross-sectoral knowledge	•	
Accurate process models	•	
Refined planning capabilities		•
Accessible market for flexibility and DR programs	•	•
Attractive tariff structure, including pre-qualification requirements	•	•
Relaxed availability requirements		•
Standards for IT systems and interconnection	•	
Promotion across industry		•
Matching time horizon for planning		•
Regulations should be less strict		•
Transparent and timely information about prices, mechanisms, and requirements		•

Economic requirements

In order for flexibility to be cost-effective for the industry, there needs to be a *business case*, a level playing field between conventional, continuous operation and flexible operation [34, 87, 95]. This is influenced by the market price of the product, the electricity price, and the service payments from the grid operator, if applicable. Additional investment costs and fixed costs are relevant for the assessment of a business case, as well [15], and it has to be taken into account that efficiency of production might go down [*a*] and that losses in production need to be balanced by the revenues [*f*]. Due to long investment cycles, *bridging technologies* are needed that are economically feasible even for a short period of operation [*f*].

Organisational requirements

For assessing the potential capacity a plant can allocate for flexible operation, detailed *knowledge of the process* (including its nonlinear behaviour [36]) and *understanding of power system economics* are required [33]. It is often claimed that in market design models the consumer's perspective needs to be considered, and integration and dependencies must be accounted for [33]. As stated in [29], studies often focus either on device physics and simplify the power grid side of the challenge, or represent the power grid in great detail, but oversimplify the technical behaviour of the device, when it is required to consider both. *Accurate modelling* of flexibility and integration of production and energy management is required on the industry side [33], together with *refined planning capabilities* as most processes in the chemical industry are currently running continuously [23].
In order to facilitate the contribution of flexible plants to grid reliability under the condition of an existing business case for the offering party, there needs to be a *market for flexibility*, and plant operators should have *access to DR programs* [23]. The former depends on the electricity market design, while the latter depends on the regulations set by the regulator. According to [89], changes are required to attain an *attractive electricity tariff structure* that promotes participation for the industry, as it is currently partly disincentivising flexible operation by offering tariff discount for stable consumption patterns [23]. For a study on different tariffs and their impact on the amount of flexibility offered by the industry, and the investments in flexibility that can be expected we refer to [19]. An important criterion for access to the market is the minimum capacity that needs to be offered to the grid operator [21], and it would be beneficial to *relax the availability requirements* for the plant [*c*]. In this regard, marketing the flexibility via an aggregator is seen as an advantageous option as they have access to a portfolio of available flexibility [*c*] and because aggregators provide know-how. *Technical standards* for connecting the two parties would help reduce the complexity of, e.g., the required IT systems [21]. *Participation needs to be promoted* and metering and pre-qualification requirements should be designed in such a way that these requirements do not discourage participation in DR programs [23].
Another requirement is the alignment of the grid operators' *time horizon for planning* grid stabilising services to the time horizon of plant operators, as this is currently an issue [*a*], [86]. The requirements for such cooperation should become more flexible [*a*].

Transparency and timely information about prices [23] is required, and participants need to be informed about hardware and software requirements timely [86].

Comparison of requirements identified in literature and industry

Table 2.4 shows that there is large agreement on technical requirements, namely on the core requirements for flexibility, the ability to vary the power load and ramp processes up and down at a required rate. Excess capacities and/or storage facilities as flexibility strategies were also named by stakeholders and literature. The remaining technical requirements discussed in the previous sections were named by either the industry or in literature, but were not contradictory. Both groups agree that a business case is required for the implementation of flexibility. Due to the investment cycle duration in industry, economically feasible short-term bridging technologies were named as an economic requirement by one industrial stakeholder. Organisational requirements that were named by both groups are the need for a market for flexibility, and for industries to have access to this market and to DR programs. An attractive tariff structure, including pre-qualification requirements that do not disincentivise participation, is also regarded as a requirement from both sides. Literature considers the need for further promotion in the industry as a requirement for the deployment of flexibility, while industrial stakeholders rather referred to the need to redesign standards and regulations, and advocated for more transparency and security for planning ahead of time.

2.3.3. Expected limitations and trade-offs

Resulting from the requirements, there are limitations to flexibility, and resulting trade-offs that need to be considered, as shown in Table 2.5.

Technical limitations

Most chemical processes are designed to operate continuously. Deviating from the nominal operational mode can impose *safety risks* [23]. Often, already installed processes might not be able to increase their electric load because they are already operating at their maximum production capacity during nominal operational mode [21], so there is *limited available capacity* for a further increase. There is also a limit as to whether the process can be shut down, which is the amount of *time required to start up* a process again [*d*]. For increasing or decreasing electricity consumption according to external signals, the *ramping time* of the plants could be limiting if it is not sufficiently fast [*c*], [23]. Ramping times differ per process and depend on the time that is required to stabilise the process after ramping up or down. Especially thermal process units are subject to these limitations, for the time required to heat up or cool down and to reach equilibrium conditions.

Another limitation to offering DR capacity lies in the *complexity of the implementation* of flexibility [*b, f*], including the requirement to schedule different operational modes to integrate production planning and operation [23]. Studies that investigated scheduling [37] found that the availability of the plant might not match with the moments in time when the grid requires the load change. [12] emphasises that the

Table 2.5.: Identified limitations and trade-offs according to peer-reviewed/grey literature and industry publications/interviews. Bold text indicates an agreement between the two

	Literature	Industry perspective
	technical	
Safety risks		•
Limited available capacity	•	
Ramping and start-up times		•
Complexity of implementation	•	•
Industrial symbiosis	•	
	economic	
Value of relinquished production and investment costs	•	•
Uncertainties in markets	•	•
Low financial compensation	•	•
Degradation of equipment	•	
Decreased process efficiency	•	•
Resulting increase in electricity consumption	•	•
Unstable efficiencies	•	
Degradation of product quality	•	
	organisational	
Delivery obligations	•	
Confidentiality concerns	•	
Safety of IT connection to grid operator		•
Dependence on external service provider	•	
Lack of insight into bidding strategies of competitors	•	
Timing of investment cycles	•	•
Low awareness of opportunities of DR		•
	regulatory	
Required minimum power bid size	•	•
Qualification of metering		•

operation requires integrated planning, scheduling and control due to operational limitations of the plant, which requires a complex IT system [21]. The uncertainty in electricity price forecasts poses an additional difficulty for the planning of operation if electricity prices are taken into account, as the planning might need to be changed spontaneously if the forecast was not correct.

Industrial symbiosis is another limitation to flexibility that is often overlooked. Chemical production is often clustered, and in such clusters, production plants are highly interlinked with one another, which leads to interdependencies. This increases the complexity [88] and must be taken into consideration [33, 39] by evaluating if there are downstream processes that are designed for a constant specific mass flow that would not be supplied during flexible operation.

Economic limitations and trade-offs

As described previously, there are two types of demand response. If load shifting is not possible, there is a clear trade-off, namely the *value of relinquished production* versus the value of offering the demand reduction as a service [21] or decreasing electricity costs [*d*], [23]. When considering a potential increase in electricity consumption when there is surplus electricity available, another trade-off is observed. Since chemical processes are commonly operated at their maximum capacity, *financial investment* would be needed for the installation of additional equipment or storage capacities, or for replacing the old units with bigger ones [11]. [41, 42] found that the economic performance of a process that was modified to increase flexibility depends strongly on the investment costs that were required. The higher the investment costs, the longer the payback times. The two economic trade-offs discussed here were also identified in [15], one of the first studies that investigated the balancing requirements in the German electricity market and analysed the potential contribution of DR from industrial electricity consumers, including chlorine production.

As mentioned before, *uncertainty in market prices* increases the difficulty of planning flexible operation. Uncertainties are therefore a barrier for the industry to consider flexible operation as valuable for them [53]. Such uncertainties include first, the electricity price and long-term development in the price [42], second, the amount of money paid for grid-balancing services [21], third, the hydrogen price, in case of operation with auxiliary units [41], and last, the development of the markets they are involved in [33]. These uncertainties impose a risk on the process operators, because payback times are difficult to determine [*c*], and the *financial compensation* from electricity cost savings might be too low to make a positive business case for flexible operation [21]. This was also mentioned in the *Power to Products* project report on industrial DR in the Netherlands [84].

Another trade-off is that non-optimal operation can *degrade the equipment* and lead to a *decrease in efficiency* [*a*], [94]. The latter can imply *higher electricity consumption*, and would therefore reduce the potential financial benefit of flexible operation [*d*]. [53] added that the absence of an adaptive control architecture for flexible operation also increases the *difficulty to maintain a stable efficiency*. Deviation from optimal operating conditions can also *degrade the quality of the product* [21], which can lead to additional economic losses.

Since doubts exist about the business case of flexibly operating production, industries' disposition to consider flexible operation appears currently limited, with some industrial stakeholders pointing out that 'normal' production would likely be prioritised over operation for DR [*b, c*].

Organisational limitations

If companies alter the production volume in order to adjust their electricity consumption according to the availability of electricity, they might not be able to fulfil *delivery obligations* set by their customers. In addition to the doubts about the economic performance mentioned before, organisational obligations can be another reason for companies to prioritise 'normal' production over offering DR [21].

For the assessment of potential participation in DR programs of the grid operator, accurate modelling of the process is required. If this assessment is done by a third party, companies might need to share data, but it is doubtful that industries are willing to share data with third parties due to *confidentiality concerns* [33, 38]. For participation in DR programs, the grid operator requires to set up an IT connection with collaborating entities, and it is reported that industrial partners were concerned about the *safety* of such an IT connection because it could allow other entities to interfere with their processes [*c*].

Additionally, knowledge of energy markets is required. If this knowledge is not available within the company, an external service provider could be necessary. Some companies might object to a potential *dependency on this service provider* [21]. It was reported that companies perceive the *lack of information about bidding strategies* of competing parties as a barrier to offering grid stabilising services [21].

Another organisational limitation is related to the innovations that are required when flexibility should be implemented. The (physical) implementation of innovations happens mostly during the construction phase, so opportunities are bound to the *investment cycle* of the respective plants [94] and companies are hesitant to abandon these cycles because otherwise the lifetime of existing assets would be reduced, which has economic disadvantages [*f*].

One grid operator claimed that the *awareness of the opportunities* of offering DR is low among industrial stakeholders in general [23].

Regulatory limitations

Although there is not much information available yet, regulations can also be a barrier to the deployment of flexibility. An example is the *minimum power requirement* for the provision of grid stability services. If that is considerably high (like 1 MW in the case of Belgium [53]), it will not be met by all parties [23] and constitutes a barrier to offering flexibility. The required installation of *qualified metering equipment* for participation in DR programs is also regarded as an additional effort [23]. Even though some regulatory requirements and limitations were mentioned, regulations seem to be a minor concern. We believe this might be because stakeholders from the chemical industry focused on financial, organisational and technical aspects since they were closer to their expertise, although several of the aspects named are partly a direct consequence of regulation.

2.4. Conclusion and outlook

This study provided insights into how the flexibility of chemical processes is considered in the context of the energy transition and identified key benefits and bottlenecks.

The main drivers to consider the industries' flexibility potential are, first, the contribution to energy system reliability by balancing electricity generation and demand, and second, potential cost savings for the industry due to the possibility to adapt the production to fluctuations in the electricity price. The main limitations are, a) the uncertain economic performance of flexible processes due to investment costs, reduced production and uncertain revenues from flexible operation, and b) the complexity of the implementation. The interest in flexibility is expected to grow as the increasing electrification of the chemical industry is considered. However, it is uncertain whether the benefits outweigh the limitations, and to what extent the benefits are worth the effort that has to be made to fulfil the requirements of the flexible operation of chemical processes.

Despite large expectations in literature, the techno-economic feasibility of flexible operation in the chemical industry is still unclear. It is also unclear what revenue models for flexibility could look like, including required CO_2 price levels and network tariffs or monetary incentives, and how companies can cope with uncertainties of market prices that affect their decision-making regarding whether to invest in flexibility.

Even though some frameworks have been proposed to quantify the flexibility of chemical processes, an established methodology is still lacking. Local interconnections of the process need to be included in the assessment to account for industrial symbiosis and interdependencies between single industries, and to get insights into whether these interconnections could provide opportunities to exploit synergies.

There is a lack of knowledge on how the flexibility of current chemical processes can be increased, beyond electrolysis-based industries, such as chlorine production or water electrolysis. It has been suggested to investigate options for electrification of process heat for flexible use and to consider strategies to increase the flexibility of future processes, such as distributing production.

The impact of future technologies and alternative process designs on the flexibility potential is unknown, too. It is important to close this knowledge gap due to the upcoming changes in the industry that are necessary for meeting GHG emission targets and because this knowledge is needed to assess future developments in the electricity market.

The limitations and open questions should be addressed in future research, to explore if and how flexibility in the chemical industry can play a role in achieving future grid reliability.

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3

The potential for electrifying industrial utility systems in existing chemical plants

The electrification of utility systems of energy-intensive plants is a promising measure for decarbonising the chemical industry in the short term. However, with the increasing deployment of renewable energy sources, the variability of electricity prices will become a challenge for plants with continuous and constant energy demand. It is thus unknown whether electrification can become financially viable. This work models the electrification of utility systems in combination with storage technologies for five chemical plants with existing fossil fuel-based utility generation and uses historical data as energy price scenarios. The results show that partial electrification is cost-effective when using electricity is cheaper than natural gas for more than 600 hours. Regarding the portfolio of technologies, electric boilers are installed first, followed by thermal energy storage and batteries. Hydrogen is not cost-effective in any of the scenarios explored. This is independent of the type of plant, the available grid connection capacity, and the minimal load of existing fossil fuel-based utility generation. This chapter thus highlights the potential for electrifying industrial utility systems and the role that electric boilers and energy storage units can play in electrification.

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3.1. Introduction

Anthropogenic climate change is caused by the accumulation of greenhouse gases (GHG) in the atmosphere. Today, almost one-fourth of globally emitted energy-related GHG emissions are caused by industry [1] due to the high usage of fossil fuels like oil and gas. The chemical industry has the highest final energy demand in the industrial sector because fossil fuels are used for energy generation and as feedstock [2], and emissions from the chemical industry are estimated to make up 10% of global GHG emissions [3]. Therefore, the deployment of measures to cut down on the emissions from the chemical industry needs to speed up to achieve climate targets.

The electrification of industrial processes is a measure that is gaining increasing attention [4–7]. The ongoing decarbonization of electricity generation has led to an increasing use of renewable energy sources (RES) such as wind and solar power, the availability of which is variable in nature. With significant penetration of RES in the power grid, average prices are decreasing, but the uncertainty of electricity prices increases, which imposes a financial risk on the industry if it were to electrify processes because most existing chemical processes are built to operate at their nominal level and need a constant energy supply [8, 9].

One measure to cope with variability is demand side management (DSM), where the electricity demand is adjusted to the availability of electricity supply. The possibility of engaging the chemical industry in DSM is receiving increasing attention in literature [10–14]. Electrification will lead to a steep increase in the chemical industry's demand for electricity. The demand from the European chemical industry is estimated to increase to 135% of the expected EU electricity production in 2050 [15] and estimations for the global chemical industry indicate a future demand 6 times larger than the current global energy demand [16]. Therefore, DSM in the chemical industry is also a topic of interest for the power sector [17–19].

A requirement for DSM is flexibility. Flexibility in chemical plants can be achieved via flexible process operation. However, the flexibility potential of most chemical processes is still unclear, and previous work showed that stakeholders see opportunities but also plenty of potential limitations [20].

Flexibility in chemical plants can also be achieved by operating the plant's utility system (the in-situ system that delivers the electricity, heat and cooling required by the plant as depicted in Figure 3.1) flexibly. About one-third of GHG emissions from the chemical industry stem from energy use [3], indicating that the electrification of utility systems combined with the adoption of storage technologies could allow for a first step towards emission reduction and DSM while ensuring a constant delivery of energy to the processes.

Many studies have presented models which design utility systems for chemical processes (see Table C.1 in Appendix C). However, the electrification of utility systems has received limited attention (see Appendix C for a literature review). Therefore, it is still unclear which technology portfolio could best enable electrification and how electrified systems would perform in terms of cost and CO_2 emissions compared to utility systems based on fossil sources.

Currently, incentives to electrify utility generation are limited because most industries have long-term energy contracts with a fixed, constant price for energy. In this work,

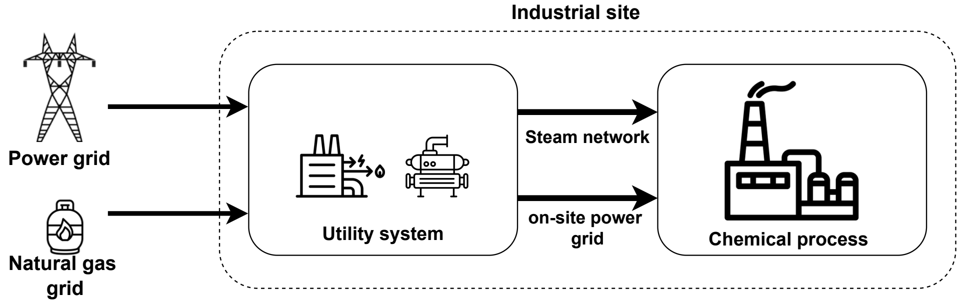


Figure 3.1.: Sketch of an industrial site including a utility system.

a scenario is considered in which companies need to pay (fluctuating) market prices for the energy they consume and consider electrifying their fossil-based utility system. The aim is to 1) understand how the electrification of utility systems could look under different combinations of fluctuating electricity, natural gas and CO_2 emission allowance prices and 2) examine if, and to what extent, cost-optimal systems lead to CO_2 emission reductions while delivering constant utilities.

Different processes from the ethylene value chain, an important branch of the petrochemical industry, are analysed. As a base chemical, ethylene is a building block for, among others, plastics such as polyethylene (PE) and polyvinyl chloride (PVC). Global production of Ethylene was approximately 230 million metric tons in 2023 and is expected to reach around 290 million metric tons in 2030 [21]. Today, Ethylene is produced from fossil feedstock like naphtha or ethane, which is produced from natural gas or petroleum. The most common production process for ethylene is steam cracking, the most energy-intensive process within the chemical industry [22]. Therefore, the ethylene industry is a highly polluting industry with global CO_2 emissions of 366 million tons every year [23], and emission reduction is crucial if the chemical industry wants to meet emission reduction targets. To understand how the utility demand (i.e., the heat and power demand) of a plant impacts its (potential) electrification, the analysis includes four additional plants from an ethylene value chain located at the chemical cluster in the Port of Rotterdam: An ethylene oxide plant, an ethylbenzene plant, an ethylene glycol plant and a PET plant.

3.1.1. Contributions

Based on the knowledge gaps discussed above, the contribution of the study to the existing literature is threefold.

- It is unknown to what extent electrification can become a cost-effective decarbonisation strategy for utility systems in existing chemical plants. To address this gap, five plants from an ethylene value chain were studied. Six years of historical energy price data were used to assess how energy prices could lead to cost-efficient electrification of utility systems. The results are considered representative beyond the 5 processes studied in this chapter, as chemical processes tend to have similar conditions to the ones studied in this work (i.e., low- to high-level temperature demand and low levels of flexibility).

- The results show which portfolio of technologies is selected to replace fossil-based technologies and how utility demand, legacy technologies, fuel costs, technology costs, and the grid connection capacity affect the choice.
- Hydrogen is a required feedstock for many chemical processes, but it is not yet understood if hydrogen could also be an alternative energy carrier for utility systems. This work investigates whether including hydrogen in the energy carrier mix is economically beneficial, considering the current and decreased technology cost scenarios.

The remainder of this chapter is structured as follows. Following the introduction, the methods and the model used are described in detail in Section 2. Section 3 presents the results, and Section 4 discusses them and their limitations. Section 5 provides the conclusion of the findings presented in this chapter.

3.2. Methods

Utility systems that allow for a continuous energy supply are modelled under six different combinations of market prices for electricity, natural gas and ETS emission allowances and their techno-economic performance is analysed for five industrial processes with constant utility demands.
Following the current situation in the chemical industry in the Port of Rotterdam, the utility systems are assumed to have a fossil-based utility generation technology already in place. Electricity-based generation and storage units can be added to the technology in place. Since many combinations of generation and storage units are possible, mathematical optimisation is used to find the cost-optimal design of the new utility system. Figure 3.2 provides information about the inputs and outputs of the optimisation model. The mathematical formulation of the model is described in the following section, followed by a brief presentation of the technologies with which the utility systems can be extended. Section 3.2.3 describes the benchmark system modelling, section 3.2.4 presents the price scenarios considered, section 3.2.5 discusses the conducted sensitivity analyses, and section 3.2.6 describes the industrial processes which serve as the case study in this work.

3.2.1. Optimisation model

The following section presents the model that is used to determine the technology portfolio and operation of cost-optimal utility systems for chemical plants. The following assumptions are made. Each utility system supplies one individual plant. The heat and power demands of the plant have to be fulfilled at all times. A legacy technology (a CHP or a gas boiler) can be operated at no additional investment cost. If the heat demand of the plant is similar to the power demand, a CHP is assumed as the legacy technology. For processes with a much higher heat than power demand, a gas boiler is assumed to be the legacy technology. The capacity of the legacy

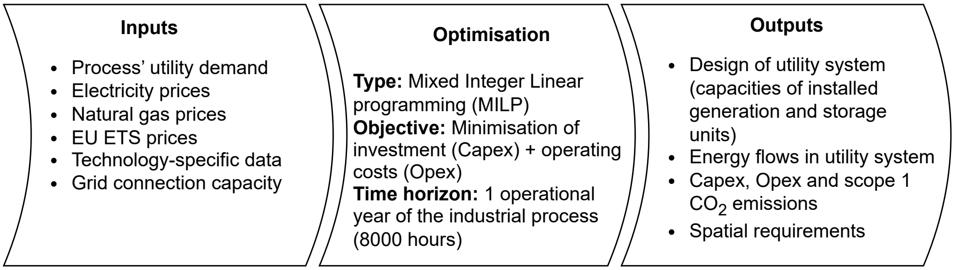


Figure 3.2.: The optimisation model used to design cost-optimal utility systems.

technology is equal to the heat demand of the plant. If the legacy technology is a CHP, power can be sold to the grid at the current market price. Selling steam is not considered. Electricity and natural gas are available at all times and have to be bought at the (fluctuating) market price of the respective national markets. No new fossil-based utility technologies can be installed, only non-fossil-based technologies and storage capacity for electricity and heat can be added to the existing utility systems. The assumed grid connection capacity limits the maximum power flow from the grid but comes at no additional cost. The cost of electricity consumption peaks is not considered.
The model is formulated in Python, using the 'Pyomo' package for optimisation. It is a mixed-integer linear programming problem (MILP) solved using Gurobi's solvers. The objective of the optimisation is to minimise the sum of the required investment CapEx_i for newly installed technology i and the operational cost OpEx(t) of the utility system over the 8000 annual operating hours of the chemical plant, according to Eq. (D.47).

$$min \sum_{t=0}^{t=8000} \text{OpEx}(t) + \sum_i \text{CaPex}_i \tag{3.1}$$

The OpEx is calculated according to Eq.(5.2) and consists of three components: first, the cost of consuming grid electricity minus the potential revenue from selling excess electricity from the CHP to the grid, if applicable. Second, the cost of consuming natural gas and third, the payments for purchasing CO_2 emission allowances within the European Emission Trading System (EU ETS).

$$\begin{aligned} \text{OpEx}(t) = \; & \text{p}_{\text{el, grid}}(t) \cdot \sum (P_{gr,i}(t) - P_{i,gr}(t)) \cdot \Delta t \\ & + \text{p}_{\text{NG}}(t) \cdot NG_{in}(t) \cdot \Delta t \\ & + \text{p}_{\text{EUA}}(t) \cdot NG_{in}(t) \cdot \Delta t \cdot \text{EF}_{\text{NG}}, \end{aligned} \tag{3.2}$$

The first component is the cost of purchasing electricity from the grid, with $\text{p}_{\text{el, grid}}(t)$ being the hourly market price in [eur/MWh]. Power flow from the grid to technology i is denoted as $P_{gr,i}(t)$ and power flow from technology i back to the grid as $P_{i,gr}(t)$. Both are expressed in [MW], and Δt is $1h$. Note that taxes and other fees for selling power back to the grid are neglected. The second component of the operating cost is

the cost of purchasing natural gas with market price $p_{NG}(t)$ at time t in [eur/MWh], required to fuel the legacy technology. The quantity of gas consumed over time is denoted by $NG_{in}(t)$ and measured in [MW]. The last component is the cost for emission allowances for the CO_2 emissions produced by the legacy technology (scope 1 emissions). The price per ton of CO_2 emitted at time t is $p_{EUA}(t)$ in [eur/ton$_{CO_2}$]. The emissions caused per MWh of combusted natural gas are calculated with the emission factor $EF_{NG} = 0.2\,t_{CO_2}/\mathrm{MWh}$.
The CaPex for each technology i is calculated in Eq.(5.3), where s_i denotes the size of an equipment and c_i the cost per unit of equipment size. Since the model is run for only one year, the required investment for added technologies is annualised using an annualisation factor AF_i, which is calculated as stated in Eq.(5.4).

$$\mathrm{CaPex}_i = s_i \cdot c_i \cdot \mathrm{AF}_i \tag{3.3}$$

$$\mathrm{AF}_i = \frac{r}{1-(1+r)^{-\mathrm{LT}_i}} \tag{3.4}$$

With the annualisation factor, the costs are annualised over the lifetime LT_i of equipment i. The discount rate r is set to 10%, as in [24].
Since most chemical plants are designed to operate at their rated capacity continuously, the electricity demand P_{dem} and the heat demand H_{dem} of the plants need to be fulfilled at all times. Eq. (3.5) and Eq.(3.6) describe the equality constraints that ensure a constant supply of utilities, where $P_{dem,\ plant}(t) = \mathrm{const.}$ and $H_{dem,\ plant}(t) = \mathrm{const.}$

$$\mathrm{P}_{\mathrm{dem,\ plant}}(t) = \sum P_{i,\mathrm{plant}}(t) \tag{3.5}$$

$$\mathrm{H}_{\mathrm{dem,\ plant}}(t) = \sum H_{i,\mathrm{plant}}(t) \tag{3.6}$$

$P_{i,\mathrm{plant}}(t)$ are electricity flows from equipment i to the plant. $H_{i,\mathrm{plant}}(t)$ are heat flows from equipment i to the plant.
How much heat or electricity can be delivered by the generation technologies is determined by their size s_i in Eq.(3.7), where $P_{i,j}(t)$ is the power flow from technology i to technology j, and $H_{i,j}(t)$ the respective heat flow.

$$\begin{aligned} s_i &\geq \sum P_{i,j}(t) \text{ or} \\ s_i &\geq \sum H_{i,j}(t) \end{aligned} \tag{3.7}$$

The required inflow into the equipment is calculated using Eq.(3.8). The energy type input and output depend on the equipment. For example, the CHP's energy input is natural gas, and the energy output is heat or electricity.

$$\sum \mathrm{Energy}_{i,in}(t) \cdot \eta_i = \sum \mathrm{Energy}_{i,out}(t) \tag{3.8}$$

The flexibility of the legacy technologies is limited. To avoid damage, cold starts are avoided by defining a minimal load under which the load of the unit cannot drop, as described in Eq.(3.9).

$$\sum \text{Energy}_{\text{CHP/GB},out}(t) \leq s_{\text{CHP/GB}} \cdot \eta_{\text{CHP/GB}} \cdot \text{MinLoadFactor}_{\text{CHP/GB}} \tag{3.9}$$

How much energy can be taken from the storage units depends on their state of energy SOE_i. All storage units are empty at the beginning of the optimisation. For $t > 0$, the state of energy is found by Eq.(3.10).

$$SOE_i(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_i(t-1) \ + \sum \text{Energy}_{j,i}(t-1) \cdot \eta_{\text{charge},i} - & \\ \sum \text{Energy}_{i,j}(t-1)/\eta_{\text{discharge},i}, & \text{otherwise} \end{cases} \tag{3.10}$$

The maximum state of energy is constrained by the unit's size s_i according to Eq.(3.11).

$$SOE_i(t) \leq s_i \tag{3.11}$$

For the battery and the thermal energy storage, the charge and discharge power are constrained by a charge rate (crate_i) of the technology, as described in Eq.(3.12) and Eq.(3.13), respectively. To prevent simultaneous charging and discharging, a binary variable b_i is implemented as described in Eq.(3.12) and Eq.(3.13). If $b_i(t) = 1$, the discharge power can only be 0, if $b_i(t) = 0$, the charge power can only be 0.

$$\begin{aligned} P_{j,i}(t) &= 0, \quad \text{if } t = 0 \\ P_{j,i}(t) &\leq s_i \cdot \text{crate}_i / \Delta t \cdot b_i(t), \quad \text{if } t \geq 0 \end{aligned} \tag{3.12}$$

$$\begin{aligned} P_{i,j}(t) &= 0, \quad \text{if } t = 0 \\ P_{i,j}(t) &\leq s_i \cdot \text{crate}_i / \Delta t \cdot (1 - b_i(t)), \quad \text{if } t \geq 0 \end{aligned} \tag{3.13}$$

Since the utility systems are connected to the national power grid, the total power flow from the grid to the utility system and from the utility system to the grid is constrained by the capacity of the utility system's connection to the grid cap_{gr}. This is reflected in Eq.(3.14) and Eq.(3.15).

$$\sum P_{gr,i}(t) \leq \text{cap}_{\text{gr}} \tag{3.14}$$

$$\sum P_{i,gr}(t) \leq \text{cap}_{\text{gr}} \tag{3.15}$$

A complete formulation of the model and the nomenclature are listed in Appendix D.

To validate the model, it was run with the (fixed) energy prices that energy-intensive industries are paying at the moment. No new technologies were installed in the resulting cost-optimal utility systems, and the utility generation was fully fossil fuel-based. This mirrors the current situation in the chemical industry.

3.2.2. Technologies

The technologies included in the optimisation model have been selected based on their suitability to supply the required utilities and their technological maturity. Only commercially available technologies are considered. The following subsection describes the technological options, while Tables 5.1 and 5.2 provide an overview of the data used for modelling those technologies.

Utility generation technologies

In many existing utility systems, the energy demand is supplied by a CHP or a gas boiler fuelled by natural gas [8]. Therefore, it is assumed that either a CHP or a gas boiler has been installed in the past and can operate without any additional investment cost or spatial requirement. Electricity from the CHP can be sold to the power grid. An electricity-based alternative for heat generation is an electric boiler. Electric boilers are frequently mentioned in literature as a key technology for the electrification of industrial heat demand [15, 25, 26], and companies are running pilot projects with electric boilers [27]. Electric boilers are a mature technology [28], can start up quickly, and have high ramp rates [29]. They can produce saturated steam of up to 350°C [30]. Another alternative technology for steam production is a hydrogen boiler (H2 boiler). Hydrogen boilers have been implemented in various industrial sectors [31], for example, in the chlorine industry to increase the economic performance of the plant by using the by-product hydrogen energetically instead of venting it into the atmosphere [32, 33]. In the model, the hydrogen that fuels the hydrogen boiler is produced on-site from water electrolysis. The electrolyser is assumed to be a proton exchange membrane (PEM) electrolyser because its flexibility is higher than that of alkaline electrolysers [34]. Note that even though existing electrolysers have limited capacity (operating PEM electrolysers have reached capacities around 20 MW), the capacity of the electrolyser is not limited in our model. Table 5.1 lists the data used to model the generation technologies.

Table 3.1.: Data used to model conversion technologies

	CHP	Gas boiler	Electric boiler	Electrolyser	H2 boiler
Capacity thermal [MW_{th}]	H_{dem}	H_{dem}	decision variable	decision variable	decision variable
electric [MW_{el}]	$H_{dem}/\eta_{th,\text{CHP}} \cdot \eta_{el,\text{CHP}}$				
Efficiency η [%]	$\eta_{th} = 40$, $\eta_{el} = 30$ [35, 36]	$\eta_{th} = 90$ [24]	99 [25, 26, 29]	69 [34]	92 (based on [37, 38])
Minimal load factor [% of max. load]	50 [39]		0	0	0
Cost [Eur/kW]	not included in model		70 [29]	700 [34]	35 [31]
Lifetime lt [years]	not included in model		20 [29]	15	20 [31]

Storage units

To allow the utility system to use energy at a different time than generated or procured, three storage units are included in the utility system models: Lithium-ion batteries, high-temperature sensible thermal energy storage and hydrogen storage tanks (H2 Storage). Table 5.2 provides the data used to model the storage units.
Figure 3.3 depicts how the technologies presented above can be interconnected in the case of a plant with an existing CHP. Electricity flows are depicted in yellow, natural gas flows in grey, hydrogen flows in blue and steam flows in red.

Table 3.2.: Data used to model storage technologies

	Battery	Thermal energy storage	H2 Storage[a)]
Capacity [MWh]	decision variable	decision variable	decision variable
Efficiency			
η_{ch} [%]	95 [24]	90 [40]	90 [24]
η_{disch} [%]	95 [24]	100	100
Ramp rate rr [% of max. load]	100	100	100
Cost [Eur/kWh]	300[41]	23 [40]	10[40]
Lifetime [years]	15 [41]	25 [42]	20 (based on [43])

[a)] A type I tank (the most simple storage tank version [44]) that stores hydrogen at 200 bar.

3.2.3. *Benchmark utility system*

In this study, the benchmark utility systems consist of a connection to the national power grid and a natural gas-fuelled CHP if the plant's heat demand is approximately the same as its power demand or a gas boiler if the heat demand is much higher than the power demand. The thermal capacity of the CHP or gas boiler is assumed to be just enough to fulfil the heat demand of the respective plant, and the ratio between heat and electricity generation of the CHP is assumed constant. This can result in a mismatch between the plants' electricity demand and the electricity generated by the CHP, which is why additional electricity is bought, or excess electricity is sold via the connection to the national power grid.
The benchmark systems operate under the same energy market price scenarios as the new utility systems (Table 3.3). The resulting operational costs and CO_2 emissions are calculated using the equations described in Appedix D.2.

3.2.4. *Energy price scenarios*

This study considers several combinations of market price data for electricity, natural gas and CO_2 emissions allowances. Six different independent years are explored, and an operational time of 8000 hours is considered for a plant. The combinations of price data correspond to historical data from 2018 to 2023. Even though those years include the COVID pandemic and increased gas prices due to Russia's invasion of Ukraine, they are considered interesting to assess because the rise in gas prices and

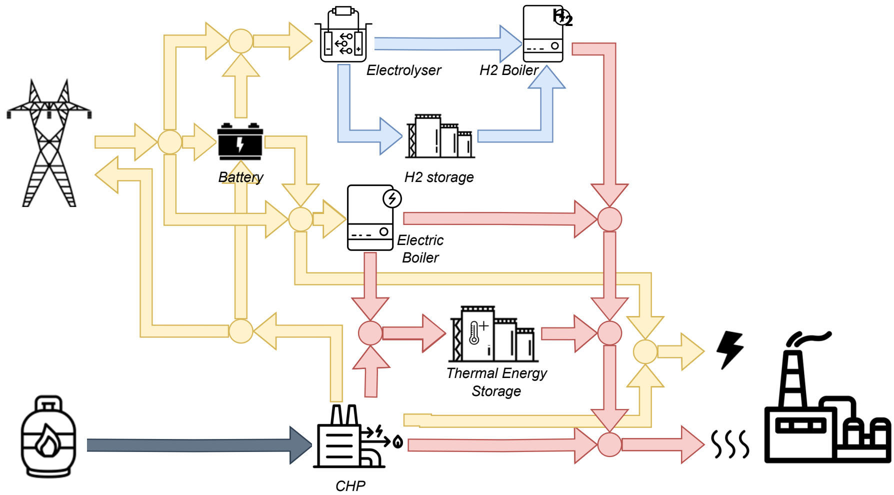


Figure 3.3.: Illustration of the options to configure the utility system with a CHP as legacy technology. A connection to the national power grid and a natural gas-fuelled CHP are assumed to be in place. In addition, the model can choose to add a battery, an electric boiler for steam generation, thermal energy storage, a hydrogen tank and/or a hydrogen boiler. Electricity flows are yellow, natural gas flows grey, hydrogen flows blue and steam flows red.

electricity price fluctuations is likely to continue with the increasing decarbonisation of the global economy. Data of the Dutch Day-ahead electricity market was retrieved from the ENTSO-E transparency platform [45], data for the natural gas market (Dutch TTF) was retrieved from an online source [46], and EU ETS emission allowance prices were obtained from Ember [47] and Sandbag [48]. Since the gas price data was only available per day and because the market is not operating on the weekends, the data had to be treated before running the optimisation. The opening price of the day was assumed to last for all 24 hours of the day, and the previous existing value replaced non-existing values. The EU ETS emission allowance data was also only available in daily resolution and treated the same way as the natural gas price data.
Table 3.3 shows the mean and the variance of the electricity price and the cost of using natural gas (the sum of the natural gas price and the EU ETS emission allowance price per MWh of natural gas used) per scenario. Of all years, 2020 has the lowest mean prices, but the variance is the lowest in 2019. 2022 shows the highest mean prices and variance in electricity and gas use costs. While mean prices are similar in 2021 and 2023, the variance in 2021 is higher than in 2023, especially in the cost of using natural gas. The table also shows the number of hours during

which using electricity is cheaper than using natural gas[1]. This number increases significantly after 2019 (more than fivefold), and 2023 has the highest amount of hours favouring electricity use. Note that while the mean and variance of electricity price and cost for gas use are somewhat similar in 2021 and 2023, the respective number of hours with lower electricity prices differs almost by a factor of 2.

Table 3.3.: Average and variance of the considered prices for electricity and the cost of using natural gas (equal to natural gas price + cost for EU ETS CO_2 allowance) and number of hours during which the electricity price is lower than the cost of using natural gas. Based on [45–48].

	Electricity price		**Cost of using natural gas**		**Electricity price < using natural gas**
	Mean	Variance	Mean	Variance	Number of hours
Year	[Eur/MWh]	[(Eur/MWh)^2]	[Eur/MWh]	[(Eur/MWh)^2]	[hours]
2018	52	233	25	16	99
2019	42	128	20	10	62
2020	31	199	14	13	518
2021	90	3263	51	783	611
2022	240	16886	150	2813	1280
2023	98	2383	59	120	1153

3.2.5. Sensitivity analyses

The sensitivity of the results to three parameters is tested. First, the available grid connection capacity; second, the minimal load of the legacy technology; and third, the technology cost for batteries, thermal energy storage, and electrolysers.

Grid connection capacity

Sufficient grid connection capacity is key for electrification, but it might not be readily available to industrial sites. In the Netherlands, for example, the current situation of the power grid imposes a barrier to electrification plans which require additional connection capacity [49]. Therefore, it is important to examine if/how the conclusions of this work are affected by the assumed grid connection capacity. Hence, the model is run for different grid connection capacities as follows.
If the parameter f_{grcap} in Eq.(3.16) is equal to 1, the grid connection capacity cap_{gr} in Eq.(3.14) and Eq.(3.15) is big enough, yet not larger than necessary, to allow for a fully electrified utility supply in the utility generation "chain" with the lowest conversion efficiency.

$$cap_{gr} = f_{grcap} \cdot \frac{P_{dem} + H_{dem}}{\eta_{bat} \cdot \eta_{bat} \cdot \eta_{H2E} \cdot \eta_{H2S} \cdot \eta_{H2B}} \tag{3.16}$$

For the sensitivity analysis, f_{grcap} takes values between 0.5 and 1.2, which represent grid connection capacities between 50% and 120% of what is required for a fully electrified utility system, respectively.

[1]The number of hours when $p_{el,\ grid}(t) < p_{NG}(t) + p_{EUA}(t) \cdot EF_{NG}$.

Minimal load of the legacy technology

Since the new utility systems include a fossil-based legacy technology, they might depend on the flexibility of the latter, which is limited by the minimal load. As described in 3.2.1, the legacy technology is assumed to be unable to shut down and to operate at a minimum of 50% of its capacity to avoid damage. Therefore, it is explored if/how the conclusions of this work would change if a more optimistic value of 30% for the minimal load factor $MinLoadFactor_{\text{CHP/GB}}$ in Eq.(3.9) is chosen.

Cost of new utility equipment

The costs for batteries, thermal energy storage and water electrolysers are considered the most uncertain among the technology portfolio. Hence, the sensitivity of the results to those parameters is tested by repeating the model runs with distinct technology cost (TC) scenarios. Per run, the cost of one technology was either increased or decreased by 25%. This resulted in the six TC scenarios described in table 3.4.

Table 3.4.: Technology cost data per technology cost (TC) scenario

TC scenario	Electric boiler [Euro/kW$_{th}$]	Battery [Euro/kWh]	TES [Euro/kWh]	Electrolyser [Euro/kW]	H2 boiler [Euro/kW$_{th}$]	H2 storage [Euro/kWh]
Bat-High	70	375	23	700	35	10
Bat-Low	70	225	23	700	35	10
TES-High	70	300	28.75	700	35	10
TES-Low	70	300	17.25	700	35	10
H2E-High	70	300	23	875	35	10
H2E-Low	70	300	23	525	35	10

3.2.6. Case study

In this work, the model presented above is run for plants from an ethylene value chain. The case study includes five plants: An olefins plant, an ethylbenzene plant, an ethylene oxide plant, an ethylene glycol plant, and a PET plant. The processes have different utility demands (in magnitude and ratio of power to heat demand), which allows analysis of the impact of the 'demand profile' on the technology portfolio of the new utility system. Table 3.5 provides an overview of the plants' utility demand and their production capacities. Energy demand data was obtained from existing Aspen Plus twin models of an Ethylene value chain located in the chemical cluster of the Port of Rotterdam, the Netherlands [50]. Currently, the energy demand from the plants in the cluster is supplied by natural gas combustion and, in the case of the olefins plant, by the combustion of waste gases from the process itself for the generation of very high-pressure steam required in the steam cracker. For this study, the utility generated from waste gas combustion is not considered since it is assumed that the core processes remain unchanged, and therefore, waste gases continue to be available. The remaining steam requirements do not exceed medium-pressure steam at 265°C. Note that the model data might overestimate utility demands compared to

data from real plants since heat integration is likely more advanced in practice than in the models.
As shown in the table, the olefins plant has the highest production capacity (in terms of kilotons per year) and the highest energy demand. Electricity demand and heat demand are almost equal. The remaining plants have a higher heat demand than electricity demand. In terms of energy intensity per unit of product, the olefins plant has the highest specific energy intensity, and the ethylbenzene plant has the lowest.

Table 3.5.: Overview of the chemical plants analysed in this study, including their production capacities, utility demands, and assumed legacy technologies

	Capacity	**Electricity demand**		**Heat demand**[a]			
		Power	Cooling	LPS	MPS	HPS	
Chemical plant	[kilotons/ year]	[MW]	[MW]	[MW]	[MW]	[MW]	Legacy technology
Olefins	878 (ethylene)	37.67	138.48	180.85	0	0	CHP
Ethylene oxide	293	5.13	15.04	30.07	0	0	CHP
Ethylbenzene	758	0.3	0.6	0	2.3	41.06	Gas boiler
Ethylene glycol	113	1.06	1.14	0	44.32	0	Gas boiler
PET	231	0.67	0.49	0	0	24.49	Gas boiler

[a] LPS at 155°C, 5.5 bar; MPS at 214°C, 12 bar; HPS at 265°C, 51 bar

Table 3.5 also shows the assumed fossil fuel-based legacy technology for each plant. As explained in 3.2.3, the legacy depends on the ratio of the plant's heat and power demand. If the demand is in the same order of magnitude, a CHP is assumed to supply the plant's demand. If the heat demand is higher than the power demand, the legacy technology is assumed to be a gas boiler. In both cases, a connection to the national power grid is required to supply electricity to the plant. This is because the electricity generation by the CHP does not match the plant's demand. Table 3.6 provides the thermal and electric capacities of the benchmark systems consisting of a CHP and the mismatch between electricity demand and generation.

Table 3.6.: Thermal and electric capacity of the CHP and the mismatch between the process's electricity demand and the electricity generated by the CHP, which has to be supplied by or sold to the national power grid

System	Thermal capacity CHP [MW_{th}]	Electric capacity CHP [MW_{el}]	Electricity mismatch $P_{dem} - P_{\mathrm{CHP}}$ [MW_{el}]
CHP Olefins	181	136	40
CHP Ethylene oxide	30	23	-2

3.3. Results

3.3.1. Cost-optimal utility systems for different Opex scenarios

This section presents the cost-optimal utility systems for all plants and (individual) years considered. The results show which technology portfolios are chosen per plant and year, and how the economic and environmental performance of the new utility systems compares to the respective benchmark system. First, the results are presented for the plants with an existing CHP and subsequently for those with an existing gas boiler. Note that the new utility systems have enough grid connection capacity available for complete electrification of the utility demand of the respective plant, and that the minimal load of the fossil-based legacy technology is set to 50% of its maximum capacity.

Plants with an existing CHP

Tables 3.7 and 3.8 show that the utility systems remain fossil-based for 2018 and 2019 because the energy and ETS prices are not incentivising new investments. In the remaining four years, a partially electrified system results in lower total costs than the Opex of the benchmark system (which is equal to the total cost since no Capex is required).
In 2020 and 2021, an electric boiler is installed to supply the remaining heat demand of the plant when the CHP is operating at its minimum load because consuming natural gas is more expensive than electricity. The costs of using natural gas include its market price and the price for the required CO_2 emission allowances. In 2022, the mean prices and fluctuations of natural gas and electricity are high enough to install a battery that shifts fuel use to hours with low electricity prices and enables cheap heat generation with the electric boiler.

Table 3.7.: Additionally installed utility technologies for cost-optimal utility system for an Olefins plant for six energy price years and a grid connection capacity of 692.4 MW

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2018	0.0	0.0	0.0	0.0	0.0	0.0
2019	0.0	0.0	0.0	0.0	0.0	0.0
2020	90.4	0.0	0.0	0.0	0.0	0.0
2021	90.4	0.0	0.0	0.0	0.0	0.0
2022	423.6	741.7	2591.7	0.0	0.0	0.0
2023	511.1	0.0	2103.2	0.0	0.0	0.0

Table 3.8.: Total cost and scope 1 CO_2 emissions of the benchmark and new utility system for the Olefins plant for distinct energy price data and a grid connection capacity of 692.4 MW

	Total cost [Million euro]			Scope 1 CO_2 emissions [kiloton]		
Year	CHP-based system	New system	Reduction [%]	CHP-based system	New system	Reduction [%]
2018	107.8	107.8	0.0	723.4	723.4	0.0
2019	84.7	84.7	0.0	723.4	723.4	0.0
2020	59.4	58.9	0.8	723.4	684.2	5.4
2021	212.9	207.5	2.5	723.4	659.6	8.8
2022	619.5	559.9	9.6	723.4	548.9	24.1
2023	245.0	227.2	7.3	723.4	554.2	23.4

In 2023, no more battery capacity is installed because prices have fallen to lower

levels than those for prices from 2022. Mean prices are lower than in 2021, but the variance is lower. However, the number of hours during which using electricity is cheaper than using gas is higher than in 2021. Therefore, heat storage is financially beneficial. The boiler size equals the grid capacity minus the power demand of the process, which has to be supplied by the grid when the gas boiler is not operating during hours with negative electricity prices. Since no battery is installed, more grid capacity is available for the electric boiler, and hence, its capacity is bigger than in 2022.
The results show that with an increasing number of hours during which using electricity is cheaper than using natural gas, electric boiler capacity is installed first. Next is TES capacity and, third, battery capacity. Hydrogen technologies are not installed for any of the years considered at the assumed technology costs. Partial electrification of the utility system leads to reductions in scope 1 CO_2 emissions of the olefins plant of minimum 5 and maximum 24%.
For the utility system of the ethylene oxide plant, the trends regarding which technologies are installed in which year are similar to those for the utility system of the olefins plant. The results can be found in tables E.1 and E.2 in Appendix E. Compared to the benchmark system, CO_2 emission reduction (scope 1) ranges from 5 to 24%.

Plants with an existing gas boiler

Tables 3.9 and 3.10 show results similar to the results for the olefins plant with the difference that no additional technologies are installed for the utility system in 2020. For the sole production of steam, the gas boiler is more efficient than a CHP. Hence, increased natural gas use costs have a lower impact on a system with a gas boiler than on a system with a CHP. In 2020, the gas use costs are not sufficiently high (and/or the power prices are not often enough cheaper than the gas use costs) for installing a power-to-heat unit.
A cost-efficient partial electrification of utility systems enables CO_2 emission reductions between 5 and 19% compared to the benchmark utility system for the ethylbenzene plant.

Table 3.9.: Additionally installed utility technologies for cost-optimal utility system for an ethylbenzene plant for six years' energy price data and a grid connection capacity of 85.8 MW

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2018	0.0	0.0	0.0	0.0	0.0	0.0
2019	0.0	0.0	0.0	0.0	0.0	0.0
2020	0.0	0.0	0.0	0.0	0.0	0.0
2021	21.7	0.0	0.0	0.0	0.0	0.0
2022	83.3	3.8	385.4	0.0	0.0	0.0
2023	84.1	0.0	361.3	0.0	0.0	0.0

The technology portfolio in the different years for the ethylene glycol and the PET plant is the same as for the ethylbenzene plant, only the capacities are different, as shown in Appendix E, tables E.3 and E.5. The economic and environmental

Table 3.10.: Total cost and scope 1 CO_2 emissions of the benchmark and new utility system for an ethylbenzene plant for distinct energy price years and a grid connection capacity of 85.8 MW

	Total cost [Million euro]			Scope 1 CO_2 emissions [kiloton]		
Year	GB-based system	New system	Reduction [%]	GB-based system	New system	Reduction [%]
2018	10.1	10.1	0.0	77.1	77.1	0.0
2019	7.9	7.9	0.0	77.1	77.1	0.0
2020	5.5	5.5	0.0	77.1	77.1	0.0
2021	20.2	20.0	1	77.1	73.5	4.7
2022	59.5	55.7	6.4	77.1	62.6	18.8
2023	23.5	21.5	8.5	77.1	62.7	18.7

performance of the new utility systems is presented in tables E.4 and E.6 in Appendix E. CO_2 emission reduction differs per plant in terms of absolute numbers but remains between 5 and 19% compared to the benchmark system.

3.3.2. *Sensitivity analyses*

Grid connection capacity

Plants with an existing CHP Independent of the grid connection capacity, no additional capacity is installed in 2018 and 2019, and no hydrogen-based technology is installed in any year for the olefins plant. The newly installed capacities in 2020 and 2021 are not affected by the grid connection capacity, either. Figure 3.4 shows only the results affected by the grid connection capacity. The complete results are presented in the Appendix E.

Figure 3.4 shows that although the grid connection capacity does not impact which technologies are installed in which year, it affects the capacities of the newly installed technologies. When the connection capacity is lower than required for a fully electrified utility supply, the capacities decrease because of the limited power inflow from the grid. When the grid connection capacity increases after it has reached a capacity at which a fully electrified supply is possible, the installed capacities of the electric boiler and the TES increase, but the battery capacity remains stable. The findings support the previous observation that the grid connection capacity is the limiting factor for the electric boiler capacity and that the TES capacity depends on it in 2022 and 2023. If more grid connection capacity is available, investments into higher electric boiler and TES capacities pay off from shifting energy consumption in time. Since this is not the case for battery capacity, battery capacity is likely too expensive for energy-shifting purposes. The results for utility systems for the ethylene oxide plant differ in terms of capacities but reveal the same findings (see Appendix E).

Plants with an existing GB The results for plants with existing gas boilers support the findings described above. As an example, the results for the ethylbenzene plant are shown in Figure 3.5. In the years with the highest number of hours during which using electricity is cheaper than using gas, 2022 and 2023, the electric boiler and TES

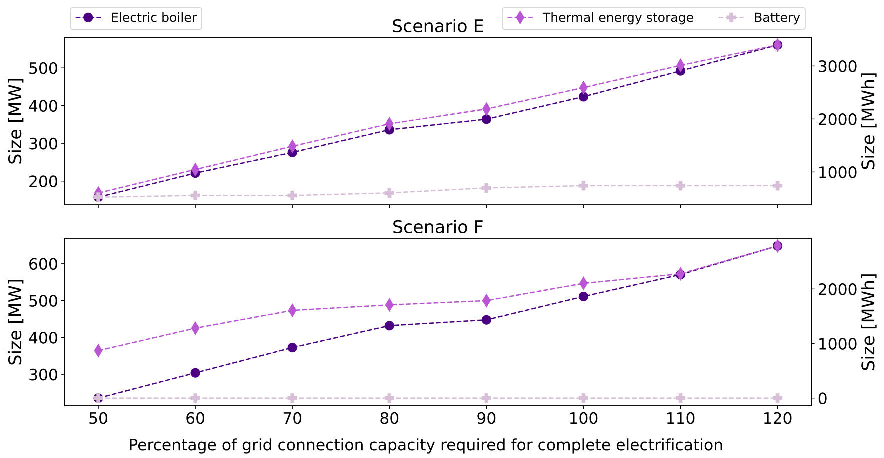


Figure 3.4.: Newly installed capacity for the olefins plant under different grid connection capacity values. f_{grcap} is the percentage of the connection capacity required for a fully electrified utility supply.

capacity increases with increasing grid connection capacity, but the battery capacity remains constant. The complete results are shown in Appendix E.

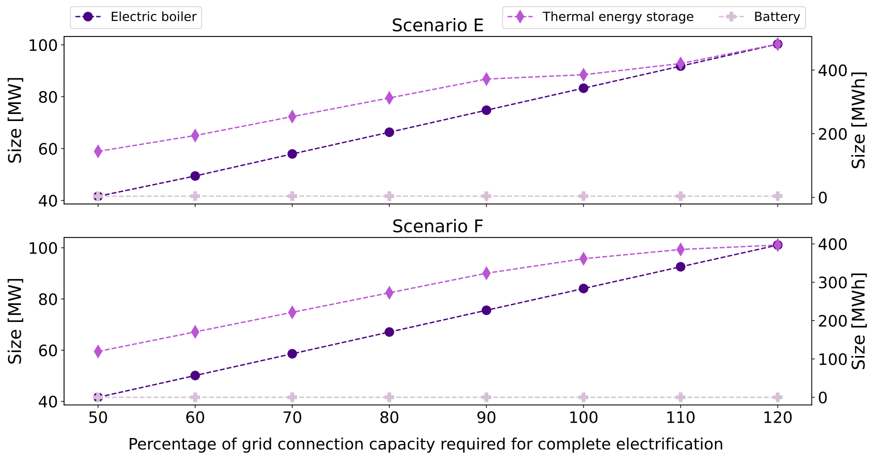


Figure 3.5.: Newly installed capacity for the ethylbenzene plant under different grid connection capacity values. f_{grcap} is the percentage of the connection capacity required for a fully electrified utility supply.

Minimal load of legacy technology

Plants with an existing CHP A lower minimal load of the CHP (which means an increase in flexibility) does not lead to additional capacity for the utility system for the Olefins plant in 2018 and 2019, and none of the years leads to using hydrogen-based technologies. The results in table 3.11 show that a lower minimal load of the CHP does also not affect the 'merit order' in which the technologies are installed (electric boiler first, then TES capacity and then battery capacity). Compared to the utility systems with a higher minimal load of the CHP, the reduced minimal load leads to lower total cost and CO_2 emissions (see table 3.12) and different capacities of the newly installed technologies.

For prices from 2020, 2021, 2022 and 2023, the electric boiler capacity increases because the CHP can be operated at a lower load than in previous utility systems. With 2022 prices, the lower minimal load of the CHP leads to a smaller battery and TES. Since the CHP can supply less heat to the plant when natural gas is expensive, more heat has to be supplied by the electric boiler. Since most of the heat from the boiler goes to the plant, less can go to the TES, which explains why the TES capacity is lower than in the runs with a higher minimal load of the CHP. Since the electric boiler requires more grid power, less power flow is available to charge the battery, and hence, the battery capacity is also smaller. With 2023 prices, the TES capacity is higher than in the run with a higher minimal load of the CHP. If the CHP can be operated at a lower minimal load, more money is saved when the gas price is high. These savings in OPEX are available to be invested in capacity that enables shifting from natural gas to electricity (like the electric boiler) and shifting heat generation in time (like the TES). As the results for the ethylene oxide plant are in line with the discussion above, they are shown in Appendix E.

Table 3.11.: Additionally installed utility technologies for cost-optimal utility system for an Olefins plant for four energy price years, a grid connection capacity of 692.4 MW and lower minimal load of the CHP

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2020	126.6	0.0	0.0	0.0	0.0	0.0
2021	126.6	0.0	0.0	0.0	0.0	0.0
2022	445.4	609.8	2531.9	0.0	0.0	0.0
2023	551.3	0.0	2391.2	0.0	0.0	0.0

Table 3.12.: Total cost and scope 1 CO_2 emissions of the benchmark and new utility system for the Olefins plant under distinct energy prices, a grid connection capacity of 692.4 MW and a lower minimal load of the CHP

	Total cost [Million euro]			Scope 1 CO_2 emissions [kiloton]		
Year	CHP-based system	New system	Reduction [%]	CHP-based system	New system	Reduction [%]
2020	59.4	58.7	1.2	723.4	668.6	7.6
2021	212.9	205.3	3.6	723.4	634.1	12.3
2022	619.5	547.8	11.6	723.4	496.1	31.4
2023	245.0	219.0	10.6	723.4	501.7	30.6

Plants with an existing gas boiler The results for the plants with an existing gas boiler lead to findings similar to those for the olefins plant. The change in minimal load does not affect the energy price years for which it is cost-effective to install new technologies. Neither does it affect which technology portfolio is installed in which year. Nevertheless, the lower minimal load impacts the capacities of the electric boiler and TES, as table 3.13 shows for the ethylbenzene plant. For the electric boiler, the effect differs depending on the year. In 2021, the capacity increases because when the GB operates at its minimal load, additional electric boiler capacity must supply the remaining heat. In 2022, the lower minimal load of the GB leads to a) less fossil- and more electricity-based heat delivered to the plant and b) less fossil- and more electricity-based heat delivered to the TES. Despite the smaller capacity of the TES, the overall energy delivered to the plant by the TES slightly increases compared to the system with a CHP with a higher minimal load. The Sankey diagrams in Figure 3.6 show the energy flows in the respective systems in 2023.

In 2023, the electric boiler capacity remains the same as in the utility system with a less flexible GB, but the TES capacity decreases. Less heat is sent to the TES from the GB. Slightly more heat is sent to the TES by the electric boiler, but overall, the TES supplies the plant with a slightly lower amount of heat while the heat supplied by the electric boiler increases.

The reduced minimal load leads to higher savings in total cost and CO_2 emissions (see table 3.10). The complete results for the plants with existing gas boiler are shown in Appendix E.

Table 3.13.: Additionally installed utility technologies for cost-optimal utility system for an ethylbenzene plant for three energy price years, a grid connection capacity of 692.4 MW and lower minimal load of the GB

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2021	30.4	0.0	0.0	0.0	0.0	0.0
2022	83.4	3.8	371.5	0.0	0.0	0.0
2023	84.1	0.0	322.4	0.0	0.0	0.0

Table 3.14.: Total cost and scope 1 CO_2 emissions of the benchmark and new utility system for the ethylbenzene plant for distinct energy price years, a grid connection capacity of 85.8 MW and a lower minimal load of the GB

	Total cost [Million euro]			Scope 1 CO_2 emissions [kiloton]		
Year	CHP-based system	New system	Reduction [%]	CHP-based system	New system	Reduction [%]
2021	20.2	19.9	1.5	77.1	72.1	6.5
2022	59.5	54.9	7.7	77.1	59.6	22.7
2023	23.5	21.1	10.2	77.1	60.6	21.4

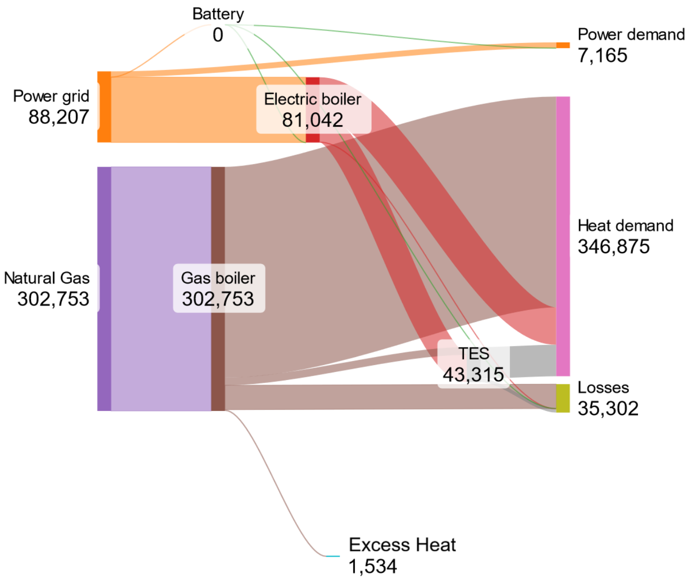
Technology cost scenarios

In the following, results from the utility system model runs with the technology cost data in table 3.4 are presented to show how changes in the investment cost required for battery, TES, and electrolyser capacity impact the previous findings. The data underlying those findings is presented in Appendix E.

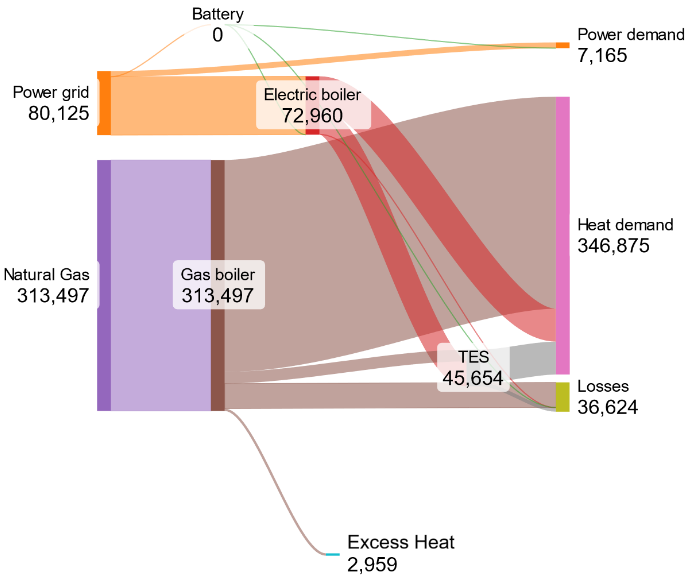
Plants with an existing CHP The technology portfolio per year is not affected by the technology cost (TC) scenarios 'Bat-High', 'TES-High', 'H2E-High' and 'H2E-Low' in 2018, 2019, 2020 and 2021. No additional investment is made in 2018 and 2019, and electric boiler capacity is installed to supply 50% of the plant's heat demand while the CHP is operating at its minimal load in 2020 and 2021. In 2022 and 2023, the technology selection remains the same, but the capacities change for the scenarios 'Bat-High' and 'TES-High': TES capacity is added to the electric boiler in 2022 and 2023, and battery storage is cost-effective only in 2023 in both TC scenarios. However, less TES capacity is installed in' TES-High' compared to the previous results. Furthermore, less battery capacity is installed in 'Bat-High' in 2023, and the electric boiler and TES capacities increase, compared to previous results.

TC scenarios 'Bat-Low' and 'TES-Low' with a 25% decrease in the battery price and TES price, respectively, lead to changes in the technology portfolio in one year, as a battery is added to the technology portfolio in 'Bat-Low' in 2023, and the electric boiler and TES capacity are decreased. An example of the resulting energy flows in the utility system for the olefins plant is shown in Figure 3.7. The Figure shows that the battery is mainly charged from the grid, but also the CHP when the difference between the gas use and electricity cost is small enough for a cost-effective power supply to the plant by the grid (indicated by the beige dots). The battery enables the utility system to sell power back to the grid when the electricity price is high because it supplies the power demand of the plant (indicated by khaki squares), while the CHP supplies the heat but sells the electricity it produces (indicated by the brown stars). The electric boiler capacity is decreased because the battery takes up part of the grid connection capacity. Hence, less power can flow from the grid to the electric boiler. Since the electric boiler is smaller, the TES can decrease in size, too, enabling savings in investment costs.

In 'TES-Low', TES capacity and the required additional electric boiler capacity are added to the technology portfolio installed in 2021 for plants with an existing CHP. The TES is charged during hours with a low electricity price, when the additional electric boiler is operating at its maximum. This allows for more heat generated from electricity during those hours, enabling savings in operational costs (and CO_2 emissions).



(a) Minimal load of GB = 30% of its capacity.



(b) Minimal load of GB = 50% of its capacity.

Figure 3.6.: Sankey diagrams visualising the accumulated energy flows in the cost-optimal utility system for the ethylbenzene plant in 2023 with GBs with different minimal load constraints. The grid connection capacity is 85.8 MW, enough to electrify the plant's utility demand completely.

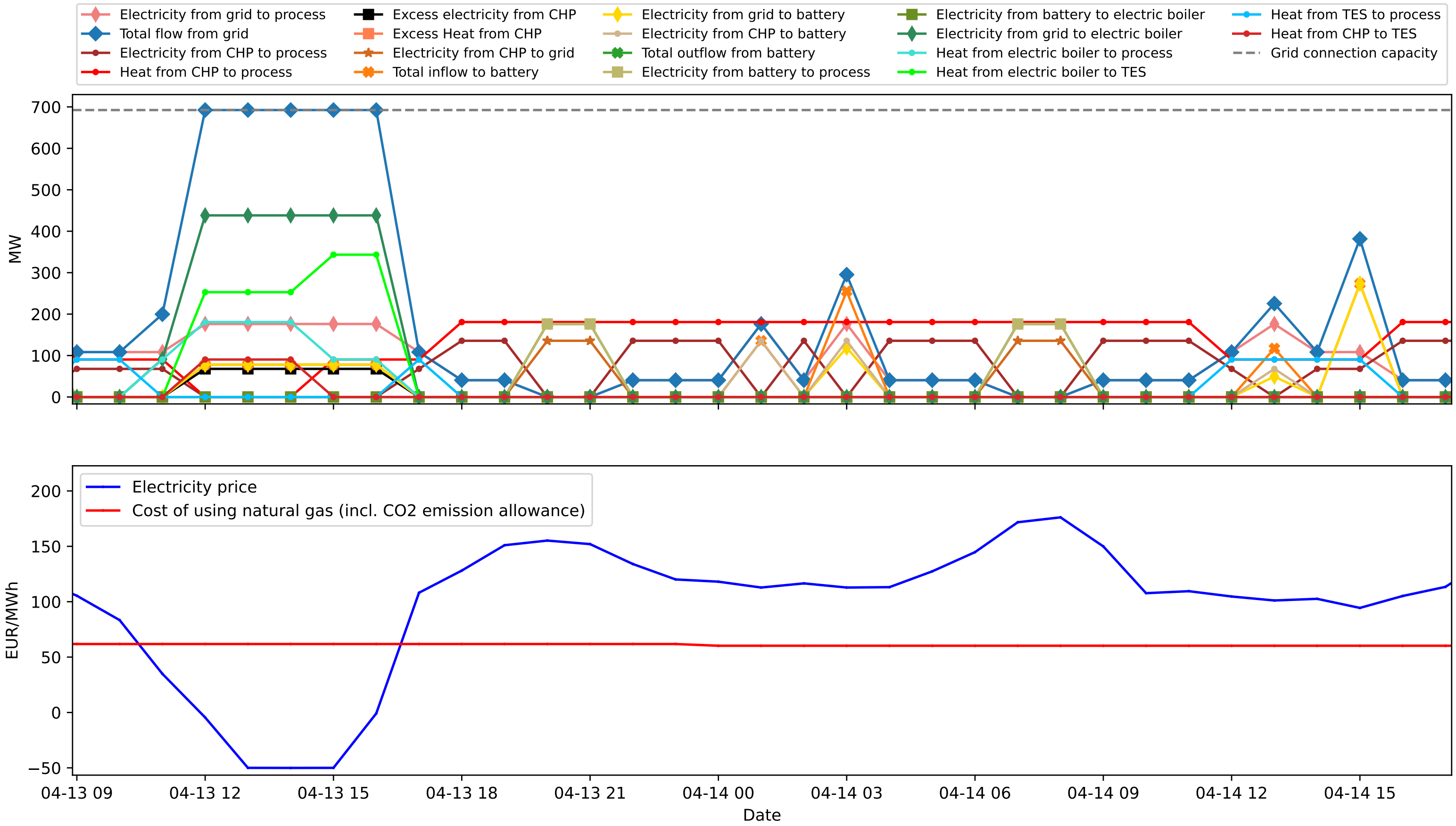


Figure 3.7.: The energy flows of the cost-optimal utility system for an olefins plant in 2023 and technology cost scenario 'Bat-Low'.

Plants with an existing gas boiler For the plants with an existing gas boiler, all observations made about the results for the plants with a CHP are made for the plants with gas boilers, except in TC scenarios ’Bat-Low’ and ’TES-Low’. In ’Bat-Low’, the additional battery capacity in 2023 is small compared to the remaining capacities, as shown in the Sankey diagram for the aggregated energy flows in the utility system for the ethylbenzene plant in Figure 3.8. This is because its role is to supply the power demand of the plant (less than 1 MW) when electricity is expensive.

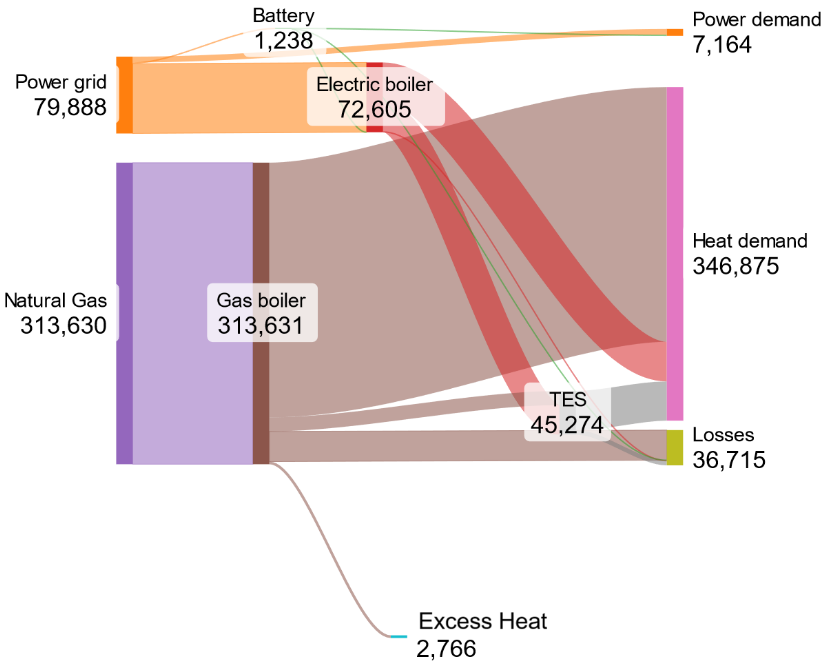


Figure 3.8.: Sankey diagram visualising the accumulated energy flows in the cost-optimal utility system for an ethylbenzene plant in 2023 and technology cost scenario ’Bat-Low’.

No additional TES capacity is added to the cost-optimal utility system in TC scenario ’TES-Low’ in 2021. The savings in operational costs enabled by the additional electric boiler and TES capacity are not enough to pay off the required investment because the share of the operational cost in the total cost is lower than in the case of plants with a CHP. This is because of the gas boiler’s higher efficiency than the CHP.

Results including hydrogen in the energy mix As hydrogen technologies have not been included in the utility systems presented in the previous sections, the technology cost for the electrolyser was decreased further to explore how much the cost would need to decrease until is cost-optimal to invest in hydrogen.

Table 3.15.: Additionally installed utility technologies for cost-optimal utility system for an olefins plant with a grid connection capacity of 692.4 MW and electrolyser technology cost of 68 euro/kW. Note that hydrogen was only part of the energy mix with 2023 energy prices

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2023	492.3	0.0	2009.4	18.9	5.4	130.7

Table 3.16.: Additionally installed utility technologies for cost-optimal utility system for an ethylbenzene plant with a grid connection capacity of 85.8 MW and electrolyser technology cost of 48 euro/kW

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2023	77.9	0.0	337.2	6.3	1.3	31.8

Tables 3.15 and 3.16 show that hydrogen technologies are installed in the utility system for the olefins plant when the cost for the electrolyser falls to 68 euro/kW and for the ethylbenzene plant when the cost falls to 48 euro/kW. For both plants, this only happens for 2023 energy prices. Note that these prices are an order of magnitude lower than the electrolyser costs assumed in previous model runs.

3.4. Discussion and limitations

The results presented show that if industries are subject to fluctuating costs for their utilities, using a mix of electricity and gas and investing in electric boilers and electricity and heat storage is economically and environmentally beneficial in years when the number of hours of cheaper electricity than gas is higher than 600 (7.5% of the plant's operational hours in a year). This is independent of the ratio of their heat to power demand, the available grid connection capacity, and technology cost developments. However, there are limitations in the chosen methodology and scenarios, which need to be considered before drawing strong conclusions from these findings.

An optimisation model has perfect foresight of market prices. In reality, perfect foresight is impossible. Hence, the numbers presented are likely too optimistic. Furthermore, the optimisation model does not capture the practical difficulties of managing fluctuations which do not follow the predicted price dynamics. Therefore, the presented model can show the potential but not the actual flexibility of the system. Future studies should explore how the proposed cost-optimal systems would perform in actual (uncertain) operational conditions. In addition, optimisation results in a single result. Analysing sub-optimal results would allow an understanding of the impact of the type and sizing of new investments on the total cost and indicate which investments are less risky.

Since the model optimises the total cost of the utility system for one operational year, the discount rate is a parameter that influences the model outcomes. The discount rate of 10% was chosen because, to the authors' knowledge, 10% is common practice for considering investments in industry. A lower discount rate would lead to lower Capex and, therefore, higher capacities for newly installed technologies. Hence, it would favour electrification and support our conclusion about the financial viability of electrification.

From the energy flows in the cost-optimal utility systems follows that the use of the generation and storage units fluctuates strongly. Degradation and part-load efficiencies could be added to the model, where applicable, to increase the accuracy of our model. Both lead to cost changes; degradation leads to an increase in Capex, and part load efficiencies affect the Opex. Since we considered scenarios with increased technology cost (i.e., increased Capex) and energy price data that result in a wide Opex range, the main conclusions of this work (i.e., the potential for cost-effective electrification and the 'merit order' of newly installed technologies) would likely remain unaffected if the degradation and part load efficiencies were accounted for.

The CHP was modelled in a simplified way, i.e., without backup and integration boilers and with a fixed ratio between heat and power generation. A more flexible CHP model could lead to different results, potentially decreasing the extent to which electrification is economically optimal. Further work should address this limitation.

Costs resulting from retrofitting the legacy technologies are not included in the total cost, nor are system integration costs or costs for additional spatial requirements. Adding the investment cost required for retrofitting the legacy technologies would likely increase electricity use and might result in larger electric boilers. Adding system integration costs or costs for additional land use would likely reduce the capacities of new technologies.

Maintenance costs are not considered in the Opex as they were found to be negligible for the electric boiler, thermal energy storage and battery [24, 29]. Since the model selects no hydrogen technologies, adding their maintenance cost would not change the study's findings.

The energy demand data of the plants is subject to uncertainty and might be higher than in existing plants because heat integration was not the focus of the process modelling work conducted in-house. Since the conclusions discussed above are the same for all five plants considered in this work, even though their utility demand ranges from approximately 25MW to 350 MW, they are not expected to be affected by the potential overestimations in the demand data.

As this work looks mainly at the cost-effectiveness of electrification from an industry's perspective, the chosen energy price data are considered to represent a wide enough range in terms of absolute prices and price variability to gain insights relevant to industries. However, they do not allow to draw conclusions about the role of each of the individual cost components, i.e., the role of the electricity prices versus the role of the price for CO_2 emissions allowances versus the role of the natural gas price. In the future, the model could be used for such an analysis, which could be helpful for policymakers who want to promote CO_2 emission savings. Extending the analysis from solely looking at scope 1 CO_2 emissions to, e.g., including scope 2 emissions

would enhance the environmental assessment.
The sensitivity of the results toward the technology cost of, among others, electrolysers was tested but did not result in changes in the results, i.e., the installation of hydrogen equipment. To understand when using hydrogen could become economically feasible, additional model runs were done, and it was found that hydrogen started appearing in the energy mix when the cost for the electrolyser fell below 70 euro/kW for plants with an existing CHP and below 50 euro/kW for plants with an existing gas boiler. This is in the range of the minimum cost studies predict for future PEM electrolyser costs [34]. The results thus indicate that, as long as the temperatures required by the process do not exceed what electric boilers or alternative power-to-heat technologies can deliver, electrolyser costs must decrease significantly for hydrogen to become a cost-optimal option for utility electrification. In the explored case studies, hydrogen is also not required as a feedstock. If processes with a hydrogen feedstock demand were to be included in the analysis, the results and conclusions would likely be different.
Heat pumps are not considered in this work for two reasons. Firstly, employment at the required scale is still rare. Second, the integration of heat pumps is specific to the respective plant and its available excess heat and needs to be modelled with greater detail than the model in this work allows. However, their deployment is advancing rapidly. Hence, future work should extend the model and consider heat pumps. Industries could also decide to invest in power generation from renewable sources and build, i.e., a wind or solar park. Future work could consider this investment instead of buying electricity and fuel from the market.
Flexibility in demand or variable demand is not considered in this work because plants in the ethylene value chain commonly run continuously at capacity. Considering plants with a more variable demand would allow us to expand the conclusions of this work to plants or industries beyond those with a continuous and constant utility demand.
Furthermore, instead of planning utility systems for individual plants, centralising utility generation in industrial clusters could be beneficial because of improved utilisation of the generation technologies and storage units. Since larger capacities are required when more plants are supplied with utilities, centralised utility systems could benefit from reduced technology costs due to economies of scale.
Finally, the findings in this study cannot be extended to greenfield situations or future processes with different utility 'profiles', especially when electricity-based processes are considered, e.g., ethylene production via electrolysis.

3.5. Conclusion

This work examined the potential for electrifying industrial utility systems in scenarios with highly fluctuating energy prices, using five existing chemical plants as a case study. For this purpose, utility systems for a continuous energy supply were modelled for six independent years of historical market prices for electricity, natural gas and ETS emission allowances (2018 to 2023). The utility systems consisted of a fossil fuel-based legacy technology to which the model could add electricity-based technologies and storage units. The utility systems of the five industrial processes were compared, a

techno-economic analysis was conducted and their CO_2 emissions were calculated.
The results show that electrification and storage technologies enable the cost-effective decarbonisation of utility systems in a scenario where industries were to pay increasingly variable gas and electricity prices. For plants with a heat and power demand which are of the same order of magnitude and an existing CHP, years with more than 500 hours during which using electricity for heat generation is cheaper than burning natural gas resulted in a cost-effective partial electrification of the utility system, despite electricity prices being on average twice as expensive as using natural gas in some of these years. For plants with a power demand one order of magnitude lower than their heat demand and an existing gas boiler, partial electrification was cost-effective in years with more than 600 hours of cheaper electricity than natural gas use.

The results also show that electric boilers, thermal energy storage, and batteries were selected for the cost-optimal utility systems. This was independent of the type of plant, the available grid connection capacity, and the minimal load of the CHP or gas boiler. The combination of those three technologies that was chosen depended on the energy price data. With an increasing number of hours during which using electricity is cheaper than using natural gas, electric boiler capacity was installed first. Next was TES capacity, and third was battery capacity. Changes in the investment costs for thermal energy storage and batteries led to minor changes in the capacities of the chosen technologies and changed the technology portfolio in particular years. Power-to-hydrogen-to-power or heat was not selected for any of the plants and years unless electrolyser costs were below 50 euro/kW.
This work thus highlights the potential for electrifying industrial utility systems and the role of electric boilers and energy storage units in pursuing CO_2 emission reduction in existing plants.

List of Abbreviations

Bat	Battery
CapEx	Capital expenditure
CHP	Combined heat and power plant
DSM	Demand-side management
EU ETS	EU Emissions Trading System
GB	Gas boiler
GHG	Greenhouse gases
H2 boiler	Hydrogen boiler
H2 storage	Hydrogen storage tank
MILP	Mixed-integer linear programming problem
OpEx	Operating expense
PEM electrolyser	Proton exchange membrane electrolyser
RES	Renewable energy sources
TC scenarios	Technology cost scenarios
TES	Thermal energy storage

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4

The Impact of Heat Pump Integration on the Electrification of Industrial Utility Systems

Power-to-heat technologies decarbonise heat generation by using electricity instead of fossil fuels, and storage technologies can help deal with price fluctuations, which are expected to increase with a rising share of renewable sources in power generation. However, selecting the adequate type and combination of power-to-heat and storage technologies is challenging due to the differences in cost, conversion and storage efficiencies, especially when high temperatures are required. It is unclear whether the potential reduction in operational costs associated with high-efficiency technologies, such as heat pumps, outweighs the investment requirements, and how the ideal technology portfolio changes in response to distinct energy price developments. This also applies to choosing the integration strategy for heat pumps, as several options are often possible in the industrial context. This chapter provides insights into the trade-off between investment and operational costs by modelling technology portfolios with several heat pump integration options for energy price profiles with different price mean and variance. Two scenarios are explored. First, a case with an existing natural gas boiler, and second, a scenario where natural gas use is no longer allowed. The results indicate that, in most cases, high levels of heat pump integration are not a worthwhile investment. The results also show that the energy price and the availability of natural gas have a limited influence on the result.

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4.1. Introduction

Combatting climate change requires a reduction of greenhouse gas emissions, including carbon dioxide (CO_2) emissions. Industrial activities, particularly the production of chemicals, contribute about 25% to global CO_2 emissions, most of which result from fossil fuel combustion [1]. Therefore, finding alternative ways for industrial heat generation would significantly reduce global CO_2 emissions [2].
Power-to-heat (PtH) technologies enable heat generation from electricity. Electric boilers, for example, produce heat directly from electricity, while heat pumps use power to upgrade heat from lower to higher temperatures. Electric boilers require less investment but are less efficient than heat pumps [3–5], especially when heat pumps only need to pump heat over a small temperature lift. However, a small temperature lift often requires integrating the heat pump into the core process, resulting in higher integration costs compared to a heat pump that uses the environment as a heat source. When selecting the optimal technology portfolio for heat electrification, it is crucial to consider the trade-off between required investment and efficiency, particularly when electricity prices are uncertain and access to grid connection capacity is limited.

Previous work has shown that combining PtH technologies with energy storage technologies can decrease the total annual cost (TAC) of industrial heat generation, due to their flexibility to adapt energy consumption to external signals, such as the availability or price of energy [6, 7]. The importance of the flexibility offered by storage is expected to increase along with the share of variable power production from sources such as wind and solar power. An additional aspect that increases the need for storage is that most industrial processes require continuous heat. Therefore, energy storage technologies should be an integral part of assessing trade-offs between the required investment and the efficiency of different PtH options.
Studies that incorporate alternative PtH and storage technologies when evaluating optimal levels of heat pump integration are currently lacking in the literature. For instance, literature on electrifying utility systems, which explores a combination of several PtH with storage technologies, like [6, 8, 9], does not explore different heat pump integration options. On the other hand, studies that focus on integrating HPs into industrial processes, aiming to achieve the highest possible efficiency of the heat pump, either exclude electric boilers and energy storage from their analysis (see [10–13]) or fail to consider energy price fluctuations and investment cost [14]. To the best of the authors' knowledge, it is unknown how the techno-economic performance of HPs with different integration levels compares when combined with alternative PtH technologies, and to what extent optimal heat pump integration options depend on mean energy prices and their fluctuations. Moreover, it has not been explored which technology portfolio is cost-optimal if natural gas can no longer be used.
This chapter addresses these knowledge gaps. It aims to identify the impact of heat pump integration options on the electrification of an industrial utility system. Thereby, it bridges the gap between the existing literature on a) the technology portfolio required for industrial heat electrification that includes only one heat pump integration option and b) the existing literature that focuses on heat pump placement based on process integration, neglecting alternative PtH and storage technologies.

In this work, an existing utility system (a plant's onsite system for heat and power generation) is modelled. The model can choose to install a less or more integrated heat pump, and/or electric boilers, hydrogen boilers, and storage technologies. Optimisation is used to find the technology portfolio that results in the lowest possible total annual cost, including the required investment and operational costs. The study's contributions to the existing literature are as follows.

- The results provide insights into the trade-off between the cost and efficiency of electric boilers and heat pump integration options. By exploring energy price profiles with different levels of price mean and variance, and scenarios with and without natural gas use, the study generates insights into whether increasing efficiency outweighs the required additional investment under these conditions.
- The fully electrified utility systems illustrate which technology portfolios can lead to the best economic performance for different energy price profiles when natural gas can no longer be used.

4.2. Methods

This section describes the research approach used in this work. Section 4.2.1 elaborates on the overall approach. Section 4.2.2 introduces the utility system model, and Section 4.2.3 presents the industrial plant that served as a case study.

4.2.1. Overall approach

To identify the impact of heat pump integration options on the electrification of an industrial utility system, a model was developed to minimise the TAC of the utility system. This cost comprises operational costs (cost for energy and CO_2 emission allowances) and capital expenditure for newly installed technologies. To explore the impact of mean prices and price fluctuations, the energy prices presented in Section 4.2.3 were used.
The optimisation was executed for all considered heat pump integration options individually, rather than using a single superstructure that contains all possible integration options. This allows to analyse the difference between these options (as opposed to finding the overall optimal technology portfolio), enabling a deeper understanding of the trade-offs between different system configurations and the performance of suboptimal solutions.
The portfolio of technologies that the model could choose from included an electric boiler (ElB), a heat pump (HP), mechanical vapour recompression (MVR) units, and a power-to-gas-to-heat system composed of an electrolyser (H2E), a hydrogen storage tank (H2S), and a hydrogen boiler (H2B). In the model, electricity could be stored in batteries (Bat) and heat in two different types of thermal energy storage (TES). Electrical power was supplied via a connection to the local power grid, which is assumed to have limited capacity, and heat could be extracted from and delivered to the production process. In the scenario where natural gas (NG) was assumed to be available, an NG boiler with a thermal capacity equal to the maximum heat demand was considered available without additional capital expenditure, mimicking existing

conditions in industrial settings where the units are available and already paid off. To model the limited flexibility of the equipment, the minimal output of the NG boiler was capped at 20% [15].

4.2.2. Utility system model

The utility system model is a linear mixed-integer model formulated in Python, using the 'Pyomo' package. It is based on the model presented in [6] and solved for 8000 hours (the yearly operational hours of the plant, excluding downtime for maintenance). The time resolution is 1 hour. Compared to the previous model, two main changes were made. Firstly, the fossil fuel-based legacy technology is an NG boiler since no CHP is operational in the plant used as a case study, and secondly, an HP and an MVR were added to the technology portfolio.

4

Model formulation

The model's objective is to minimise the sum of operational costs (OpEx) and required (annualised) capital investment (CaPex) as described in Eq. (D.47).

$$min \sum_{t=0}^{t=8000} \mathrm{OpEx}(t) + \sum_{i} \mathrm{CaPex}_i \tag{4.1}$$

The OpEx (Eq. (5.2)) includes the costs for consumed grid power and natural gas, and the allowances for all emitted CO_2, which are included in the cost for natural gas consumption. In Eq. (5.2), $\mathrm{p_{el,\ grid}}(t)$ is the hourly electricity price at time t in €/MWh; $P_{gr,i}(t)$ is the power flowing from the grid to technology i in MW; $P_{bat,gr}(t)$ is the power from the battery (if installed) to the grid in MW; $\mathrm{p_{NG}}(t)$ is the cost of natural gas at time t in €/MWh; $NG_{in}(t)$ is the consumed natural gas in MW; $\mathrm{p_{EUA}}(t)$ is the cost of CO_2 emission allowances in €/tonne$_{CO_2}$, and $\mathrm{EF_{NG}}$ is the emission factor of natural gas in tonne$_{CO_2}$/MWh$_{NG}$.

$$\begin{aligned}\mathrm{OpEx}(t) = {} & \mathrm{p_{el,\ grid}}(t) \cdot \sum (P_{gr,i}(t) - P_{i,gr}(t)) \cdot \Delta t \\ & + \mathrm{p_{NG}}(t) \cdot NG_{in}(t) \cdot \Delta t \\ & + \mathrm{p_{EUA}}(t) \cdot NG_{in}(t) \cdot \Delta t \cdot \mathrm{EF_{NG}},\end{aligned} \tag{4.2}$$

All conversion technologies are modelled using energy flow balances and the respective technological constraints, which are reported in Appendix F.
The HP model is described by Eq. (5.6), where, $H_{\mathrm{HP,out}}(t)$ is the HP's heat output at t in MW, $P_{\mathrm{HP,in}}(t)$ is the inflowing power at t in MW, and $\mathrm{COP_{ideal}}$ is the HP's Carnot coefficient of performance (COP). The $\mathrm{COP_{ideal}}$ is multiplied by a factor of 0.5 because mechanical closed-cycle HPs work at about 50% of their ideal COP [16, 17]. $\mathrm{COP_{ideal}}$ is calculated using Eq. (5.7), where T_{sink} is the temperature of the heat sink and T_{source} is the heat source's temperature. The MVR is modelled as the HP model, with the difference that it works at 70% of its ideal COP. This exergetic efficiency is derived from comparing the Carnot COP with the COP based on an MVR with an

isentropic efficiency of 70% operating at steam pressures between 1 and 5 bar [18].

$$H_{\text{HP,out}}(t) = P_{\text{HP,in}}(t) \cdot \text{COP}_{\text{ideal}} \cdot 0.5 \tag{4.3}$$

$$\text{COP}_{ideal} = \text{T}_{sink} / (\text{T}_{sink} - \text{T}_{source}) \tag{4.4}$$

In case the HP sources heat from a finite heat source, its energy balance is constrained by the capacity of that heat source in the model H_{source}, as described by Eq. (4.5).

$$H_{\text{HP,out}}(t) \leq \text{H}_{\text{source}} \cdot 1 - \frac{1}{\text{COP}_{\text{ideal}} \cdot 0.5} \tag{4.5}$$

Technical parameters

The capital investment was estimated using the product of bare equipment cost (Table 4.1) and installation cost (Lang) factors (Table 4.2). Tables 4.3 and 4.4 show the data used to model the conversion and storage technologies, respectively.

4

Table 4.1.: Technology cost per unit capacity

Technology	**Cost per unit capacity [1000€/Unit]**	**Unit**	**Source**
Electric boiler	70	MW	[4]
Battery	300	MW	[19]
Sensible TES	23	MWh	[20]
Latent TES 1	40	MWh	[20, 21]
Latent TES 2	40	MWh	[20, 21]
Electrolyser	760	MWel	[22]
Hydrogen boiler	35	MWth	[23]
Hydrogen storage	10	MWh	[20]
Stand-alone heat pump	400	MWth	[5]
Integrated heat pump	300	MWth	[5]
Mechanical vapor recompression	100	MWth	[5]

4.2.3. *Case study*

In this work, a biodiesel production plant was used as a case study. This case represents a typical industrial process characterised by mild operational temperatures and CO_2 emissions resulting from heating requirements. Furthermore, this process has a well-documented process layout ([24–26]), which facilitated the modelling. Despite the use of batch reactors, the heating requirements are approximately constant over time and were considered as such in the model.

Synthesis of technology configurations

The approach to derive possible technology configurations followed in this study requires data on the process's heat demand and on the existing heating (steam)

infrastructure's temperature levels and quantities.
Pinch analysis was used to map the net heating requirements of the biodiesel process. Here, all the heat required by and available from the process was aggregated into a hot and a cold composite curve. These curves were used to identify the heat integration bottleneck in the process, the pinch point, where heat exchange is no longer economically viable. This lack of available heat at the pinch point and the net heat available (below the pinch) or required (above the pinch) at a certain temperature is plotted in a grand composite curve (GCC), shown by the blue line in Fig. 4.1.

Table 4.2.: Overview of installation cost factors used in the model[a)]. Based on [27].

Technology	Installation cost factor	Note
Electric boiler	1	Installed cost
Battery	2.5	Miscellaneous equipment
Sensible TES	2.5	Miscellaneous equipment
Latent TES 1	2.5	Miscellaneous equipment
Latent TES 2	2.5	Miscellaneous equipment
Electrolyser	–	Included in equipment cost in [22]
Hydrogen boiler	2	Based on fired heaters
Hydrogen storage	4	Pressurised vessels
Mechanical vapor recompression	2.5	Stand-alone compressors

[a)] The installation cost factors for the heat pumps are presented in Table 4.8

Table 4.3.: Data used to model conversion technologies. References for the data are shown in brackets next to the data.

	NG boiler	Electric boiler	Heat pump	MVR	Electrolyser	H2 boiler
Thermal or electric Capacity [MW_{th}/MW_e]	100% of heat demand	Decision variable	Decision variable	Decision variable	Decision variable	Decision variable
Efficiency [%]	82	99 [3]	0.5 COP_{ideal} [28]	0.7 COP_{ideal} [18]	69 [29]	92 [30]
Min. load factor [%]	20 [15]	0	0	0	0	0
Lifetime [years]	–[b)]	20 [4]	20 [5]	20 [5]	15	20 [23]

[b)] Not included in the model

Figure 4.1 shows that a) the net heat required above the pinch point (at 108 °C), is 2012 kW at 113 °C (orange bar labelled 'Process sink'); b) there is additional 360 kW at 120 °C (orange bar labelled 'Low-temperature steam network'), and an additional 250 kW at 250 °C (orange bar labelled 'High-temperature steam network'); c) 1450 kW of heat is available at 55 °C from a process source (blue bar labelled 'Process source'), and from the air from inside the process hall at 30 °C (blue bar labelled 'Environment'), which is considered to be infinitely available. Data related to

Table 4.4.: Parameters used to model storage technologies. References for the data are shown in brackets next to the data.

	Battery	TES	Hydrogen tank
Efficiency [%]	90 [8]	90 [20]	90 [8]
Max. output [% of capacity]	70 [8]	50 [8]	100
Lifetime [years]	20 [8]	25[31]	23 [32]

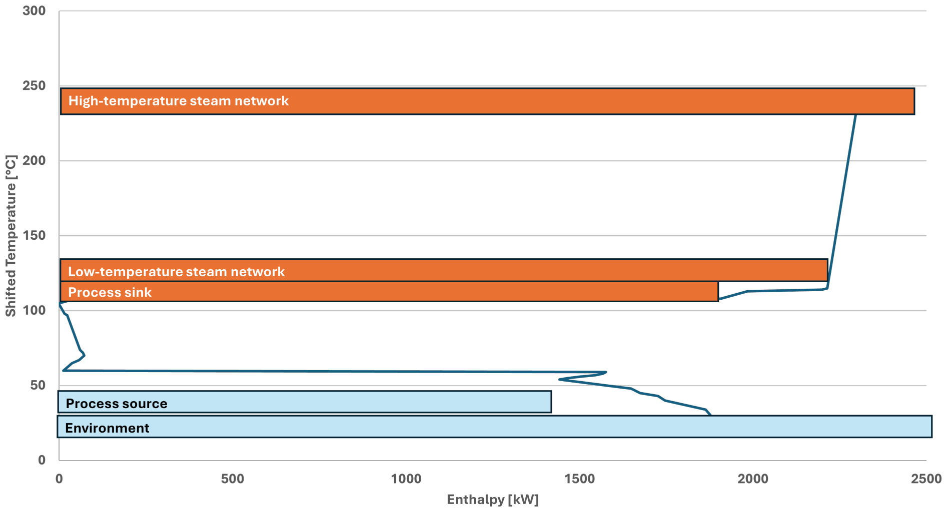


Figure 4.1.: Grand composite curve of the biodiesel production process based on [25] with highlighted heat sinks as orange bars and heat sources as blue bars. The blue line represents the original grand composite curve, which illustrates the exchangeable heat flows at the respective temperatures.

the connections and the existing heating infrastructure is summarised in Table 4.5. Using the data shown in Table 4.5, possible technology configurations for the utility

Table 4.5.: Heat requirements of the case study

Name	Temperature [°C]	Capacity [MW]	Type
Process source	55	1.450	Source
Environment	30	∞	Source
High-temp steam network	250	2.622	Sink
Low-temp steam network	120	2.048	Sink
Process sink	113	2.012	Sink

system were synthesised as follows. All boilers (GB/ElB/H2B) were connected to the high-temperature, or pressure, steam network (HT-steam). In the model, the boilers supply heat that is either used directly to fulfil the high-temperature demand of the

plant or cascaded down to the low-temperature steam network, which supplies heat to the plant's low-temperature processes. Similarly, the heat pump can supply heat either to the largest heat sink just above the pinch temperature ('Process sink') or to the low-temperature steam network (LT-steam). The HP's heat source can either be the air inside the process hall ('environment') or the largest heat source (in terms of quantity of available heat) just below the pinch temperature ('Process source').
For the case study, this resulted in the five heat pump integration options listed in Table 4.6. Note that it is currently impossible to directly connect the process source to the HT-steam demand with state-of-the-art HPs [5], which is why this option is missing in the table. The temperature lift that the HPs in options 1 to 4 cannot realise is complemented using MVRs. Two types of thermal energy storage

Table 4.6.: Heat pump integration options with the respective heat source and heat sink

Heat source	**HT-steam**	**LT-steam**	**Process sink**
Environment	No integration	Integration 1	Integration 3
Process source	–	Integration 2	Integration 4

were considered, latent thermal energy storage (LT-TES) and sensible thermal energy storage (SS-TES). SS-TES is less expensive than LT-TES [20], but it can only be charged with heat at high temperatures [20]. Therefore, the high-temperature steam network was connected to the SS-TES, and the LT-TES was selected as the energy storage option for the low-temperature steam network and the largest heat sink just above the pinch temperature.

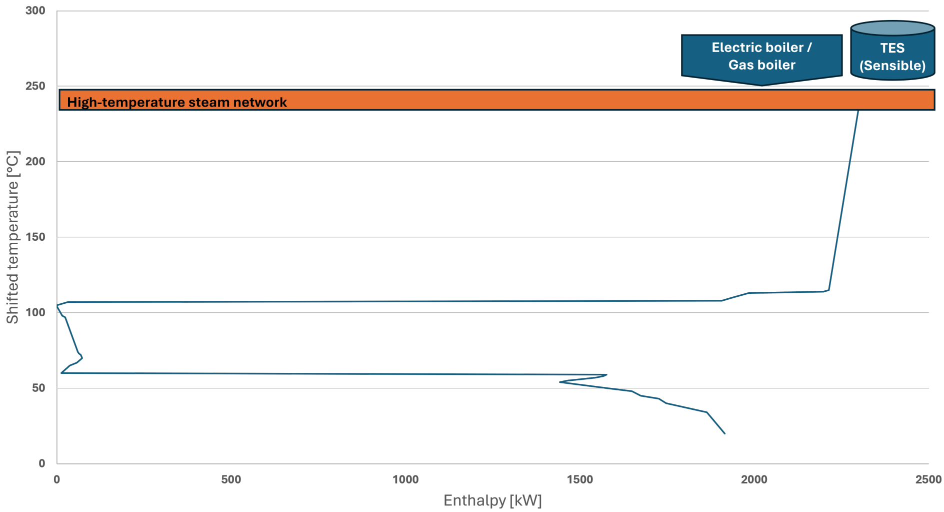
Resulting heat pump integration options

Figure 4.3 shows the resulting technology configurations for each HP integration option. A minimal temperature difference of 2.5 °C was used to transfer heat to and from the heat pump. As indicated in Fig. 4.2a, the reference system did not include a heat pump. In this case, the technology portfolio is composed of the existing GB and potential ElB and TES capacity.
The HP used in the 'No integration' HP system (Fig. 4.2b was assumed to be a combination of a closed-cycle HP that produces low-pressure steam and an MVR that increases the steam pressure up to the required temperature. For the remaining systems, high-temperature closed-cycles HPs were considered based on data provided in [5]. Table 4.7 shows the ideal COPs for the HP in each system. As discussed

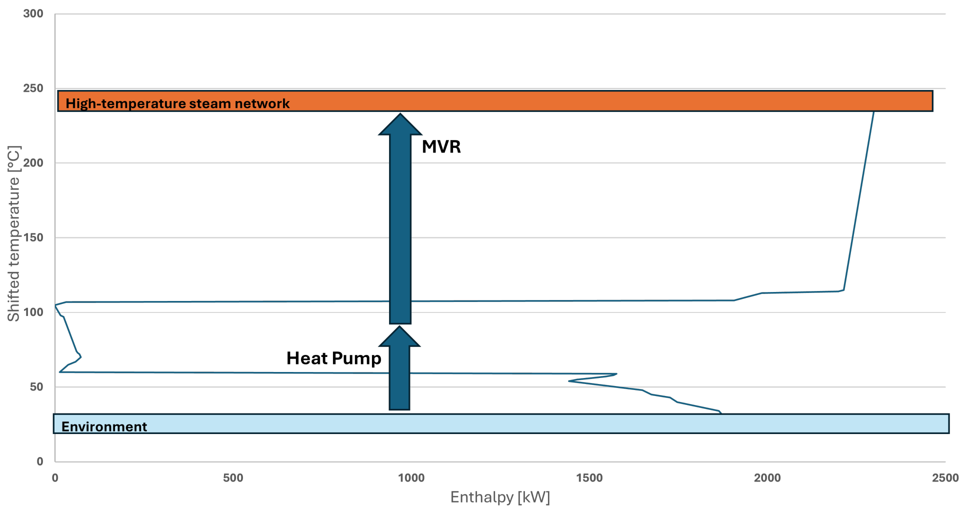
Table 4.7.: Ideal COPs for the heat pump in each integration option

	No integration	**Integration option 1**	**Integration option 2**	**Integration option 3**	**Integration option 4**
COP_{ideal}	1.2	2.2	3.0	2.3	3.3

previously, increasing the heat pump's integration in the process leads to higher investment costs because the installation is more costly. This is reflected in the installation cost factor, see Table 4.8.

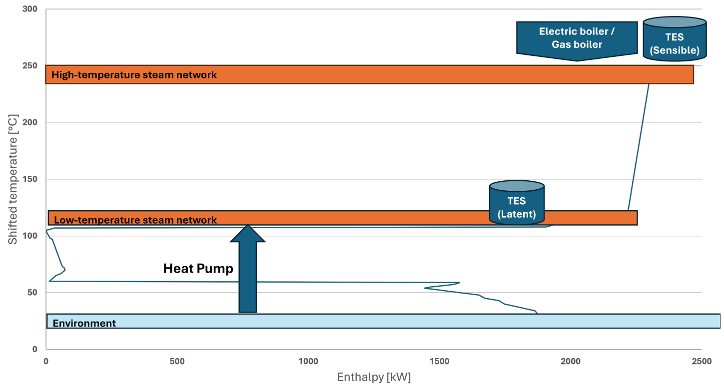


(a) Reference system

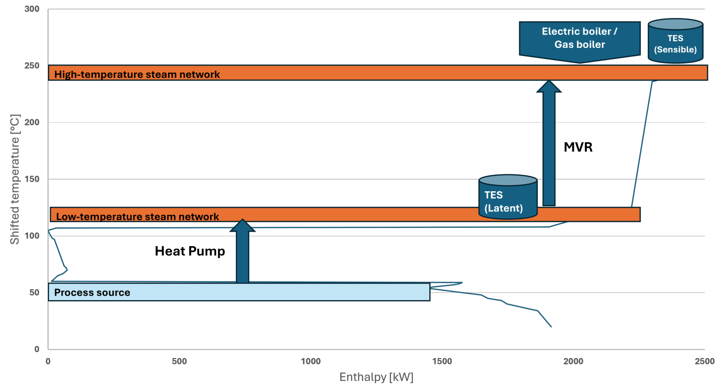


(b) No heat pump integration

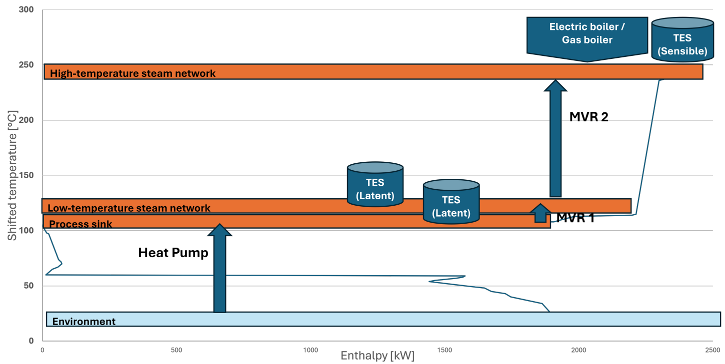
Figure 4.2.: Outline of technology configurations in the reference system and for the non-integrated heat pump.



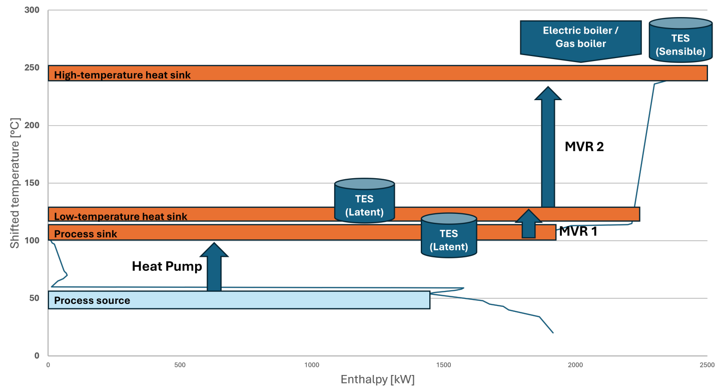
(a) Integration option 1



(b) Integration option 2



(c) Integration option 3



(d) Integration option 4

Figure 4.3.: Outline of technology configurations for the explored heat pump integration options.

Table 4.8.: Installation cost factor for the heat pump in each integration option. Installation factors are based on [27]

HP integration option	Installation cost factor	Based on
No integration	2.5	stand-alone compressors
Option 1	3.3	standard changes to a fluids processing plant
Option 2	4.5	standard changes to a fluids processing plant, including contingency
Option 3	6.0	standard changes to fluid processing plants when considering inside battery limits for intermittent operation
Option 4	7.8	standard changes to a fluid processing plant, including inside battery limits cost, requiring mostly new piping, but no civil, or structure and buildings work.

Table 4.8 shows that the integration factor increases from the 'No integration' heat pump to heat pump integration option 4. However, the ideal COP does not increase, as shown in Table 4.7. The COP_{ideal} of HP integration option 3 is lower than that of option 2. Therefore, HP integration option 3 is not considered further in this study. The remaining integration options and their names are presented in Table 4.9.

Table 4.9.: Names of the explored heat pump integration options with the respective heat source and heat sink

Heat source	Heat sink		
	HT-steam	LT-steam	Process sink
Environment	No integration	Option 1: 'Low integration'	Option 3: Not considered further
Process source		Option 2: 'Medium integration'	Option 4: 'High integration'

Energy price profiles

Three energy price profiles were used to explore the potential impact of the price mean and variance on the integration of the HP that results in the lowest TAC (i.e., the cost-optimal technology portfolio for the utility system):

- Base profile: a profile with low price variance and a high mean price
- Lower mean profile: a profile with the same variance as the base profile but a lower mean
- Higher variance profile: a profile with a higher price variance but the same mean as the base profile

The ‘Lower mean’ profile was based on 2019 prices, and the ’Higher variance’ profile on 2023 prices. For the ‘Base’ profile, the mean price is based on 2023 data, while its variance is taken from 2019 data, to represent an in-between of the two historical price years, to ensure comparability. Data on the three energy price profiles are presented in Table 11, and the full price profiles are shown in G.
Electricity price data for the Dutch Day-Ahead market was sourced from the ENTSO-E transparency platform [33], price data of the Dutch gas market (‘Dutch TTF market’) was used for the cost of natural gas [34], and EU-ETS prices were used for the CO_2 allowance prices [35, 36]. Electricity prices change on an hourly basis, while natural gas prices and CO_2 allowance prices change on a daily basis. Missing natural gas price data, due to market closure during weekends, was assumed to remain the same as it was on the day before the closure. The same approach was used for missing EU-ETS price data. It was also assumed that CO_2 emission allowances have to be purchased for 100% of the emissions (no free allocation was considered). The prices in Table 4.10 were used to identify optimal utility configurations for two scenarios: one with and one without natural gas availability.

Table 4.10.: Energy prices by price type and energy profile

Energy price profile	Base	Lower mean	Higher variance
Electricity price			
mean [€/MWh]	96.2	41.5	97.7
variance [(€/MWh)^2]	127.5	127.5	2382.7
Natural gas price			
mean [€/MWh]	41.7	14.7	42.0
variance [(€/MWh)^2]	11.1	11.1	120.5
EU ETS price			
mean [€/tonne$_{CO_2}$]	85.0	24.9	86.0
variance [(€/tonne$_{CO_2}$)^2]	4.4	4.4	30.6

4.3. Results and discussion

In the following sections, the results of the utility system model runs are presented. First, for the scenario in which using natural gas is possible, then for the scenario in which the system has to be fully electrified.

4.3.1. Scenario with an existing natural gas boiler

Table 4.11 shows the TAC of the utility systems with the different heat pump integrations. For energy prices with a lower mean than in the base profile, all heat demand is supplied from the existing natural gas boiler, as electrification of the utility system does not decrease the TAC. As shown in Table 4.11, this is independent of the HP integration option. Table 4.12 shows the technology portfolio of the cost-optimal utility systems in the different cases for the base energy prices and prices with increased variance, respectively. Tables 4.11 and 4.12 show that only integrated heat pumps enable TAC savings (if electrification is cost-optimal). The highest savings are shown for the utility system with medium heat pump integration. The systems with a low HP integration perform better in terms of the TAC than the systems with a high HP integration. This is the case for both energy price profiles that enable electrification. Figures 4.4 and 4.5 show that all integrated heat pumps lower the

Table 4.11.: Total annual cost of the utility systems in the reference case, with no, low, medium, and high heat pump integration. Results for the scenario with an existing NG boiler for the 'Base', 'Lower mean', and 'Higher variance' profiles

	Reference case	**'No integration'**		**'Low integration'**		**'Medium integration'**		**'High integration'**	
Energy profile	TAC [Million €]	TAC [Million €]	Savings [%]	TAC [Million €]	Savings [%]	TAC [Million €]	Savings [%]	TAC [Million €]	Savings [%]
Base	1.50	1.50	0	1.28	14	1.17	22	1.37	9
Lower mean	0.50	0.50	0	0.50	0	0.50	0	0.50	0
Higher variance	1.37	1.37	0	1.29	6	1.18	14	1.36	0.4

natural gas consumption significantly compared to the reference system, even when an electric boiler is installed (see results for the 'Higher variance' profile). For the 'Base' profile shown in Figure 4.4, the utility system that leads to the lowest TAC (Medium integration) operates the heat pump as the only PtH technology alongside the NG boiler (Table 4.12). In this case, the NG boiler operates at its minimal load while the HP supplies the remaining share of low-temperature heat demand.

In the utility system with the lowest TAC for energy prices with a higher variance ('Medium integration'), a heat pump of the same size as for the Base energy price profile is installed alongside a small electric boiler, which works together with the NG boiler to minimise the cost of high-temperature heat (Table 4.12). Note that in this case, no TES is installed, despite high price fluctuations. Since the electric boiler capacity is small, there is only a minor difference in natural gas consumption between the utility system in the 'Base' and the 'Higher variance' profiles (compare Figures 4.4 and 4.5).

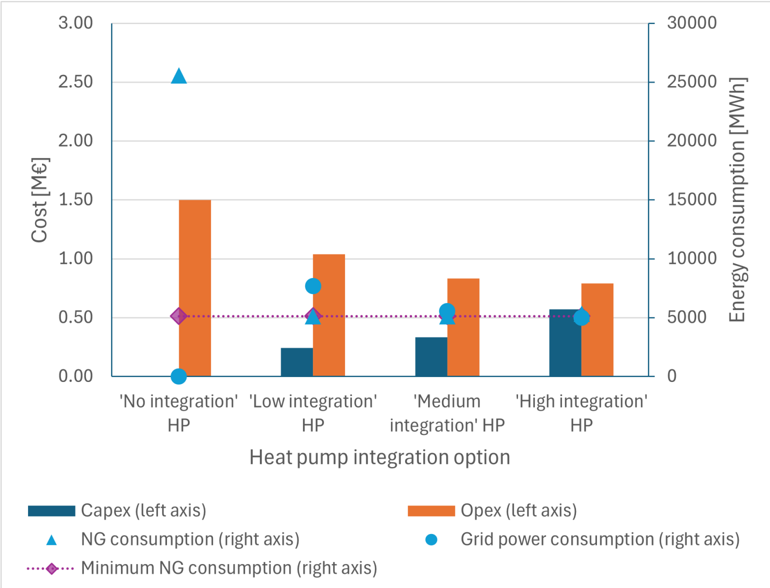


Figure 4.4.: CaPex, Opex, NG and grid power consumption for the utility systems with the different HP integrations for the 'Base' energy price profile.

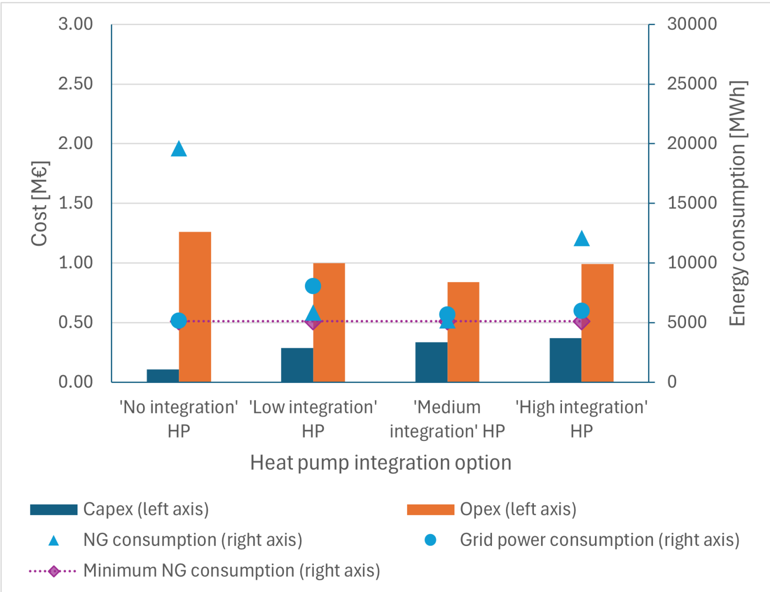


Figure 4.5.: CaPex, Opex, NG and grid power consumption for the utility systems with the different HP integrations for the 'Higher variance' energy price profile.

Table 4.12.: Installed capacities in the scenario with an existing natural gas boiler for the explored energy price profiles. TES250 indicates that heat is stored at 250°C. MVR120-250 indicates that the MVR lifts heat from 120°C to 250°C. Bold font indicates the technology profile of the system with the lowest TAC. 'NA' means that the technology was not available in this technology configuration.

	Electric boiler [MWth]	**Heat pump [MWth]**	**MVR120-250 [MWth]**	**MVR120-113 [MWth]**	**TES250 [MWh]**	**TES120 [MWh]**	**TES113 [MWh]**
			'Base' energy price profile				
Reference system	0	NA	NA	NA	0	NA	NA
'No integration'	0	0	NA	NA	0	NA	NA
'Low integration'	0	2.10	0	NA	0	0	NA
'Medium integration'	**0.00**	**2.10**	**0**	**0**	**0**	**0**	**0**
'High integration'	0.00	2.07	0	0	0	0	0
			'Higher variance' energy price profile				
Reference system	4.95	NA	NA	NA	10.49	NA	NA
'No integration'	4.95	0	NA	NA	10.49	NA	NA
'Low integration'	2.00	2.10	0	NA	4.20	0	NA
'Medium integration'	**0.52**	**2.10**	**0**	**0**	**0**	**0**	**0**
'High integration'	4.66	0.98	0	0	10.09	0	0

4.3.2. Fully electrified scenario

Table 4.13 shows the results if the use of NG would no longer be possible. Table 4.14 shows the installed capacities that lead to the cost-optimal utility systems. As in the scenario where NG was possible (section 4.3.1), all options with integrated heat pumps lead to utility systems with lower TAC than the reference system with an electric boiler. The systems with a non-integrated HP lead to the lowest reduction or no reduction in TAC (see Tables 4.13 and 4.14). The only exception is observed for energy prices that have a lower mean. In this case, also the 'High integration' heat pump cannot compete with the electric boiler, and thus no HP is installed (see Table 4.14). Tables 4.13 and 4.14 show that the utility system with medium HP integration

4

Table 4.13.: Total annual cost of the utility systems in the reference case, with no, low, medium, and high heat pump integration. Results for the scenario without natural gas use for the 'Base', 'Lower mean', and 'Higher variance' profiles

	Reference case	**'No integration'**		**'Low integration'**		**'Medium integration'**		**'High integration'**	
Energy profile	TAC [Million €]	TAC [Million €]	Savings [%]	TAC [Million €]	Savings [%]	TAC [Million €]	Savings [%]	TAC [Million €]	Savings [%]
Base	2.06	2.00	3	1.26	39	1.25	39	1.48	28
Lower mean	0.90	0.90	0	0.72	21	0.74	18	0.90	0
Higher variance	1.80	1.80	0	1.28	29	1.17	35	1.38	23

performs best in terms of TAC reduction for the 'Base' and the 'Higher variance' profiles, similar to the scenario with the existing NG boiler. However, the systems with a low HP integration lead to similar levels of TAC. The minor difference between the 'Low' and 'Medium' HP integration is because in the system with the medium HP integration, the HP capacity is limited by the available heat from the process heat source. Since heat from the NG boiler is no longer available in this scenario, the system is forced to install an ElB to meet the remaining heat demand. This inhibits the model from selecting a more efficient MVR, which would upgrade heat from the HP using less electricity. In the system with low HP integration, which results in the same or lower TAC, the heat source is unlimited, and an MVR can be installed instead of an ElB.

In both systems ('low' and 'medium HP integration'), the heat pump is the main heat supplier. The other components, either a small ElB or MVR, do not lead to a significant difference in TAC, unless energy price fluctuations increase. Figures 4.6 and 4.7 visualise the similarity in system operation between systems with 'Low' and 'Medium' HP integration, while Figure 4.8 shows a larger difference in the case of energy prices with a higher variance. In this case, large ElB and TES capacities are used to increase the flexibility of the utility system to benefit from low and negative electricity prices. This is notably different from the technology portfolio when the NG boiler could be used (see Table 4.12).

A comparison of the TAC of the utility systems and the ideal HP integration for both scenarios (Tables 4.11 and 4.13) shows that the HP enables a complete electrification at almost the same TAC. This can be explained by the missing NG boiler with its minimal load constraint, as the fully electrified system is not forced to use natural gas anymore. This shows that a limited flexibility of a fossil fuel-based technology can be a limitation to the potential cost-optimal electrification of utility systems.

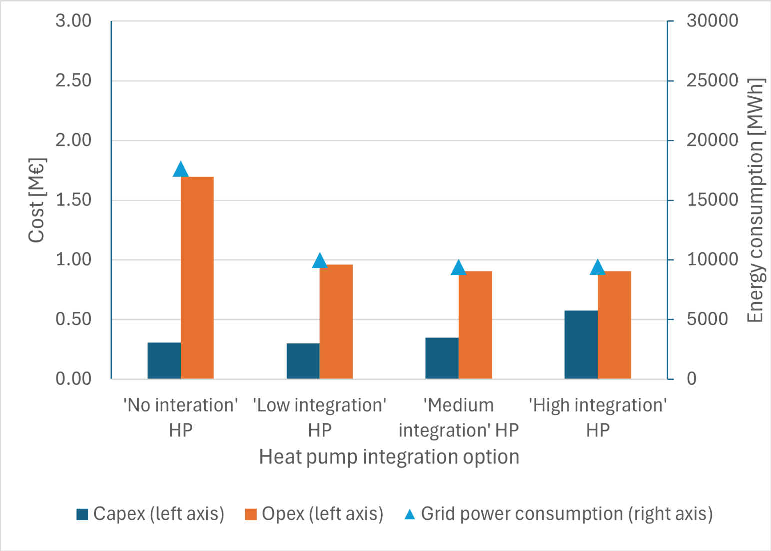


Figure 4.6.: CaPex, Opex, and electricity consumption from the power grid for all heat pump integration options for the 'Base' energy price profile.

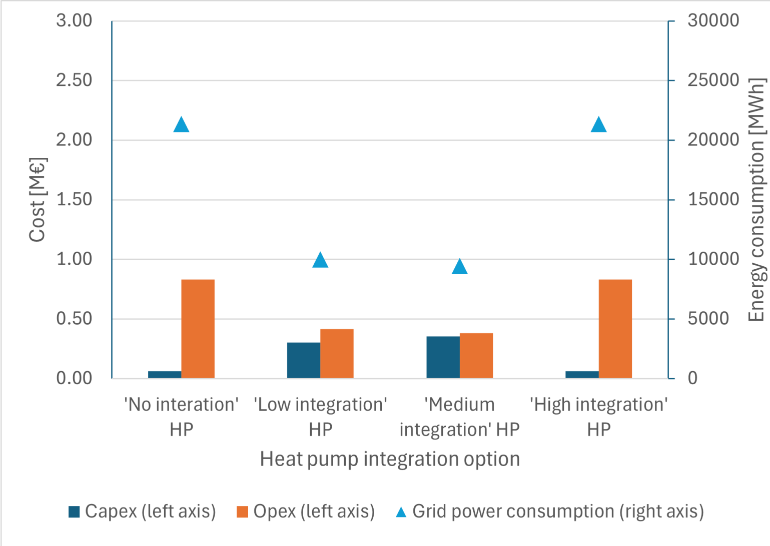


Figure 4.7.: CaPex, Opex, and electricity consumption from the power grid for all heat pump integration options for the 'Lower mean' energy price profile.

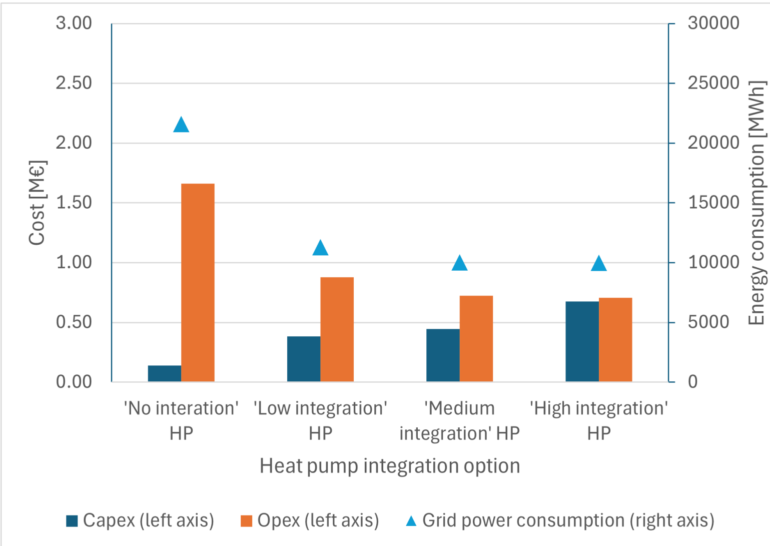


Figure 4.8.: CaPex, Opex, and electricity consumption from the power grid for all heat pump integration options for the 'Higher variance' energy price profile.

Table 4.14.: Installed capacities in the scenario with an existing natural gas boiler for the explored energy price profiles. TES250 indicates that heat is stored at 250°C. MVR120-250 indicates that the MVR lifts heat from 120°C to 250°C. Bold font indicates the technology profile of the system with the lowest TAC. ’NA’ means that the technology was not available in this technology configuration.

	Electric boiler [MWth]	**Heat pump [MWth]**	**MVR120-250 [MWth]**	**MVR113-120 [MWth]**	**TES250 [MWh]**	**TES120 [MWh]**	**TES113 [MWh]**
			‘Base’ energy price profile				
Reference system	2.62	NA	NA	NA	0.00	NA	NA
‘No integration’	0.00	2.62	NA	NA	0.00	NA	NA
‘Low’ integration’	**0.00**	**2.53**	**0.25**	**NA**	**0.00**	**0.00**	**NA**
‘Medium’ integration’	**0.46**	**2.17**	**0.00**	**NA**	**0.00**	**0.00**	**NA**
‘High integration’	0.55	2.07	0.00	0.06	0.00	0.00	0.00
			‘Lower mean’ energy price profile				
Reference system	3.73	NA	NA	NA	5.24	NA	NA
‘No integration’	3.73	0	NA	NA	5.24	NA	NA
‘Low’ integration’	**0**	**2.53**	**0.25**	**NA**	**0**	**0**	**NA**
‘Medium’ integration’	**0.65**	**2.17**	**0**	**NA**	**0.91**	**0**	**NA**
‘High integration’	3.73	0	0	0	5.24	0	0
			‘Higher variance’ energy price profile				
Reference system	4.95	NA	NA	NA	15.73	NA	NA
‘No integration’	4.95	0	NA	NA	15.73	NA	NA
‘Low integration’	**3.82**	**2.43**	**0.09**	**NA**	**10.42**	**0**	**NA**
‘Medium’ integration’	**4.24**	**2.17**	**0**	**NA**	**10.79**	**0**	**NA**
‘High integration’	4.33	2.07	0	0.06	10.79	0	0

4.3.3. Discussion

Table 4.15 shows the level of HP integration that results in the utility system with the lowest TAC for each energy price profile and scenario. As shown, a low and/or medium integration of the HP leads to the system with the lowest TAC in all cases, provided electrification is cost-optimal. When NG can be used, medium HP integration leads to better results than low levels. When NG cannot be used, the difference in TAC reduction between these two systems is minor. The results in Table 4.15 show that the optimal heat pump integration remains unchanged for the different energy price profiles, as long as electrification is cost-optimal. This indicates that the effect of energy price variance on the extent to which higher COPs outweigh higher integration costs is minimal. Since there is an overlap between the cost-optimal integration of systems with and without natural gas use, the effect of natural gas availability appears to be weak as well. Independent of whether NG can

Table 4.15.: Level of HP integration that results in the utility system with the lowest TAC for each energy price profile and scenario

	'Base' profile	**'Lower mean' profile**	**'Higher variance' profile**
With Natural Gas	'Medium integration'	— (no electrification)	'Medium integration'
Without Natural Gas	'Low/Medium integration'	'Low/Medium integration'	'Low/Medium integration'

still be used or not, the results indicate that more ElB and TES capacity is installed for the 'Higher variance' profile than in the 'Base' or 'Lower mean' profiles, because, in the model, investing in excess ElB and TES capacity pays off when energy prices fluctuate strongly.

The electrified cost-optimal utility systems that lead to the lowest TAC enable a significant reduction of (scope 1) CO_2 emissions compared to the respective reference system (80% for the 'Base', and 74% for the 'Higher variance' energy price profile, respectively). Note that while the reference system for the 'Base' profile generates all heat using natural gas, 4.95MW ElB and 10.5MWh TES capacity are installed in the reference for the 'Higher variance' profile. Since the reduction of emissions is shown compared to the reference system, significantly less CO_2 is emitted when an HP is installed compared to when ElB and TES are installed.

4.4. Limitations of the study

Before drawing final conclusions from the presented results, it is important to consider the limitations of the methodology, scope, and case study chosen in this work.

The methodology has the following limitations. Deterministic optimisation with a single objective does not show how robust the results are to uncertainties inherent to parameters such as energy prices, installation cost factor and equipment cost. Unreported model runs with a higher optimality gap (as small as 1%) resulted in different capacities in the technology portfolios, tending to be more favourable for

HP and MVR, and had lower ElB and TES capacities than the reported solutions in the model runs with an optimality gap of 0.1%. If the model is used for energy system planning, future work should include robust optimisation and/or modelling to generate alternatives [37] to test the robustness of the utility system design to uncertainties. However, as this work aimed to explore and compare different integration strategies, deterministic optimisation and scenario analysis were deemed adequate as they allowed to assess the extent to which different HP integrations enhanced savings in the TAC with limited computational effort. With minor changes, the developed model could be used to test the robustness of the proposed utility system designs for additional energy price profiles by fixing the installed capacities, optimising the operation of utility system only and analysing the performance of the system under varying conditions.

Considering the technology models, two key limitations are identified. Firstly, the fixed minimal load of the GB might underestimate the flexibility of GBs in the real world. Increasing the flexibility of the GB would likely lead to changes in installed capacities, as indicated by the results from the scenario without a natural gas boiler, where fully electrified systems had similar TAC compared to the systems with a natural gas boiler that were forced to run at minimal load at all times. HP capacities could be increased to maximise the use of their heat source; otherwise, ElBs could be added to the installed HP capacity. Secondly, off-design efficiencies of the HP were not considered, which would increase the accuracy of the HP model. Including off-design operation in the model could influence the installed capacities and add the possibility to use the HP for charging the TES without installing additional HP capacity.

Regarding the scope of this work, three limitations are identified. Firstly, the selected energy price profiles were considered sufficient to explore the impact of the price profile on whether increasing efficiency outweighs additional integration costs. However, additional energy prices could be used to explore the point at which the results would change and allow to determine the individual impact of price mean and price variance. Secondly, optimising for TAC and including CO_2 emissions only indirectly via the cost for scope 1 emission allowances set the focus of this work on the economic performance of electrified utility systems. Including emission reduction as a second optimisation objective would reveal whether the cost-optimal technology portfolios would also be the preferred solution from an environmental perspective and generate insights about potential trade-offs. Thirdly, grid use costs (e.g., peak tariffs) were not included in the model because they are country-specific and may vary depending on the contract between the plant and the grid operator. Adding grid use costs to the price of electricity might limit the extent to which electrification is cost-optimal. At the same time, grid use costs would steer the system to use electricity as efficiently as possible, as they would increase the cost of electricity. Therefore, including peak use tariffs might reduce the benefits of ElB (peak) capacity, lead to decreased TES capacities and lead to an increase in HP (base-load) capacity. The model could be used to assess the impact of different tariffs that grid operators offer and support industries in deciding whether to invest in additional flexibility or not.

Finally, the heat which can be sourced from the process in the case study is not enough to meet the demand. A possible result of this is that MVRs were not part of any cost-optimal technology portfolio, as the effective COP of transferring environmental heat to high-temperature process demands is close to the performance of an ElB, which is cheaper. An additional integration option could be a hybrid between the low and medium integration to use all excess heat from the process and supply the remaining heat demand by utilising environmental heat.

4.5. Conclusions and recommendations for future work

This study aimed to identify the impact of heat pump integration options on the electrification of an industrial utility system. To this end, it modelled an existing utility system with the option to invest in power-to-heat technologies, such as a less or more integrated heat pump, electric boilers, hydrogen boilers, and storage technologies. Optimisation is used to find the technology portfolio that results in the lowest possible total annual cost when energy prices vary in terms of mean and variance, and when natural gas use is no longer allowed. The analysis was conducted for a continuously operating biodiesel production plant with heating requirements in the range of 100°C – 250°C, and heat sources available at 55°C and 30°C. This is a typical industrial process characterised by mild operational temperatures and CO_2 emissions that are caused by heating requirements.

The results show that the model prefers to utilise environmental or process heat and existing heating infrastructure by installing a heat pump with low or medium levels of integration. This shows that the reduction in operational cost outweighs the additional integration cost compared to a non-integrated heat pump with a lower COP. However, a high level of heat pump integration does not further decrease the total annual costs of the system because the installation becomes then too costly. Furthermore, the transition from a utility system with natural gas to a fully electric system does not significantly affect the optimal level of heat pump integration.

When energy price fluctuations increase, electric boilers and thermal energy storage are installed to reduce operational costs by shifting power use to times of low electricity prices. However, heat from the heat pump is never directly used for this purpose. In the model, heat pumps are never oversized and always scaled to either the process heat demand or the size of the heat source. As a result, heat pumps are also never connected to thermal energy storage. This indicates that thermal energy storage can only be used when electric boilers are installed, which are less expensive than heat pumps.

Overall, the results show that a) thoughtful (but limited) integration of a heat pump can significantly improve its economic performance; b) the use of existing heating infrastructure is key to an economically viable solution, and c) there is a limited impact of energy price volatility and availability of natural gas on those findings. Future studies should explore modelling to generate alternatives [37] to test the robustness of the proposed utility system designs, identify tipping points in the economic viability of electrification, and assess the impact of grid tariffs on the proposed utility systems.

List of Abbreviations

Bat	Battery
CaPex	Capital expenditure
CCG	Grand composite curve
CO_2	Carbon Dioxide
COP	Coefficient of performance
ElB	Electric boiler
EU ETS	EU Emissions Trading System
GB	Natural gas boiler
GHG	Greenhouse gases
H2	Hydrogen
H2B	Hydrogen boiler
H2E	Electrolyzer
H2S	Hydrogen storage tank
HP	Heat pump
HT steam	High-temperature steam
LT steam	Low-temperature steam
LT-TES	Latent thermal energy storage
MVR	Mechanical vapour recompression
NG	Natural gas
OpEx	Operating expense
PtH	Power-to-heat
SS-TES	Sensible thermal energy storage
TAC	Total Annual Cost
TES	Thermal energy storage
Dutch TTF	Dutch Title Transfer Facility

4

Nomenclature

4.5.1. Nomenclature of parameters and variables

Symbol	Explanation	Unit
Time-dependent variables (per time step)		
$P_{\mathrm{gr,i}}(t)$	Power from the electricity grid to technology i	MW
$P_{\mathrm{i,gr}}(t)$	Power from technology i to the electricity grid	MW
$NG_{\mathrm{in}}(t)$	quantity of natural gas consumption	MW
$P_{\mathrm{HP,in}}(t)$	Power flow to the heat pump	MW
$H_{\mathrm{HP,out}}(t)$	Heat output from the heat pump	MW
Time-dependent parameters		
$\mathrm{p_{el,grid}}(t)$	Electricity price at time t	Eur/MWh
$\mathrm{p_{NG}}(t)$	Natural gas price at time t	Eur/MWh
$\mathrm{p_{EUA}}(t)$	Emission allowance price at time t	Eur/tonne$_{CO_2}$
Constants		
Δt	Time step duration	h
$\mathrm{EF_{NG}}$	Emission factor of natural gas	tonne$_{CO_2}$/MWh$_{NG}$
$\mathrm{COP_{ideal}}$	Carnot Coefficient of Performance	-
$\mathrm{T_{sink}}$	Temperature of the heat sink of the heat pump	K
$\mathrm{T_{source}}$	Temperature of the heat source of the heat pump	K
$\mathrm{H_{source}}$	Heat source of the heat pump	MW

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5

The impact of energy prices on the electrification of utility systems in industries with fluctuating energy demand

Industrial greenhouse gas emissions, primarily carbon dioxide, constitute about one-third of global emissions, and 75% are caused by the generation of heat from fossil fuels. Therefore, a key decarbonisation strategy is electrifying heat generation using renewable sources and power-to-heat technologies. This chapter explores the impact of the energy price on the optimal choice and sizing of power-to-heat and storage technologies in existing energy-intensive industries with a variable heat demand. A mixed integer linear program is used to determine the technology portfolio and size of the equipment that leads to the lowest total annual cost of the utility system while ensuring that heat demand is always fulfilled. The results of a case study in the Netherlands show that adding power-to-heat and storage technologies to a fossil fuel-based combined heat and power plant is economically viable under all explored scenarios. The mean and the variance of electricity prices significantly influence the sizing of heat pumps, electric boilers, and thermal energy storage. High and stable electricity prices lead to larger heat pump capacities compared to scenarios with low and more variable electricity prices. Electric boilers are primarily sized based on the variance of electricity prices and the capacity of thermal energy storage, which plays a crucial role in managing electricity price fluctuations. The study emphasises the potential for cost-effective electrification and provides valuable insights for reducing industrial CO_2 *emissions.*

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5.1. Introduction

International commitments aim to reduce greenhouse gas (GHG) emissions significantly [1]. Approximately one-third of global GHG emissions stem from the industry and consist mainly of CO_2 emissions [2]. Roughly 75% of these emissions are related to the combustion of fossil fuels for fulfilling heating requirements [3]. Therefore, electrifying heat generation with renewable sources is considered a key pathway to reducing industrial CO_2 emissions [4].

Power-to-heat (PtH) technologies have gained attention as they can a) directly convert electrical power into heat (using, e.g., an electric boiler (ElB)), b) use electrical power to produce an intermediate energy carrier, such as hydrogen (H2), that can be stored and thereafter converted into heat, or c) use electrical power to upgrade waste heat streams (with, e.g., a heat pump (HP)) [5]. Among the three options, waste heat-upgrading technologies such as heat pumps require the least electricity to generate heat [6]. Yet, the technical performance of a heat pump is highly dependent on the temperature at which heat is demanded and available [7].

Combining PtH technologies with energy storage can increase the use of renewable electricity, reduce CO_2 emissions and improve the economic performance of an industrial plant's energy conversion facility (utility system), as they enable energy use when it is abundant and cheap [8]. However, identifying cost-effective combinations of PtH and storage technologies is challenging due to varying and uncertain equipment costs and efficiencies, as well as the fluctuating availability and cost of renewable electricity.

This challenge has been studied from different perspectives in the literature, and studies can be categorised into three groups. The first compares different PtH technologies with each other in scenarios with a constant energy price, excluding the option of energy storage. Son et al. [5], for example, study the potential role of PtH technologies in an oil refinery with a pinch analysis and identify economically feasible HP and ElB solutions. Wiertzema et al. used the same approach to study the impact of electrifying the utility system on the heat integration of a chemical process and found that replacing a gas boiler with an electric boiler reduces the waste heat and therefore the potential for heat integration. However, they also found that the operational cost of the selected electric boiler halved in 2040, compared to a 2030 energy market scenario [9]. Kim et al. used pinch analysis at the site level and found several electrification options, but excluded an assessment of their economic performance [10]. Walden and Stathapopoulos used a time-sliced pinch approach to study the impact of a fluctuating heat demand on the optimal integration of a heat pump and found that a heat pump can provide flexibility up to a point at which part-load behaviour leads to diminishing returns [11].

The second group of studies considers fluctuating energy prices, but explores the use of only one PtH and storage technology. Walden et al. [12], for example, used optimisation to study the operation of a high-temperature heat pump and a sensible thermal energy storage with electricity coming from the power grid and a wind turbine in a process with a constant heat demand. Trevisan et al. used mixed integer linear optimisation to study the techno-economic feasibility of molten salt-based thermal energy storage with embedded electrical heaters for a process with a variable heat demand and different electricity spot market prices [13].

The third group considers multiple PtH and storage technologies and fluctuating energy prices. Baumgaertner et al. [14], for example, studied the impact of time-dependent grid emissions on the design and operation of an electrified utility system with a mixed integer linear model for a pharmaceutical facility with a fluctuating energy demand. While they include varying electricity prices in their study, the gas price is kept constant. Reinert et al. [15] expanded this work and added the possibility of pumped thermal energy storage. However, again, gas prices were kept constant. Previous work by some of the authors of this study explored the potential for cost-optimal electrification of existing utility systems for chemical plants with fluctuating electricity and gas prices. Direct and indirect electrification with electric and hydrogen boilers was considered, but the option to upgrade waste heat with a heat pump was not included [16]. Fleschutz et al. [17] studied using the combination of an ElB, hydrogen as an energy carrier, a heat pump and forms of energy storage for electrification for industrial applications. However, the assessment was carried out for low-temperature heat requirements, for which the performance of the heat pump is significantly different from the performance in the case of high-temperature applications.

The studies presented thus far do not analyse the impact of energy price profiles on the combination of PtH and storage technologies under fluctuating energy prices and operational conditions for existing high-temperature industrial applications. Insight into the potential role of electrification technologies under these circumstances is needed to enable cost-effective electrification of current fossil industrial heating systems.

The aim of this work is thus to evaluate the impact of variable energy prices on deploying PtH and storage technologies in an energy-intensive industry with variable high-temperature heat demand and existing heating infrastructure. Herein, the trade-off between options with a higher efficiency and a higher cost, i.e., heat pumps, and options with lower efficiency and cost, i.e., electric boilers, is explored. The contribution to the existing literature on electrified utility systems for industrial plants is twofold.

1. This work presents a feasibility assessment of technology portfolios that enable cost-effective electrification of fluctuating high-temperature heat demand requiring minimal changes to the plant's existing infrastructure.

2. The impact of the mean and variance of energy prices and the electricity to gas price-ratio on the selection and sizing of technologies, specifically on heat pumps, is shown.

5.2. Methods

This section introduces the model used to design and simulate the utility system and the energy price and technology cost scenarios that were explored (sections 5.2.1 and 5.2.5). Then, the industrial plant that served as a case study is presented (section 5.2.3.

5.2.1. Existing utility system and potential investment options

The model used to design and assess cost-optimal electrified utility systems is based on an existing utility system fuelled by natural gas (NG). This system, shown in Figure 5.1, comprises a bidirectional connection to the local power grid, a gas-fired gas turbine (GT) and a heat recovery steam generator (HRSG) with additional natural gas co-firing in a gas boiler (GB). The co-firing allows additional heat generation without producing power and enables the system to react to fluctuations in process heat demand. The GT, HRSG, and GB are referred to as combined heat and power plant (CHP) for the remainder of this chapter. Since the CHP has already been installed, it is assumed that it does not require further investments. Investments due to maintenance are also not included.

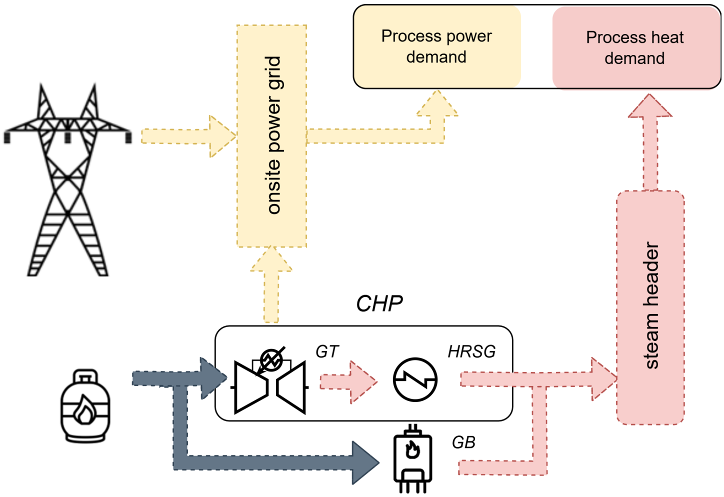

Figure 5.1.: Fossil fuel-based utility system assumed to be the existing utility system for the plant considered in this study. Note that the onsite power grid and steam header are added to the figure for better readability, but are not included in the model. The heat demand is supplied by a CHP, which consists of a gas turbine (GT) and a heat recovery steam generator (HRSG) with additional natural gas co-firing in a gas boiler (GB). The power demand is supplied by the power produced by the GT or by electricity from the national power grid.

To electrify the utility system, PtH technologies and storage technologies can be added to the system as shown in Figure 5.2. The PtH technologies considered in this study include an HP, which utilises excess heat from a heat recovery unit, an electric boiler (ElB), and a hydrogen boiler (H2B) fuelled with hydrogen generated by a proton exchange membrane water electrolyser (H2E). The decision to include hydrogen is based on low-cost storage opportunities in hydrogen tanks (see Table 5.5). The storage units considered are a Li-Ion battery (Bat), a sensible TES and a hydrogen storage tank (H2S). Due to the different temperature levels at which the PtH technologies produce heat, in practice, they would not be connected to the same TES unit. To reduce complexity, the TES is considered one unit in the model. Furthermore, it is assumed that the HP and the TES produce heat at the temperature required by the process and that the heat from the ElB is cascaded down to the required level by using throttling valves. The cost of these valves is not included in the model as it is considered minor compared to the cost of the PtH and storage equipment.

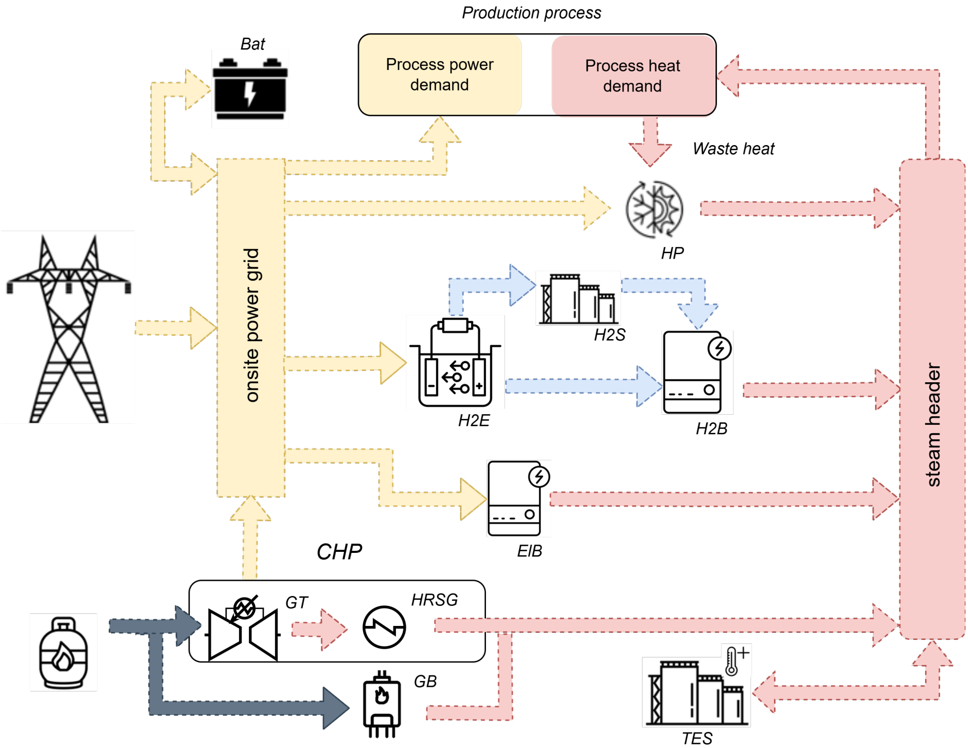

Figure 5.2.: Potential utility system design including a fossil-based legacy utility system (CHP) consisting of a gas turbine (GT) with a heat recovery steam generator (HRSG) and a gas boiler (GB), and an electric boiler (ELB), a heat pump (HP), and a power-to-gas-to-heat system consisting of an electrolyser (H2E), a hydrogen storage tank (H2S), and a hydrogen boiler (H2B). Energy can be stored in batteries (Bat) and thermal energy storage (TES). Note that the onsite power grid and steam header are used to improve the visualisation. In the model, all interconnections between technologies and from the technologies to the gas or power grid are modelled separately.

5.2.2. Model formulation

This work explores how changes in the electricity price affect the technology portfolio and economic performance of the system. Deterministic optimisation in combination with scenario analysis is used, as this study does not aim to find the best solution for all uncertain parameters but rather to understand the model's response to them. The model is implemented using the Python-based optimisation package 'Pyomo' and solved using Gurobi solvers. Its time resolution is $\Delta t = 0.5\ h$, following the resolution of the demand data of the case study. The solving time depends on the scenario. Some scenarios could not be solved to full optimality on a laptop (with Intel CORE i7 vPRO processor) and had to be solved on a supercomputing cluster. The default optimality gap was set to 0.005%.

The model departs from a model presented in [16] and was extended to include an HP and a more flexible CHP. The objective of the optimisation is to minimise the total cost of the utility system for the duration of one operational year, including the investment cost (CapEx) and the operational costs (OpEx), see Eq. (D.47). Since the model runs in half-hourly steps and the operational time of the process is 8000 hours, assuming 760 hours of downtime per year, the model includes 16000 time steps.

$$min \sum_{t=0}^{t=16000} \mathrm{OpEx}(t) + \mathrm{CaPex} \tag{5.1}$$

The OpEx is calculated using Eq.(5.2). It consists of the cost of consuming grid electricity minus the potential revenue from selling electricity from the CHP back to the grid and the cost of consuming natural gas (including the cost of purchasing CO_2 emission allowances within the European Emission Trading System (EU ETS)). Taxes and other fees for selling power back to the grid are not included in the model. In Eq.(5.2), $\mathrm{p_{el,\ grid}}(t)$ is the electricity price at time t in [euro/MWh]. Power flow from the grid to technology i is denoted as $P_{gr,i}(t)$ and power flow from technology i back to the grid as $P_{i,gr}(t)$. Both are expressed in [MW]. $\mathrm{p_{NG}}(t)$ is the cost of using natural gas at time t in [euro/MWh]. The quantity of gas consumed per time step is denoted by $NG_{in}(t)$ in [MW].

$$\begin{aligned} \mathrm{OpEx}(t) = \ & \mathrm{p_{el,\ grid}}(t) \cdot \sum (P_{gr,i}(t) - P_{i,gr}(t)) \cdot \Delta t \\ & + \mathrm{p_{NG}}(t) \cdot NG_{in}(t) \cdot \Delta t \end{aligned} \tag{5.2}$$

The CapEx (Eq. (5.3)) includes the investment required for all newly installed technologies i and is a product of their technology cost c_i (in [euro/MW] or [euro/MWh]), their installation factor Inf_i and their size s_i (in [MW] or [MWh]).

$$\mathrm{CaPex} = \sum_i \mathrm{c}_i \times \mathrm{Inf}_i \times s_i \times \mathrm{AF}_i \tag{5.3}$$

Since the model only considers one operational year, the investment is annualised using an annualisation factor of the respective technology AF_i, which is calculated using Eq.(5.4). LT_i is the lifetime of equipment i, and the discount rate r is set to

10%, as in [17].

$$\mathrm{AF}_i = \frac{\mathrm{r}}{1-(1+\mathrm{r})^{-\mathrm{LT}_i}} \tag{5.4}$$

The power or heat generation and storage technologies are represented by energy flow balances and the respective technological constraints, as described in section 2.1 of [16]. The CHP in this study is modelled as a combination of a gas turbine, a heat recovery steam generator, and a gas boiler. Mirroring the situation of the case study, the operational flexibility of the GT is based on the combined operation of two gas turbines, which both have the ability to operate at 60-100% of their capacity. It is assumed that one turbine can be shut down completely. One GT, or 30% of the total GT capacity, has to operate at all times to limit the number of cold starts, which damage the equipment. Therefore, the minimal load of the CHP is assumed to be 30% of its capacity. The heat generation of the CHP is calculated using Eq. (5.5), where $NG_{\mathrm{GT,in}}(t)$ is the amount of natural gas converted in the gas turbine, $\eta_{\mathrm{GT,th}}$ the thermal conversion efficiency of the gas turbine, $NG_{\mathrm{GB,in}}(t)$ the amount of natural gas going to the gas boiler, η_{GB} the conversion efficiency of the gas boiler and $H_{\mathrm{CHP,out}}(t)$ the heat output of the CHP.

$$\left(NG_{\mathrm{GT,in}}(t)\cdot\eta_{\mathrm{GT,th}} + NG_{\mathrm{GB,in}}(t)\right)\cdot\eta_{\mathrm{GB}} = H_{\mathrm{CHP,out}}(t) \tag{5.5}$$

The energy conversion of the HP is modelled as stated in Eq. (5.6), where $H_{\mathrm{HP,out}}(t)$ is the heat output of the HP, which is a function of the power input $P_{\mathrm{HP,in}}(t)$ and the ideal, or Carnot, coefficient of performance (COP) COP_{ideal} multiplied by 0.5 because a mechanical closed-cycle HP is expected to operate at 50% of its ideal COP [18, 19].

$$H_{\mathrm{HP,out}}(t) = P_{\mathrm{HP,in}}(t)\cdot \mathrm{COP}_{ideal}\cdot 0.5 \tag{5.6}$$

The ideal COP is calculated using Eq. (5.7).

$$\mathrm{COP}_{ideal} = T_{sink}/(T_{sink} - T_{source}) \tag{5.7}$$

All equations of the model are presented in D.

5.2.3. Case study

This study explores the electrification of the utility supply for the energy-intensive industry with a highly fluctuating electricity and (high-temperature) heat demand. These conditions are commonly observed in sectors with a large product portfolio, batch processing, and or cleaning-in-place processes such as in the food and beverage, the chemical and pharmaceutical, the textile and the paper and pulp industry. An existing paper mill in the Netherlands with various paper recipes is used as a representative case study for this group of discontinuous processes.

Of the considered paper mill, only the heat demand of the drying section was considered, as it requires over 80% of the total heat demand. The heat demand, between 100 °C and 160 °C, varies in capacity every 30 minutes. The maximum heat demand is 21.5 MW, the average 13.7 MW and the minimum 1.1 MW. Figure 5.3 shows the demand duration curve of the process (in blue) and the heat delivered by the CHP when it operates at its minimal load (in orange). For confidentiality reasons, a more detailed description of the underlying demand data cannot be disclosed.

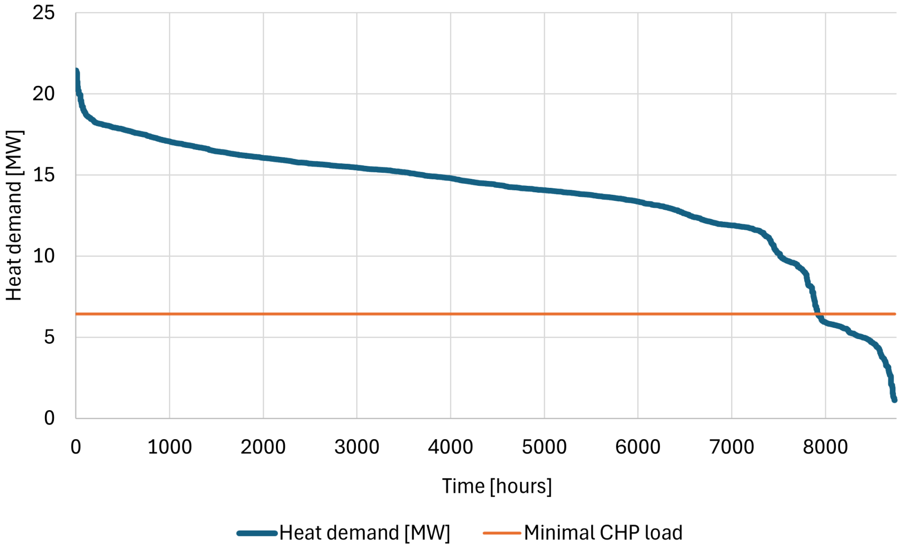

Figure 5.3.: Heat demand duration curve of the process in the case study and the demand that the CHP supplies at its minimal possible load.

Excess heat can be recovered from the drying hood at T = 55 °C and fed to a HP. Since the HP is required to generate heat at 160 °C, the COP of the HP for this paper mill is 2 based on a second law efficiency of 50%. The electricity demand is assumed to be 10% of the heat demand based on information obtained from the plant operator. The grid connection capacity that limits the power flow from or to the local power grid was assumed to be 30 MW based on the capacity of the actual grid connection of the case study plant.

Technical parameters

The parameters used to model the technologies are shown in Tables 5.1 and 5.2. Except for the minimal load factor of the CHP, the data is derived from literature. The minimal load factor of the gas turbine is dictated by the equipment installed in the paper mill, and in line with the proposed 50% operational flexibility by Voll et al. [20]. I.2 shows how the results would look like for more flexible CHPs.

Table 5.1.: Data used to model conversion technologies

	Gas turbine	Gas boiler	ElB	HP	Electrolyser	H2 boiler
Capacity thermal [MW_{th}] electric [MW_{el}]	$H_{dem,max}/\eta_{GB}$	20% of GT	decision variable	decision variable	decision variable	decision variable
Efficiency η [%]	$\eta_{\text{thermal}} = 60$, [a] $\eta_{el} = 30$	82	99 [6, 21]	$0.5 \cdot COP_{ideal}$	69 [22]	92 [23, 24]
Minimal load factor [% of max. load]	0.5·60	0	0	0	0	0
Lifetime LT [years]	not included in model		20 [21]	20 [7]	15	20 [25]

[a] Note that η_{thermal} concerns the generation of heat from natural gas

Table 5.2.: Data used to model storage technologies

	Battery	TES	Hydrogen tank
Capacity	decision variable	decision variable	decision variable
Efficiency η [%]	90 [17]	90 [26]	90 [17]
Maximum energy output [% of capacity/Δt]	70 [17]	50 [17]	100
Lifetime LT [years]	15 [27]	25 [28]	20 [29]

5.2.4. Reference utility system

The fossil fuel-based legacy utility system described in 2.1 is the reference system of this study. The reference system's total cost is its operational cost, which is calculated according to the cost-optimal operation of the system as described in Eq. (5.8). The total cost of the reference system is the sum of the costs for grid power and NG use. The cost for grid power use is a function of the electricity price at time t and the difference between electricity consumed by the process $P_{\text{gr,process}}(t)$ minus the power generated by the GT and sold to the grid, $P_{\text{GT,gr}}(t)$. The cost for NG consumption is a function of the natural gas price at t and the gas used by the gas turbine and the boiler, $NG_{\text{GT,in}}(t)$ and $NG_{\text{GB,in}}(t)$.

$$\text{Total Cost} = min \sum_{t=0}^{t=16000} \Big(\mathrm{p}_{\text{el, grid}}(t) \cdot \Delta t \cdot \big(P_{\text{gr,process}}(t) - P_{\text{GT,gr}}(t)\big) + \mathrm{p}_{\text{NG}}(t) \cdot \Delta t \cdot \big(NG_{\text{GT,in}}(t) + NG_{\text{GB,in}}(t)\big)\Big) \tag{5.8}$$

The same technical parameters and constraints are used as in the optimisation model described in 5.2.1.

5.2.5. Scenarios with differing techno-economic assumptions

The optimisation model is run for a number of energy price scenarios and technology cost (TC) scenarios since the design of an electrified utility system depends on capital and operational costs, and both are subject to uncertainties. The scenario tree containing all explored scenarios is included in the Appendix (Figure H.5).

Energy price scenarios

Three uncertainties have been addressed in this chapter, namely 1) the average energy price because of the trade-off between investment and operational cost, 2) energy price variability because of the potential value of flexibility in the utility system, and 3) the electricity-to-gas price ratio (EGR) because PtH technologies compete with existing gas-based technologies. To understand the impact of these uncertainties, several energy price scenarios were designed.

The average electricity price for the 'low mean' scenario is 30 euro/MWh and is based on the average price of electricity on the Dutch day-ahead market in 2020 [30]. The mean electricity price of the 'high mean' scenario is 100 euro/MWh and is based on 2023 data from the same market [30]. The electricity price volatility (its variance) is included via two scenarios, i.e. with a low variance, based on 2019 data, and with a high variance, based on 2023 (Dutch day-ahead market) data [30]. A combination of the two mean and the two variance scenarios leads to four electricity price scenarios. The abbreviations used in the first column of Tables 5.3 and 5.4 are based on the mean price and the level of price variance of the respective scenario. The scenario with a low mean price and high levels of price variance, for example, is named 'LMHV' ('Low Mean High Variance').

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Two gas price scenarios are added to each electricity price scenario to explore the impact of the EGR. One scenario has cheaper gas than electricity prices, based on the average EGR (including EU ETS allowance price) in 2023 of 1.6 (see data in [30–32]). Note that companies in the Netherlands did not have to pay for all of their CO_2 emissions and that including free allocation rights would result in an EGR of >2 in 2023. For the second scenario, an EGR of 1 was assumed to simulate scenarios with increased gas use prices. The gas price profiles are based on Dutch TTF market data [31] and were adapted to have a mean price matching the desired EGR. To avoid negative gas prices, the gas price is capped at 10 euro/MWh, which aligns with the lowest price in the period 2021 to 2024 (see data in [31, 33]). 17 euro/MWh_{NG} (85 euro/ton_{CO_2}) are added to the gas price, mimicking prices in 2023, to include the cost of purchasing CO_2 emission certificates to the cost of using natural gas [34]. This CO_2 price is used in all gas price scenarios.

Tables 5.3 and 5.4 provide information about the resulting price scenarios. All price profiles are shown in Figures H.1 to H.4 in H.

Technology cost scenarios

In this study, the cost for new equipment is the product of the technology cost and its installation cost factor. The technology cost was based on a literature review and is shown in Table 5.5. The installation cost factors were taken from Sinnot and Towler [35]. HPs were considered to be a collection of compressors (2.5) and heat exchangers (3.5), storage technologies miscellaneous equipment (2.5). The hydrogen boiler was considered a gas-fired boiler (2), and the hydrogen storage a pressure vessel (4). For

Table 5.3.: Electricity price and negative price statistics in the energy price scenarios.

Scenario	EGR	Electricity Price: Mean (Euro/MWh)	Electricity Price: Variance $(\text{Euro/MWh})^2$	Negative Prices: Number of hours	Negative Prices: Average Value (Euro/MWh)
LMLV	1.6	30	127	30	-6.82
	1	30	127	30	-6.82
LMHV	1.6	30	2,405	1,641	-43.67
	1	30	2,405	1,641	-43.67
HMLV	1.6	100	127	-	-
	1	100	127	-	-
HMHV	1.6	100	2,405	155	-47.46
	1	100	2,405	155	-47.46

Table 5.4.: Natural gas use cost and hours when the electricity price is lower than the gas cost (including the price for emitting CO_2).

Scenario	EGR	Natural Gas Use Cost: Mean (Euro/MWh)	Natural Gas Use Cost: Variance $(\text{Euro/MWh})^2$	Electricity Price < Gas Cost: Number of hours
LMLV	1.6	35.75	10	6,649
	1	47	10	8,269
LMHV	1.6	35.75	113	4,431
	1	47	113	5,814
HMLV	1.6	79.5	10	121
	1	117	10	8,269
HMHV	1.6	79.5	113	1,945
	1	117	113	5,816

the ElB and the electrolyser, a factor of 1 was used as the technology cost was derived from a reference, which had already included the installation cost.

Two technology cost scenarios (TC scenarios) are explored to account for the uncertainty of the TC of Bat, TES, H2E and HP. The technology cost of the ElB, the H2B and the H2S were kept the same for both the high- and low technology cost scenarios, as these technologies are mature and less price development is expected than for the remaining technologies. The first scenario favours installing HPs by assuming low HP costs and high costs for other equipment ('LowHP-HighRest'). In the second scenario, it is the other way around, i.e. HP costs are high, and the cost of the remaining equipment is low ('HighHP-LowRest'). The ranges in technology cost deliberately span a wide range for the purpose of exploring the impact of these cost scenarios on the operation and sizing of the utility system.

5.3. Results and discussion

In sections 5.3.1 to 5.3.4, the cost-optimal utility systems for the energy price scenarios are presented, and it is discussed how they differ from each other and the

Table 5.5.: Technology cost scenarios

Technology	**Technology cost per scenario**		**Reference**	**Lang Factor**
	'HighHP-LowRest'	**'LowHP-HighRest'**		
ElB	60 euro/kW	60 euro/kW	[21]	1
HP	500 euro/kW	300 euro/kW	[7]	3
Battery	180 euro/kWh	320 euro/kWh	[27]	2.5
Thermal Energy Storage	15 euro/kWh	40 euro/kWh	[36]	2.5
Electrolyser	760 euro/kW	980 euro/kW	[22, 37]	1
Hydrogen boiler	35 euro/kW	35 euro/kW	[25]	2
Hydrogen storage	10 euro/kWh	10 euro/kWh	[26]	4

respective reference systems. In section 5.3.5, the sizing of new equipment across scenarios is discussed.

5

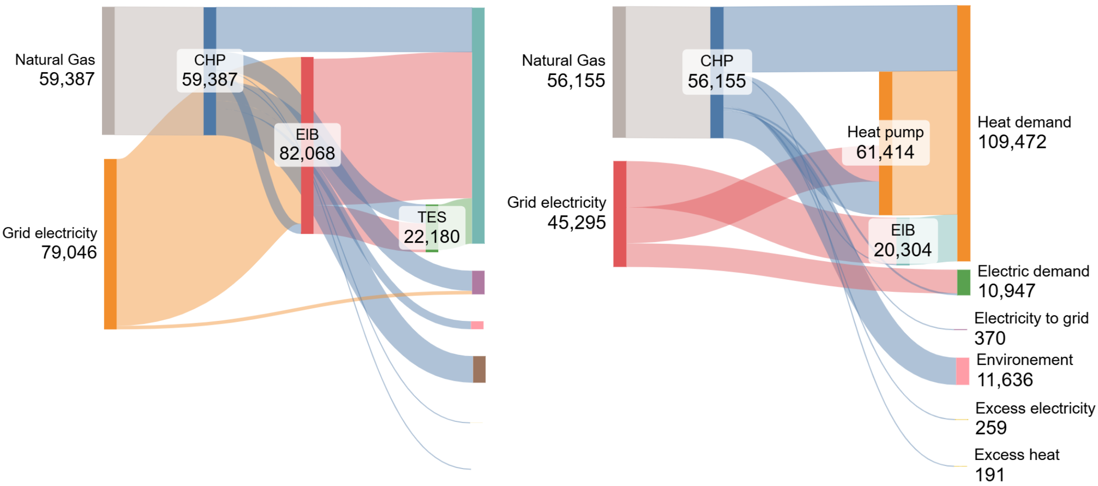
5.3.1. Cost-optimal utility systems for energy price scenarios with low mean and low variance

This scenario explores the electrification of the utility system if the prices are low and have low fluctuations. Table 5.6 shows that, while ElB and TES are installed for all values of the EGR and TC scenarios, HPs are only installed in the 'LowHP-HighRest' scenarios. No HPs are installed in the 'HighHP-LowRest' scenario. Since the same trends in technology choice and sizing can be observed in both EGR scenarios, only the operation of the systems in the 'EGR 1.6' scenarios is discussed in detail.

Table 5.6.: Installed PtH and storage capacities in the energy price scenarios with low mean and variance

EGR	TC scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	14	24	0
	LowHP-HighRest	6	5	5
1	HighHP-LowRest	14	28	0
	LowHP-HighRest	6	6	5

In the TC scenario with high HP cost ('HighHP-LowRest'), shown in Figure 5.4a, the CHP operates 97% of the time at its minimum possible load (30% of its capacity) and ramps up to full capacity only when electricity prices are higher than 3 times the average price. The power generated by the CHP is either sold to the power grid when electricity prices are high or directly fed to the paper mill (herein referred to as the process) and the ElB when electricity prices are low. The heat generated by the CHP goes to the process, and excess heat goes to the TES. 6% of the time, when electricity prices are very low, all energy from the CHP goes to the TES (directly or via the ElB). Power and heat are wasted (neither used nor stored) when the electricity price reaches its negative peak, to consume as much electricity as possible with the ElB. The ElB operates 68% of the time and supplies roughly 50% of the total heat demand, as Figure 5.4a shows. It charges the TES when either heat demand is low enough and



(a) TC scenario 'HighHP-LowRest'

(b) TC scenario 'LowHP-HighRest'

Figure 5.4.: Energy exchange in [MWh] in the utility systems for the energy price scenario with low mean prices, low variance and EGR 1.6.

excess heat is available, electricity is cheap enough to allow for cost-effective use of the maximum capacity of the ElB, or when electricity prices are negative. Around 25% of the power for the ElB is supplied by the CHP (see Figure 5.4a). The TES supplies heat to the process during hours with a heat demand exceeding the minimal heat output by the CHP and electricity prices that render using the ElB unfavourable.

When an HP is installed, like in the 'LowHP-HighRest' TC scenario shown in Figure 5.4b, the CHP still operates at its minimal load 97% of the time. In this scenario, the HP is the main heat supplier next to the CHP, as Figure 5.4b shows. It operates 94% of the time, mostly at full capacity (its load factor, i.e. the total energy supplied in one operational year over the installed capacity times the number of operational hours, is 92%). Only during peak heat demand and a relatively high electricity-to-gas price ratio, e.g., 2, is the HP turned off, and the CHP delivers all heat required by the process. This, however, only happens 3% of the time. As Figure 5.4b shows, the CHP supplies approximately two-thirds of the power the HP requires to run and delivers almost half of the power the ElB uses. The TES supplies heat to the process at peak heat demand. It is charged mainly by the CHP and the HP. The ElB charges the TES only when electricity prices are very low, and the HP is operating at full capacity, which happens 5% of the time. The ElB operates for a similar amount of hours as in the previous scenario but contributes less to the heat demand of the process than before (compare the two diagrams in Figure 5.4) as it supplies heat to the process during peak demand when the electricity prices are low, or the TES is empty. The gas boiler is used only 2% of the time and operates for two reasons. Either to supply heat demand exceeding what the ElB, TES, HP and CHP operating at minimal load combined can deliver (maximum 16 MW) and electricity prices or PtH capacities do not allow storing the additional power from the CHP, or it is used instead of the ElB when electricity prices are much higher than gas prices (e.g., 1.5 times higher).

Table 5.7.: Total annual cost (TAC), savings in TAC compared to the reference system, energy consumption including gas and power from the grid, and power sold to the grid in the energy price scenarios with low mean and variance

EGR	System	TC scenario	TAC [Million euro]	Savings [%]	NG to system [GWh]	Power Power grid to system [GWh]	System to power grid [GWh]
1.6	Ref.	-	5.9		196.5	0.02	35.1
	New	HighHP-LowRest	4.9	16.9	109.9	43.4	8.6
	New	LowHP-HighRest	4.9	16.9	107.9	21.1	3.8
1	Ref.	-	8.1		195.2	0.02	34.2
	New	HighHP-LowRest	6.1	24.7	105.3	45.7	7.2
	New	LowHP-HighRest	6.1	24.7	105	20.5	2.7

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Finally, compared to the reference utility system, less power is sold to the grid in the new systems, as Table 5.7 shows. The combination of PtH technologies and TES would enable an economically more efficient use of the power generated by the CHP. This is also illustrated by the reduced total use of energy (see Table 5.7) and the consequent cost savings.

5.3.2. Cost-optimal utility systems for energy price scenarios with low mean and high variance

As Table 5.8 shows, only ElBs and TES are installed in the scenarios with low mean and high variance energy prices. The capacities of the installed ElBs come close to the available grid connection capacity of 30 MW to exploit periods of low electricity prices. Note that the lowest price peaks are stronger than in the scenario discussed in the previous section (see 'Negative Price' column in Table 5.3 and Figures H.1 to H.4). The high price variance also results in TES units from 55 to 112 MWh, a strong increase compared to the TES capacities in the scenarios in 5.3.1. The cost of the TES has a strong impact on its size as its capacity in the 'HighHP-LowRest' scenarios is about twice as big as in the 'LowHP-HighRest' scenarios.

Table 5.8.: Installed PtH and storage capacities in the energy price scenarios with low mean and high variance

EGR	TC scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	29	103	0
	LowHP-HighRest	28	55	0
1	HighHP-LowRest	29	112	0
	LowHP-HighRest	28	61	0

Scenario 'EGR 1, HighHP-LowRest' is shown in Figure 5.5 as an exemplary scenario of the energy price scenarios with low mean and high variance. The CHP operates similarly to the 'HighHP-LowRest' scenario in 5.3.1. The TES enables selling excess power from the CHP to the grid when electricity prices are high, while the CHP operates at its minimum possible load as the TES supplies heat to the process when the demand exceeds what the CHP can generate at minimal load. The TES is either charged by the CHP when demand is lower than the heat generated by the CHP at minimal load or by the ElB when electricity prices are low. Figure 5.5 shows that the ElB is predominantly used to charge the TES. Table 5.9 shows that an increase in

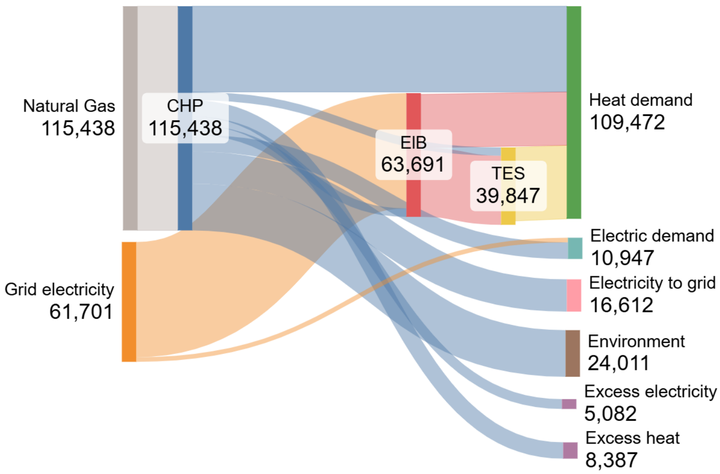

Figure 5.5.: Energy exchange in [MWh] in the utility systems for the energy price scenario with low mean prices, high variance, EGR 1 and TC scenario 'HighHP-LowRest'.

gas prices leads to a decreased use of the CHP. This explains the slightly larger TES capacities in the 'EGR 1' scenarios compared to those in the 'EGR 1.6' scenarios. The electrified utility systems lead to a higher reduction in TAC than the scenarios with a low price variance (compare Tables 5.7 and 5.9). This illustrates that the value of the flexibility to choose the energy carrier is higher than in the scenarios with lower price variance. Since ElB capacity is cheaper than HP capacity, the model chooses to install large over-capacities of ElB combined with large storage capacities to maximise the flexibility of the utility systems. Finally, more power is sold to the grid than in the scenarios with a low variance because the peaks of the electricity price profile are higher (see Table 5.9).

5.3.3. Cost-optimal utility systems for energy price scenarios with high mean and high variance

Table 5.10 shows the installed technologies for the scenarios with high variance and high average prices. Compared to the scenarios discussed previously, additional investments are made, and the capacities installed show larger differences between

Table 5.9.: Total annual cost (TAC), savings in TAC compared to the reference system, energy consumption including gas and power from the grid, and power sold to the grid in the energy price scenarios with low mean and high variance

EGR	System	TC scenario	TAC [Million euro]	Savings [%]	NG to system [GWh]	Power grid to system [GWh]	System to power grid [GWh]
1.6	Reference	-	5.4		207.1	1.9	36.4
	New	HighHP-LowRest	2.6	51.9	134.8	53.5	23.5
	New	LowHP-HighRest	3.1	42.6	139.7	50.6	24.0
1	Reference	-	7.7		201.1	1.9	32.5
	New	HighHP-LowRest	4.0	48.1	115.4	61.7	15.8
	New	LowHP-HighRest	4.5	41.6	117.5	60.2	16.6

the sub-scenarios. HP capacities range from 2 to 9 MW_{th}, TES from 15 to 113 MWh and ElB from 9 to 31 MW_{th}.

Table 5.10.: Installed PtH and storage capacities in the energy price scenarios with high mean and high variance

EGR	TC scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	31	113	2
	LowHP-HighRest	10	15	8
1	HighHP-LowRest	26	97	6
	LowHP-HighRest	9	17	9

The combination of a high HP price and low gas cost in the 'EGR 1.6, HighHP-LowRest' sub-scenario results in the highest consumption of natural gas among all cost-optimal utility systems. The resulting energy flows are shown in Figure 5.6. The figure shows that most electricity generated by the CHP is sold to the grid, which can be explained by the high electricity prices in this scenario (price peaks reach 470 euro/MWh), which make selling power economically more attractive than storing it in the form of heat for later use. The figure also shows that the ElB supplies more heat than the HP, unlike in other scenarios with ElB and HP instalments, such as the one shown in Figure 5.4b in 5.3.1. This is because the combination of ElB and TES allows more flexibility at lower costs than a combination of HP and TES, as explained in the previous section. As a result, only a small HP of 2 MW_{th} is installed. When electricity prices are negative, the ElB operates at full capacity instead of the HP because the ElB is less efficient and consumes more electricity, which is beneficial when prices are negative.

The technology portfolio and operation of the utility system in the 'EGR 1, LowHP-HighRest' sub-scenario is very different, as Figure 5.7 shows. In this scenario, the CHP delivers half of what it did in the HighHP-LowRest scenario depicted in Figure 5.6, as the thermal output by the ElB doubles and that of the HP nearly triples.

The energy use across the sub-scenarios differs greatly, as shown in Table 5.11. Even more power is sold to the grid than in the scenario discussed in 5.3.2, because

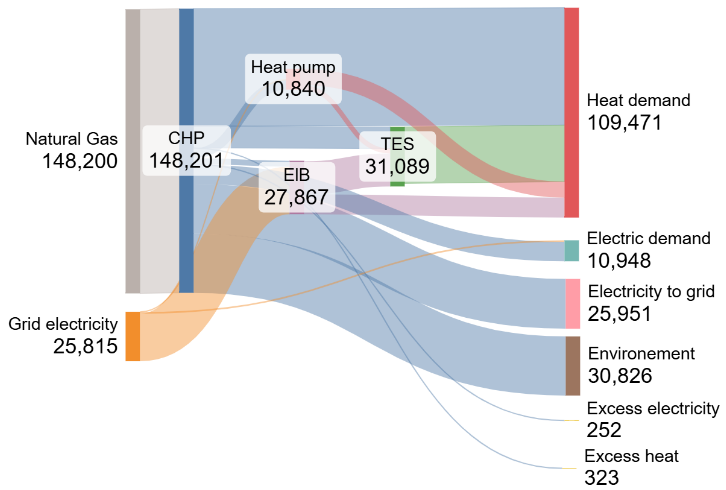

Figure 5.6.: Energy exchange in [MWh] in the utility systems for the energy price scenario with high mean prices, high variance, EGR 1.6 and TC scenario 'HighHP-LowRest'.

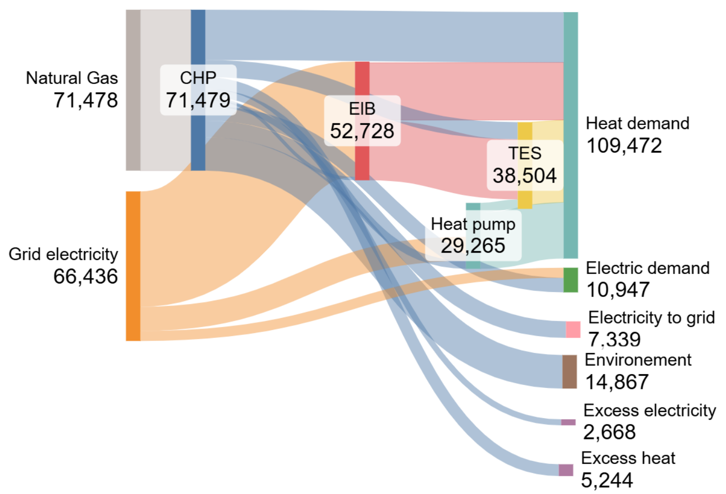

Figure 5.7.: Energy exchange in [MWh] in the utility systems for the energy price scenario with high mean prices, high variance, EGR 1 and TC scenario 'LowHP-HighRest'.

(mean and peak) electricity prices have increased. In the 'EGR 1.6 HighHP-LowRest' sub-scenario, this results in more power being sold to the grid than consumed. The relative savings in TAC differ by a factor of almost 2 between the EGR scenarios.

Table 5.11.: Total annual cost (TAC), savings in TAC compared to the reference system, energy consumption including gas and power from the grid, and power sold to the grid in the energy price scenarios with high mean and high variance

EGR	System	TC scenario	TAC [Million euro]	Savings [%]	NG to system [GWh]	Power grid to system [GWh]	System to power grid [GWh]
1.6	Reference	-	11.8		210.5	0.2	45.0
	New	HighHP-LowRest	9.9	16.1	148.2	25.8	26.0
	New	LowHP-HighRest	9.9	16.1	121.0	11.3	26.0
1	Reference	-	19.4		196.8	0.2	34.8
	New	HighHP-LowRest	14.2	26.8	105.5	22.0	3.7
	New	LowHP-HighRest	14.0	27.8	105.2	14.7	4.1

5.3.4. Cost-optimal utility systems for energy price scenarios with high mean and low variance

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In the scenarios with high mean price and low variance, HPs and TES units are installed in all scenarios, with capacities ranging from 7 to 9 MW and 6 to 32 MWh, respectively. ElBs are only installed in scenarios with an electricity-to-gas price ratio of 1 and their capacity is limited to 2 MW.

Table 5.12.: Installed PtH and storage capacities in the energy price scenarios with high mean and low variance

EGR	TC scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	0	19	8
	LowHP-HighRest	0	6	9
1	HighHP-LowRest	2	24	8
	LowHP-HighRest	2	7	9

The CHP operates at minimal capacity most (i.e. 95-100%) of the time across all sub-scenarios. The heat from the CHP is fed to the process, whereas its power is used to drive the HP, the process itself and the ElB, if installed. When the process demands little heat and power, power from the CHP is sold to the grid because electricity prices are high and storage capacity is limited. The HP operates as a baseload heat supply next to the CHP, as shown for scenario 'EGR 1, HighHP-LowRest' in Figure 5.8. When heat demand is low, the HP is used to charge the TES. About 8% of the time, the HP is off because the CHP alone provides enough heat. In the 'LowHP-HighRest' scenarios, HP capacity increases while the TES capacity decreases. Since the load factor of the HP in this scenario is up to 10% lower than in the scenario discussed in 5.3.1, this means that the HP becomes economically viable at high mean electricity prices even when it is not operated at maximum capacity throughout the year.

Table 5.13 shows that in all sub-scenarios, around 3 GWh are sold to the grid, which is less than in all other scenarios and less than one-tenth of the amount sold by the CHP in the reference model. This is due to the use of electricity from the CHP to power the HP. Like in the energy price scenario with high mean and variance (section

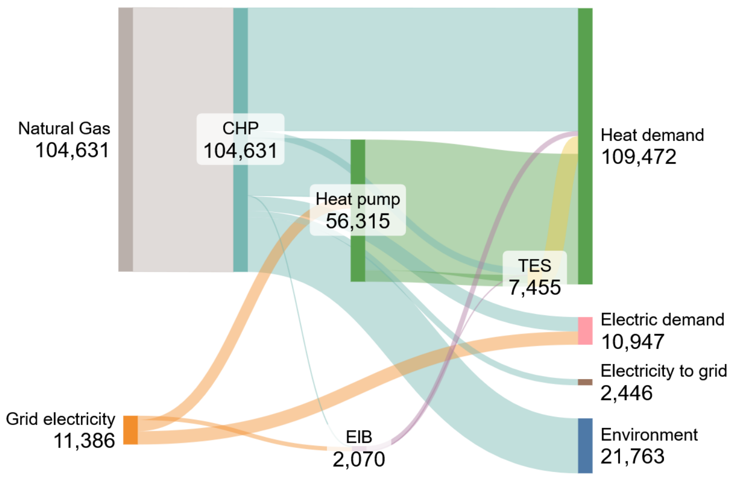

Figure 5.8.: Energy exchange in [MWh] in the utility systems for the energy price scenario with high mean prices, low variance, EGR 1 and TC scenario 'HighHP-LowRest'.

5.3.3), the relative savings in TAC differ by a factor of 2 between the EGR scenarios, reflecting the difference in gas prices. This can be explained by the amount of natural gas consumed, which is relatively similar in both scenarios (see Table 5.13).

Table 5.13.: Total annual cost (TAC), savings in TAC compared to the reference system, energy consumption including gas and power from the grid, and power sold to the grid in the energy price scenarios with high mean and low variance

EGR	System	TC scenario	TAC [Million euro]	Savings [%]	NG to system [GWh]	Power grid to system [GWh]	System to power grid [GWh]
1.6	Reference	-	12.0		202.1	0	39.5
	New	HighHP-LowRest	10.7	11.3	109.3	8.5	2.9
	New	LowHP-HighRest	10.2	15.4	107.5	10.1	3.5
1	Reference	-	19.4		195.0	0	34.1
	New	HighHP-LowRest	14.6	24.6	104.6	11.4	2.5
	New	LowHP-HighRest	14.1	27.2	104.6	12.0	3.5

5.3.5. Equipment sizing

Fig. 5.9 shows the normalised equipment sizing of the ElBs, the HPs and the TESs in all considered scenarios. The small overlap between the PtH technologies shows that, in most cases, either HPs or ElBs are installed, and rarely both. Large HPs are predominantly installed in scenarios with high mean prices on the left side of Fig. 5.9, and large ElBs are predominantly installed in the case of low and volatile energy prices, depicted on the right side of the figure. The large ElBs are combined with large TES, sized according to equipment cost. The highest HPs are installed when prices are, on average, high and show small fluctuations ('High mean low variance' scenarios). In these scenarios, neither the relative HP cost nor the electricity-to-gas price ratio leads to significant changes in the HP capacity. The large HPs in these scenarios are economically viable despite lower load factors because higher mean electricity prices lead to overall higher operational costs, which in turn leave more room for additional investment that enables operational cost savings.

Figure 5.9 shows that Elb and HP capacities are combined in the energy price scenarios with a low mean and low variance (LMLV), and with a high mean and a high variance (HMHV). In the LMLV scenarios, HP and ElB capacities are low, as energy prices are too low to justify the investment in HPs and too stable for large ElBs. In the HMHV scenarios, the large positive and negative price peaks lead to a large (26 MW) ElB capacity alongside a 6 MW HP and a 97 MWh TES when the equipment cost of the HP is high ('HMHV HighHP-LowRest'). The HP load factor ranges from 78 to 92%, which means that the HP operates as base load technology next to the CHP and confirms that high mean energy prices are required for the installation of HPs.

When an HP is installed, its size is affected by the EGR when HP capacities are below 5 MW, as seen in Table 5.10. Higher capacities of the HP are installed when the mean gas price is equal to the electricity price because switching from gas to electricity use leads to higher cost savings than in the scenarios with a lower gas price. The observed threshold of 5 MW can be explained by looking at Figure 5.10. The curve declines sharply around 12 MW. Since the CHP has to operate at minimal load at all times, the steady heat output of the CHP of around 6.5 MW reduces the heat that is required during around 7000 hours per year to 5.5 MW. HPs that operate above 5.5 MW, therefore, operate with a lower load factor and are only economically viable under HP-favourable conditions, i.e. high mean electricity prices. HPs that operate under those conditions are less sensitive to the EGR.

5.4. Limitations of the study

Though the results provide valuable insights for electrifying utility systems for the energy-intensive industry with fluctuating energy demand, the chosen method, assumptions, and scenarios have limitations. This section addresses them, offering important considerations for interpreting the results of this study.

The selected energy price scenarios are based on the assumption that companies pay for all their CO_2 emissions. Allowing free allocation of CO_2 permits would increase the EGR and likely limit the electrification technologies' economic viability. Additional price scenarios could be added to the analysis to explore "tipping points"

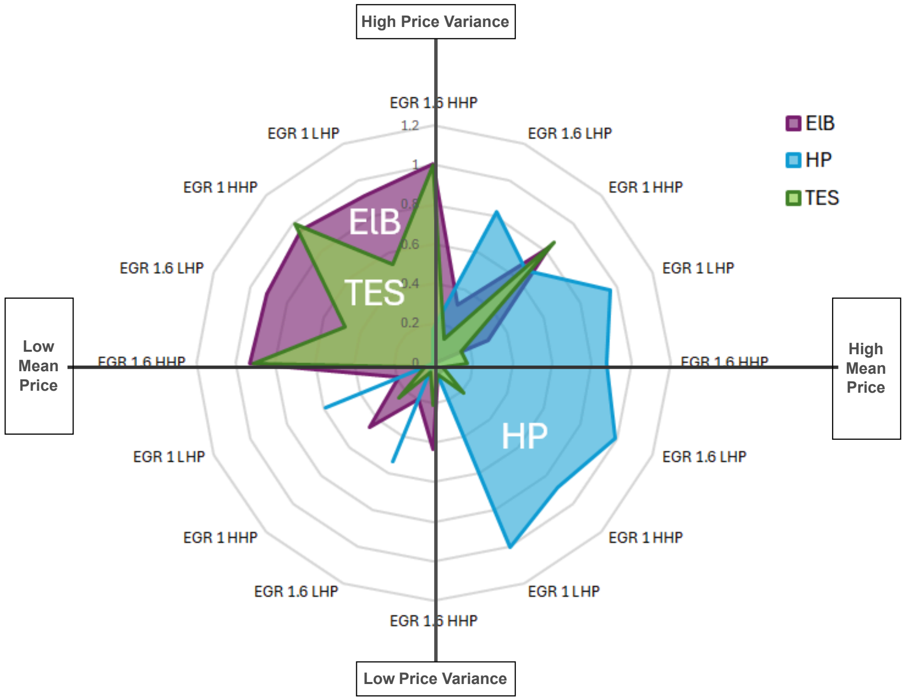

Figure 5.9.: Overview of normalised installed capacities across all scenarios. The right half of the diagram shows the installed capacities in energy price scenarios with a high mean price, and the upper half for scenarios with a high price variance.

for increasing levels of electrification.
Including the cost of energy transport in the model, such as network cost and peak tariffs, is also likely to affect the capacities and may reduce the share of electrification seen in the results. The authors expect that the effect would be more significant for the ElB capacity due to its less efficient use of electricity compared to an HP. Peak tariffs would likely lead to decreased ElB and TES capacities because they disincentivise the consumption of large amounts of power. However, transport costs would not need to be added to the consumption of power generated by the CHP. Therefore, it would not affect the power exchange between the CHP and the PtH technologies, which is high in the systems presented. Hence, (partial) electrification of utility systems is likely still cost-optimal if grid use costs were included in the model.
The explored energy price scenarios do not account for energy price uncertainty since the system has perfect foresight. Accounting for operational difficulties any system encounters in the real world, where prices might deviate from the forecast, would result in capacities different from those presented, especially those of the storage

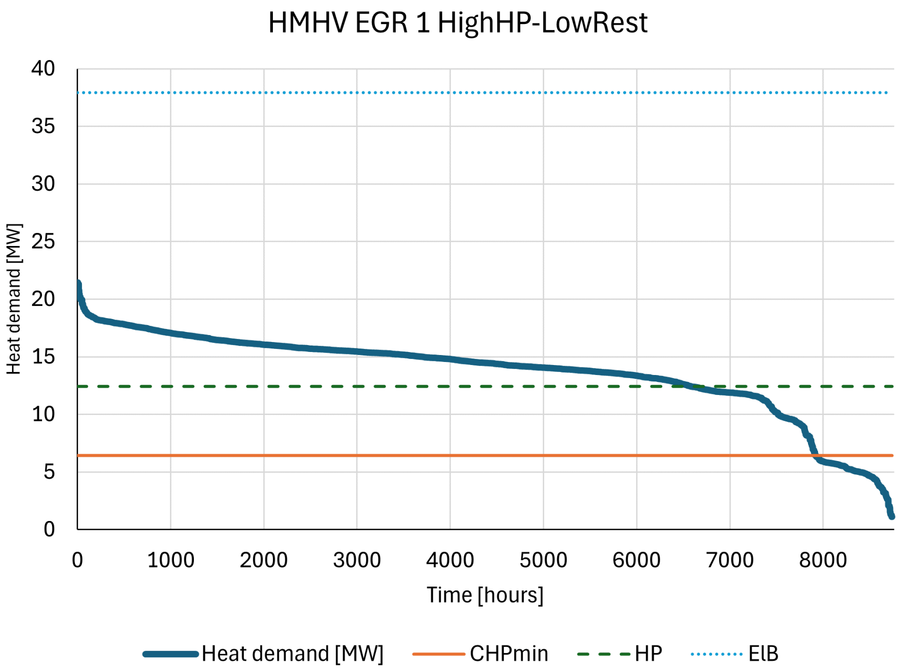

Figure 5.10.: Heat demand duration curve with the minimal heat output by the CHP and the added capacities by the HP and ElB in the HMHV EGR 1 HighHP-LowRest scenario

units. Stochastic programming could be used to explore this aspect in future studies. The main objective of the model is to minimise the total annual cost of the utility system. While this performance indicator provides valuable insights, other aspects, such as payback time and environmental impact, have not been considered, despite their importance to industry [38]. Including these indicators will likely result in other optimal solutions. The CO_2 emissions related to grid electricity (scope 2 emissions) are currently not considered in the model as they are case-specific and subject to change due to the ongoing decarbonisation of the national power generation. The model could be extended to include multiple objectives to explore the trade-offs between CO_2 emission reduction and TAC. This would likely result in higher PtH capacities, especially HP capacity, because of their conversion efficiency.
The sizing of the HP, ElB and other technologies also depends on the selected discount rate of 10%, and the absence of eventual retrofitting costs for the CHP in the model. A lower discount rate would incentivise investments and lead to larger installed capacities. The need to invest in the CHP due to required maintenance or retrofitting would likely have a similar effect. Larger PtH and storage capacities were also observed in model runs without the constraint limiting the CHP's operation to a minimum of 30% of its capacity. These results and a brief discussion are included in

I.2. They indicate that more flexible CHPs would likely supply less energy to the process lead to higher levels of electrification in the utility system.
In this study, a CHP exists before electrifying the utility system. Since the results show that PtH and storage technologies use power generated by the CHP, the results would change if the CHP did not exist.
The model was used to study the optimal electrification of a utility system for a paper mill with a grid connection capacity of 30 MW, which exists because of the plant's previous role as energy supplier. The size of the grid connection affects the sizing of the PtH technologies. The results show that the ElB is sized to this capacity when energy prices are highly volatile. Hence, a smaller connection capacity would result in a smaller ElB. As a consequence, the TES would be charged less and potentially scaled down. The size of the grid connection is likely to also affect the sizing of the HP, but only in cases when the HP's size exceeds that of the grid connection.
The variable operation of the utility system result in part-load operation of the PtH technologies. While this is not expected to affect the ElB, it would lead to a suboptimal efficiency of the HP. However, a change in the HP's efficiency in part load operation is neglected in the model to decrease its complexity. Accounting for it could lead to changes in HP capacity. Either the capacity would decrease while operation at full capacity would be increased, or the capacities would remain, but the share of heat generation of the HP would increase by reducing the use of any of the other technologies.
Finally, the TES in this study is modelled based on a latent heat storage unit with isothermal operation. This technology was selected based on the isothermal temperature supply by the HP for effective implementation [39]. When multiple TES systems were to be considered, the high-temperature potential of direct electrification could be combined with sensible heat storage that comes at a lower cost than latent heat storage [26]. The option for cheaper TES capacity might lead to higher ElB capacities.

5.5. Conclusions and recommendations for future work

This study presented an analysis of the influence of energy prices on the electrification of industrial utility systems for processes with highly variable energy demand. To this end, energy price profiles with differing average prices and variances and technology cost scenarios were explored. The analyses were carried out for a paper mill in the Netherlands with an existing utility system comprising a CHP and a connection to the national power grid of 30 MW.
The results show that under the assumed technical and economic conditions (presented in Tables 5.3, 5.4 and 5.5), electrification reduces the total annual cost by between 11 and 52 per cent. The model added heat pumps and/or electric boilers and thermal energy storage to the existing utility system; batteries and hydrogen technologies were not selected. A sensitivity analysis, presented and briefly discussed in I.1, shows that the cost for the electrolyser capacity has to decrease by between one and more than three orders of magnitude (depending on the energy price scenario) to become part of the cost-optimal technology portfolio. The difference between the

scenarios is likely due to the number of hours with negative electricity prices, which allow the system to generate revenues because of the losses in hydrogen production. The fact that hydrogen is not picked up by the model can thus be explained by the high upfront cost. Therefore, we conclude that for the explored energy price and technology cost scenarios, hydrogen as an energy carrier is not required for cost-optimal electrification, as long as temperature requirements do not exceed what electric boilers and heat pumps can deliver. Using hydrogen might become more interesting when energy prices are high for extended periods of time, and the required storage capacity would become larger, as hydrogen storage costs are lower than the cost for alternative means of energy storage.

The heat supplied by the CHP is reduced to the minimum possible amount in most scenarios and replaced by power-to-heat and storage technologies. By using a large share of the power generated by the CHP to run the power-to-heat technologies, the amount of power sold to the grid is reduced compared to the reference case without power-to-heat and storage technologies.

Heat pumps are sized based on the process's heat demand duration curve, the minimal load of the CHP and the mean energy price. High and stable energy prices lead to the largest installed heat pump capacities. Lower energy prices limit the profitability of the investment-intensive heat pump and result in smaller capacities. The impact of the relative technology cost of heat pumps on their size increases with the variance of energy prices because the heat pump competes with the electric boiler and thermal energy storage, which have a lower cost and are, therefore, the cheaper peak technology.

The size of the electric boiler is mainly defined by the variance of electricity prices and is limited by the size of the grid connection and the thermal energy storage capacity. The operation of all components is a function of the electricity-to-gas price ratio and the absolute electricity price.

It is recommended to further study utility system electrification. The presented model can serve as a basis for future research, which should explore valuing flexibility by a) assessing different energy markets (e.g., imbalance markets) and b) providing grid services. Moreover, including uncertainty in the analysis would add further understanding of optimal electrification strategies for industries with fluctuating energy demand.

List of Abbreviations

Bat	Battery
CaPex	Capital expenditure
CHP	Combined heat and power plant
CO_2	Carbon Dioxide
COP	Coefficient of performance
EGR	Electricity-to-gas price ratio
ElB	Electric boiler
EU ETS	EU Emissions Trading System
GB	Gas boiler
GHG	Greenhouse gases
GT	Gas turbine
H2	Hydrogen
H2B	Hydrogen boiler
H2E	Electrolyzer
H2S	Hydrogen storage tank
HMHV	High Mean High Variance
HMLV	High Mean Low Variance
HP	Heat pump
HRSG	Heat recovery steam generator
LMHV	Low Mean High Variance
LMLV	Low Mean Low Variance
NG	Natural gas
OpEx	Operating expense
PtH	Power-to-heat
TAC	Total Annual Cost
TC	Technology Cost
TES	Thermal energy storage
TTF	Title Transfer Facility

Nomenclature

Symbol	Explanation	Unit
Time-dependent variables (per time step)		
$H_{\text{CHP,out}}(t)$	Heat output from the Combined heat and power unit	MW
$H_{\text{HP,out}}(t)$	Heat output from the heat pump	MW
$H_{\text{HP,out}}(t)$	Heat produced by the Combined heat and power unit	MW
$NG_{\text{in}}(t)$	quantity of natural gas consumption	MW
$NG_{\text{GT,in}}(t)$	Natural gas input to the gas turbine	MW
$NG_{\text{GB,in}}(t)$	Natural gas input to the gas boiler	MW
$P_{\text{gr,i}}(t)$	Power from the electricity grid to technology i	MW
$P_{\text{i,gr}}(t)$	Power from technology i to the electricity grid	MW
$P_{\text{gr,process}}(t)$	Power from the electricity grid to the process	MW
$P_{\text{GT,gr}}(t)$	Power from the gas turbine to the electricity grid	MW
$P_{\text{GT,process}}(t)$	Power from the gas turbine to the process	MW
$P_{\text{GT,bat}}(t)$	Power from the gas turbine to the battery	MW
$P_{\text{HP,in}}(t)$	Power flow to the heat pump	MW
Sizing variables		
s_{i}	size of technology i	MW or MWh
Time-dependent parameters		
$\text{p}_{\text{el,grid}}(t)$	Electricity price at time t	Eur/MWh
$\text{p}_{\text{NG}}(t)$	Natural gas price at time t	Eur/MWh
$H_{\text{dem}}(t)$	heat demand of the process at time t	MW
$P_{\text{dem}}(t)$	power demand of the process at time t	MW
Constants		
AF_{i}	Annualization factor of technology i	-
c_i	Capital cost of component i	Eur/unit
$\text{COP}_{\text{ideal}}$	Carnot Coefficient of Performance	-
$\text{H}_{\text{dem,max}}$	Maximal heat demand	MW
Inf_{i}	Installation or Lang factor of technology i	-
LT_i	Lifetime of component i	years
r	Discount rate	%
T_{sink}	Temperature of the heat sink of the heat pump	K
T_{source}	Temperature of the heat source of the heat pump	K
Δt	Time step duration	h
η	efficiency	-
$\eta_{\text{i,th}}$	Thermal efficiency of technology i	-
$\eta_{\text{i,el}}$	Electric efficiency of technology i	-

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Addendum

Tables 5.15 to 5.18 were not included in the published version of this Chapter. Since the data presented in the tables is relevant for the answer to the research questions, they are presented as an Addendum to this Chapter.

Table 5.15.: Total annual cost (TAC), savings in TAC compared to the reference system, scope 1 CO_2 emissions, and scope 1 CO_2 emission reduction in the energy price scenarios with low mean and variance when the minimal load constraint of the CHP is removed from the model.

EGR	System	TC scenario	TAC [Million euro]	TAC savings [%]	scope 1 CO_2 emissions [kiloton]	CO_2 emission savings [%]
1.6	Ref.	-	5.9	-	39.0	-
	New	HighHP-LowRest	3.6	39.0	1.9	95.1
	New	LowHP-HighRest	3.5	40.7	0.7	98.1
1	Ref.	-	8.1	-	39.0	-
	New	HighHP-LowRest	3.7	24.7	0.2	99.4
	New	LowHP-HighRest	3.6	24.7	0.1	99.8

Table 5.16.: Total annual cost (TAC), savings in TAC compared to the reference system, scope 1 CO_2 emissions, and scope 1 CO_2 emission reduction in the energy price scenarios with low mean and high variance when the minimal load constraint of the CHP is removed from the model.

EGR	System	TC scenario	TAC [Million euro]	TAC savings [%]	scope 1 CO_2 emissions [kiloton]	CO_2 emission savings [%]
1.6	Ref.	-	5.4	-	41.4	-
	New	HighHP-LowRest	1.1	79.6	13.0	68.6
	New	LowHP-HighRest	1.7	68.5	14.0	66.2
1	Ref.	-	7.7	-	40.2	-
	New	HighHP-LowRest	1.6	79.2	4.9	87.8
	New	LowHP-HighRest	2.2	71.4	5.6	86.1

Table 5.17.: Total annual cost (TAC), savings in TAC compared to the reference system, scope 1 CO_2 emissions, and scope 1 CO_2 emission reduction in the energy price scenarios with high mean and variance when the minimal load constraint of the CHP is removed from the model.

EGR	System	TC scenario	TAC [Million euro]	TAC savings [%]	scope 1 CO_2 emissions [kiloton]	CO_2 emission savings [%]
1.6	Ref.	-	11.8	-	42.2	-
	New	HighHP-LowRest	8.3	29.7	10.5	75.1
	New	LowHP-HighRest	7.8	33.9	5.1	87.8
1	Ref.	-	19.4	-	39.4	-
	New	HighHP-LowRest	8.8	54.6	0.2	99.5
	New	LowHP-HighRest	8.1	58.2	0.2	99.5

Table 5.18.: Total annual cost (TAC), savings in TAC compared to the reference system, scope 1 CO_2 emissions, and scope 1 CO_2 emission reduction in the energy price scenarios with high mean and low variance when the minimal load constraint of the CHP is removed from the model.

EGR	System	TC scenario	TAC [Million euro]	TAC savings [%]	scope 1 CO_2 emissions [kiloton]	CO_2 emission savings [%]
1.6	Ref.	-	12.0	-	40.4	-
	New	HighHP-LowRest	9.1	24.1	0.9	97.7
	New	LowHP-HighRest	8.2	84.5	0.6	98.5
1	Ref.	-	19.4	-	39.0	-
	New	HighHP-LowRest	9.2	52.8	0.0	100.0
	New	LowHP-HighRest	8.2	57.7	0.0	100.0

6
Conclusion

This thesis aimed to explore the conditions for mitigating the impacts of intermittency in the chemical industry, specifically by electrifying existing utility systems. It started with identifying benefits, limitations, and requirements for exploiting flexibility in the chemical industry by conducting a literature review and stakeholder interviews in Chapter 2. Chapter 3 explored the potential for electrifying utility systems in existing chemical plants using a utility system model. Five chemical processes served as case studies, and the model was run for six (individual) historical energy price years. In addition, the sensitivity to the grid connection capacity was tested. Chapter 4 studied the use of heat pumps for utility system integration. Since heat pumps can be added to the utility systems either as a standalone or as an integrated heat pump, to increase their COP, the chapter investigated which 'type' of heat pump leads to the highest savings in total annual cost. It was investigated how the result changed when energy prices decreased in average and increased in variance. Finally, Chapter 5 analysed the impact of energy prices on cost-optimal technology portfolios when electric boilers and heat pumps are available for utility system electrification.

This chapter presents the conclusions of this thesis. It starts with answering the research questions presented in Chapter 1, before discussing the overarching conclusions and their implications in sections 6.1 and 6.2, respectively. Limitations of the chosen methodology and scope are discussed in section 6.3. Section 6.4 concludes this chapter and the thesis with recommendations for future research.

6.1. Research outcomes

This section presents the research outcomes by answering the questions that guided the research.

6.1.1. Research question 1

What requirements and limitations should be considered to implement flexibility in the chemical industry?

Chapter 2 addressed this question by studying peer-reviewed and grey literature that discussed flexible chemical production as a measure for mitigating the impact of intermittency in power generation. The literature review was complemented with a series of stakeholder interviews, which contributed several requirements and limitations that had not been mentioned in the literature. Technical, economic, organisational, and regulatory requirements and limitations were identified.

Examples of technical requirements are sufficient grid capacity, the need to vary the electrical load within the specified time, and the availability of excess capacity for a potential ramp-up of production in times of excess power. Technical limitations of flexible process operation include potential safety risks, long start-up times of processes, and the complexity of implementation in general.
There has to be a business case for flexibility, but there are a number of economic limitations. Typical limitations are potentially high investment costs, economic losses due to relinquished production, potential damage to the equipment, and a potential decrease in product quality. Moreover, the financial compensation is low, and the uncertainty inherent to energy markets requires knowledge on how to cope with market uncertainty.
Organisational requirements are diverse, and include cross-sectoral knowledge, refined planning capabilities, and matching time horizons for planning between the chemical plant and the grid operators. Markets for flexibility have to be accessible, and tariff structures must be attractive for the chemical industry to participate in grid-balancing services. Examples of organisational limitations include delivery obligations of chemical plants, concerns about confidentiality, and security of the IT connection to the grid operator. Moreover, the awareness of opportunities of Demand Response within the chemical industry is low, which might be a reason why flexibility is barely mentioned in energy transition roadmaps from chemical companies, as shown in Figure 6.1.
Regulatory limitations highlighted by stakeholders are the required minimum power bid size and the installation of qualified metering equipment.

The chapter shows the complexity of flexibility in the chemical industry and the need to explore potential solutions. Note that while the chapter points out limitations at various levels, the thesis will focus on the techno-economic limitations.

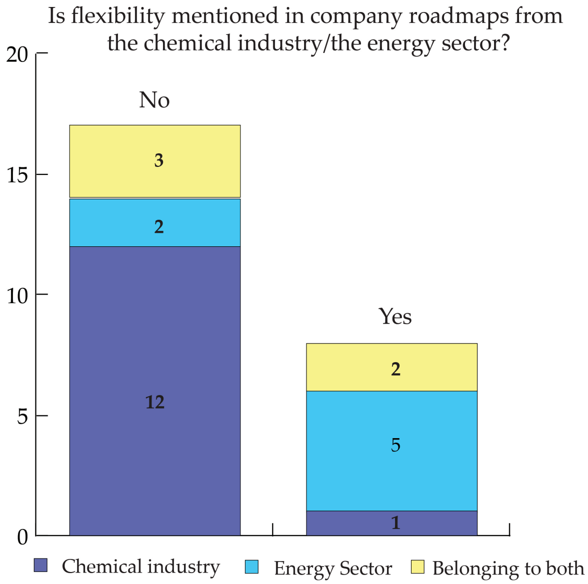

Figure 6.1.: Consideration of flexibility in companies' sustainability roadmaps, and company domains. Figure originally shown in Chapter 2.

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6.1.2. Research question 2

To what extent and under which conditions can flexible utility systems enhance the electrification of chemical plants?

Next to flexible process operation, increasing the flexibility of existing utility systems by installing power-to-heat (PtH) and storage technologies can be a measure to mitigate the impact of an intermittent power supply on chemical plants. To answer research question 2, Chapters 3 to 5 presented cost-optimally electrified utility systems for a range of conditions, including energy prices, technology cost, the available grid connection capacity, and the flexibility of fossil-fuel-based technologies [1].

In Chapter 3, the extent to which electrification can be cost-optimal was explored using historical energy price data and five existing chemical plants as case studies. The results show that partial electrification, and hence, an increase in the flexibility to choose between electricity and natural gas, can be cost-optimal under two conditions. 1) the electricity-to-gas price ratio is approximately 2, and 2) the number of hours during which it is cheaper to use electricity than natural gas[2] (referred to as 'hsE<NG' in the remainder of this chapter) is greater than 500 hours for plants with existing CHPs. For plants with existing natural gas boiler, the hsE<NG has to be greater than 600 hours. These findings do not change for the explored values of grid connection capacity, technology costs, and minimal load of the CHP or gas boiler.

[1] represented by their minimal load

[2] including the costs of the required CO_2 emission allowances

Additional flexibility in the form of energy storage is added to the utility system when the hsE<NG doubles compared to the hsE<NG in years for which no energy storage is installed (while the electricity-to-gas price ratio remains similar). The results of the sensitivity analysis on technology cost show that the model installs energy storage for those years that have a lower hsE<NG, when the investment required for thermal energy storage decreases.

In Chapter 5, a heat pump was added to the technology options the model could choose from. The explored energy price scenarios were more favourable for electrification than the historical price data (the electricity-to-gas price ratio was assumed to be lower) to assess utility system electrification in a scenario with decreased electricity prices and increased natural gas and CO_2 emission allowance prices. The resulting utility systems show that under these conditions, installing a heat pump leads to cost savings even in an energy price scenario with only 100 hsE<NG. In this scenario, the average electricity price is twice, and the natural gas price is three times as high as in a historical price year, while having a similar hsE<NG as in Chapter 3. The explored technology cost scenarios have little impact on the potential for cost-optimal electrification.

The results of both chapters show that the conditions for electrification cannot be described as a set of fixed values for, e.g., the electricity-to-gas price ratio. Instead, they are a combination of the following parameters.

- The hsE<NG (number of hours during which using electricity is cheaper than using natural gas),
- the conversion efficiency of the PtH technology,
- the conversion efficiency of the existing fossil fuel-based technologies,
- average energy and CO_2 emission allowance prices, and
- the electricity-to-gas price ratio[3].

The extent of electrification, measured as the resulting reduction of natural gas consumption that is achieved, ranges from 5% when electric boilers are installed to 24% when energy storage and excess electric boiler capacity are added, assuming historical energy price data in Chapter 3. When the flexibility of the existing CHP and gas boiler is increased in the model, CO_2 emissions are reduced by up to 31% (because in the model, the flexibility of the fossil fuel-based technology determines the minimum possible NG consumption). The impact of the CHPs' or gas boilers' flexibility on the potential natural gas consumption reduction is also clearly visible in the results in Chapter 5. There, the natural gas consumption reduction of the electrified utility systems does not exceed 50% even in energy price scenarios in which using electricity is cheaper than using natural gas up to 94% of the time. As shown in the Addendum to Chapter 5, the cost and emission savings are much higher when the minimal load constraint is removed from the model.

[3] The yearly average

6.1.3. Research question 3

How do changing conditions affect cost-optimal technology portfolios of electrified utility systems for chemical plants?

Comparing the technology portfolios of cost-optimal systems presented in Chapters 3 to 5 allows to assess the impact of changing energy prices, technology costs, and conversion efficiencies on the technology portfolios.

Chapter 3 shows that with an increasing hsE<NG, the model installs electric boilers first. Note that heat pumps were not included in the model used in this chapter. When, due to a higher price variance, the hsE<NG doubles compared to the hsE<NG that leads to utility systems with electric boilers, thermal energy storage is added. When mean prices increase about 2.5-fold, the model installs batteries. Under the conditions explored in the chapter, the electricity-to-gas price ratio does not affect the technology portfolio, provided that electrification is cost-optimal.
Changes to the technology costs of batteries and thermal energy storage lead to differences in their sizing, but do not affect the model's choice of installed technologies. Electrolysers, hydrogen boilers and/or storage are not part of the cost-optimal technology portfolios, unless the technology cost of the electrolyser decreases by about an order of magnitude.
If installed, the electric boiler and thermal energy storage capacities increase with increasing grid connection capacity, while the battery capacity remains unchanged.

If heat pumps are included in the utility system model, as in Chapter 5, technology portfolios change. Figure 6.2 shows that the model prefers to install heat pumps and small thermal energy storage capacities over electric boilers when average energy prices are high (as in the scenarios shown in the right half of the Figure). However, electric boilers combined with large thermal energy storage capacities are the preferred technology choice when energy prices are low and variable (as shown for the scenarios in the top left of the Figure).
The results confirm that the technology cost has an impact on the installed capacities, but affects the technology choices the model makes much less (only in a scenario with low and stable energy prices, as shown in the bottom left of Figure 6.2). The results also confirm that while the electricity-to-gas price ratio is important to determine whether or not electrification is cost-optimal, it has a limited impact on the technology portfolio. It is important to note that the process studied in Chapter 5 has a variable heat demand. This explains that thermal energy storage is installed even when energy prices are stable.

Concerning the choice of the level of integration of the heat pump with the process, Chapter 4 analysed the extent to which a more complex heat pump integration resulting in a higher COP of the heat pump led to lower costs of the utility system. The results in Chapter 4 show that only low and medium levels of integration are worth the additional investment under the conditions assumed in the study. Price mean and variance have little impact on this conclusion. Whether or not existing fossil fuel-based technologies can be used for heat generation in the model does not

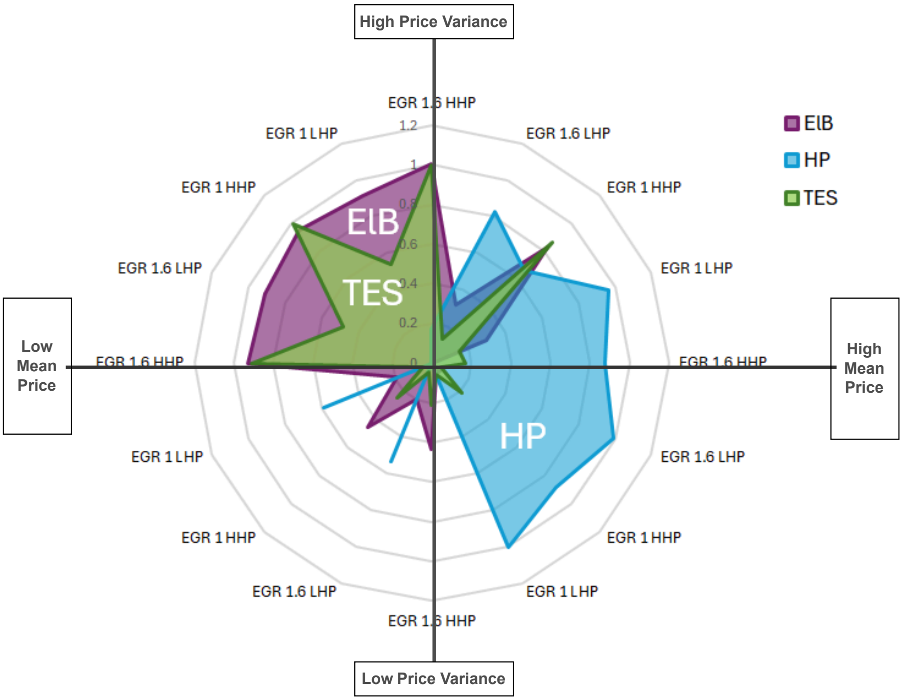

Figure 6.2.: Cost-optimal technology portfolios for different energy price and technology cost scenarios. 'EGR' is the energy-to-gas-price ratio, 'HHP' refers to a technology cost scenario with a high, and 'LHP' with a low heat pump cost. 'ElB' stands for electric boiler, 'TES' for thermal energy storage, and 'HP' for heat pump. Figure originally shown in Chapter 5.

change this finding, either. Thermal energy storage capacity is only installed in the fully-electrified utility system, and only when energy price fluctuations increase.

6.2. Overarching conclusions and implications of the research outcomes

The aim of this thesis was to explore the conditions for handling intermittency in the chemical industry by exploiting flexibility in chemical plants, specifically through electrifying existing utility systems. The results show that (partial) electrification of utility systems can lead to cost savings for industrial plants and allow for the synthesis of the following conditions.

A prerequisite is that industries have sufficient grid connection capacity. This implies that industries need to assess the extent to which their existing connection to the grid allows electrification. Note that, in this thesis, it was assumed that fossil-fuel-based technologies were already installed and could continue to be used in most cases.

Energy prices determine the potential for cost-optimal electrification and the required technology portfolios. However, there is no single indicator which determines the potential and cost-optimal technology portfolio. As described in Section 6.1.2, important indicators include the number of hours during which using electricity is cheaper than using natural gas (hsE<NG), the type of PtH technology that is available to the model, and the average electricity-to-gas price ratio in a year. The hsE<NG is found to be a good indicator for the potential for cost-optimal electrification when heat pumps are not included in the model, and the electricity-to-gas-price-ratio is between 1.6 and 2.2. Under the conditions assessed in Chapter 3, for example, electrification is cost-optimal if the hsE<NG is greater than 600. This shows that electrification of existing utility systems can be cost-optimal even when electricity is cheaper than natural gas for only 7% of the time.
Electrification is shown to be cost-optimal in all cases, independent of the hsE<NG, when the electricity-to-gas-price-ratio decreases to between 1 and 1.6, and heat pumps are included in the model. The bespoken conditions imply that the potential for cost-optimal electrification increases with increasing natural gas and CO_2 emission allowance prices, decreasing electricity prices, and with an increase in price volatility.[4]

6

Which PtH technology is ultimately the best choice for a company is uncertain and depends on the development of energy prices.
The model installs heat pumps instead of electric boilers when energy prices are high, while electric boilers combined with (mostly thermal) energy storage are installed when the price variance is high and requires excess capacity for additional flexibility in the utility system. This implies that companies should evaluate the extent to which they will be exposed to, or seek to benefit from, price fluctuations before deciding whether to invest in heat pumps or electric boilers.
The development of energy prices is less critical for thermal energy storage when the heat demand is variable, as thermal energy storage is installed by the model under all energy price and technology cost conditions. When heat demand is constant, however, thermal energy storage is installed only when price fluctuations are high, and never in combination with heat pumps, unless the utility system is forced to be fully electrified under highly variable energy prices. This implies that thermal energy storage is not needed when heat demand and energy prices are stable. Note that batteries are not installed, either.

The extent to which electrification reduces CO_2 emissions depends on the energy prices, the conversion efficiency of the installed PtH technology, and the flexibility of the fossil fuel-based legacy technology.
The emission reduction that is observed for historical energy price data in Chapter 3 does not exceed 24%. This implies that, if energy prices were to be similar to

[4] Given that price peaks and valleys do not occur simultaneously in natural gas and electricity prices.

the historical data, additional incentives or natural gas reduction regulations are needed to achieve higher levels of emission reduction. Still, electrification can be a step towards introducing an alternative for the industry so that later on, when tighter emission regulations are introduced, companies have already installed PtH and storage capacities and gained experience with them. The emission reduction values reported in this thesis also imply that the operational strategy of fossil fuel-based technologies has a significant impact on the emission reduction potential.

6.3. Limitations of the research

While important insights for handling intermittency in the chemical industry were gained through this dissertation, it exhibits a number of limitations.

The modelling choices have the following limitations.
Deterministic modelling has the inherent limitation of perfect foresight. While this was considered an acceptable limitation in the exploratory research conducted in this thesis, it might not allow for capturing uncertainties with a sufficient level of detail for companies to use the model as is for their utility system design (or operation). However, the model can help industries in deciding which technologies to install and show the impacts of, e.g., energy price developments, on the performance of their potential utility system design.
The choice was made to represent the intermittency of renewable energy sources in the model by using variable electricity prices. This assumes that electricity is always available. An alternative approach could have been to assess the option to install renewable power plants onsite. This might have resulted in technology portfolios with more storage capacity, if economically feasible, or a higher natural gas consumption. Concerning the electricity prices, prices were assumed to be those from the day-ahead market, as they are known to the buyer one day in advance, which facilitates scheduling. However, plants could use their utility system to participate in shorter-term markets, too, to increase the potential savings or create additional revenues. On the other hand, long-term contracts could be used for hedging. Then, intermittency would not be an issue (or opportunity), and the electricity-to-gas price ratio would determine the potential for cost-optimal electrification.

The chosen case studies exhibit the following limitations.
First, very-high temperature demand was supplied from burning off-gases from the processes and therefore not included in the heat demand. If very-high temperature demand were to be supplied by using electricity, additional PtH technologies might be required, as electric boilers can supply steam only up to 500°C [4].
Second, chemical plants were considered individually, even though they are often part of a larger chemical cluster, like the plants from the Port of Rotterdam studied in Chapter 3. Potential obligations to deliver heat or power to other plants in the cluster might impose a constraint on the flexibility of utility systems. However, potential revenues from selling heat or power could enable the installation of PtH and storage units. If utility systems for entire clusters were to be considered, economies of scale

might lead to lower technology costs for PtH and storage units, which could be favourable for the electrification of the utility system.
Last, future processes have not been included in the case studies. As discussed in Chapter 1, utility system electrification can reduce up to one-third of the emissions of the chemical industry. Therefore, processes need to be developed which use alternative feedstocks to reduce the industry's emissions further. These processes might have different utility demands than the ones studied, for example, a much higher demand for electricity than heat. Investing in PtH technologies without considering potential changes to the core process might lead to utility systems not fit for purpose when new processes are installed. In the worst case, this could challenge decisions to invest in new, low-emission processes and hinder progress toward further emission reductions.

6.4. Recommendations for future research

The models used in Chapters 3 to 5 of this thesis have been built to conduct exploratory studies, and the uncertainty of different parameters has been addressed in the research by using scenario analysis. For exploring the robustness of the proposed utility systems to a wider range of uncertain conditions, to, for example, find potential 'low-regret' technology portfolios, stochastic programming is recommended. For increasing the level of detail in which the technologies are represented in the model, it is recommended to include the option for complete shutdowns of the CHPs or gas boilers, while ensuring that the impact of cold-starts on the lifetime of the equipment is accounted for in the model. A third recommendation concerning the modelling is to add CO_2 emission reduction as a second optimisation objective, as it would add further insights into the potential tradeoff between cost and emission reduction. This could help companies in their decision-making and policymakers in designing potential subsidies.
Concerning future case studies, it is recommended to study future processes which use non-fossil feedstocks. As discussed earlier, these processes might have a utility demand different from the processes studied in this thesis. Therefore, different technology portfolios might be required. Comparing the findings of such a study to the findings from this thesis could address the question of whether or how electrification of utility systems can be a short- and long-term measure for emission reduction in the chemical industry.
This thesis showed that key barriers to exploiting flexibility in the chemical industry were found to be the uncertainty about the business case of flexibility and the limited awareness of the potential benefits of flexibility in the chemical industry. To foster the deployment of flexibility, the uncertainty of the business case should be addressed by investigating potential collaboration schemes (such as special tariffs or grid balancing services) between the power sector and the chemical industry. This could also tackle the low levels of awareness of potential benefits among stakeholders from the chemical industry, as stakeholders from both sectors would need to be engaged in this type of research.
Last but not least, other CO_2 emissions reduction options, for example, carbon capture

and storage (CCS), could be an alternative and/or complement to electrification. To assess which options would lead to a faster reduction of comparable amounts of emissions, it is recommended to study a combination of options, including the use of existing utility systems with CCS under the condition of a low-carbon electricity supply.

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A

Appendix A: Sustainability roadmaps review in Chapter 2

A

Table A.1 provides a list of company roadmaps that are included in the analysis shown in Figure 2.1 and described in Section 3 of Chapter 2. Some roadmaps are joint roadmaps from several companies, such as the one published by Gasunie and Tennet, or by Netbeheer Nederland.

Table A.1.: Supplementary information to Figure 1 in section 3: Consideration of flexibility in companies' roadmaps towards sustainability. Roadmaps included in the analysis and respective domain. Some companies are involved in more than one roadmap

Roadmap from	Chemical industry	Energy sector
Gasunie & Tennet		•
Tennet		•
Eneco		•
RWE		•
Uniper		•
Nobian		•
BP	•	•
Netbeheer Nederland		•
Engie		•
Total	•	•
DOW	•	
Huntsman	•	
Eastman	•	
BASF	•	
ExxonMobil	•	•
SABIC	•	
Dupont	•	
LyondellBasell	•	
Shell	•	•
Yara	•	
Avantium	•	
Air Liquide	•	
Shin-Etsu Chemical Co. Ltd.	•	
Air Products and Chemicals Inc.	•	
Vattenfall		•

B

Appendix B: Questions and notes of the stakeholder interviews in Chapter 2

The questions asked during the stakeholder interviews and notes of their answers are available in the 4TU Research Data repository belonging to this thesis (doi: 10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb). The repository is accessible online using this link: https://doi.org/10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb.v1.

C

Appendix C: Literature review belonging to Chapter 3

Many studies have presented models which design utility systems for chemical processes (see Table C.1). Among those, some focus on utility systems for the petrochemical industry [1–8]. Table C.1 shows that most studies focus on reducing CO_2 emissions. However, only some [6, 9, 10] address the electrification of utility systems as CO_2 emission reduction strategy. For instance, Bauer et al. [10] model a utility system consisting of a CHP for baseload energy generation with an additional electric boiler. Options to replace the CHP for baseline energy supply are qualitatively discussed but not quantitatively studied. Hofmann et al. [9] study a flexible utility system for batch production consisting of an electric boiler, a biomass boiler, a thermal energy storage unit (TES) and a heat exchanger network. The study considers that flexibility is required due to variations in production but assumes no variation in prices for electricity and gas. Only one paper [6] was found that considers fully electrified scenarios: The author presents two case studies with electrified core processes and utility systems. While the paper proposes design strategies for the long-term goal of completely electrifying chemical production, solutions to reduce emissions in the short term are not considered. The study also does not include energy storage. According to Hofmann et al., energy storage might benefit a fully electrified system [9]. The papers just discussed are the only literature found on the electrification of utility systems for chemical plants as a measure to decrease CO_2 emissions in the chemical sector.

In the literature on utility systems for other industrial sectors, there is more attention on electricity-based technologies such as electric boilers, batteries, and heat pumps. Atabay presents a model for capacity-expansion planning which allows energy export and considers CHPs, gas boilers, immersive heaters, batteries and TES [11]. The study focuses on a green field and shows that batteries are not invested in with the assumed technology cost. In another study, Baumgaertner et al. consider a wide range of technological options (among others, electric boilers, heat pumps, compression chillers, batteries and TES) for a pharmaceutical facility [12]. Unlike Atabay, Baumgaertner et al. do consider time-dependent electricity prices, but gas prices are assumed to be constant. The technology portfolio in Baumgaertner et al. was extended to include pumped heat storage (a power-to-heat-to-power system) in a study by Reinert et al. [13]. Neither Baumgaertner et al. nor Reinert et al. include hydrogen in their scope.

Two studies on utility systems for other industries consider using hydrogen as an energy carrier. In the first study, Kostelack et al. analyse four utility system concepts based on hydrogen produced with power from a PV plant [14]. They show that hydrogen can reduce operational costs if electricity prices are lower than natural gas prices and that hydrogen reduces risks due to decreased exposure to energy price increases. However, capital expenditures for hydrogen technologies are neglected, and the study assumes some flexibility in the processes' energy demand, which is unlikely to be available in the chemical industry. The second study that includes hydrogen is presented by Fleschutz et al. [15]. In their utility system model, they consider a natural gas-fuelled CHP and boiler, a hydrogen-based system consisting of electrolyser, hydrogen storage, and fuel cell and a heat pump, a solar power plant, a wind turbine and storage units for electricity and thermal energy, including battery electric vehicles. The study shows that the system's flexibility (provided by the storage units and the coupling of the energy system and the mobility demands) leads to significant cost savings for carbon emission-free utility systems. Only some of the presented systems are cost-competitive with their reference system. However, varying prices for purchasing natural gas and ETS emission allowances are not considered, which could lead to increased costs with the inflexible reference system.

To the authors' knowledge, no study has considered using a combination of electric boilers, the generation and use of hydrogen, and storage units to electrify fuel-based utility systems for chemical plants. Therefore, it is still unclear which combinations of those technologies can best enable electrification and how electrified systems would perform in terms of cost and CO_2 emissions compared to utility systems based on fossil sources.

Table C.1.: Literature on the design of utility systems for the chemical industry

Study	Case study	CO_2 emission reduction strategy and/or implemented technologies	Fully decarbonised?
Mitra et al. (2013) [16]	Chemical park	None	No
Luo et al. (2014) [1]	Petrochemical complex	Optimising exergy efficiency	No
Han and Lee (2014) [2]	Petrochemical complex	Increasing efficiency & CCS	No
Klasing et al. (2018) [17]	No specific process	Electric boilers and heaters and TES	No
Leenders et al. (2019) [18]	No specific process	None	No
Hofmann et al. (2019) [9]	No specific process	Heat exchanger-network, biomass boiler, electric boiler, and TES	No
Zhang and You (2019) [19]	No specific process	None	No
Quian et al. (2021) [3]	Petrochemical complex	Wind and PV for power supply, TES and electric chiller	No
Wang et al. (2021) [20]	Refinery	Wind and PV integration, electrolyser and energy storage	No
Bauer et al. (2022) [10]	No specific process	Electric boiler	No
Ghiasi et al. (2022) [4]	Petrochemical complex	Heat exchanger network	No
Hwangbo et al. (2022) [5]	Petrochemical clusters	Wind, PV and CCS	No
Kim (2022) [21]	Refinery	Full electrification	Yes
Kim (2022) [6]	Methyl acetate and ethylbenzene	Full electrification	Yes
Wang et al. (2022) [22]	Chemical plant	Wind, solar thermal energy, TES	No
Su et al. (2023) [8]	Petrochemical sites	Power from renewable sources, biomass fuels, CCS	No
Li and Zhao (2023) [7]	Ethylene plant	None	No
Jimenez-Romero et al. (2023) [23]	Chemical plant	None	No

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D

Appendix D: Modelling code belonging to Chapter 3

Note: The code is also available online on GitHub, via `https://github.com/SvenjaBie/ElectrUtilEtyhlInd_Open`.

D.1. Nomenclature of parameters and variables

Symbol	Explanation	Unit
Time-dependent variables		
$P_{\mathrm{gr,ElB}}(t)$	Grid power to the electric boiler	MW
$P_{\mathrm{gr,plant}}(t)$	Grid power to the plant	MW
$P_{\mathrm{gr,bat}}(t)$	Grid power to the battery	MW
$P_{\mathrm{gr,H2E}}(t)$	Grid power to the electrolyser	MW
$P_{\mathrm{CHP,gr}}(t)$	Power from CHP plant to the grid	MW
$P_{\mathrm{CHP,plant}}(t)$	Power from CHP to the plant	MW
$P_{\mathrm{CHP,bat}}(t)$	Power from CHP to the battery	MW
$P_{\mathrm{bat,plant}}(t)$	Power from battery to the plant	MW
$P_{\mathrm{bat,ElB}}(t)$	Power from battery to the electric boiler	MW
$P_{\mathrm{bat,H2E}}(t)$	Power from battery to the electrolyser	MW
$H_{\mathrm{ElB,plant}}(t)$	Heat generated by electric boiler for the plant	MW
$H_{\mathrm{CHP,plant}}(t)$	Heat generated by the CHP for the plant	MW
$H_{\mathrm{TES,plant}}(t)$	Heat from thermal energy storage to the plant	MW
$H_{\mathrm{H2B,plant}}(t)$	Heat from the hydrogen boiler to the plant	MW
$H_{\mathrm{CHP,TES}}(t)$	Heat from CHP to thermal energy storage	MW
$H_{\mathrm{ElB,TES}}(t)$	Heat from electric boiler to thermal energy storage	MW
$H_{\mathrm{GB,plant}}(t)$	Heat from gas boiler to the plant	MW
$H_{\mathrm{GB,TES}}(t)$	Heat from gas boiler to thermal energy storage	MW
$NG_{\mathrm{in}}(t)$	Natural gas input to the utility system	MW
$H_{2,\mathrm{H2E,H2B}}(t)$	Hydrogen from electrolyser to the boiler	MW
$H_{2,\mathrm{H2E,H2S}}(t)$	Hydrogen from electrolyser to storage	MW
$H_{2,\mathrm{H2S,H2B}}(t)$	Hydrogen from storage to the boiler	MW
$SOE_{\mathrm{bat}}(t)$	State of energy of the battery	MWh
$SOE_{\mathrm{TES}}(t)$	State of energy in the thermal energy storage	MWh
$SOE_{\mathrm{H2S}}(t)$	State of energy in hydrogen storage	kg
$b_1(t)$	Binary variable for battery charging	Binary (0/1)
$b_2(t)$	Binary variable for thermal energy storage charging	Binary (0/1)
$b_3(t)$	Binary variable for hydrogen storage tank	Binary (0/1)
$b_4(t)$	Binary variable for grid connection	Binary (0/1)

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Symbol	**Explanation**	**Unit**
Sizing variables		
s_{ElB}	Electric boiler size	MW_{th}
s_{H2E}	Electrolyser size	MW_{th}
s_{H2B}	Hydrogen boiler size	MW_{th}
s_{TES}	Thermal energy storage size	MWh
s_{H2S}	Hydrogen storage size	MWh
s_{bat}	Battery size	MWh
Time-dependent parameters		
$\mathrm{p}_{\mathrm{el,grid}}(t)$	Electricity price at time t	Eur/MWh
$\mathrm{p}_{\mathrm{NG}}(t)$	Natural gas price at time t	Eur/MWh
$\mathrm{p}_{\mathrm{EUA}}(t)$	CO_2 allowance price at time t	Eur/ton
$H_{\mathrm{dem}}(t)$	(Constant) heat demand of the plant at time t	MW
$P_{\mathrm{dem}}(t)$	(Constant) power demand of the plant at time t	MW
Constants		
s_{CHP}	CHP size	MW
s_{GB}	Gas boiler size	MW
$\mathrm{EF}_{\mathrm{NG}}$	Emission factor for natural gas	kg CO_2/MWh
r_{disc}	Discount rate	%
Δt	Time step duration	h
$\eta_{\mathrm{CHP,el}}$	CHP electric efficiency	-
$\eta_{\mathrm{CHP,th}}$	CHP thermal efficiency	-
η_{GB}	Gas boiler efficiency	-
η_{ElB}	Electric boiler efficiency	-
η_{H2E}	Hydrogen electrolyser efficiency	-
η_{H2B}	Hydrogen boiler efficiency	-
η_{bat}	Battery charge and discharge efficiency	-
η_{TES}	Thermal energy storage efficiency	-
η_{H2S}	Hydrogen storage efficiency	-
$\mathrm{MinLoadFactor}_{\mathrm{CHP}}$	Minimum load factor for CHP	% of capacity
$\mathrm{MinLoadFactor}_{\mathrm{GP}}$	Minimum load factor for GB	% of capacity
$\mathrm{crate}_{\mathrm{bat}}$	Charge/discharge rate of battery	MW/MWh
$\mathrm{crate}_{\mathrm{TES}}$	Charge/discharge rate of thermal energy storage	MW/MWh
$\mathrm{cap}_{\mathrm{gr}}$	Grid connection capacity	MW
$\mathrm{area}_{\mathrm{available}}$	Available area for system installation	m^2
c_i	Capital cost of component i	Eur/unit
LT_i	Lifetime of component i	years

D.2. Mathematical formulations of the benchmark models

The following equations are used to calculate the performance of the benchmark models.

Objective function

$$min \sum_{t=0}^{t=8000} \mathrm{OpEx}(t), \tag{D.1}$$

where

$$\begin{aligned}\mathrm{OpEx}(t) =& \mathrm{p}_{\mathrm{el,grid}}(t) \cdot \Delta t \cdot \left(P_{\mathrm{gr,\ plant}}(t) - P_{\mathrm{CHP,\ gr}}(t)\right)\\ &+ NG_{\mathrm{in}}(t) \cdot \Delta t \cdot \left(\mathrm{p}_{\mathrm{NG}}(t) + \mathrm{p}_{\mathrm{EUA}}(t) \cdot \mathrm{EF}_{\mathrm{NG}}\right)\end{aligned}$$

if the benchmark utility system consists of a CHP and

$$\begin{aligned}\mathrm{OpEx}(t) =& \mathrm{p}_{\mathrm{el,grid}}(t) \cdot \Delta t \cdot P_{\mathrm{gr,\ plant}}(t)\\ &+ NG_{\mathrm{in}}(t) \cdot \Delta t \cdot \left(\mathrm{p}_{\mathrm{NG}}(t) + \mathrm{p}_{\mathrm{EUA}}(t) \cdot \mathrm{EF}_{\mathrm{NG}}\right)\end{aligned}$$

if the benchmark utility system consists of a gas boiler.

Energy balance equality constraints
Heat balance:

$$H_{\mathrm{dem}} = H_{\mathrm{CHP,plant}}(t), \tag{D.2}$$

or

$$H_{\mathrm{dem}} = H_{\mathrm{GB,plant}}(t), \tag{D.3}$$

Power balance:

$$P_{\mathrm{dem}} = P_{\mathrm{gr,plant}}(t) + P_{\mathrm{CHP,plant}}(t) \tag{D.4}$$

or

$$P_{\mathrm{dem}} = P_{\mathrm{gr,plant}}(t) \tag{D.5}$$

CHP constraints
Power generation constraint:

$$NG_{\mathrm{in}}(t) = \frac{P_{\mathrm{CHP,plant}}(t) + P_{\mathrm{CHP,excess}}(t) + P_{\mathrm{CHP,gr}}(t)}{\eta_{\mathrm{CHP,el}}} \tag{D.6}$$

Heat generation constraint:

$$NG_{\mathrm{in}}(t) = \frac{H_{\mathrm{CHP,plant}}(t) + H_{\mathrm{CHP,excess}}(t)}{\eta_{\mathrm{CHP,th}}} \tag{D.7}$$

Maximum heat generation:

$$H_{\text{CHP,plant}}(t) + H_{\text{CHP,excess}}(t) \leq s_{\text{CHP}} \cdot \eta_{\text{CHP,th}} \tag{D.8}$$

Minimum heat generation:

$$H_{\text{CHP,plant}}(t) + H_{\text{CHP,excess}}(t) \geq s_{\text{CHP}} \cdot \eta_{\text{CHP,th}} \cdot \text{MinLoadFactor}_{\text{CHP}} \tag{D.9}$$

Gas boiler constraints
Heat generation constraint:

$$NG_{\text{GB,in}}(t) = \frac{H_{\text{GB,plant}}(t) + H_{\text{GB,excess}}(t)}{\eta_{\text{GB}}} \tag{D.10}$$

Maximum heat generation:

$$H_{\text{GB,plant}}(t) + H_{\text{GB,excess}}(t) \leq s_{\text{GB}} \cdot \eta_{\text{GB}} \tag{D.11}$$

Minimum heat generation:

$$H_{\text{GB,plant}}(t) + H_{\text{GB,excess}}(t) \geq s_{\text{GB}} \cdot \eta_{\text{GB}} \cdot \text{MinLoadFactor}_{\text{GB}} \tag{D.12}$$

Grid connection capacity
Maximum inflow constraint:

$$\text{cap}_{\text{gr}} \cdot b_3(t) \geq P_{\text{gr,plant}}(t) \tag{D.13}$$

Maximum outflow constraint for systems with a CHP:

$$P_{\text{CHP,gr}}(t) \leq \text{cap}_{\text{gr}} \cdot (1 - b_3(t)) \tag{D.14}$$

D.3. Mathematical formulation of the model with an existing CHP

The following equations represent the mathematical formulation of the model for the utility system with an existing CHP.

Objective function

$$min \sum_{t=0}^{t=8000} \mathrm{OpEx}(t) + \mathrm{CaPex}, \tag{D.15}$$

where

$$\begin{aligned}\mathrm{OpEx}(t) =& \mathrm{p}_{\mathrm{el,grid}}(t) \cdot \Delta t \cdot \Big(\\ & P_{\mathrm{gr,\ ElB}}(t) + P_{\mathrm{gr,\ plant}}(t) + P_{\mathrm{gr,\ bat}}(t) + P_{\mathrm{gr,\ H2E}}(t) - P_{\mathrm{CHP,\ gr}}(t)\Big) \\ & + NG_{\mathrm{in}}(t) \cdot \Delta t \cdot \left(\mathrm{p}_{\mathrm{NG}}(t) + \mathrm{p}_{\mathrm{EUA}}(t) \cdot \mathrm{EF}_{\mathrm{NG}}\right)\end{aligned} \tag{D.16}$$

and

$$\mathrm{CaPex} = \sum_{i \in \{\mathrm{bat,ElB,TES,H2E,H2B,H2S}\}} \frac{m_i \cdot c_i \cdot r_{\mathrm{disc}}}{1 - (1 + r_{\mathrm{disc}})^{-\mathrm{lt}_i}} \tag{D.17}$$

Energy balance equality constraints
Heat balance:

$$H_{\mathrm{dem}} = H_{\mathrm{ElB,plant}}(t) + H_{\mathrm{CHP,plant}}(t) + H_{\mathrm{TES,plant}}(t) + H_{\mathrm{H2B,plant}}(t) \tag{D.18}$$

Power balance:

$$P_{\mathrm{dem}} = P_{\mathrm{gr,plant}}(t) + P_{\mathrm{CHP,plant}}(t) + P_{\mathrm{bat,plant}}(t) \tag{D.19}$$

CHP constraints
Power generation constraint:

$$NG_{\mathrm{in}}(t) = \frac{P_{\mathrm{CHP,plant}}(t) + P_{\mathrm{CHP,excess}}(t) + P_{\mathrm{CHP,bat}}(t) + P_{\mathrm{CHP,gr}}(t)}{\eta_{\mathrm{CHP,el}}} \tag{D.20}$$

Heat generation constraint:

$$NG_{\mathrm{in}}(t) = \frac{H_{\mathrm{CHP,plant}}(t) + H_{\mathrm{CHP,TES}}(t) + H_{\mathrm{CHP,excess}}(t)}{\eta_{\mathrm{CHP,th}}} \tag{D.21}$$

Maximum heat generation:

$$H_{\mathrm{CHP,plant}}(t) + H_{\mathrm{CHP,TES}}(t) + H_{\mathrm{CHP,excess}}(t) \leq s_{\mathrm{CHP}} \cdot \eta_{\mathrm{CHP,th}} \quad \text{(D.22)}$$

Minimum heat generation:

$$H_{\mathrm{CHP,plant}}(t) + H_{\mathrm{CHP,TES}}(t) + H_{\mathrm{CHP,excess}}(t) \geq s_{\mathrm{CHP}} \cdot \eta_{\mathrm{CHP,th}} \cdot \mathrm{MinLoadFactor}_{\mathrm{CHP}} \quad \text{(D.23)}$$

D

Electric boiler
Heat generation constraint:

$$H_{\mathrm{ElB,plant}}(t) + H_{\mathrm{ElB,TES}}(t) = \left(P_{\mathrm{gr,ElB}}(t) + P_{\mathrm{bat,ElB}}(t)\right) \cdot \eta_{\mathrm{ElB}} \quad \text{(D.24)}$$

Sizing constraint:

$$H_{\mathrm{ElB,plant}}(t) + H_{\mathrm{ElB,TES}}(t) \leq s_{\mathrm{ElB}} \quad \text{(D.25)}$$

Water electrolyser
Hydrogen production constraint:

$$\left(P_{\mathrm{gr,H2E}}(t) + P_{\mathrm{bat,H2E}}(t)\right) \cdot \eta_{\mathrm{H2E}} = H_{2,\mathrm{H2E,H2B}}(t) + H_{2,\mathrm{H2E,H2S}}(t) \quad \text{(D.26)}$$

Sizing constraint:

$$P_{\mathrm{gr,H2E}}(t) + P_{\mathrm{bat,H2E}}(t) \leq s_{\mathrm{H2E}} \quad \text{(D.27)}$$

Hydrogen boiler
Heat generation constraint:

$$\left(H_{2,\mathrm{H2E,H2B}}(t) + H_{2,\mathrm{H2S,H2B}}(t)\right) \cdot \eta_{\mathrm{H2B}} = H_{\mathrm{H2B,plant}}(t) \quad \text{(D.28)}$$

Sizing constraint:

$$H_{\mathrm{H2B,plant}}(t) \leq s_{\mathrm{H2B}} \quad \text{(D.29)}$$

D

Battery
State of energy:

$$\mathrm{SOE}_{\mathrm{bat}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\mathrm{bat}}(t-1) + \\ \eta_{\mathrm{bat}} \cdot \Delta t \cdot \big(P_{\mathrm{gr,bat}}(t-1) + P_{\mathrm{CHP,bat}}(t-1)\big) - \\ \frac{1}{\eta_{\mathrm{bat}}} \cdot \Delta t \cdot \big(P_{\mathrm{bat,plant}}(t-1) + P_{\mathrm{bat,ElB}}(t-1) + P_{\mathrm{bat,H2E}}(t-1)\big), & \text{otherwise} \end{cases} \tag{D.30}$$

Maximum charge constraint:

$$P_{\mathrm{gr,bat}}(t) + P_{\mathrm{CHP,bat}}(t) \leq \frac{s_{\mathrm{bat}}}{\eta_{\mathrm{bat}}} \cdot \frac{\mathrm{crate}_{\mathrm{bat}}}{\Delta t} \cdot b_1(t) \tag{D.31}$$

Maximum discharge constraint: Discharging for $t = 0$:

$$P_{\mathrm{bat,plant}}(0) + P_{\mathrm{bat,ElB}}(0) + P_{\mathrm{bat,H2E}}(0) = 0 \tag{D.32}$$

Discharging for $t > 0$:

$$P_{\mathrm{bat,plant}}(t) + P_{\mathrm{bat,ElB}}(t) + P_{\mathrm{bat,H2E}}(t) \leq s_{\mathrm{bat}} \cdot \eta_{\mathrm{bat}} \cdot \frac{\mathrm{crate}_{\mathrm{bat}}}{\Delta t} \cdot (1 - b_1(t)) \tag{D.33}$$

Sizing constraint:

$$SOE_{\mathrm{bat}}(t) \leq s_{\mathrm{bat}} \tag{D.34}$$

Thermal energy storage
State of energy (SOE):

$$SOE_{\mathrm{TES}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\mathrm{TES}}(t-1) + \\ \big(H_{\mathrm{CHP,TES}}(t-1) + H_{\mathrm{ElB,TES}}(t-1)\big) \cdot \Delta t - \\ \frac{H_{\mathrm{TES,plant}}(t-1)}{\eta_{\mathrm{TES}}} \cdot \Delta t, & \text{otherwise} \end{cases} \tag{D.35}$$

Maximum charge constraint

$$H_{\mathrm{CHP,TES}}(t) + H_{\mathrm{ElB,TES}}(t) \leq \frac{s_{\mathrm{TES}} \cdot \mathrm{crate}_{\mathrm{TES}}}{\Delta t} \cdot b_2(t) \tag{D.36}$$

Maximum discharge constraint: Discharging for $t = 0$:

$$H_{\mathrm{TES,plant}}(0) = 0 \tag{D.37}$$

Discharging for $t > 0$:

$$H_{\text{TES,plant}}(t) \leq \frac{s_{\text{TES}} \cdot \eta_{\text{TES}} \cdot \text{crate}_{\text{TES}}}{\Delta t} \cdot (1 - b_2(t)) \tag{D.38}$$

Sizing constraint:

$$SOE_{\text{TES}}(t) \leq s_{\text{TES}} \tag{D.39}$$

Hydrogen storage
State of energy:

$$\text{SOE}_{\text{H2S}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\text{H2S}}(t-1) + \left(H_{2,\text{H2E,H2S}}(t-1) - \frac{H_{2,\text{H2S,H2B}}(t-1)}{\eta_{\text{H2S}}}\right) \cdot \Delta t, & \text{otherwise} \end{cases} \tag{D.40}$$

Charge constraint

$$H_{2,\text{H2E,H2S}}(t) \leq s_{\text{H2S}} \cdot b_3(t) \tag{D.41}$$

Discharge constraint: Discharging for $t = 0$:

$$H_{2,\text{H2S,H2B}}(0) = 0 \tag{D.42}$$

Discharging for $t > 0$:

$$H_{2,\text{H2S,H2B}}(t) \leq \frac{s_{\text{H2S}} \cdot \eta_{\text{H2S}}}{\Delta t} \cdot (1 - b_3(t)) \tag{D.43}$$

Sizing constraint:

$$SOE_{\text{H2S}}(t) \leq s_{\text{H2S}} \tag{D.44}$$

Grid connection capacity
Maximum inflow constraint:

$$\text{cap}_{\text{gr}} \cdot b_4(t) \geq P_{\text{gr,plant}}(t) + P_{\text{gr,ElB}}(t) + P_{\text{gr,bat}}(t) + P_{\text{gr,H2E}}(t) \tag{D.45}$$

Maximum outflow constraint:

$$P_{\text{CHP,gr}}(t) \leq \text{cap}_{\text{gr}} \cdot (1 - b_4(t)) \tag{D.46}$$

D.4. Mathematical formulation of the model with an existing gas boiler

The following equations represent the mathematical formulation of the model for the utility system with an existing gas boiler.

Objective function

$$min \sum_{t=0}^{t=8000} \mathrm{OpEx}(t) + \mathrm{CaPex}, \tag{D.47}$$

where

$$\begin{aligned} \mathrm{OpEx}(t) =& \mathrm{p}_{\mathrm{el,grid}}(t) \cdot \Delta t \cdot \Big(\\ & P_{\mathrm{gr,\ ElB}}(t) + P_{\mathrm{gr,\ plant}}(t) + P_{\mathrm{gr,\ bat}}(t) + P_{\mathrm{gr,\ H2E}}(t)\Big) \\ & + NG_{\mathrm{in}}(t) \cdot \Delta t \cdot \left(\mathrm{p}_{\mathrm{NG}}(t) + \mathrm{p}_{\mathrm{EUA}}(t) \cdot \mathrm{EF}_{\mathrm{NG}}\right) \end{aligned} \tag{D.48}$$

and

$$\mathrm{CaPex} = \sum_{i \in \{\mathrm{bat,ElB,TES,H2E,H2B,H2S}\}} \frac{m_i \cdot c_i \cdot r_{\mathrm{disc}}}{1-(1+r_{\mathrm{disc}})^{-\mathrm{lt}_i}} \tag{D.49}$$

Energy balance equality constraints

Heat balance:

$$H_{\mathrm{dem}} = H_{\mathrm{ElB,plant}}(t) + H_{\mathrm{GB,plant}}(t) + H_{\mathrm{TES,plant}}(t) + H_{\mathrm{H2B,plant}}(t) \tag{D.50}$$

Power balance:

$$P_{\mathrm{dem}} = P_{\mathrm{gr,plant}}(t) + P_{\mathrm{bat,plant}}(t) \tag{D.51}$$

Gas boiler constraints

Heat generation constraint:

$$NG_{\mathrm{GB,in}}(t) = \frac{H_{\mathrm{GB,plant}}(t) + H_{\mathrm{GB,TES}}(t) + H_{\mathrm{GB,excess}}(t)}{\eta_{\mathrm{GB}}} \tag{D.52}$$

Maximum heat generation:

$$H_{\mathrm{GB,plant}}(t) + H_{\mathrm{GB,TES}}(t) + H_{\mathrm{GB,excess}}(t) \leq \mathrm{s}_{\mathrm{GB}} \cdot \eta_{\mathrm{GB}} \tag{D.53}$$

Minimum heat generation:

$$H_{\text{GB,plant}}(t) + H_{\text{GB,TES}}(t) + H_{\text{GB,excess}}(t) \geq s_{\text{GB}} \cdot \eta_{\text{GB}} \cdot \text{MinLoadFactor}_{\text{GB}} \tag{D.54}$$

Electric boiler
Same as in D.3.

Water electrolyser
Hydrogen production constraint: Same as in D.3.

Hydrogen boiler
Same as in D.3.

Battery
State of energy:

$$\text{SOE}_{\text{bat}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\text{bat}}(t-1) + & \\ \eta_{\text{bat}} \cdot \Delta t \cdot P_{\text{gr,bat}}(t-1) - & \\ \frac{1}{\eta_{\text{bat}}} \cdot \Delta t \cdot \left(P_{\text{bat,plant}}(t-1) + P_{\text{bat,ElB}}(t-1) + P_{\text{bat,H2E}}(t-1)\right), & \text{otherwise} \end{cases} \tag{D.55}$$

Maximum charge constraint:

$$P_{\text{gr,bat}}(t) \leq \frac{bat_{\text{cap}}}{\eta_{\text{bat}}} \cdot \frac{crate_{\text{bat}}}{\Delta t} \cdot b_1(t) \tag{D.56}$$

Maximum discharge constraint: Same as in D.3.
Sizing constraint: Same as in D.3.

Thermal energy storage
State of energy (SOE):

$$SOE_{\text{TES}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\text{TES}}(t-1) + & \\ \left(H_{\text{GB,TES}}(t-1) + H_{\text{ElB,TES}}(t-1)\right) \cdot \Delta t - & \\ \frac{H_{\text{TES,plant}}(t-1)}{\eta_{\text{TES}}} \cdot \Delta t, & \text{otherwise} \end{cases} \tag{D.57}$$

Maximum charge constraint

$$H_{\mathrm{GB,TES}}(t) + H_{\mathrm{ElB,TES}}(t) \leq \frac{s_{\mathrm{TES}} \cdot \mathrm{crate}_{\mathrm{TES}}}{\Delta t} \cdot b_2(t) \tag{D.58}$$

Maximum discharge constraint: Same as in D.3.
Sizing constraint: Same as in D.3.

Hydrogen storage
Same as in D.3.

Grid connection capacity
Maximum inflow constraint: Same as in D.3. Maximum outflow constraint: Not required because no electricity can be sold to the grid.

E

Appendix E: Remaining results from Chapter 3

Cost-optimal utility systems for different Opex scenarios

Table E.1.: Additionally installed utility technologies for cost-optimal utility system for an ethylene oxide plant for six different years and a grid connection capacity of 97.4 MW

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2018	0.0	0.0	0.0	0.0	0.0	0.0
2019	0.0	0.0	0.0	0.0	0.0	0.0
2020	15.0	0.0	0.0	0.0	0.0	0.0
2021	15.0	0.0	0.0	0.0	0.0	0.0
2022	70.0	84.9	420.2	0.0	0.0	0.0
2023	76.5	0.0	307.3	0.0	0.0	0.0

Table E.2.: Total cost and scope 1 CO_2 emissions of benchmark and new utility system for the ethylene oxide plant for distinct years and a grid connection capacity of 97.4 MW

	Total cost [million euro]			Scope 1 CO_2 emissions [kiloton]		
Year	CHP-based system	New system	Reduction [%]	CHP-based system	New system	Reduction [%]
2018	14.1	14.1	0.0	120.3	120.3	0.0
2019	11.1	11.1	0.0	120.3	120.3	0.0
2020	7.6	7.6	0.0	113.8	120.3	5.4
2021	27.9	28.8	3.1	109.7	120.3	8.8
2022	76.5	85.5	10.5	91.2	120.3	24.2
2023	30.7	33.6	8.6	93.3	120.3	22.3

Table E.3.: Additionally installed utility technologies for cost-optimal utility system for an ethylene glycol plant for six different years and a grid connection capacity of 90.2 MW

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2018	0.0	0.0	0.0	0.0	0.0	0.0
2019	0.0	0.0	0.0	0.0	0.0	0.0
2020	0.0	0.0	0.0	0.0	0.0	0.0
2021	22.2	0.0	0.0	0.0	0.0	0.0
2022	85.2	9.3	393.9	0.0	0.0	0.0
2023	87.1	0.0	369.3	0.0	0.0	0.0

Table E.4.: Total cost and scope 1 CO_2 emissions of benchmark and new utility system for the ethylene glycol plant for distinct years and a grid connection capacity of 90.2 MW

	Total cost [million euro]			Scope 1 CO_2 emissions [kiloton]		
Year	CHP-based system	New system	Reduction [%]	CHP-based system	New system	Reduction [%]
2018	10.8	10.8	0.0	78.8	78.8	0.0
2019	8.5	8.5	0.0	78.8	78.8	0.0
2020	5.9	5.9	0.0	78.8	78.8	0.0
2021	21.4	21.6	1.1	75.1	78.8	4.7
2022	59.2	63.3	6.4	64.0	78.8	18.7
2023	23.0	25.0	8.2	64.0	78.8	18.7

Table E.5.: Additionally installed utility technologies for cost-optimal utility system for a PET plant for six different years and a grid connection capacity of 49.7 MW

Year	Electric boiler [MW]	Battery [MWh]	TES [MWh]	Electrolyser [MW]	H2 boiler [MW]	H2 storage [MWh]
2018	0.0	0.0	0.0	0.0	0.0	0.0
2019	0.0	0.0	0.0	0.0	0.0	0.0
2020	0.0	0.0	0.0	0.0	0.0	0.0
2021	12.2	0.0	0.0	0.0	0.0	0.0
2022	47.1	4.9	217.7	0.0	0.0	0.0
2023	48.1	0.0	204.1	0.0	0.0	0.0

Table E.6.: Total cost and scope 1 CO_2 emissions of benchmark and new utility system for the PET plant for distinct years and a grid connection capacity of 49.7 MW

	Total cost [million euro]			Scope 1 CO_2 emissions [kiloton]		
Year	CHP-based system	New system	Reduction [%]	CHP-based system	New system	Reduction [%]
2018	6.0	6.0	0.0	43.5	43.5	0.0
2019	4.7	4.7	0.0	43.5	43.5	0.0
2020	3.3	3.3	0.0	43.5	43.5	0.0
2021	11.8	11.9	1.1	41.5	43.5	4.7
2022	32.6	34.8	6.4	35.4	43.5	18.7
2023	12.7	13.8	8.2	35.4	43.5	18.7

Grid connection capacity

The remaining results of the grid connection capacity sensitivity analysis can be found in the Appendix of the published version of this chapter, and in the repository of this thesis. The repository with the doi 10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb is available via `https://doi.org/10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb.v1`.

Impact of different technology cost scenarios

The remaining results of the technology cost sensitivity analysis can be found in the Appendix of the published version of this chapter and in the repository of this thesis.

The repository with the doi 10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb is available via https://doi.org/10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb.v1.

Impact of the minimal load of the legacy technology

The remaining results of the sensitivity analysis on the minimal load of the legacy technology can be found in the Appendix of the published version of this chapter and in the repository of this thesis. The repository with the doi 10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb is available via https://doi.org/10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb.v1.

F

Appendix F: Modelling code used in Chapter 4

Since not all code used in this thesis can be included in the thesis, I refer the reader to the repository. The repository with the doi 10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb is available via `https://doi.org/10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb.v1`. The code is also available online on GitHub, via `https://github.com/SvenjaBie/HPInteg_Open`.

G

Appendix G: Energy price scenarios explored in Chapter 4

The explored electricity and EU ETS prices are shown in Figures G.1 to G.3. Unfortunately, natural gas prices cannot be disclosed.

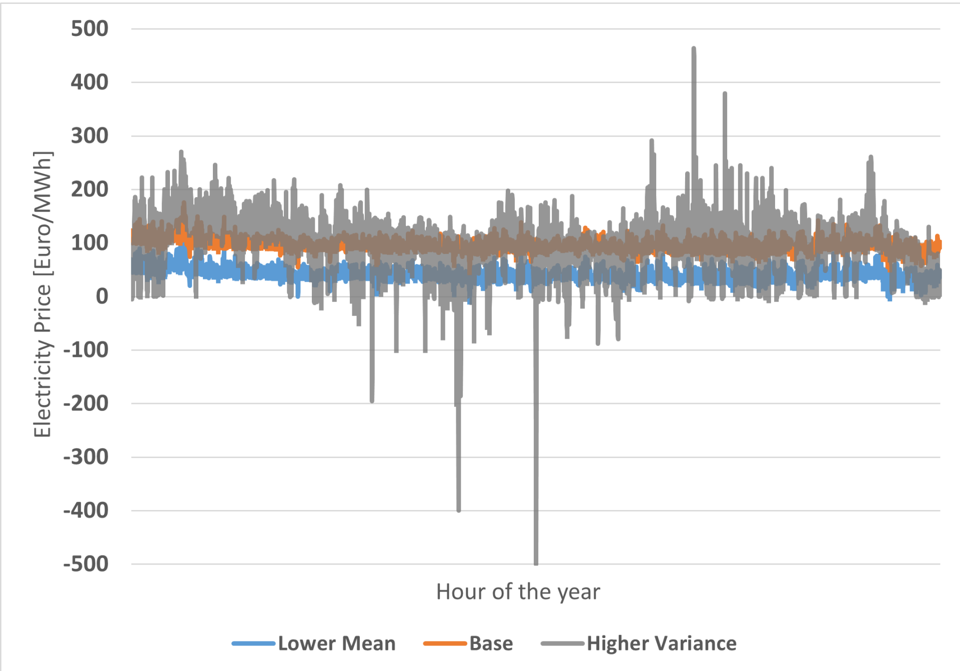

Figure G.1.: Electricity prices explored in this study. Based on data obtained through [24].

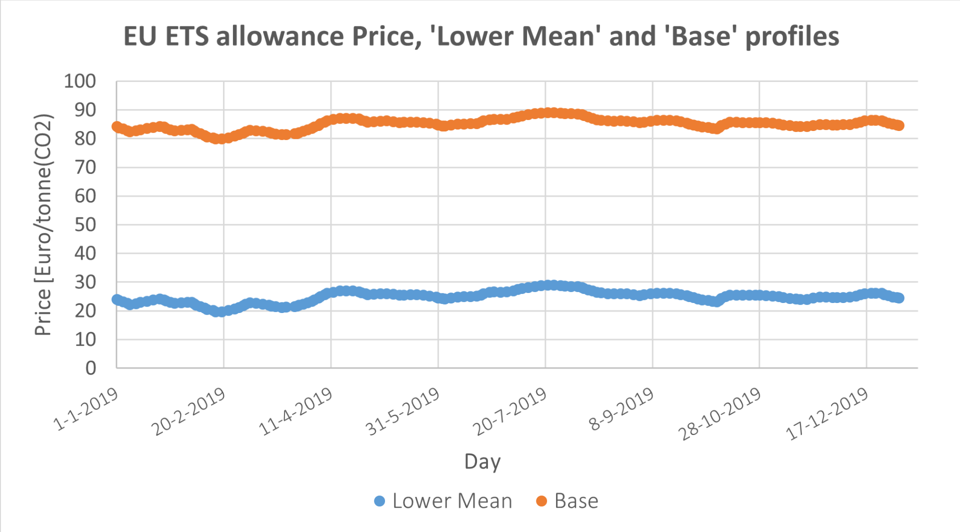

Figure G.2.: Co_2 allowance prices explored in the 'Lower Mean' and 'Base' energy price profiles in this study. Based on data obtained from [25].

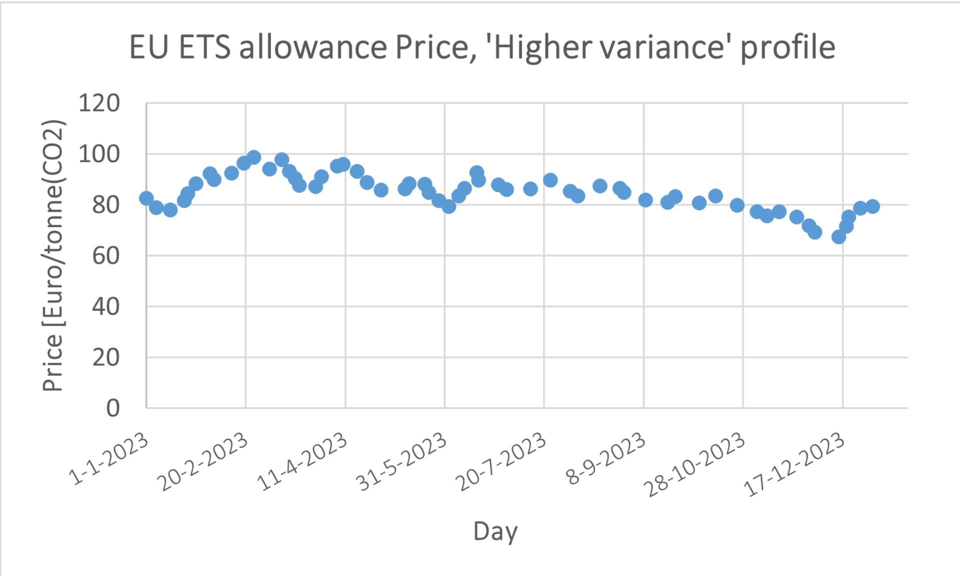

Figure G.3.: Co_2 allowance prices explored in the 'Higher Variance' energy price profile in this study. Based on data obtained from [26].

H

Appendix H: Energy price and technology cost scenarios explored in Chapter 5

To study the impact of changes in the energy and technology cost on the results of the model sixteen scenarios were formulated. Figures H.1 to H.4 show the energy price profiles in these scenarios, presented in 5.2.5. Figure H.1 depicts the energy prices in the LMLV scenario. It clearly shows the difference in volatility between the electricity prices (EP) and the gas prices (GP). Moreover, it shows how the two gas prices differ in the EGR scenarios, with the 'EGR 1' being the scenario with the highest average price. The ratio between the GP in EGR 1 and the GP in EGR 1.6 is the same in Figures H.2 to H.4. Figure H.5 shows how the different energy price scenarios are combined with the technology cost scenarios.

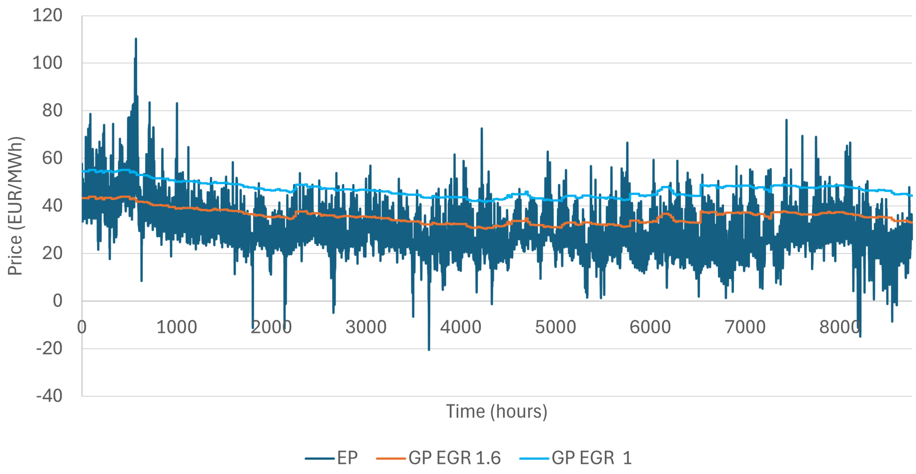

Figure H.1.: The electricity (EP) and gas (GP) prices for the electricity-to-gas price ratio (EGR) of 1.6 and 1 for the 'Low Mean Low Variance' scenario

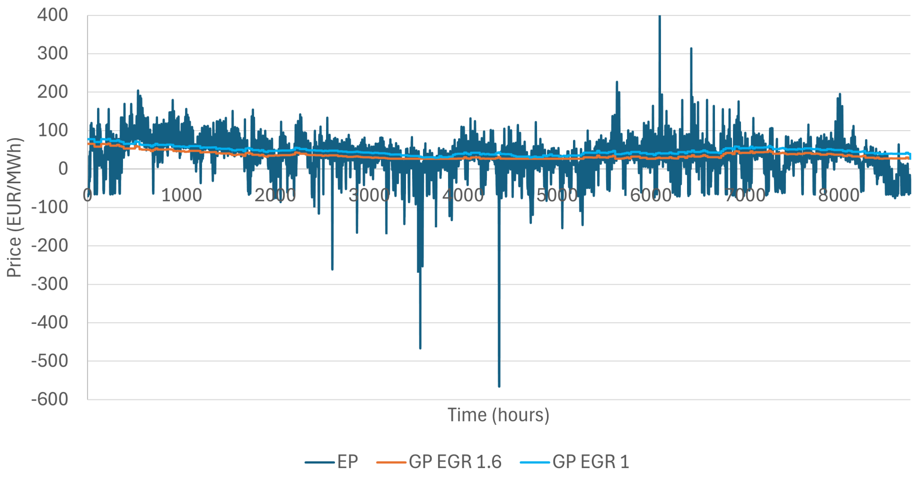

Figure H.2.: The electricity (EP) and gas (GP) prices for the electricity-to-gas price ratio (EGR) of 1.6 and 1 for the 'Low Mean High Variance' scenario

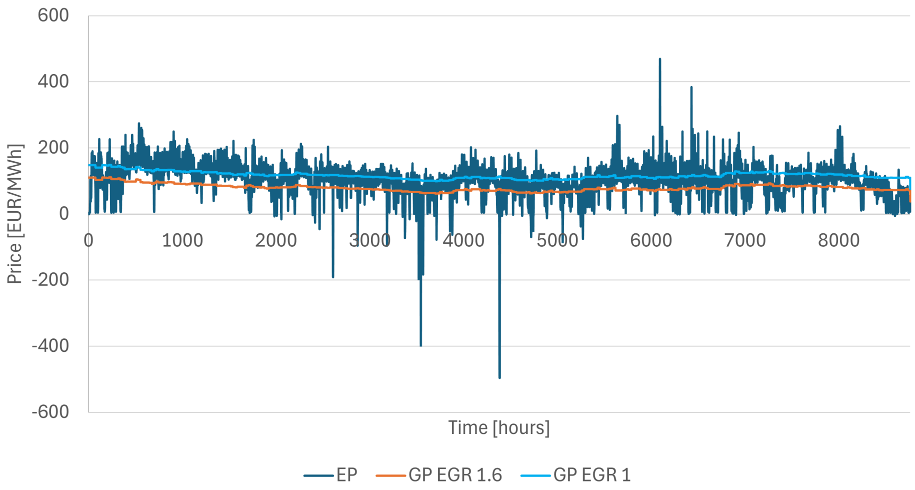

Figure H.3.: The electricity (EP) and gas (GP) prices for the electricity-to-gas price ratio (EGR) of 1.6 and 1 for the 'High Mean High Variance' scenario

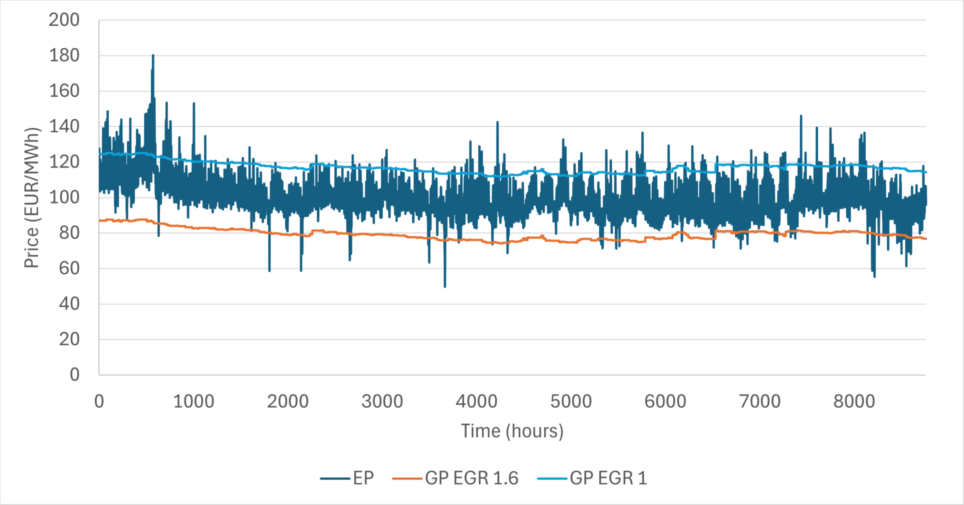

Figure H.4.: The electricity (EP) and gas (GP) prices for the electricity-to-gas price ratio (EGR) of 1.6 and 1 for the 'High Mean Low Variance' scenario

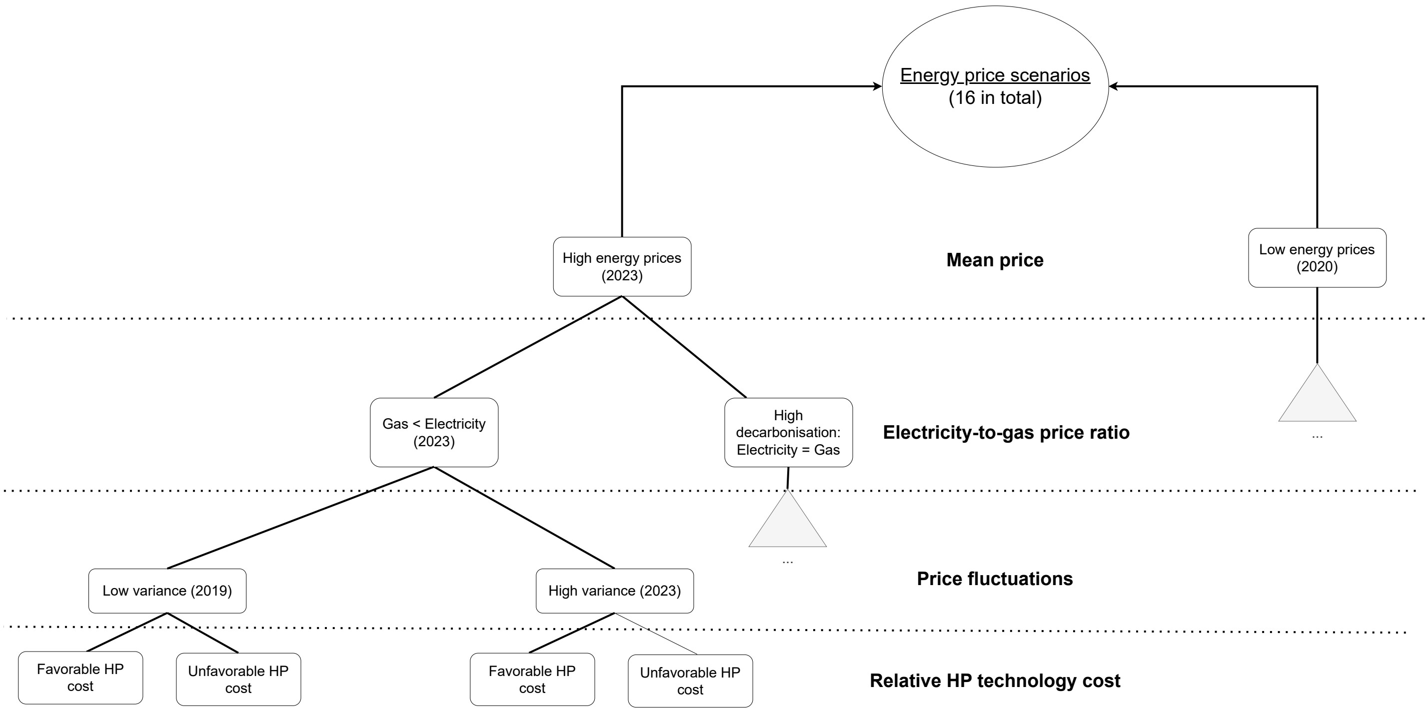

Figure H.5.: Scenario tree considering the mean energy price, the electricity-to-gas price ratio, the energy price fluctuations and the technology cost

I

Appendix I: Remaining results from Chapter 5

I.1. Electrolyser technology cost sensitivity analysis

To enhance the understanding of why hydrogen is not selected by the model in any of the results presented in Section 5.3, a sensitivity analysis of the electrolyser cost was carried out. The two energy cost scenarios with the highest deviation in terms of electricity prices were selected for the analysis: 'Low Mean High Variance' with EGR 1.6 and 'High Mean High Variance' with EGR 1. In both cases, the TC scenario unfavourable for HPs and favourable for alternative technologies, such as the electrolyser, was chosen. The technology cost of the electrolyser was decreased until hydrogen was picked up by the model. The cost was decreased by one order of magnitude at the time until hydrogen started appearing in the technology portfolio. Then, the price was increased again. For the 'Low Mean High Variance' scenario, the step size was increased by halving the cost difference between the steps until the tipping point was found to be at 9% of the original technology cost. For the 'High Mean High Variance' scenario, the cost first had to be decreased to 0.1% of the original cost (76 euro/MW). Subsequently, the cost was doubled, and then decreased by steps of 50 euro/kW. The results of the sensitivity analysis for which hydrogen is and is not part of the cost-optimal technology portfolio are presented in Tables I.1 and I.2. For the 'Low Mean High Variance' energy price scenario, with relatively many negative electricity price hours, the cost has to decrease more than one order of magnitude, from 760 euro/kW to 68.4 euro/kW. For the 'High Mean High Variance' scenario, the cost has to be as low as 0.2 euro/kW.

Table I.1.: Installed PtH and storage capacities in the energy price scenario with low mean and high variance for different electrolyser technology costs

TC_{H2E} [euro/MW]	EGR	TC cost scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]	H2E [MW]	H2B [MW]	H2S [MWh]
68400	1.6	'HighHP-LowRest'	28.4	100.5	0	0.3	0.2	0
76000	1.6	'HighHP-LowRest'	29	103	0	0	0	0

Table I.2.: Installed PtH and storage capacities in the energy price scenario with high mean and high variance for different electrolyser technology costs

TC_{H2E} [euro/MW]	EGR	TC cost scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]	H2E [MW]	H2B [MW]	H2S [MWh]
200	1	'HighHP-LowRest'	22.3	85.7	6.1	7.6	0.4	7.5
250	1	'HighHP-LowRest'	26.5	92.2	6.1	0	0	0

I.2. Results without the minimal load constraint of the CHP

Tables I.3, I.4, I.5, and I.6 show the technology portfolio of the cost-optimal utility system if the CHP operation is not constrained and can shut down completely. Omitting this constraint and accepting it, though not accounting for the increase in maintenance cost, results in the following changes to the sizing and operation of the PtH technologies. For low and stable electricity prices, more PtH technologies are installed. The size of the HP increases with the previous minimal capacity of the CHP. The combined capacity of TES and ElB increases by a factor of 2. When price fluctuations increase, the change in capacities is limited as the size of ElB and the TES are already limited by the grid connection capacity of the system. Nevertheless, less natural gas is consumed overall. When the mean energy price increases, the size of the ElB reduces, the capacity of the TES remains the same, and the size of the HP increases compared to the scenario with the CHP constraint. Reducing price fluctuations whilst maintaining the high mean energy price results in the same increase in HP capacity, whilst the capacities of the TES and ElB remain relatively unchanged. Though the total natural gas consumption is reduced in all scenarios when the CHP is allowed to shut down completely, complete electrification is only cost-optimal in the scenario with high mean prices, low price fluctuations and a low electricity-to-gas price ratio.

Table I.3.: Installed PtH and storage capacities in the energy price scenarios with low mean and variance

EGR	TC cost scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	24	42	0
	LowHP-HighRest	6	5	11
1	HighHP-LowRest	25	49	0
	LowHP-HighRest	6	6	12

Table I.4.: Installed PtH and storage capacities in the energy price scenarios with low mean and high variance

EGR	TC cost scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	29	103	0
	LowHP-HighRest	28	62	0
1	HighHP-LowRest	29	113	0
	LowHP-HighRest	28	68	0

Table I.5.: Installed PtH and storage capacities in the energy price scenarios with high mean and high variance

EGR	TC cost scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	24	94	8
	LowHP-HighRest	7	15	14
1	HighHP-LowRest	22	96	13
	LowHP-HighRest	6	18	15

Table I.6.: Installed PtH and storage capacities in the energy price scenarios with high mean and low variance

EGR	TC cost scenario	ElB [MW_{th}]	TES [MWh]	HP [MW_{th}]
1.6	HighHP-LowRest	0	19	14
	LowHP-HighRest	0	6	15
1	HighHP-LowRest	2	22	14
	LowHP-HighRest	2	6	16

J

Appendix J: Modelling code used in Chapter 5

Since not all code used in this thesis can be included in the thesis, I refer the reader to the Appendix of the published version of this chapter or to the repository. The repository with the doi 10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb is available via `https://doi.org/10.4121/c95f553c-a4af-47ae-84b8-e13675a65ccb.v1`. The code is also available online on GitHub, via `https://github.com/SvenjaBie/ElectrUtilPapInd_Open`.

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To Tonny, Inna, Michael, Fien, Thijmen, Jessie, Brendon, and Eric: I am grateful that we did our PhD almost in parallel. Thank you for sharing your knowledge on chemical processes, thermodynamics, coding, writing, publishing, and many other things. Thank you also for the warmth and support that we gave each other. I am curious to see how and where each of us will contribute to the defossilisation of the industry. Brendon, thank you for teaming up on three great projects. Our regular meetings first thing in the morning (for me ;)) made it easy to start the day. Thank you for sharing your expertise with me and for adding your insights about the practical challenges of heat electrification to my model. I will miss working together.
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Several people helped me develop the model that I used throughout the research. A big thank you especially to Anya, Roman, Ivan, Thijmen, Justin, and Brendon.

When I had moved back to Germany, I found a temporary home every time I returned to Delft. Thank you for welcoming me, Fra and Anna, Ivan, Hannia and Emilia, Laurens and Deborah, Salma and Abdalla, Lins and Ilker, Inna and Kartik, Fien and Theo.
Back in Germany, I'd like to thank the Library of the Germanic National Museum in Nuremberg for providing me with a workspace. Without it, I would have taken much longer to finish.

To my friends and family: Thank you for taking my thoughts away from work, which was not always easy, especially during the last year. Thank you for all the fun and support, and that I could still always discuss the hardships with you. Chiari, thank you also for designing the beautiful cover for this book, despite your busy life. Sevil, thank you so much for your guidance on navigating the difficulties of the PhD and other facets of life.

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Thank you to you, dear reader, for your interest in my work. How can you contribute to the changes that are necessary for limiting climate change?

About the author

Svenja has been passionate about the Energy Transition ever since high school. She studied Renewable Energies and received her Bachelor's degree from Stuttgart University. Afterwards, she joined Robert Bosch GmbH for the 'PreMaster' program. There, she worked on battery cell manufacturing and on simulating a fuel cell drive train. In 2020, Svenja earned her Master's degree in Sustainable Energy Technology from TU Delft. After a brief period working as a Junior Development Engineer, she began her PhD research at the Energy & Industry group, Faculty of Technology, Policy and Management at TU Delft. Before she moved on to her current job as Senior Consultant for Energy Systems at Siemens Energy, she worked as an independent consultant, using the model presented in Chapters 3 to 5 of this thesis.

Next to sustainable energy engineering, Svenja enjoys immersing herself in foreign cultures and political engagement. She spent one year volunteering in Peru, did a project in Namibia, and studied in Germany, Italy and the Netherlands. She's fluent in German, English, Spanish, Dutch, and Italian, experiencing language as a key to culture. From early on, active civil engagement was important to Svenja. She held a scholarship from the Friedrich Ebert Foundation for the duration of her studies, which allowed her to participate in seminars and workshops related, but not limited to, energy politics. She was a co-founder of the Energy working group of the foundation's scholarship program. During her PhD, Svenja was an active member of Volt Rotterdam, where she co-led the development of the party's election program for the regional elections. Also, she represented students' and employees' interests in higher management decision making as part of the faculty works councils at Stuttgart University and TU Delft.

List of Publications

Chapters 2 to 5 of the dissertation are based on the following publications.

- S. Bielefeld, M. Cvetković, and A. Ramírez. “Should we exploit flexibility of chemical processes for demand response? Differing perspectives on potential benefits and limitations”. In: *Frontiers in Energy Research* 11 (June 2023). ISSN: 2296-598X. DOI: 10.3389/fenrg.2023.1190174. URL: https://www.frontiersin.org/articles/10.3389/fenrg.2023.1190174/full
- S. Bielefeld, M. Cvetković, and A. Ramírez. “The potential for electrifying industrial utility systems in existing chemical plants”. In: *Applied Energy* 392 (Aug. 2025). ISSN: 03062619. DOI: 10.1016/j.apenergy.2025.125988
- Prepared for submission:
  S. Bielefeld, B. de Raad, C. Cvetcović, and A. Ramírez. "The Impact of Heat Pump Integration on the Electrification of Industrial Utility Systems."
- S. Bielefeld, B. de Raad, L. Stougie, M. Cvetković, M. v. Lieshout, and A. Ramírez. “The impact of energy prices on the electrification of utility systems in industries with fluctuating energy demand”. In: *Energy* 335 (Oct. 2025). ISSN: 18736785. DOI: 10.1016/j.energy.2025.137679