Chair of Energy Network Technology

Doctoral Thesis

Application of an integrated life cycle assessment approach toward a carbon-neutral industry

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AFFIDAVIT

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"Sustainable development is a fundamental break that's going to reshuffle the entire deck. There are companies today that are going to dominate in the future simply because they understand that."

– Francois-Henri Pinault

ABSTRACT

Mitigating climate change and achieving industry-wide decarbonization by 2050 are critical challenges for humanity. Energy-intensive industries that rely mainly on fossil fuels are compelled to reshape their energy systems and production processes to achieve climate neutrality by adopting innovative low-emission technologies and approaches. Given the need for a swift transition toward sustainable industries, it is crucial to develop effective methods that can accurately assess the sustainability potential of various measures at an early stage.

To ease the transition to climate-neutral energy systems, an integrated life cycle assessment (LCA) method was developed to comprehensively evaluate the environmental, economic, and energetic implications of sustainability measures. This method was developed and demonstrated based on research findings from specific sustainability approaches at four selected industrial sites in energy-intensive industries: pulp, paper, and print; chemical and petrochemical; cement; and magnesia. Within the integrated LCA framework, a scenario analysis is embedded to identify optimal solutions by varying design parameters such as energy supply alternatives, by-product use, or flexibility options. This allows for establishing an optimization hierarchy based on environmental, techno-economic, and energetic indicators, facilitating decision-making using multi-criteria decision methods. Given the expected increase in the share of renewable energy sources in the future, emissions from energy production are anticipated to exhibit greater fluctuations throughout days and seasons, making previous approaches based on aggregated annual values less accurate. To address this, the integrated LCA framework incorporates a novel dynamic energy modeling approach that considers the dynamics of energy generation and merges it with industrial load profiles, resulting in a time-resolved emission profile. This approach enables a more precise assessment of the ecological footprint of products, which is becoming increasingly important to customers.

The integrated LCA method was used for site-specific analysis in various industries. In the paper industry, the implementation of production flexibility and the integration of low-emission technologies, such as storage, power purchase agreements (PPAs), electric boilers, and heat pumps, resulted in a greenhouse gas (GHG) mitigation potential of up to 32.3% per ton of paper. Energy costs were reduced by 44%, renewable primary energy demand (PED) increased by 156%, and fossil PED decreased by 32%. In the chemical industry, a GHG mitigation potential of up to 80% was achieved for 1 MJ of sustainable aviation fuel (SAF) compared with the fossil benchmark. This was accomplished by utilizing the by-product lignin as fuel and integrating renewable electricity. Renewable energy accounted for up to 82% of the PED. Utilizing all by-products was necessary to achieve exergetic system efficiencies of up to 57%. The cement industry demonstrated a GHG reduction potential of 245 tons of CO_2 per GWh of recovered waste heat. However, waste heat utilization as process steam in a dairy in the proximity was economically unviable, regardless of whether thermal storage was implemented to balance supply and demand fluctuations. In the magnesia industry, a GHG reduction potential of up to 38.2% was achieved for producing 1 ton of MgO by co-firing locally available biomass with pet coke. The operational production costs could be decreased by 9.75%.

The examined case studies have demonstrated the importance of holistic assessments for industrial implementations of novel low-emission technologies and sustainability approaches. Although the eventual goal is decarbonization, the viability of the measures depends on their economic feasibility. Therefore, the accurate quantification of various indicators is crucial, and using multi-criteria decision-making methods can help strike a balance among different considerations. However, future flagship projects and success stories will be pivotal in driving industrial transformation and facilitating replication of measures, ultimately leading to a climate-neutral and prosperous European Union.

KURZFASSUNG

Die Eindämmung des Klimawandels und die Dekarbonisierung der Industrie bis 2050 sind entscheidende Herausforderungen für die Menschheit. Energieintensive Industrien basieren primär auf fossilen Ressourcen, müssen aber nun ihre Energiesysteme und Produktionsmuster anpassen, um durch die Einführung von innovativen emissionsarmen Technologien und Ansätzen Klimaneutralität zu erreichen. Da dieser Wandel hin zu umweltfreundlichen Industrien rasch vollzogen werden muss, werden wirksame Methoden benötigt, mit denen das Nachhaltigkeitspotenzial verschiedener Maßnahmen bereits in einem frühen Stadium treffsicher bewertet werden kann.

Zur Unterstützung der Energietransformation, wurde eine integrierte Lebenszyklusanalyse entwickelt, um die ökologischen, ökonomischen und energetischen Auswirkungen von Nachhaltigkeitsmaßnahmen umfassend zu untersuchen. Diese Methode wurde auf der Grundlage von Forschungsergebnissen zu spezifischen Nachhaltigkeitsansätzen an vier ausgewählten Industriestandorten in energieintensiven Industrien entwickelt und demonstriert: Zellstoff, Papier und Druck; Chemie und Petrochemie; Zement; und Magnesium. In der integrierten Lebenszyklusanalyse ist eine Szenarioanalyse eingebettet, um optimale Lösungen durch Variation von Gestaltungsparametern wie Energieversorgungsalternativen, Nebenproduktnutzung oder Flexibilitätsoptionen zu ermitteln. Dies ermöglicht die Ableitung einer Optimierungshierarchie in Bezug auf ökologische, techno-ökonomische und energetische Indikatoren, welche die Entscheidungsfindung mit Hilfe von multikriteriellen Entscheidungsmethoden erleichtert. Da der Anteil der erneuerbaren Energien in der Energieversorgung in Zukunft erheblich steigen wird, werden die Emissionen aus der Energieerzeugung voraussichtlich größere tages- und jahreszeitliche Schwankungen aufweisen, sodass bisherige Ansätze über aggregierte Jahreswerte zunehmend ungenau werden. Daher beinhaltet die integrierte Lebenszyklusanalyse einen neuartigen dynamischen Energiemodellierungsansatz, der die Dynamik der Energieerzeugung berücksichtigt und diese mit industriellen Lastprofilen zu einem zeitlich aufgelösten Emissionsprofil zusammenführt. Dies führt zu einer genaueren Bestimmung des ökologischen Fußabdrucks von Produkten, welcher für Kund:innen immer mehr an Bedeutung gewinnt.

Die entwickelte Methode wurde für standortspezifische Analysen in verschiedenen Branchen eingesetzt. In der Papierindustrie wurde durch die Nutzung von Produktionsflexibilitäten und der Integration emissionsarmer Technologien wie Speicher, Stromabnahmeverträgen, Elektrokessel und Wärmepumpen, ein Treibhausgas (THG)-Einsparungspotenzial von bis zu 32.3% pro Tonne Papier erreicht. Die Energiekosten sanken um 44%, der Anteil der erneuerbaren Energien am Primärenergiebedarf stieg um 156%, und der Anteil des fossilen

Primärenergiebedarfs sank um 32%. In der chemischen Industrie wurde ein THG-Minderungspotenzial von bis zu 80% für die Produktion von 1 MJ nachhaltigem Flugzeugtreibstoff im Vergleich zum fossilen Benchmark ermittelt. Dies wurde durch die Nutzung des Nebenprodukts Lignin als Brennstoff und die Integration von erneuerbarem Strom erreicht. Bis zu 82% des Primärenergiebedarfs werden durch erneuerbare Energie gedeckt. Exergetische Systemeffizienzen von bis zu 57% sind realisierbar, sofern alle Nebenprodukte entlang der Wertschöpfungskette verwertet werden. In der Zementindustrie ergab sich ein THG-Reduktionspotenzial von 245 Tonnen CO_2 pro GWh rückgewonnener Abwärme. Die Rückgewinnung von Abwärme und die Nutzung als Prozessdampf für eine in der Nähe gelegene Molkerei waren jedoch unwirtschaftlich, unabhängig davon, ob thermische Speicher zum Ausgleich von Versorgungs- und Bedarfsschwankungen eingesetzt wurden. In der Magnesiumbranche wurde bei der Produktion von 1 Tonne MgO durch die Mitverbrennung von lokal verfügbarer Biomasse zu Petrolkoks ein THG-Minderungspotenzial von bis zu 38.2% erreicht. Die betrieblichen Produktionskosten sanken dabei um 9.75%.

Die untersuchten Fallstudien haben gezeigt, dass ganzheitliche Bewertungen für die industrielle Umsetzung neuer emissionsarmer Technologien und Nachhaltigkeitsansätzen unerlässlich sind. Obwohl die Dekarbonisierung das vorrangige Ziel ist, werden die Maßnahmen nur dann umgesetzt, wenn sie wirtschaftlich tragfähig sind. Die Quantifizierung verschiedener Indikatoren ist von entscheidender Bedeutung, wobei multikriterielle Entscheidungsfindungsmethoden helfen können, die verschiedenen Aspekte gegeneinander abzuwägen. Zukünftige Leuchtturmprojekte und Erfolgsgeschichten werden jedoch der Schlüssel zum industriellen Wandel und zur Replikation von Maßnahmen sein, um ein klimaneutrales und wohlhabendes Europa zu erreichen.

FOREWORD

The completion of this thesis represents an essential personal milestone and has greatly contributed to my personal growth, both in the research field and in my private life. I would like to take this opportunity to express my gratitude to all the individuals who have supported me throughout this challenging endeavor over the past years.

First and foremost, I am deeply grateful to my loved ones in my personal environment. Juggling the demands of commuting between my hometown of Großklein, Leoben, and Linz often limited my free time and required meticulous planning to attend various appointments. I sincerely thank my parents, Adelheid and Georg, who have supported me from the beginning, nurturing my personal growth and encouraging my academic pursuits. A special appreciation goes to my girlfriend, Helene, who has consistently motivated me to pursue my goals and was understanding of the time constraints. I am also grateful to my friends and the associations in my hometown, who have shown great understanding when I was occasionally unavailable. The unwavering support from my personal network has undeniably played a pivotal role in my academic success.

Secondly, I would like to express my gratitude to my employer, the association *Energieinstitut an der JKU Linz*, under the current leadership of Robert Tichler, before Horst Steinmüller, for granting me the opportunity to conduct this thesis. Through engagements in national and international research projects spanning a wide range of topics, I have had the privilege to engage in insightful discussions on energy-related matters with experienced researchers and industrial experts, thereby gaining a comprehensive understanding of energy-related subjects. Therefore, I extend my gratitude to the entire team at Energieinstitut for the daily exchange of experiences and outstanding team dynamics. I would like to offer my special thanks to my project leaders, Johannes, Karin, and Simon, who have consistently supported me with their invaluable advice and assistance, providing me with a wealth of valuable skills and professional attributes. I would also like to thank my office colleagues Hans, Andreas, Valerie, Daniel, and Lukas, with whom I have had the opportunity to discuss various problems. This collaboration has been crucial in the context of research and, of course, in a personal context as well.

Lastly, I would like to express my gratitude to my supervisor, Thomas Kienberger, for enabling me to undertake this thesis at the *Montanuniversität Leoben at the Chair of Energy Network Technology*. In this context, I would also like to acknowledge the mentorship of Markus Lehner during this thesis. Through numerous conversations, they have guided me on my scientific journey and consistently provided me with valuable feedback on energy-related topics.

In conclusion, I am filled with great anticipation as I embark on the next phase of my research journey, eager to discover where it will lead me and what other exciting opportunities life has in store for me.

Stefan Puschnigg, July 2023

CONTENTS

NOMENCLATURE

Abbreviations

ADP	Abiotic depletion
AHP	Analytic Hierarchy Process
AGCS	Austrian Gas Clearing and Settlement
AP	Acidification potential
BAU	Business-as-usual
BREF	Best Available Technology Reference Document
CAPEX	Capital expenditure
CCM	Caustic calcinated magnesia
CCS	Carbon capture and storage
CCU	Carbon capture and utilization
CED	Cumulative energy demand
CHP	Combined heat and power
CML	Centrum voor Milieukunde Leiden
CORSIA	Carbon Offsetting and Reduction Scheme for International Aviation
DBM	Dead burnt magnesia
DSM	Demand-side management
EEX	European Energy Exchange
EP	Eutrophication potential
EPEX	European Power Exchange
EU	European Union
EU-27	European Union - 27 member states
EUA	European Union Emission Allowances
EU ETS	European Union Emission Trading System
EXAA	Energy Exchange Austria

FAETP	Freshwater aquatic ecotoxicity potential
GaBi	Ganzheitliche Bilanzierung
GHG	Greenhouse gas
GWP	Global warming potential
GW	Groundwood
HOB	Heat-only-boiler
HTP	Human toxicity potential
ILCD	International Life Cycle Data system
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
KPI	Key performance indicator
LCA	Life cycle assessment
LCC	Life cycle costing
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LCOE	Levelized cost of energy
LCOP	Levelized cost of product
LCSA	Life cycle sustainability assessment
LI	Lignin
MAETP	Marine aquatic ecotoxicity potential
MCDM	Multi-criteria decision making
NG	Natural gas
NG-B	Natural gas boiler
NPV	Net present value
ODP	Ozone layer depletion potential
OK	Olive kernels

OPEX	Operational expenditure
ORC	Organic Rankine Cycle
PED	Primary energy demand
PGW	Pressurized groundwood
PM	Paper mill
PPA	Power purchase agreement
PtG	Power-to-Gas
PtX	Power-to-X
POCP	Photochemical ozone creation potential
RED	Renewable energy directive
RES	Renewable energy sources
ROI	Return on investment
SAF	Sustainable aviation fuel
Sb	Antimony
SHP	Sunflower husk pellets
S-LCA	Social life cycle assessment
SNG	Synthetic natural gas
TEA	Techno-economic assessment
TES	Thermal energy storage
TETP	Terrestrial ecotoxicity potential
TRACI	Tool for the Reduction and Assessment of Chemical and other environmental Impacts
TRL	Technology readiness level
UNFCCC	United Nations Framework Convention on Climate Change
VBC	Virtual battery concept
VDI	Verein Deutscher Ingenieure
WSD	Wood sawdust

Indices

bio	biomass
bp	by-product
c	capital
d	demand
DCB	Dichlorobenzene
en	energetic
eq.	equivalent
ex	exergetic
geo	geothermal
HHV	Higher heating value
I	irreversible
in	input
l	losses
m	miscellaneous
MP	Main product
n.d.	not-defined
nuc	nuclear
O	operation
out	output
p	proceeds
pr	product
pv	photovoltaic
Q	thermal flow
sys	System
t	period
W	work

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1 INTRODUCTION

Climate change is a central concern that will essentially impact the forthcoming decades. This pressing issue is predominantly caused by the extensive use of fossil fuels, resulting in an alarming rise in greenhouse gas (GHG) concentrations in the atmosphere and adverse climatic effects. The escalating occurrence of weather anomalies and extreme events, such as heatwaves and flooding, presents multifaceted challenges to human populations and ecosystems worldwide. To effectively combat the anthropogenic greenhouse effect and actively mitigate climate change, it is imperative to adopt efficient measures to minimize GHG emissions. Implementing these measures is crucial for achieving the target set by the Paris Agreement, which aims to restrict the global average temperature increase to below 2 °C, ideally 1.5 °C, compared to pre-industrial levels [1].

1.1 Greenhouse gas emissions and energy demand

More than two-thirds of the GHG emissions produced by the 27 member states of the European Union (EU-27), encompassing both energetic and non-energetic uses, are attributed to three primary sectors: energy industries (24%), manufacturing industries by including construction (22%), and transportation (22%). A detailed examination of the GHG composition measured in terms of carbon dioxide equivalents (CO_2-eq.) reveals that approximately 80% of the emissions are attributed to carbon dioxide (CO_2), which primarily originate from the combustion of fossil fuels [2]. In Austria, carbon dioxide (CO_2) comprises 84% of GHG emissions, and other GHGs such as methane (CH_4), mainly originating from livestock farming and waste disposal, and nitrous oxide (N_2O) from agricultural soils contribute to a smaller portion of the emissions [3].

The primary energy consumption in the European Union (EU) has decreased by 17.5% from 2005 to 2020, with a 13% reduction in final energy consumption. Although this declining trend is generally positive, it is unlikely to achieve the established climate targets, necessitating additional measures. The transport, household, and industrial sectors are the primary consumers of final energy in Austria and EU-27 (Figure 1-1). Notably, the industrial sector plays a substantial role, accounting for approximately one-third of Austria's and one-quarter of the EU-27's energy consumption. Approximately 60% of the final energy demand is attributed to energy-intensive industries such as chemical, mineral, paper and pulp, and iron and steel production [4]. These industries rely predominantly on fossil fuels as their primary energy source. However, an essential challenge lies in reducing carbon emissions to achieve carbon neutrality while maintaining competitiveness. A crucial step towards addressing this challenge is transitioning from a fossil fuel-based energy system to renewable energy sources (RES) and adapting improved energy-efficient systems [5]. To attain this transition, industries must modify their current consumption and production patterns [6] to integrate volatile RES and low-emission energy technologies [7]. Additionally, measures such as waste stream utilization and waste heat recovery [8], [9], fostering industrial symbiosis [10], promoting circular economy practices [11], adapting carbon capture, storage, and utilization technologies (CCS/CCU) [12], and use of biomass [13] and renewable gases [14] play crucial roles in achieving a climate-neutral industry.

This study primarily concentrates on energy-intensive industries, recognizing the necessity for novel technologies that reduce consumption and diminish reliance on fossil fuels. It is essential to recognize that focusing on a single sector alone is inadequate for attaining climate neutrality. Therefore, addressing climate challenges requires disruptive technologies and innovations across all sectors. Comprehensive evaluation measures encompassing environmental, economic, and energy-related aspects are essential to facilitate energy transformation. The most environmentally friendly and cost-effective energy sources are those that are not consumed at all, highlighting the importance of energy efficiency and sufficiency.

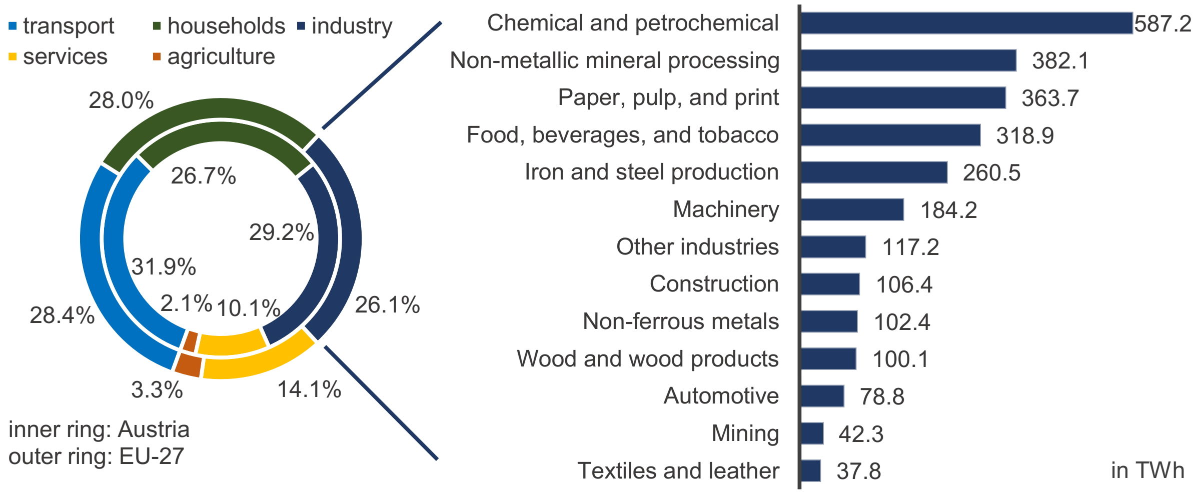

Figure 1-1: Final energy consumption by economic sectors in Austria and EU-27 in 2020(inner ring: Austria based on BMK 2021 [15]; outer ring: EU-27 based on BMK 2022 [16]) and different industries in EU-27 (based on Eurostat 2020 [4])

1.2 Legal framework for a green transition in industries

Energy-intensive industries are subjected to a fast-changing climate-policy landscape and have to constantly adjust their operations. The *European Green Deal* [5], representing the EU's long-term strategy, aims to transform the EU into the world's first climate-neutral continent and recognizes the importance of energy-intensive industries in contributing to Europe's economy. The EU has committed to reducing GHG emissions by 55% by 2030 and to achieving climate neutrality by 2050 (Figure 1-2). Therefore, in line with these goals, specific targets for

2030 have been set, including a renewable energy share of ≥ 32% [17] and an energy efficiency improvement of ≥ 32.5% [18]. Although the 20% GHG emission reduction target for 2020 was met, the outcome was affected by the COVID-19 pandemic [19]. The GHG emission projections based on historical trends indicate that future emission reduction targets for 2030 and 2050 are unlikely to be met, despite the seeming feasibility suggested by the historical trend over the past five years (2017–2021). This discrepancy can be attributed to the impact of the COVID-19 pandemic on the trendline. Consequently, a provisional agreement was made to increase the renewable energy share target by at least 42.5%, ideally 45%, by 2030. The *Fit for 55 package* is a crucial mechanism to align EU policies with the climate goals. This comprehensive package comprises a set of proposals to revise and update EU legislation and introduce new initiatives. By implementing the measures outlined in the *Fit for 55 packages*, the EU aims to effectively tackle the challenges of climate change and propel the transition towards a sustainable and climate-neutral future [20].

Several initiatives as part of the *European Green Deal* have been launched for a climate-neutral and competitive industry: In response to Russia's invasion of Ukraine, *REPowerEU* was established to save and produce clean energy and diversify energy suppliers [21]; the *Net-Zero Industry Act* was promulgated to scale-up the manufacturing of clean technologies [22]; and *The Green Deal Industrial Plan* was initiated to increase the competitiveness of Europe's net zero industries [12]. Since 2005, the *European Union Emissions Trading Scheme (EU ETS)* has regulated EU emission allowances (EUA) for the industrial, electrical, and heat generation sectors through a cap-and-trade system. It is also scheduled for reform as part of the *Fit for 55 package* [23]. However, additional measures such as future initiatives, adaptations, and disruptive technologies are necessary to achieve the desired climate targets of the EU.

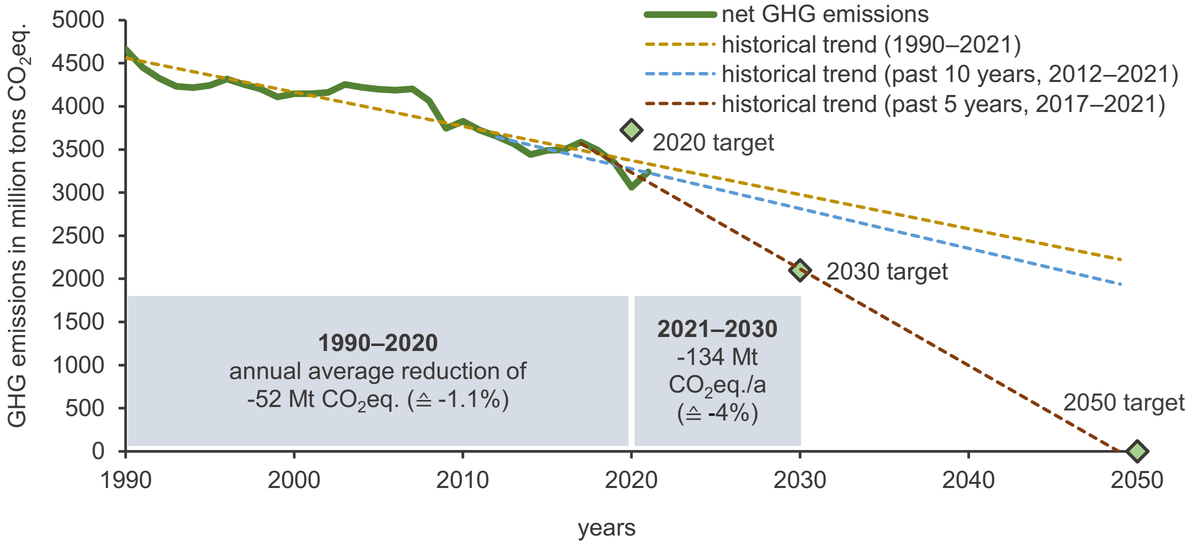

Figure 1-2: Historical trends and future projections for greenhouse gas emissions based on European Environment Agency 2022 [19] and European Environment Agency 2023 [24]

1.3 Structure of the thesis

The thesis is organized as follows: Chapter 2 provides the context and describes the research needs. Chapter 3 outlines the research approach and structure of cumulative work. This chapter also discusses research questions and objectives. Chapter 4 elaborates on the research methodology developed for a sustainable, cost-efficient, and competitive industry. Chapter 5 explains the results and discusses the research findings. Chapter 6 provides a summary of the main results. Finally, Chapter 7 presents the main conclusions based on the research questions and provides an overall outlook.

Appendix A lists the author’s participation in international research conferences. Appendix B lists the peer-reviewed publications that serve as the fundamental basis for the research and describes the author’s contributions.

2 CONTEXT AND RESEARCH NEED

The decarbonization of industries, i.e., the reduction and avoidance of carbon emissions, necessitates the adaptation of innovative technologies and approaches. Besides ecological concerns, economic and energetic factors play crucial roles in determining their potential for future integration. To effectively assess their impact across various dimensions at an early stage, there is a need for additional target-oriented methods and evaluation criteria so that the requirements of climate policy can be adequately addressed. This chapter examines the challenges of the rapidly evolving energy landscape, identifies flexible and low-emission technologies suitable for green energy transformation, and provides an overview of the existing assessment methods. Based on existing scientific knowledge, this chapter highlights areas that require further research.

2.1 Energy landscape in transition

Historically, industries have relied on fossil fuels like oil, natural gas, and coal as their primary energy sources owing to their affordability [25]. Many enterprises consider energy a peripheral concern, overshadowed by the core production value chain. However, the Russian invasion of Ukraine has brought energy procurement and its origins to the forefront. As a major energy supplier to the EU, Russia has offered abundant energy reserves at competitive prices [26]. Nonetheless, emerging bottlenecks in energy supply have led to increased energy costs and subsequent price hikes in various sectors, resulting in spillover effects. In this context, this means that high energy prices lead to price increases of products in other sectors such as food and materials. As a result, the concepts of resilience, independence, and diversity have gained significance in shaping EU energy import strategies.

In essence, resilience refers to a system’s ability to restore stability after experiencing disruptions [27]. Disruptions can be internal or external, such as the Russia-Ukraine War or the COVID-19 pandemic [28]. Enhancing energy supply’s diversity, independence, and flexibility can bolster the energy system’s resilience [27], [28]. Energy is essential to the operational cost structure, particularly in energy-intensive industries. Current events have led to a substantial increase in the inflation rate, leading to a slowdown in economic growth [29].

Figure 2-1 shows the analysis of historical spot market electricity prices from Energy Exchange Austria (EXAA), gas prices from Austrian Gas Clearing and Settlement (AGCS), and EUA from Energy Exchange Europe (EEX) until 2022, based on monthly averages. Gas and electricity prices were relatively constant and predictable until the end of 2020, ranging from 6 to 30 €/MWh (average: 18 €/MWh) and 18 to 62 €/MWh (average: 36 €/MWh), excluding taxes and fees, respectively. The COVID-19 pandemic and Russia's invasion of Ukraine had essential implications on energy prices, causing a substantial increase due to supply shortages. The peak prices occurred in mid-2022, with gas reaching 258 €/MWh and electricity reaching 482 €/MWh. Furthermore, the development of EUA within the EU ETS was examined. Although they remained relatively stable until the end of 2017, an upward trend began in 2018 and peaked in 2022, reaching prices of up to 90 €/t. Several factors contributed to this price escalation. Gas shortages led to substituting of other fossil fuels, such as coal, resulting in increased demand for EUA. Additionally, the defined emission caps within the EU ETS system played a role in driving up prices. Ongoing discussions surrounding the reform of the EU ETS, as part of the *Fit for 55 package*, further influenced these price trends [30], [31]. In addition to the EU ETS, several EU countries have implemented additional measures, such as carbon taxes, to mitigate GHG emissions [32], [33].

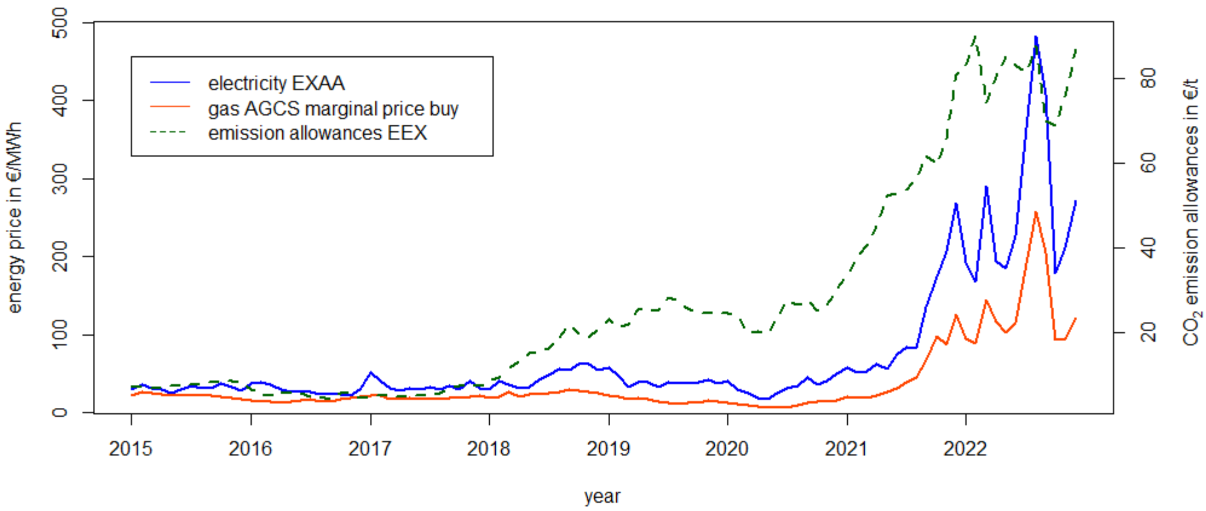

Figure 2-1: Analysis of historical energy and European Union Emission Allowance prices based on data from EXAA 2023 [34], EEX 2023 [35] and AGCS 2023 [36]

The massive change in pricing policy compared to previous years has served as a "wake-up call", driving the transition toward a renewable energy system [37]. While sustainability measures were previously implemented rather hesitantly for environmental reasons, the drastic price increases have now spurred the active pursuit of these measures. The transition to a renewable-based and energy-efficient economy represents a game-changing shift toward a more resilient, secure, flexible, competitive, independent, cleaner, and cost-effective energy system [5], [38]. The regulatory framework outlined in Section 1.2 aligns with the ambition to achieve a decarbonized EU economy. The *European Green Deal* and its associated initiatives have laid the foundation for this transformative journey, setting the course until 2050 [5].

2.2 Categorization of early-stage technologies and approaches

Assessing risks and the potential of new technologies and approaches is crucial for efficient implementation. The deployment of new technologies relies on their practicality and extensive testing to ensure their effectiveness. Any misjudgment in this process could result in a substantial cost loss and potential risks to human lives. To address this, a technology maturity rating scale was initially developed by the National Aeronautics and Space Administration (NASA) in the 1970s [39]. Over time, this scale has been adapted for various other applications, such as evaluating research projects within the *Horizon 2020 Framework Programme for Research and Innovation* [40] or the chemical industry [41]. Consequently, the scale is not only used for technologies but also concepts and sustainable approaches, reflecting a broader scope beyond individual technologies.

The primary purpose of the technology readiness level (TRL) framework is to assess the maturity of a technology or concept. It employs a numeric scale, ranging from TRL 1 (basic research) to TRL 9 (proven operation), as outlined in Table 2-1 [39]–[41]. This classification serves to enhance awareness and promote transparency, facilitating structured communication. It is worth noting that while certain established technologies may have already attained TRL 9, their ranking within the TRL framework may be substantially lower when applied in a new context or system. Therefore, defining the system boundary and establishing the corresponding TRL definition is crucial in the assessment process.

Emerging technologies and approaches can lead to significant disruptions in established industries. However, owing to the inherent uncertainty surrounding their long-term success, these technologies are typically categorized in the TRL framework during the R&D stage. These technologies and approaches often rely on funding to advance TRL and eventually reach the deployment stage.

Table 2-1: General description of technology readiness levels based on Mankins 2009 [39], European Commission 2014 [40] and Buchner et al. 2019 [41]

TRL	Stage	Description
1	Research	Basic principles observed
2		Technology concepts and/or applications formulated
3		experimental proof of concept
4	Development	Technology validated in the laboratory environment
5		Technology validated in the relevant environment
6		Technology demonstrated in the relevant environment
7	Deployment	System prototype demonstration in the operational environment
8		System complete and qualified through demonstration
9		System proven through successful operation in the relevant environment

2.3 Green energy transformation measures

The key pillars of decarbonization encompass elements such as energy efficiency, renewables, electrification, hydrogen and hydrogen-based fuels, bioenergy, CCS/CCU, and behavioral change. In the short and medium terms (up to 2030), renewable energy and energy efficiency are expected to achieve the necessary emission reductions substantially. Contrarily, electrification, hydrogen, and CCS/CCU are considered more relevant for the longer term (up to 2050) [42]. The subsequent sections of this discussion address the impact of energy efficiency measures and the integration of renewables in the industrial sector. Additionally, they provide an overview of flexible and low-emission technologies that capitalize on these measures.

2.3.1 Energy and resource efficiency

The principle of "energy efficiency first" and resource efficiency are top priorities [43] that must be implemented in all industrial sectors to mitigate climate change [44]. The rise in energy prices has increased consumer awareness, which has spurred investments in energy efficiency [45]. The Best Available Technology Reference Document (BREF) on energy efficiency elaborates on calculation methods and several measures for improvements [46]. There is a notable lack of consensus in the literature concerning the definition and measurement of energy efficiency, resulting in conflicting and misinterpreted findings. Energy efficiency can be defined and evaluated from various perspectives [47], [48] as follows:

- **Technological:** Improved energy performance of a particular technology,
- **Energy system:** Reduction of energy intensity for a plant, industrial sector, or an economy like the EU-27,
- **Economical:** Energy productivity (evaluation of energy input compared to economic output),
- **Environmental:** Mitigation of climate change, and
- **International:** Ratio of energy to gross domestic product.

The energy efficiency target in EU-27 for primary and final energy consumption was initially set at 32.5% by 2030, compared with the projected energy consumption for 2030 in 2007 [18]. The *REPowerEU* plan incorporates energy savings as one of its key pillars, emphasizing the importance of reducing energy consumption. The plan targets achieving a 13% reduction in energy compared to the levels recorded in 2020. This reduction corresponds to substantial decreases of 41.5% and 39% in primary and final energy consumption, respectively, compared to the levels in 2007 [21]. However, it is essential to consider the potential direct and indirect rebound effects when implementing economy-wide energy efficiency measures. These rebound effects have the potential to diminish the expected energy savings. The literature suggests that current global energy projection models may underestimate the growth in global energy demand [49], [50].

The industrial sector offers numerous sector-specific measures to enhance energy and resource efficiency, as detailed in specific BREFs [51]. The recovery and reuse of by-products is one of the most important general cross-sectoral measure. In the EU, the estimated annual technical waste heat potential exceeds 300 TWh, which is categorized by the temperature level and industry. This potential can be directly used, upgraded, or reused in heat-to-power applications [52]. However, it is crucial to consider the general utilization of waste heat and its suitability for specific processes based on the current temperature level and exergetic content. A cascading approach is essential for maximizing efficiency, in which space heating and hot water provision are considered the final steps on the ladder. Internal and external waste heat utilization, including district heating systems, offer pathways for improved energy efficiency. The economic feasibility of these measures is a prerequisite for successful implementations [9].

2.3.2 Renewable energy integration

RES can be integrated in different ways and adapted to the specific requirements of each industrial sector and local conditions. The use of biomass and biogas as fossil fuel substitutes and renewable electricity, such as solar, wind, and hydro, are typical approaches [44], [53]. Renewable electricity can subsequently be used to produce hydrogen or for power-to-X (PtX) applications [54]. Industrial companies have several options to increase the renewable energy share in their energy supply chain. They can opt for green electricity tariffs with a guarantee of origin, install on-site renewable assets, or explore emerging power purchase agreements (PPAs) such as those involving solar or wind energy. PPAs are long-term contracts between a supplier and a consumer, establishing either a physical or non-physical (virtual) connection to the consumer [55]–[58]. These contracts typically outline the energy price, duration of supply, and whether the supply is based on a fixed volume or "as produced [57], [59] . The latter option is often more cost-effective, but it requires greater flexibility on the consumer side to manage the fluctuations in electricity supply. Storage technologies, however, can help balance the supply and demand dynamics [60].

In the future, investments in grid infrastructure adaptation will be crucial to accommodate the growing deployment of renewable generation capacities and the increasing demand for flexibility. Owing to the increased electrification of the industry, current power grids are rapidly reaching their performance limits [61], [62]. However, physical PPAs with a private direct line to the consumer and local use of volatile energy can positively contribute to grid stability and avoid bottlenecks in transmission networks compared with non-physical PPAs.

2.3.3 Flexibility and low-emission technologies

The industrial sector requires flexible and low-emission technologies to achieve established emission-reduction targets. Fossil-fueled energy systems are typically well-suited for providing flexible energy and accommodating part-load operation. However, they emit GHG emissions that must be avoided. Innovative technologies must possess flexibility and adaptability to integrate intermittent RES effectively to reduce dependence on and consumption of fossil fuels

Despite its importance, there is currently no standardized definition of flexibility within the energy industry [63]. The literature provides various dimensions and definitions of flexibility, including the system's ability to adapt [64], to serve a higher purpose driven by incentives [65], and its role as a competitive advantage in achieving economic profitability and decarbonization [66]. Multiple definitions have been examined explicitly for power systems [67], considering characteristics such as flexible generation and operation, flexible demands, energy storage, grid infrastructure expansion, and adaptations to market design due to the increasing variability of resource capacities [68]–[70]. Recognizing the industry's significant contribution to energy flexibility, the *Verein Deutscher Ingenieure* (VDI) has released guidelines for energy-flexible factories in recent years [71], [72]. Demand-side management (DSM) measures, triggered by price signals or grid stabilization requirements, are often applied to strategically adjust loads and balance supply and demand [66], [73]. However, flexibility does not necessarily refer only to the use of electricity, but also to the generation of heat and the use of various raw materials. Consequently, based on the work of Puschnigg et al. 2023 [74], a derived interpretation of flexibility in the industrial context can be formulated as follows:

a) **Flexible products and production processes:** What is produced and when?
b) **Flexible energy supply:** How and when the energy (electricity and heat) is provided? What energy generation assets are used? How can fluctuating generation from renewables be integrated?
c) **Flexible adaption of energy assets:** How fast can they adapt to changed circumstances?
d) **Flexible resources:** Which are generally suitable? Can they be used as substitutes for fossil fuels? Are local conditions considered?

To meet decarbonization targets in the industry, adaptation of low-emission technologies and flexibility measures is crucial. As existing energy supply chains are predominantly fossil-based, a gradual transition is necessary, integrating RES, leveraging flexibility options, and implementing energy efficiency measures. A substantial amount of emissions can be reduced by fostering flexible interaction between established fossil fuels and renewable systems, setting the path towards a carbon-neutral industry.

Table 2-2 provides an overview of established flexible and new low-emission technologies. Combined heat and power (CHP) plants and heat-only boilers (HOBs) are established fossil-driven energy assets, and power-to-heat technologies such as heat pumps, electric boilers, and PPAs enable increased integration of renewables (especially surplus renewable electricity). Storage technologies (electrical, thermal, chemical, and mechanical) must be appropriately selected depending on the application and by considering typical characteristics, such as cost, storage duration, capacity, density, and efficiency. Biomass and biogas provide fuel flexibility, and can be used as substitutes for fossil fuels. In addition, Organic Rankine Cycle (ORC) can use waste heat to produce electricity.

The production of hydrogen or synthetic natural gas (SNG) via renewable power and electrolysis (i.e., power-to-gas, PtG) is widely recognized as a vital decarbonization method across various sectors, serving as both a fuel and chemical feedstock [42], [75]. However, market penetration is limited owing to the high costs associated with electrolyzers, production, transport, and necessary infrastructure investments [76]. Nevertheless, future predictions indicate substantial potential for cost reduction through upscaling effects and technological advancements [54]. Furthermore, the operation of electrolyzers can yield synergistic benefits, such as waste heat utilization in district heating networks, unlocking future possibilities for sector coupling [77].

CCS/CCU is anticipated to play an important role in decarbonizing the industries, particularly in sectors where decarbonization poses crucial challenges, such as the mineral industry [76]. Several technologies are currently in the development and demonstration stages and may be selected based on the specific stream properties of the industrial process. The TRL for diverse capture technologies is between TRL 3 and 9, for storage between TRL 2 and 9, and for utilization at TRL 6 [78].

Table 2-2: Industrial energy flexibility and low-emission technologies based on Puschnigg et al. 2023 [74]

Classification	Technology	Impact on flexibility	Description	Source
Flexible industrial generation asset	CHP (fuel-to-power-and-heat)	Possible substation units and corresponding planning, flexibility provider	Provides the main share of electricity and heat for industrial operation, part-load operation possible under certain technical limitations	[79]–[81]
	HOB (fuel-to-heat)	Possible substation units and corresponding planning, flexibility provider	Mostly used as a backup for the CHP plant, allowing for immediate operation when needed	[80], [81]
	ORC (heat-to-power)	Possible substation units and corresponding planning, flexibility provider	Utilizes wasted heat for electricity provision and part-load operation possible	[82], [83]
	Fuel resources	Possible substation units and corresponding planning, flexibility provider	Flexible input of biomass as an alternative fuel for combustion processes	[84], [85]
Flexible industrial demand asset	Electric boilers (power-to-heat)	Possible substation units and corresponding planning, flexibility provider	Usually operated in conjunction with a conventional energy supply system as a backup or support measure, frequently used for coupling to short-term energy markets or the secondary control energy market	[86]
	(High)-temperature heat pumps (power-to-heat)	Possible substation units and corresponding planning, flexibility provider	Less (electric) energy and thus less high-exergy energy sources are needed to provide the same amount of heat compared to electric boilers; suitable heat sources: ambient air, groundwater, and industrial waste heat streams; Temperatures of up to 160 °C are currently feasible.	[87]
	Flexible manufacturing assets	If free production capacities or material storages exist with corresponding planning, flexibility provider	Production on stock and demand, shutdown or partial load operation of production, demand-side management	[6], [81], [88]
Storage	Thermal	Allows temporal decoupling of supply and demand, flexibility provider	Sensible, latent, thermochemical, and sorption storage technologies	[89]

	Electrical	Allows temporal decoupling of supply and demand, flexibility provider	Batteries and supercapacitors	[68], [90]
	Mechanical	Allows temporal decoupling of supply and demand, flexibility provider	Flywheels, compressed air, and pumped hydro	[90]
	Chemical	Allows temporal Decoupling of supply and demand, flexibility provider	Power-to-X and renewable gases	[54], [91]
Contract	PPAs	Increasing need for flexibility in electricity consumption when integrated	Agreement between an electricity supplier and a consumer, such as for solar or wind electricity	[55]
Organization	Planning	Providing flexibility	Find optimal operation schedules for economic, ecologic, and other frame conditions, e.g., by optimization	[67]

2.4 Environmental life cycle assessment in industries

Life cycle assessment (LCA) is an evaluation approach and tool for determining the environmental impacts of products, services, or technologies [92]–[94]. It has become a widely recognized tool in the industrial sector to improve the sustainability of production systems [94], [95] or to compare systems and select the option with the lowest environmental burden [97]. In LCA, all flows of materials and energy, emissions, and waste are quantified and accounted for a defined system. LCA considers the following aspects [93], [98]:

- impacts throughout the life cycle (production, use, and end-of-life phases),
- impacts in upstream supply chains (resource extraction and transportation),
- impacts of emitted substances and extracted resources.

The aim of LCA is to [93], [98]–[100]:

- assist decision makers with detailed information on the environmental impacts of products, services, and technologies.
- identify the environmental impacts of green energy transition measures on the way to a decarbonized industry.
- ensure a safe and affordable future for humanity.

LCA plays a pivotal role in promoting sustainability, leading to the recommendation or requirement of its use in various regulations and directives. Typical examples include the EU directive on energy-related products [101], the EU waste framework directive [102], and the

EU framework for facilitating sustainable investment [103]. Given these circumstances, LCA has become a driving force behind government policies and the pursuit of sustainable development [95], [104]. Consequently, LCA can provide valuable insights into analyzing emerging low-emission technologies and waste utilization from a circular economy perspective. It also offers initial results on innovative approaches to decarbonizing the industry.

Different regions may adopt various LCA software applications based on their specific needs. Commonly used LCA software programs include GaBi, SimaPro, Umberto, Brightway, openLCA, eBalance, LCAiT, PEMS, TALLY, IMPACT, and eTool [104], [105].

2.4.1 Types of life cycle assessment approaches

Attributional and consequential LCA are two commonly used LCA classifications. Attributional LCAs focus on providing information about the environmental burden associated with a specific product, and aim to attribute that burden proportionally. Conversely, consequential LCAs aim to assess the environmental consequences of a decision or action by considering the broader impacts resulting from that decision [106], [107].

In traditional LCAs, static approaches are commonly employed, assuming the current situation will remain unchanged [108]. However, there is a growing interest in dynamic approaches that consider time-dependent impacts, taking into account expected technological advancements [109], variations in operation over the product's lifetime [110], changes in the life cycle inventory (LCI) [111], [112], and adjustments in impact assessment methods [113]. For future LCA studies, considering GHG emission variability resulting from expanding renewable energy technologies is recommended [114], as elaborated further in Section 2.4.3.

In addition to environmental LCA, other methods, such as life cycle costing (LCC) and social life cycle analysis (S-LCA), are used. S-LCA assesses societal impacts throughout the life cycle, while LCC considers investment and operational costs. By combining these three methods, a comprehensive life cycle sustainability assessment (LCSA) can be achieved [115], [116]. Consequently, integrated LCAs that include other methodologies like techno-economic analysis (TEA) and simulations are gaining popularity, enabling holistic analyses beyond environmental impacts [117]–[120].

2.4.2 Life cycle impact assessment

Life Cycle Impact Assessment (LCIA) is a process that assigns the mass and energy flows of a system to specific impact categories using characterization factors [121]. Initially, parameters are classified based on their impact categories, such as CO_2, CH_4, and N_2O, for global warming. Subsequently, characterization is performed, where CO_2-eq. is calculated for the global warming category. There are various approaches and methods for quantifying impacts in LCIA, depending on the impact categories and geographic region [122]. Commonly known LCIA methodologies include CML (Centrum voor Milieukunde Leiden), ReCiPe, IPCC (Intergovernmental Panel on Climate Change), TRACI (Tool for the Reduction and Assessment of Chemical and other environmental Impacts), ILCD (International Life Cycle Data system), Eco-indicator 99, World Impact+, and LCImpact [123]. The characterization can be performed using a midpoint or endpoint approach, with the midpoint approach generally recommended by the environmental guidelines [124]. Midpoint characterization focuses on environmental impacts through substance emissions, whereas endpoint categories focus on effects on ecosystems, human health, or natural resource depletion [99], [123].

Table 2-3 presents the midpoint impact categories based on the CML impact methodology utilized in this thesis. Impact categories include global warming, toxicities, acidification, eutrophication, and resource depletion. CML has undergone rigorous scientific evaluation and validation, hence providing methodological robustness. It is widely recognized and accepted within the scientific community for its comprehensive coverage of environmental impacts and is applicable to the study context, its system boundaries and geographical location.

Table 2-3: Overview of midpoint categories used in the CML method and their corresponding equivalents

Impact category	Unit
Abiotic depletion (ADP elements)	kg Sb-eq.
Abiotic depletion (ADP fossil)	MJ
Acidification potential (AP)	kg SO_2-eq.
Eutrophication potential (EP)	kg Phosphate eq.
Freshwater aquatic ecotoxicity potential (FAETP)	kg DCB-eq.
Global warming potential 100 years (GWP 100)	kg CO_2-eq.
Global warming potential 100 years excluding biogenic carbon (GWP 100 e.b.)	kg CO_2-eq.
Human toxicity potential (HTP)	kg DCB-eq.
Marine aquatic ecotoxicity potential (MAETP)	kg DCB-eq.
Ozone layer depletion potential (ODP)	kg R11-eq.
Photochemical ozone creation potential (POCP)	kg ethene eq.
Terrestrial ecotoxicity potential (TETP)	kg DCB-eq.

GWP is the most discussed indicator in the industry because of the use of carbon-intensive fossil fuels. However, other impact categories are important and must be addressed through a comprehensive analysis. An appropriate framework and tools for integrating various criteria in a comprehensive analysis are introduced in the methodology Chapter 4 in Section 4.8.

2.4.3 Energy modeling in life cycle assessment

The emissions associated with energy supply vary depending on geographical conditions. Countries with a higher ecological energy footprint (for heat or electricity) tend to have higher emissions for the corresponding products. Average static energy footprints, in this thesis obtained from the GaBi Professional database [125], are commonly used in LCA studies. For instance, the average carbon footprint of the public electricity grid in Estonia is 950 gCO_2-eq./kWh, while in Austria, it is only 291 gCO_2-eq./kWh, primarily due to the high share of hydropower [125]. Therefore, the carbon footprint of heat and electricity provision is influenced by the energy source's origin and varies among countries based on their energy source composition.

As RES are increasingly integrated into energy supply chains, carbon footprints exhibit greater seasonal and daily fluctuations. Figure 2-2 illustrates the boxplot analysis of electricity carbon footprints for selected EU countries, with a time resolution of one hour, showing their annual fluctuations in 2021. The carbon intensity indicates the amount of CO_2 emitted to generate one kWh of electricity. With its substantial hydropower capacities, Iceland has the lowest carbon footprint and minimal fluctuations, with a median of 27.9 gCO_2-eq./kWh. Spain and Austria also utilize RES but still rely on fossil fuels, resulting in median carbon footprints of 156.8 CO_2-eq./kWh and 190.4 gCO_2-eq./kWh, respectively. With a predominantly fossil-based electricity system, Estonia exhibits the highest carbon footprint, with a median of 523.5 gCO_2-eq./kWh, and experiences fluctuations mainly driven by fossil fuel use. Comparing the median values with the average values from the GaBi Professional database [125], Austria demonstrates a reduction of approximately 46%, while Estonia shows a reduction of approximately 45%.

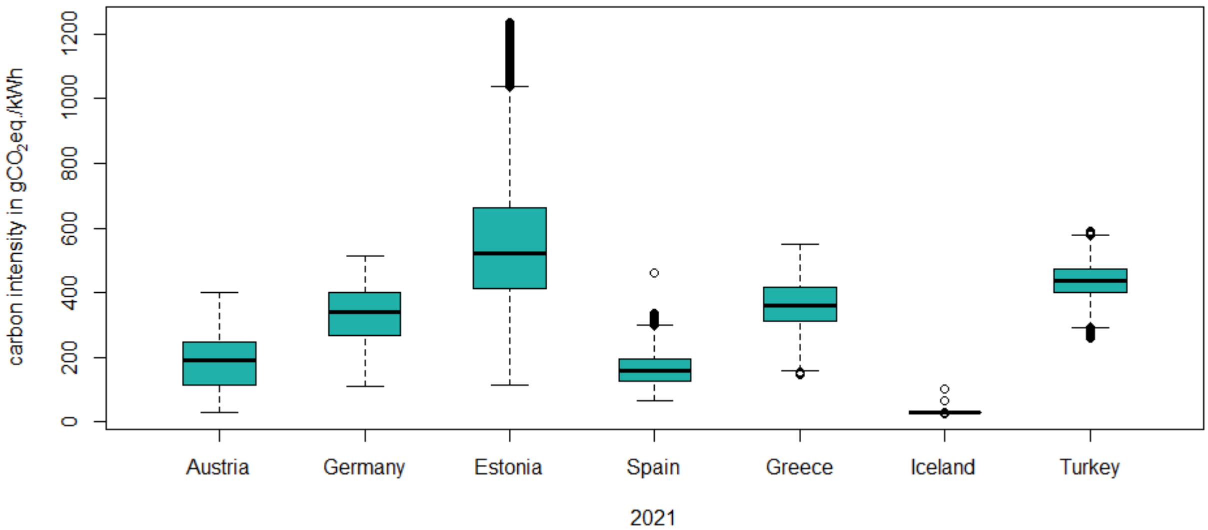

Figure 2-2: Comparison of carbon intensities in selected European countries in 2021 based on evaluated data from Electricity Map 2021 [126]

A more detailed analysis of carbon intensities was conducted in Austria. Figure 2-3 depicts the annual fluctuations in 2021, along with the day-ahead prices from European Power Exchange (EPEX SPOT) and EXAA for 2019 and 2021, respectively. The aim was to gain further insights into the variations of carbon intensities throughout the year and explore any potential correlation with prices. In the first and last months of the year, carbon intensities were high, while they decreased during the summer months. This pattern is typical for Austria, where fossil fuels are predominantly used during colder months, and RES contribute more substantially in the summer. It is evident that low prices in the early months of 2021 did not imply low carbon intensity. Although a correlation can be observed due to the price increase towards the end of 2021, it should be noted that the 2019 prices do not directly correlate with Austria's typical carbon profile. As the energy market undergoes essential changes and is characterized by uncertainties, it is important to monitor these trends as they may evolve in the future.

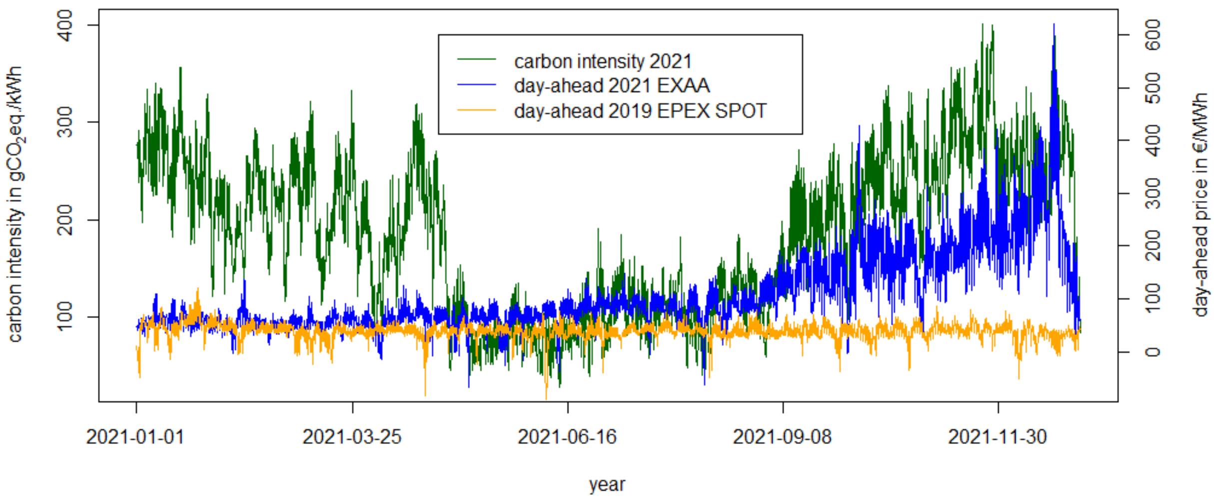

Figure 2-3: Carbon intensity of Austria and day-ahead prices based on evaluated data from Electricity Map 2021 [126]

A heat map was created for Austria and Germany to provide a deeper understanding of daily carbon fluctuations (Figure 2-4). It displays carbon intensities with a time resolution of one hour over a year, offering insights into daily and seasonal variations. This information can help industries to flexibly design and optimize their production processes by operating at full load during periods of low emissions and adjusting processes to partial load or shutdown when emissions are high. These results indicate the reduced ecological footprint of the product.

The heatmaps for Austria and Germany illustrate favorable production windows during the summer months (indicated by blue cells). However, it is important to note that extreme weather events such as floods, droughts, or cold waves can impact carbon intensities. The red cells representing high-intensity periods primarily occur in winter and at night when fossil fuels are used to meet electricity demand. Considering the wide range of carbon intensities observed, there is a need for an LCA approach that accounts for these fluctuating characteristics.

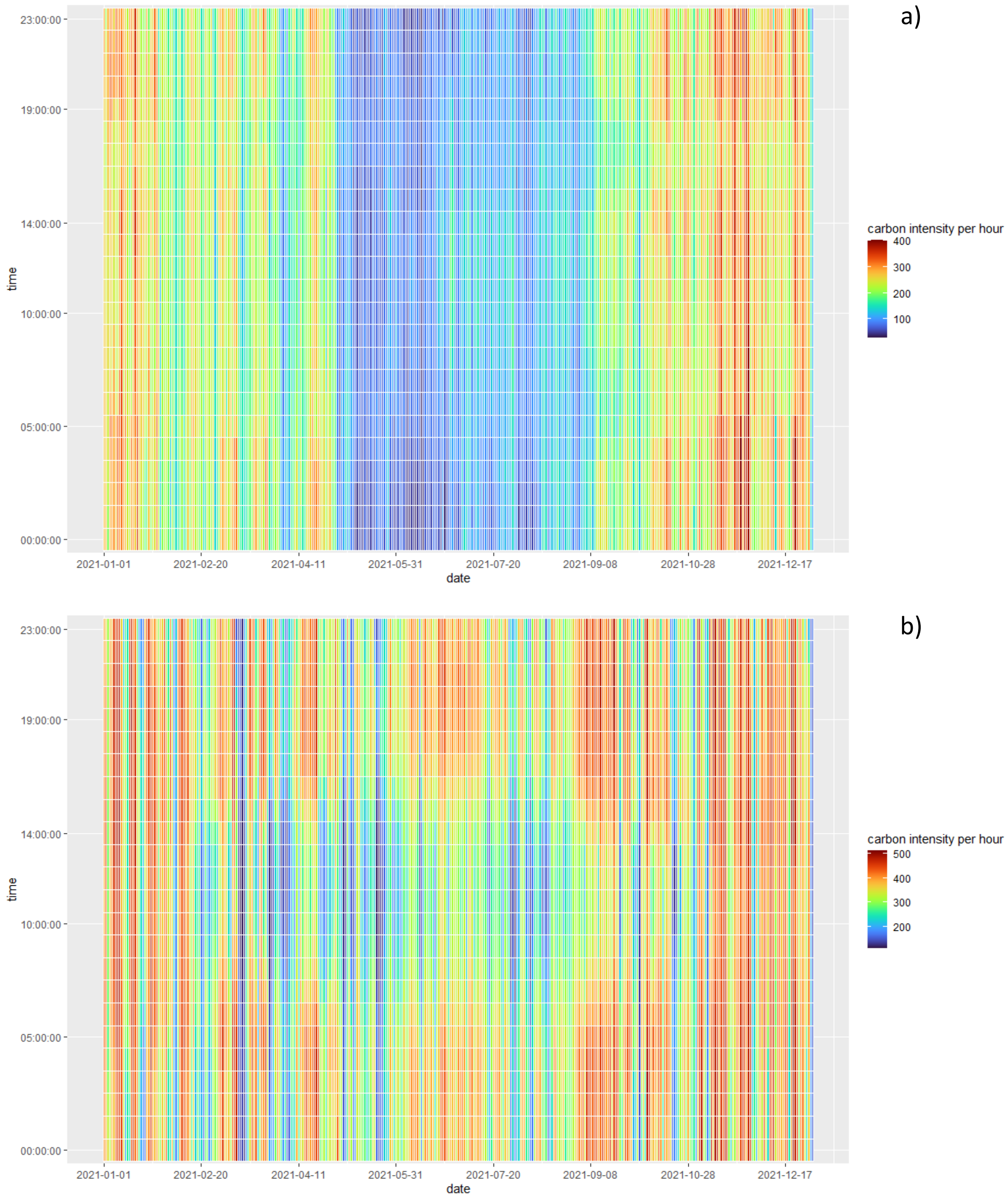

Figure 2-4: Carbon intensity of (a) Austrian and (b) German electricity production in 2021 based on Puschnigg et al. 2023 [74] and Electricity Map 2021 [126]

2.5 Energy and exergy as design criteria

Energetic and exergetic evaluations serve as design criteria for process and product developments [127], [128]. Energetic evaluations are based on the first law of thermodynamics, which ensures energy conservation. Exergetic analyses adhere to the second law of thermodynamics and consider working capacity. In this context, energy can be divided into anergy and exergy, with the sum of energies remaining constant [129].

The exergetic component represents the deviation from the thermodynamic equilibrium state of a reference system (determined by temperature and pressure), while the anergy portion is already in equilibrium with the reference system and cannot be further utilized. Exergy can be classified according to energy carriers, such as thermal energy, mechanical or electric energy, and chemical energy. The exergy from mechanical and electric energy is 100% exergy, while the exergy fraction from thermal and chemical energy is determined relative to the reference system. In material stream analyses, exergy is typically categorized as physical, chemical, kinetic, and potential exergy [130], although kinetic and potential exergy are often disregarded due to their minimal impact [131].

As an example, in Figure 2-5, the energetic and exergetic heat demand per temperature level was calculated for the Austrian industry. The exergy share of the total energy demand is approximately 57%, and the remaining share is anergy (Puschnigg et al. 2021 [89]).

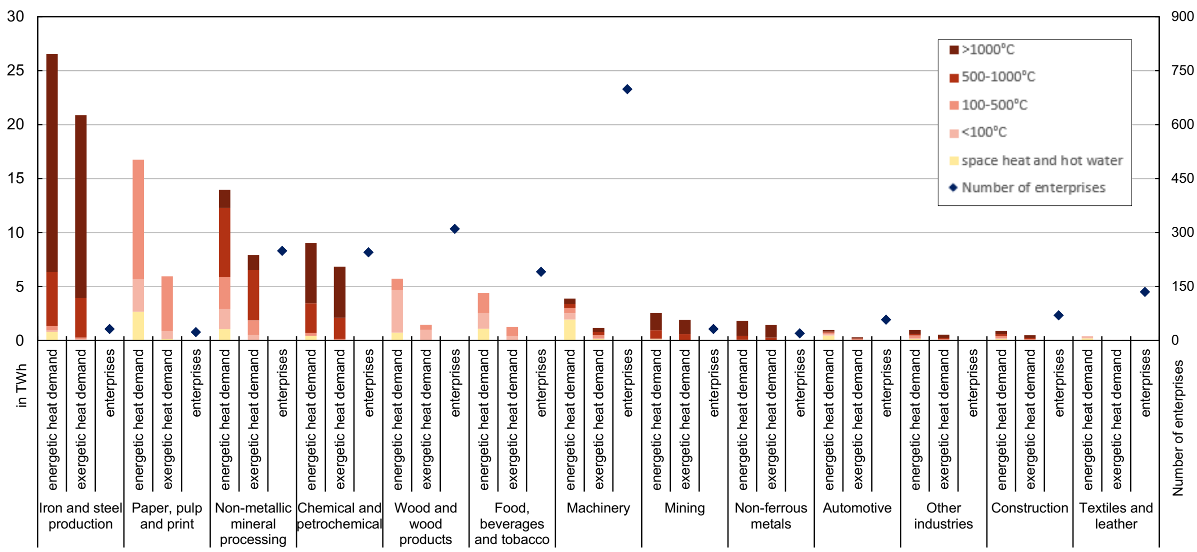

Figure 2-5: Estimated energetic and exergetic heat demand per industrial branch based on Puschnigg et al. 2021 [89]

The energy balance of a defined system is calculated according to Equation (2-1) [128]:

$$\sum_{in}\dot{E}_{en,i}+\sum_{in}\dot{E}_{en,j}^{Q}+\sum_{in}\dot{E}_{en,k}^{W}=\sum_{out}\dot{E}_{en,pr}+\dot{E}_{I.,en,l} \qquad (2\text{-}1)$$

where $\sum_{in}\dot{E}_{en,i}$ is the input energy flow for materials; $\sum_{in}\dot{E}_{en,j}^{Q}$ represents thermal energy; $\sum_{in}\dot{E}_{en,k}^{W}$ is work; and $\sum_{out}\dot{E}_{en,pr}$ are the output energy flow rates of the products; and $\dot{E}_{I,en,l}$ are the total energy losses.

Similar to the energy balance, the exergetic balance is formulated according to Equation (2-2) [127]:

$$\sum_{in}\dot{E}_{ex,i}+\sum_{in}\dot{E}_{ex,j}^{Q}+\sum_{in}\dot{E}_{ex,k}^{W}=\sum_{out}\dot{E}_{ex,pr}+\dot{E}_{I,ex,l} \qquad (2\text{-}2)$$

where $\sum_{in}\dot{E}_{ex,i}$ is the input exergy flow rate of the materials, $\sum_{in}\dot{E}_{ex,j}^{Q}$ is the thermal exergy, $\sum_{in}\dot{E}_{ex,k}^{W}$ is the work, and $\sum_{out}\dot{E}_{ex,pr}$ is the output exergy flow rate of the products, and $\dot{E}_{I,ex,l}$ is the total exergy loss.

Industrial production processes result in energy and exergy loss. However, a more detailed analysis of these losses in the respective production processes offers potential for process and system improvement. By understanding where the losses occur, more targeted measures can be derived. Exergetic evaluations go beyond energy assessments and involve in-depth work-related analyses to increase the efficiency. An appropriate framework for integrating energetic and exergetic analyses in a comprehensive evaluation framework is introduced in Chapter 4 (methodology), and discussed explicitly for decision-making based on multiple criteria in Section 4.6.

2.6 Techno-economic considerations

TEA can be used to assess the potential of new technologies, products, and approaches at an early stage [132]. An early examination of economic feasibility is advisable to avoid dead ends. TEA is a widely established tool in the industry, mainly focusing on the production phase [118]. It informs decision makers on research and development issues and enables the formation of investment decisions based on an understanding of the economic and technical perspectives [133]. Compared with the LCC methodology, which focuses heavily on life cycle costs, TEA is considered an investor tool for profitability assessment as it can vary design parameters and address technological aspects [118]. Decision-making should incorporate multiple criteria for sustainable development and not be solely based on TEA, LCC, or LCA [134]. However, it is currently common to apply TEA and LCA independently, instead of using synergies [120]. Nevertheless, weighing both advantages and disadvantages leads to better-informed decisions [135], as introduced in the integrated assessment framework in Chapter 4.

2.7 Research need

The transition of the energy landscape and the ambitious decarbonization targets set by the EU pose challenges for energy-intensive industries. Establishing sustainable, reliable, and competitive energy systems is crucial to shift from fossil-based to renewable energy systems. By diversifying energy sources, increasing the use of RES, and enhancing the flexibility of the energy supply, the dependence on fossil fuels and energy imports can be reduced. This shift is further amplified by measures that improve primary energy and resource efficiency, such as waste heat recovery and the valorization of waste streams. The industry's transformation from fossil-fueled and emission-intensive processes to green and sustainable practices relies on adopting emerging low-emission technologies and innovative approaches centered around circularity, flexibility, and renewable feedstock. Integrating RES into industrial operations is becoming increasingly important, necessitating flexible production and energy systems that can adapt to changing emissions dynamics. To effectively evaluate the environmental impacts of various sustainability measures in the industry, LCA emerges as a crucial assessment method. LCA allows the quantification of the environmental effects of different measures at an early stage, facilitating the transition toward industrial climate neutrality by 2050. However, to fully comprehend the potential of decarbonization approaches on a holistic level, a comprehensive multi-criteria assessment encompassing technological, economic, and energetic aspects is required, calling for further investigation and research. Chapter 3 outlines the research questions, targets, and approaches.

3 RESEARCH AND THESIS APPROACH

The demand for emerging low-emission technologies and innovative approaches to decarbonizing industries was outlined in the previous chapter. Appropriate methods are needed to analyze the associated environmental impacts at an early stage that can align with short-, medium-, and long-term policy targets. Complementary economic and energetic evaluations will lead to a holistic assessment of the feasibility of integration. The following chapter provides the derived research objectives, elaborates on the pursued research approach, and describes the structure of the research.

3.1 Research objective

This research aims to support the transition to green industry using suitable methods and feasibility assessments aligned with policy targets. By carrying out adequate assessments and potential analyses at the system level, sustainable transformation pathways can be identified at an early stage and dead ends can also be prevented. A comprehensive analysis from different perspectives would enable a multidisciplinary and holistic assessment approach. This enables the early identification of potential hotspots, whether caused by ecological, economic, or energetic factors, and the derivation of appropriate countermeasures. The following research questions were identified based on the research objectives:

- How can life cycle assessment methodology contribute to a more accurate analysis of measures and technologies to improve environmental performance in the industry?
- How can life cycle assessment be applied to support the engineering and set-up of sustainable industrial production facilities?
- How can increased dynamic energy generation, and hence the emission profile, be accounted for in environmental analyses of industries?
- How do energetic, exergetic, and techno-economic assessments provide conclusions complementary to environmental analyses?

3.2 Peer-reviewed research publications

This thesis adopts a cumulative approach, drawing on peer-reviewed publications, to address the research objectives and questions. Section 3.2.1. provides an overview of the selected publications that were considered relevant for discussing and answering the research questions. Section 3.2.2 lists additional publications published during this scientific work.

3.2.1 Relevant publications

The cumulative approach of this thesis is based on four articles, from A1 to A4. Throughout the sections, these published articles are labeled to ensure a coherent understanding. Stefan Puschnigg is the main author of A1, A2, and A3, while in A4, where the authors were ranked by institution, he contributed as a co-author. A comprehensive authorship statement and detailed description of each author's contribution to every article can be found in Appendix B. The published articles A1 to A4 are included in Appendix B, each presented in their respective journal styles.

The published research articles[1] are as follows:

A1 Puschnigg, Stefan; Knöttner, Sophie; Lindorfer, Johannes; Kienberger, Thomas: "Development of the virtual battery concept in the paper industry: Applying a dynamic life cycle assessment approach," Journal of Sustainable Production and Consumption, volume 40, 2023, https://doi.org/10.1016/j.spc.2023.07.013
Source: Puschnigg et al. 2023 [74]

A2 Puschnigg, Stefan; Fazeni-Fraisl, Karin; Lindorfer, Johannes; Kienberger, Thomas: "Biorefinery development for the conversion of softwood residues into sustainable aviation fuel: Implications from life cycle assessment and energetic-exergetic analyses," Journal of Cleaner Production, volume 386, 2023, https://doi.org/10.1016/j.jclepro.2022.135815
Source: Puschnigg et al. 2023 [85]

A3 Puschnigg, Stefan; Lindorfer, Johannes; Moser, Simon; Kienberger, Thomas: "Techno-economic aspects of increasing primary energy efficiency in industrial branches using thermal energy storage," Journal of Energy Storage, volume 36, 2021, https://doi.org/10.1016/j.est.2021.102344
Source: Puschnigg et al. 2021 [89]

A4 Margaritis, Nikolaos; Evaggelou, Christos; Grammelis, Panagiotis; Yiannoulakis, Haris; Papageorgiou, Polykarpos; Puschnigg, Stefan; Lindorfer, Johannes: "Use of biomass as alternative fuel in magnesia sector," Fuels, volume 3, no. 4, 2022, https://doi.org/10.3390/fuels3040039
Source: Margaritis et al. 2022 [84]

[1] The reference number at the end of each publication is only for the purpose of entry in the reference list.

3.2.2 Additional related publications

This section lists additional peer-reviewed publications by the author that were published in parallel with the research activities of this thesis. The contents of these publications also deal with sustainable energy supply systems, but in a broader and more general context and can therefore only be considered supplementary to this thesis.

(1) Zeilerbauer, Lukas; Hubmann, Felix; Puschnigg, Stefan, Lindorfer, Johannes: "Life cycle assessment and shadow cost of steam produced by an industrial-sized high-temperature heat pump," Journal of Sustainable Production and Consumption, volume 40, 2023, https://doi.org/10.1016/j.spc.2023.06.016 [136]

(2) Volkova, Anna; Reuter, Stefan; Puschnigg, Stefan; Kauko, Hanne; Schmidt, Ralf-Roman; Leitner, Benedikt; Moser, Simon: "Cascade sub-low temperature district heating networks in existing district heating systems," Smart Energy, volume 5, 2022, https://doi.org/10.1016/j.segy.2022.100064 [137]

(3) Puschnigg, Stefan; Jauschnik, Gabriela; Moser, Simon; Volkova, Anna; Linhart, Matthias: "A review of low-temperature sub-networks in existing district heating networks: Examples, conditions, replicability," Energy Reports, volume 7, 2021, The 17th International Symposium on District Heating and Cooling, https://doi.org/10.1016/j.egyr.2021.09.044 [138]

(4) Moser, Simon; Puschnigg, Stefan: "Supra-regional district heating networks: A missing infrastructure for a sustainable energy system," Energies, volume 14, no. 12, 2021, https://doi.org/10.3390/en14123380 [139]

(5) Böhm, Hans; Moser, Simon; Puschnigg, Stefan; Zauner, Andreas: "Power-to-hydrogen and district heating: Technology-based and infrastructure-oriented analysis of (future) sector coupling potentials," International Journal of Hydrogen Energy, volume 46, no. 63, 2021, https://doi.org/10.1016/j.ijhydene.2021.06.233 [77]

(6) Moser, Simon; Puschnigg, Stefan; Rodin, Valerie: "Designing the heat merit order to determine the value of industrial waste heat for district heating systems," Energy, volume 200, 2020, https://doi.org/10.1016/j.energy.2020.117579 [140]

(7) Holzleitner, Marie-Theres; Moser, Simon; Puschnigg, Stefan: "Evaluation of the impact of the new renewable energy directive 2018/2001 on third-party access to district heating networks to enforce the feed-in of industrial waste heat," Utilities Policy, volume 66, 2020, https://doi.org/10.1016/j.jup.2020.101088 [141]

3.3 Thesis approach

A cumulative thesis approach based on peer-reviewed research articles (A1 – A4) was used to address the research objectives and research questions. Based on the final energy demand analysis in Figure 1-1, the top three energy-intensive industrial sectors were selected to (i) evaluate specific sustainable and emission-saving measures and (ii) develop an integrated LCA framework by combining environmental, techno-economic, and energetic perspectives. As shown in Figure 3-1, each article deals with one industrial sector and elaborates on specific measures and methods. The pulp, paper, and print industries are represented in article A1, and the chemical and petrochemical industries are represented in article A2. For the non-metallic mineral industry, two subindustries, cement and magnesia, were considered in articles A3 and A4, respectively.

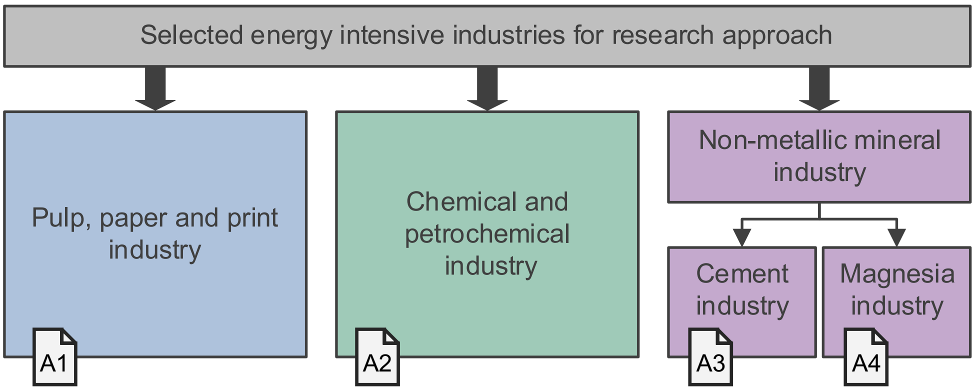

Figure 3-1: Overview of selected industries for thesis research approach

The following sections provide a compact overview of the main concepts, technological considerations, integrated measures, and main research targets for each industrial sector based on the information provided in Table 2-2. The research methods applied for different decarbonization approaches are introduced in Chapter 4.

3.3.1 Approach in the pulp, paper, and print industry

The virtual battery concept (VBC) was introduced, specifically applied for a site in the paper industry, but can be replicated in other industries as well. The main idea behind the VBC is to operate an industrial site as regional storage facility, which can either demand or supply energy based on local conditions, thereby contributing to the stability of the power grid. This involves considering the flexibility options of existing energy and production facilities at the industrial site and incorporating new flexible energy assets to increase the share of renewables, such as through PPAs. The TRL classification of the approach falls within the range of 3-5. The objective is to analyze the techno-economic and environmental impacts of various VBC scenarios on the energy supply chain and product. The VBC, paper production process, and considered system boundaries are comprehensively described in the original article A1;

therefore, the reader is referred directly to the article for more detailed information. A case study was conducted at a plant located in Germany.

3.3.2 Approach in the chemical and petrochemical industry

A lignocellulosic biorefinery was developed using softwood residues to produce isobutene, an intermediate chemical, which can be further processed into sustainable aviation fuel (SAF). The biorefinery aims to valorize all product streams along the value chain, creating additional value. The approach is classified as TRL 3-4. The main objective was to analyze the environmental sustainability of the conversion pathway and assess the impact of energy provision and by-product utilization through various biorefinery set-up scenarios. The conversion process, system design, and system boundaries are extensively described in the original article A2, and readers are referred to the article for a detailed description of the concept. The analysis was conducted using the energy characteristics of the EU-28.

3.3.3 Approach in the cement industry

The waste heat potential of a cement plant is recovered and utilized for process energy provision in a dairy located 1.5 km away. As the cement plant experiences planned and unplanned interruptions, thermal energy storage (TES) integration is considered, as the dairy operates continuously. This approach is classified as TRL 3-4. The aim is to examine the sustainability, primary energy savings, and cost-effectiveness of the concept, specifically focusing on TES compared to its fossil gas-driven benchmark. Readers are referred to the original article A3 for a detailed description of the concept. The cement plant is in Austria, so the analyses focus on Austria.

3.3.4 Approach in the magnesia industry

Pet coke is an important fossil fuel for magnesia production, leading to an essential share of GHG emissions along with carbon emissions from $MgCO_3$ decomposition. Substantial GHG savings can be achieved by substituting pet coke with alternative fuels such as biomass. The aim is to analyze the potential GHG reduction by co-firing various local biomass sources, including olive kernels (OK), wood sawdust (WSD), and sunflower husk pellets (SHP), in different mixtures and production processes. This approach is categorized as TRL 5–7. A detailed description of the process can be found article A4. The analysis was conducted on a magnesia plant in Greece.

4 METHODOLOGY

To analyze the integration potential of low-emission technologies and sustainable approaches in industries, a comprehensive evaluation of various perspectives is required, considering the environmental, techno-economic, and energetic aspects. To address these aspects, an integrated life cycle assessment (LCA) framework was developed, which is introduced in the following subsections.

4.1 Integrated life cycle assessment approach

An overview of the developed integrated LCA method is shown in Figure 4-1, which is based on the findings of research articles A1–A4. The methodology is structured into several *modules A to G*, which are elaborated in detail in subsequent sections.

In general, the methodology can be applied to:

- improve a system,
- improve a product,
- design and optimize a new or existing plant set-up.

Procedure: The method begins with *module A*, which is based on the classical LCA ISO 14040/14044 framework, after the application definition. The investigation's goal and scope are specified, and the system boundary is defined. In the subsequent life cycle inventory (LCI), the necessary mass and energy balances for the system under investigation are determined and then utilized for the life cycle impact assessment (LCIA). If data availability permits, *module B*, incorporating a dynamic energy modeling approach for electricity and heat provision, is integrated into the LCI, providing a more detailed and realistic representation of energy provision's time behavior. Once the ecological criteria are determined, additional influencing factors are evaluated in *module C*, considering energetic/exergetic aspects, techno-economic considerations, and environmental costs within the defined boundary conditions. Initial conclusions can be drawn from the preliminary results, and crucial influencing parameters are identified, which can be further analyzed through techniques like sensitivity analysis. *Module D* interprets the ecological results according to the GHG protocol commonly used in the industry. In *module E*, the comprehensively assessed criteria are qualitatively or quantitatively evaluated using multi-criteria analysis, and actionable recommendations are derived. When the specific and holistic results meet the set requirements and objectives, an improved system, product, or plant set-up is achieved. If further measures are necessary to achieve the set targets, *module F* identifies technological aspects and flexibility options. If potential modifications are identified, *module G* adjusts the processes accordingly and provides the modified data for the LCI. The adaptations in *module G* may also lead to changes in the energy load profiles in *module B*, requiring their reintegration. Through the modified LCI, a new evaluation scenario is created, and a reevaluation of the ecological, energetic/exergetic, and techno-economic implications is conducted. If, in *module E*, the findings of the new scenario indicate a further need for action, another scenario is defined and evaluated. This iterative analysis is performed until the desired results are achieved according to environmental, energetic, and techno-economic objectives.

Individual modules can also be used independently, allowing for reduced scope of work and effort. A complete iterative process does not always have to be executed. For instance, if the evaluation focuses on ecological aspects and GHG mitigation potential, applying only *module A* would be sufficient.

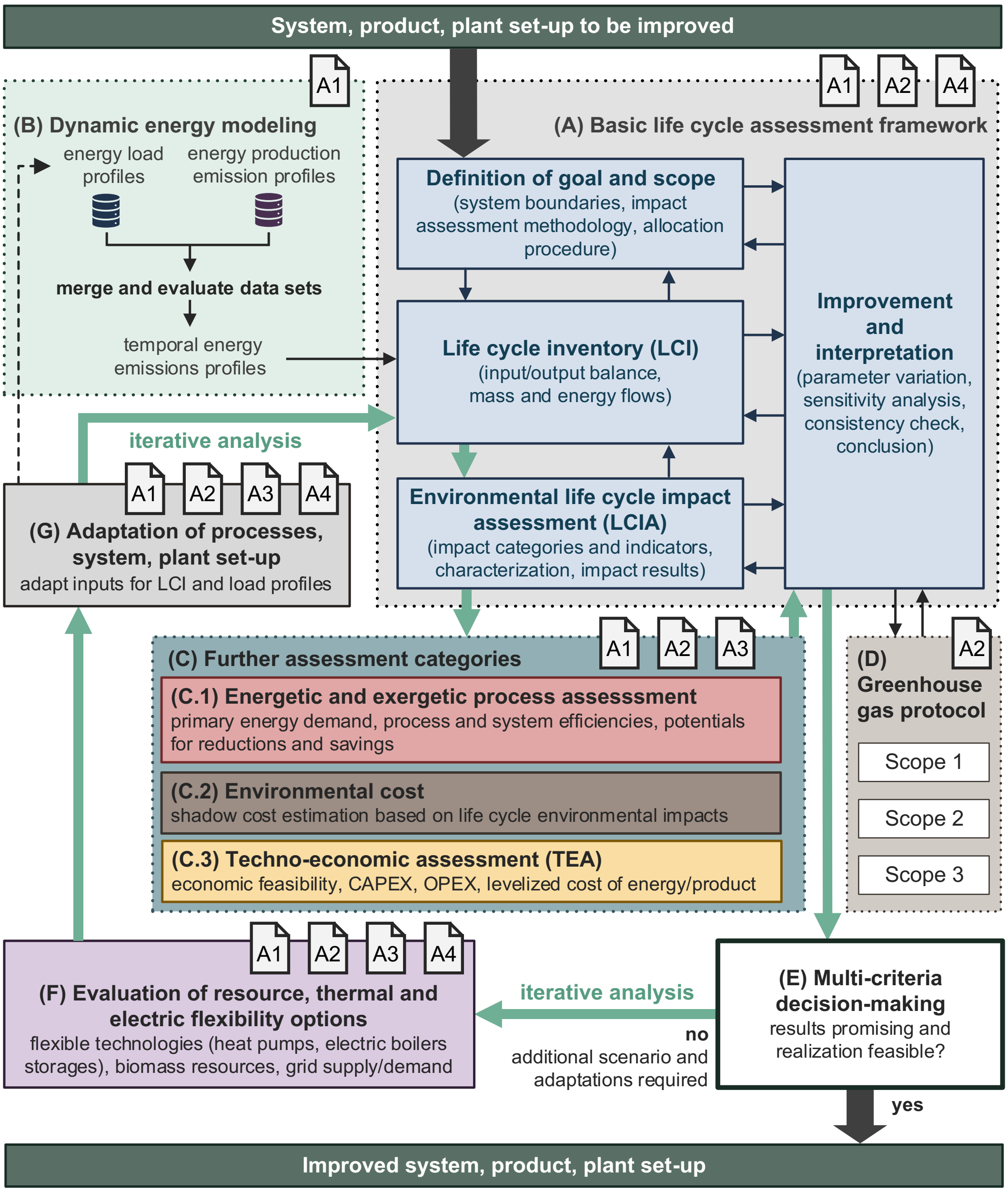

Figure 4-1: Integrated life cycle assessment framework for developing a sustainable and carbon-neutral industry

4.2 Basic life cycle assessment framework

Quantifying the environmental impacts of various sustainability measures is vital for the industry to meet climate targets. Environmental assessment is based on ISO 14040/14044 standards, which provide a LCA framework based on four steps: definition of the goal and scope, LCI, LCIA, and improvement and interpretation [93], [94]. The basic methodology is already well described in the literature [98], [121], [122], which is why only the essential information for the main steps is elaborated upon in the following sections. The software GaBi 10.6 ts by Sphera was used for environmental analysis [125].

4.2.1 Definition of goal and scope

In this step, the analysis begins by defining the goal and scope of the study and specifying the LCA. The purpose of the analysis and its intended use are explained. System boundaries are defined and additionally indicated whether it is a cradle-to-gate or cradle-to-grave analysis. The functional unit of evaluation is established, representing a specific quantity (e.g., 1 MJ, 1 kg, or 1 piece of a product). The geographical reference area is defined and allocation methods are discussed if necessary [93], [94], [98].

The functional unit is one of the most important characteristics, as all results will refer to it. As these aspects vary for each LCA and corresponding article (A1 to A4), detailed explanations can be found in the original articles in Appendix B. In short, the functional unit for the study of the paper industry was defined as 1 ton of produced paper and 1 MJ of energy provision (either electricity or heat), 1 MJ of fuel for the chemical industry, 1 ton of caustic calcinated or dead burnt magnesia (CCM or DBM) for the magnesia industry, and 1 GWh recovered waste heat for the cement industry.

Allocation procedures are applied when more than one product is produced within a LCA study (i.e., when there is a main product and by-products). Allocation and system expansion methods can be applied to allocate emissions to a specific product. The ISO 14040/14044 standards advise system expansion, but this practice leads to hardly manageable effort, as more data must be provided. Consequently, allocation methods based on energy, mass, or economic value are commonly employed in practical applications, following ISO 14040/14044 standards [93], [122], [142].

4.2.2 Life cycle inventory

The collection of all pertinent mass and energy balances within the specified system boundary is called the LCI. This step is critical, as it requires a high level of detail and transparency to produce high-quality results [93], [94]. Relevant LCI data for foreground and background processes can be sourced from established LCA databases like GaBi ts 10.6 Professional [125] and the Ecoinvent database [143], and through simulations, calculations, and demonstration cases. However, this task can be challenging since industrial data is typically sensitive and not always readily shared. Particularly for novel technologies and approaches, assumptions based on existing literature are often necessary to fill data gaps.

4.2.3 Life cycle impact assessment

As explained in Section 2.4.2, LCIA applies characterization factors to determine the environmental impacts for established impact categories, such as global warming, eutrophication, and acidification. This thesis used the established CML methodology, which is available in the applied LCA software GaBi 10.6 ts by Sphera. Special focus was given to the impact categories GWP and primary energy demand (PED), which are widely debated in the industry and are often considered key performance indicators (KPIs). As the focus in this thesis is on GWP, a robustness analysis of the results was conducted by comparing the GWP CML results with other impact assessment methods such as ReCiPe, IPCC, and TRACI for different time horizons (20, 100, and 1,000 years). The other environmental aspects were also evaluated, but are detailed only in the original articles A1, A2, and A4.

4.2.4 Improvement and interpretation

In this final step, the results are interpreted and compared with valid literature benchmarks and similar references. Furthermore, the improvement potential of the LCA study is derived. Depending on the LCA study, typical measures include parameter variations, sensitivity analyses, validations, consistency checks, and derivation of conclusions [93], [94].

4.3 Dynamic energy modeling

Because of the increased renewable uptake in energy provision, the dynamics of energy provision by energy carriers and emission fluctuations are to be considered. Section 2.4.3 explained the state-of-the-art LCA energy modeling approach that considers static datasets. This section elaborates on the developed dynamic energy modeling approach that goes beyond static observations and considers the temporal behavior of energy consumption (either electricity or heat) and emissions by energy carriers. A detailed description of the dynamic approach can be found in article A1; only key information is provided here.

4.3.1 Load profiles

To apply the dynamic energy modeling approach, a time-resolved database that includes the operating characteristics of the industrial production system is required. Load profile data containing electricity and heat consumption can be provided at the production component or system level. These load profile data are obtained from simulations or measurements. In this thesis, a one-hour time resolution was used.

4.3.2 Electricity emission modeling

The provision of electricity and heat through on-site industrial assets is directly associated with emissions, particularly when the energy carrier used is derived from sources like natural gas. When electricity is consumed from the public grid, assigning specific emissions to temporal electricity consumption becomes challenging due to the substantial variations in emissions based on the season and time of day. However, this information is crucial for accurately determining product-related emission footprints instead of relying on average static emission values. A detailed temporal electricity-related emission assignment per unit of temporal consumption is possible by merging load profiles with dynamic electricity production and emission profiles. The merging process was conducted using R software version 4.1.2.

The mathematical merging approach is detailed in article A1 and can be briefly described as follows: The annual public consumption matrix C of the industrial plant by the energy carrier was calculated based on Equation (4-1):

$$D \times P = C \tag{4-1}$$

where the public grid demand matrix D is multiplied by the production matrix P. Equation (4-2) gives a more detailed description of the matrices as follows:

$$\begin{bmatrix} D_1 & D_2 & \cdots & D_{8760} \\ D_1 & D_2 & \vdots & D_{8760} \\ \vdots & \vdots & \vdots & \vdots \\ D_1 & D_2 & \cdots & D_{8760} \end{bmatrix} \times \begin{bmatrix} x_{1,pv} & x_{1,nuc} & \cdots & x_{1,n.d} \\ x_{2,pv} & x_{2,nuc} & \vdots & x_{2,n.d} \\ \vdots & \vdots & \vdots & \vdots \\ x_{8760,pv} & x_{8760,nuc} & \cdots & x_{8760,n.d} \end{bmatrix} = \begin{bmatrix} C_{pv} \\ C_{nuc} \\ C_{bio} \\ C_{coal} \\ C_{hydro} \\ C_{oil} \\ C_{geo} \\ C_{wind} \\ C_{gas} \\ C_{n.d.} \end{bmatrix} \tag{4-2}$$

where the demand matrix D consists of the hourly load profiles of one year (x=1 to 8760); the production matrix P of the hourly shares of the public electricity production profiles by energy carrier for PV, nuclear, biomass, coal, hydro, oil, geothermal, wind, natural gas, and a not-defined share; and the calculated yearly consumption matrix C by energy carrier.

The composition of the public energy mix was calculated to determine the specific public energy carrier inputs for LCA. This is based on yearly consumption, and is calculated according to Equation (4-3):

$$E_i = \frac{C_i}{\sum_n C_n} \tag{4-3}$$

where C_i is the yearly consumption of the energy carrier, and $\sum_n C_n$ is the sum of the yearly energy consumption from the public grid.

4.4 Greenhouse gas protocol

In addition to the ISO 14040/14044 standard for LCA, the GHG protocol is another global standard for evaluating and classifying environmental impact. The emissions are divided into Scope 1, Scope 2, and Scope 3 emissions, and are often used in the industry. Scope 1 includes direct emissions from the company facilities. Scope 2 includes indirect emissions from energy purchases (electricity, steam, heating, and cooling). Scope 3 includes indirect emissions from upstream and downstream processes (e.g., purchased goods and end-of-life treatment) [144]–[147]. The results obtained from environmental LCA are classified and transformed according to the GHG Protocol, thus providing increased industrial understanding.

4.5 Environmental cost

To evaluate the economic impact of environmental emissions, the environmental cost method, often referred to as the shadow cost, was applied. The aim was to estimate the cost that would otherwise be required to prevent environmental emissions. Consequently, decision-makers and governments often use this method to support their decisions [148]–[150]. The specific environmental cost weighting factors for CML impact assessment are listed in Table 4-1 and are based on [151].

Table 4-1: Environmental cost weighting factors for CML based on Bouwkwaliteit 2019 [151]

Midpoint Category	**Unit**	**€ / kg eq.**
Abiotic depletion	kg Sb-eq.	0.16
Abiotic depletion (fuels)	MJ	7.7E-05
Acidification	kg SO_2-eq.	4
Eutrophication	kg Phosphate eq.	9
Freshwater aquatic ecotoxicity	kg 1.4-DCB eq.	0.03
Global warming potential	kg CO_2-eq.	0.05
Human toxicity	kg 1.4-DCB eq.	0.09
Marine aquatic ecotoxicity	kg 1.4-DCB eq.	0.0001
Ozone layer depletion	kg R-11 eq.	30
Photochemical oxidation	kg Ethene eq.	2
Terrestrial ecotoxicity	kg 1.4-DCB eq.	0.06

The calculation was as follows: The results per impact category was available from the LCA analysis. The specific cost for the selected impact category was calculated by multiplying each impact category by a specific environmental cost-weighting factor related to the impact category. The sum of all impact category costs resulted in the total environmental cost.

4.6 Energetic and exergetic analyses

To analyze the PED, the cumulative energy demand (CED) method was applied [152], [153]. The LCA software GaBi supports the feature of calculating the renewable, non-renewable, and total (renewable and non-renewable) PED separately based on existing LCA datasets (Table 4-2) [154]. The CED method considers the technical efficiencies of energy supply by energy source, which is elaborated in detail in VDI [153].

Table 4-2: Parameters for primary energy demand estimation

Parameter	unit
Primary energy demand, non-renewable & renewable, net calorific	MJ
Primary energy demand, non-renewable, net calorific	MJ
Primary energy demand renewable, net calorific	MJ

The energetic efficiency of the study was determined based on the energy balance introduced in Equation (2-1). The ratio of the energetic output to input determines the energy efficiency [128], [155]. Depending on whether there are by-products in addition to the main product, the efficiency can be calculated for the main product alone or for the entire system, including the by-products. The energy efficiency of the main product is calculated according to Equation (4-4):

$$\eta_{en,MP} = \left(\frac{\dot{E}_{en,MP}}{\sum_{in}\dot{E}_{en,i} + \sum_{in}\dot{E}^{Q}_{en,j} + \sum_{in}\dot{E}^{W}_{en,k}}\right) \cdot 100 \tag{4-4}$$

where $\dot{\mathrm{E}}_{\mathrm{en,MP}}$ is the main product energy flow rate, and the denominator $\sum_{\mathrm{in}}\dot{\mathrm{E}}_{\mathrm{en,i}} + \sum_{\mathrm{in}}\dot{\mathrm{E}}^{\mathrm{Q}}_{\mathrm{en,j}} + \sum_{\mathrm{in}}\dot{\mathrm{E}}^{\mathrm{W}}_{\mathrm{en,k}}$ represents the flow rates of the energetic inputs based on Equation (2-1).

To determine the energetic efficiency of the system, the numerator was extended by the energetic flow rates of the by-products $\sum_{BP}\dot{E}_{en,bp}$ and was calculated according to Equation (4-5):

$$\eta_{en,sys} = \left(\frac{\dot{E}_{en,MP} + \sum_{BP}\dot{E}_{en,bp}}{\sum_{in}\dot{E}_{en,i} + \sum_{in}\dot{E}^{Q}_{en,j} + \sum_{in}\dot{E}^{W}_{en,k}}\right) \cdot 100 \tag{4-5}$$

Similar to the energy efficiency analyses, exergetic efficiencies can be determined [127]. A distinction is made between the main product and system. The exergetic efficiency of the main product is calculated using Equation (4-6) for the system according to Equation (4-7):

$$\eta_{ex,MP} = \left(\frac{\dot{E}_{ex,MP}}{\sum_{in} \dot{E}_{ex,i} + \sum_{in} \dot{E}^{Q}_{ex,j} + \sum_{in} \dot{E}^{W}_{ex,k}} \right) \cdot 100 \tag{4-6}$$

$$\eta_{ex,sys} = \left(\frac{\dot{E}_{ex,MP} + \sum_{BP} \dot{E}_{ex,bp}}{\sum_{in} \dot{E}_{ex,i} + \sum_{in} \dot{E}^{Q}_{ex,j} + \sum_{in} \dot{E}^{W}_{ex,k}} \right) \cdot 100 \tag{4-7}$$

where $\dot{E}_{ex,MP}$ and $\sum_{BP} \dot{E}_{ex,bp}$ are the exergy flow rates of the main product and by-products, respectively, and $\sum_{in} \dot{E}_{ex,i} + \sum_{in} \dot{E}^{Q}_{ex,j} + \sum_{in} \dot{E}^{W}_{ex,k}$ are the exergy flow rates of the inputs based on Equation (2-2).

To determine the exergetic content (ex_q) of thermal energy (q), the Carnot Factor was applied. The Carnot Factor (η_C) is determined by the surrounding temperature (T_S) and the temperature level T_i of the thermal energy. Thus, the exergetic content was calculated based on Equation (4-8) [156]:

$$ex_q = q \cdot \left(1 - \frac{T_S}{T_i}\right) = q \cdot \eta_C \tag{4-8}$$

The chemical exergy of materials and streams can be calculated according to [156], but is already available in the literature for numerous materials and streams [157], [158]. The standard reference values were 25 °C and 1.01325 bar.

4.7 Techno-economic assessment

A TEA was carried out to support early decision-making and provide a comprehensive analysis in addition to environmental and energetic criteria. The cost and revenue structures are presented, the determination of the levelized cost of energy (LCOE) or product (LCOP) is demonstrated, and economic viability approaches are compactly summarized.

4.7.1 Capital and operational expenditures and proceeds

Capital expenditure (CAPEX) and operational expenditure (OPEX) are key TEA indicators. CAPEX includes the investment costs for designing, constructing, installing, and commissioning a product or system, whereas OPEX comprises the production costs, such as variable costs for raw materials or utilities, and fixed costs, such as maintenance [132]. The straightforward method to determine CAPEX for a product and system is to obtain quotes from manufacturers. CAPEX can also be calculated using experienced cost-calculation factors from *Lang and Chilton*, as elaborated in Peters et al. [158], or by the cost factors of Weber [160]. In case of novel technologies that are still in development and not yet priced in the market, CAPEX projection methods such as upscaling and technological learning can be applied for initial CAPEX estimation [54].

Proceeds are generated (i) through the sale of products or (ii) through savings in the form of fossil fuel substitution by RES and CO_2 avoidance costs for the EUA.

4.7.2 Levelized cost of energy (or a product)

The annuity method was applied to calculate LCOE or LCOP [161]. In general, total annuity (A) is calculated based on the specific annuities of proceeds (A_P), capital-related (A_C), demand-related (A_D), operation-related (A_O), and miscellaneous (A_M) costs according to Equation (4-9):

$$A = A_P - (A_C + A_D + A_O + A_M) \tag{4-9}$$

The capital-related annuity (A_C) includes the investment costs for the components of the CAPEX and is calculated according to Equation (4-10):

$$A_C = (I_0 + I_1 + \cdots + I_n - R) \cdot a \tag{4-10}$$

where $(I_0, \cdots, I_n)$ are the specific investment and replacement costs, and (R) the residual value. With annuity factor (a) according to Equation (4-11), the investment costs are split over the lifetime of a technology or plant. Therefore, the discount rate factor (q) and the depreciation period (T) must be determined.

$$a = \frac{q^T(q-1)}{q^T - 1} \tag{4-11}$$

To determine the LCOE (i.e., the generation cost), which is the ratio of the total cost to the produced energy output E_{out}, all demand- and operation-related costs (such as A_P, A_O, A_D) are considered as variable costs $\sum_i C_{var,i}$ and are calculated according to Equation (4-12) [54], [162]:

$$LCOE = \frac{A_C + \sum_i C_{var,i}}{E_{out}} \tag{4-12}$$

4.7.3 Economic viability

The net present value (NPV), amortization time, and return on investment (ROI) are typically applied to evaluate the profitability of a technology or system. Here, the aim was to determine the timing and magnitude of potential earnings compared with an alternative investment [133], [163]. NPV was calculated according to Equation (4-13) [164]:

$$NPV = -I_0 + \sum_{t=1}^{T} \frac{Z_t}{q^t} \tag{4-13}$$

where (I_0) is the initial investment and (Z_t) the net cash flow resulting from lodgments and disbursements in period (t).

The amortization period defines the recovery period for an investment. It can be calculated statically or dynamically by considering (q) and (T). The amortization period in years is defined as the ratio of investment to savings [164]. The ROI reflects the reciprocal value and is typically expressed as a percentage.

4.7.4 Top-down versus bottom-up cost approaches

The cost of a technology or system can be calculated by a bottom-up or top-down approach. While the bottom-up approach adds the costs of the individual components to determine the total cost, the top-down approach moves in the opposite direction and calculates the maximum acceptable cost of a product or system (e.g., a storage system) to be economically competitive against the benchmark system. The top-down approach was initially developed to design the heat merit order for waste heat utilization [140], but was adapted for technology and system cost calculations. By determining the fossil energy and cost savings, the maximum acceptable costs were calculated by applying the NPV method. The top-down approach is exemplarily demonstrated for the maximum cost calculation of a TES system to be applied in the investigated cement industry, as elaborated in article A3.

4.8 Multi-criteria decision making

Although decarbonization is a crucial criterion for industries striving for climate neutrality, it is equally essential to consider techno-economic and energetic aspects. Even if a new technology can achieve substantial GHG savings, its viability depends on its economic feasibility. Balancing ecological, economic, and energetic considerations is vital for informed decision-making and future success. When evaluating multiple scenarios with conflicting criteria, careful weighting is necessary to ensure comparability. Expert opinions and specific targets often drive qualitative decisions, such as achieving a minimum GHG emission-saving target for technology deployment, a defined return on investment (ROI), or a predetermined amortization goal, which ultimately determines whether to proceed or not.

Multi-criteria decision-making (MCDM) is a powerful approach for tackling complex but structured decision-making processes involving multiple criteria [165]. The process typically works as follows: first, the experts and/or laypeople select the important decision criteria; second, criteria are weighted to reflect their relative importance; third, a score is assigned to each criterion; and finally, the weighted score per scenario is determined and compared with the other scenarios [166]. The Analytic Hierarchy Process (AHP) is a widely used MCDM method, and the fuzzy set theory is often employed to address uncertainties in decision-making [165]. For more comprehensive guidance on applying MCDM, reference [166] provides further details.

While MCDM and its various assessment options and tools are considered necessary for holistic quantitative scenario assessments in the future, their practical application was outside the scope of this thesis. The focus of this thesis was on the development of the integrated LCA method and its multiple modules rather than the evaluation of all possible criteria for all selected industries.

5 RESULTS AND DISCUSSION

This chapter presents the most relevant findings of the published research articles that answer the research questions and place them in a broad context. The results are structured according to the industrial sector, which is then discussed in terms of the environmental, techno-economic, and energetic aspects. A special focus is placed on the GHG mitigation potential to achieve industrial decarbonization targets. The findings from the research articles A1 to A4 assisted in the development and design of the integrated LCA method described in Chapter 4.

5.1 Impact on the pulp, paper, and print industry

Several scenarios were elaborated to analyze the impact of diverse flexibility measures and low-emission technologies on energy provision and paper production from various perspectives. The impacts were compared to a business-as-usual (BAU) scenario, where energy was mainly provided via the fossil resources of an on-site CHP.

Compact scenario description (details in article A1):

- BAU: energy provision via natural gas CHP plant, natural gas HOB, and public grid
- Scenario S0: as BAU, but with use of existing flexibilities
- Scenario S1: as S0 but with integrating PPAs at 20€/MWh
- Scenario S2: as S0 but with integrating PPAs at 0 €/MWh
- Scenario S3: as S2 but without grid regulation
- Scenario S4: as S1 but with the electric boiler as new asset
- Scenario S5: as S4 but with heat pump, TES, and electric storage as new assets
- Scenario S6: as S5 but without grid regulation

5.1.1 Environmental analysis

The dynamic energy modeling approach conducted for the public grid of Germany has revealed substantial potential for reducing GWP in electricity provision. By comparing it to the internal static consumer grid mix dataset of the GaBi software, a GWP reduction potential of approximately 32.6% was identified in scenario S4. This reduction is attributed to the flexible and adaptive operation of the plant during periods of high renewable energy integration in the grid. Static considerations alone yield insufficient results, especially when considering the increasing integration of renewables in the future. By incorporating dynamic effects and integrating flexible technologies such as PPAs, electric boilers, and heat pumps, a GWP reduction of approximately 40% for electricity provision and around 8% for heat provision at the industrial site was achieved in scenario S6 (Figure 5-1). The main driver of these reductions is the substitution of fossil gas with RES, which reduces the operating hours of the CHP plant.

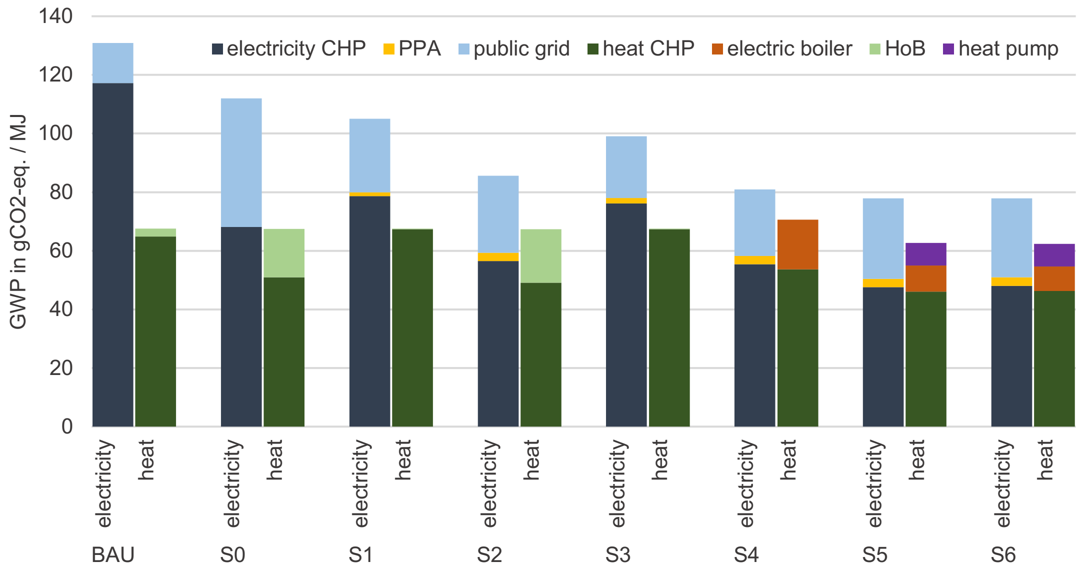

Figure 5-1: Global warming potential of 1 MJ of electricity and of 1 MJ of heat (Source: article A1)

A substantial reduction in emissions from the energy supply has a profound impact on the product's carbon footprint. Figure 5-2 illustrates a GWP reduction potential of 32.3% per ton of paper in S6, resulting in a decrease in emissions from 1,006 to 681 kgCO_2-eq. per ton of paper. More context for relating the results to other studies is given in article A1, but show similar magnitudes. The analysis conducted at the process level allows for identifying hotspots in the production chain that essentially impact emissions, such as the electricity-intensive grinders (PGW) and paper machine A (PM A). The substitution of fossil resources with RES is crucial in achieving GWP savings. As customers become more aware of the environmental footprint of purchases or demand sustainable products, LCA and scenario development can be used to consciously shape the transition to more sustainable production.

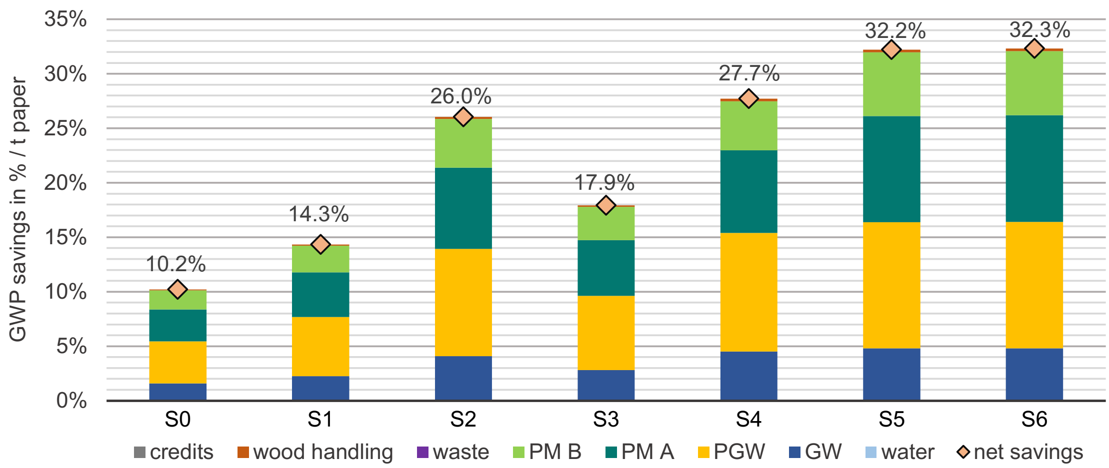

Figure 5-2: Global warming potential savings in % per ton of paper produced (Source: article A1)

A further robustness analysis was performed to compare the global warming CML results of the scenarios with other impact assessment methods such as ReCiPe, IPCC, and TRACI (Table 5-1). Different time perspectives of 20, 100, and 1,000 years were considered. The 100-year time horizon comparison indicated only minor differences between CML, ReCiPe, IPCC, and TRACI not leading to divergent conclusions. Compared to CML, ReCiPe results tend to show a 1.1−1.3% higher GWP, IPCC a 0.3% higher GWP, and TRACI a -0.3% lower GWP. However, greater differences arise when time horizon-dependent characterization factors are considered. CML does not provide the functionality for an assessment over a time horizon of 20 and 1000 years; thus, only qualitative statements based on ReCiPe and IPCC results can be drawn. For a short-term perspective of 20 years, GWP results are highest, while for a long-term perspective of 1,100 years, they are lowest.

Table 5-1: Global warming CML results comparison with different impact assessment methods and time horizons

LCIA methodologies	BAU	S0	S1	S2	S3	S4	S5	S6
CML 100 years in kgCO2 eq./t	1006	903.2	861.8	743.9	825.6	727.3	682.1	680.9
ReCiPe2016 Individualist 20 years	8.3%	7.4%	7.8%	7.9%	7.9%	7.9%	7.7%	7.7%
ReCiPe2016 Hierarchist 100 years	1.3%	1.1%	1.2%	1.2%	1.2%	1.2%	1.2%	1.2%
ReCiPe2016 Egalitarian 1,000 years	-3.8%	-3.5%	-3.7%	-3.7%	-3.7%	-3.7%	-3.7%	-3.7%
IPCC AR6 GWP 20 years	7.9%	7.1%	7.5%	7.5%	7.6%	7.5%	7.4%	7.4%
IPCC AR6 GWP 100 years	0.3%	0.2%	0.3%	0.2%	0.3%	0.3%	0.3%	0.3%
TRACI 2.1 GWP 100 years	-0.3%	-0.3%	-0.3%	-0.3%	-0.3%	-0.3%	-0.3%	-0.3%

5.1.2 Energetic analysis

The total PED required to produce one ton of paper varies between 26.2 and 34.9 GJ, with the fossil driven BAU showing the lowest demand (Figure 5-3). The higher PED in a renewable-based energy supply system results is attributed to the CED method, which considers the technical efficiencies of energy systems and where renewable energy systems are less efficient than fossil ones. However, the distinction between renewable and non-renewable energy allows for additional insights. Although the total PED increased by approximately 33% in S6 compared to the BAU, the renewable PED increased by 156%, while the non-renewable PED was reduced by 32%. The share of renewable PED reached up to 67% of the total PED in scenarios S5 and S6. This reduces dependence on imported fossil fuels and mitigates associated supply security risks. Consequently, the transition to a renewable energy system not only provides environmental benefits through GWP savings, but also enhances the resilience of the energy supply system. The increased integration of locally available RES at the industrial site, such as through PPAs, can contribute positively to local grid stability by avoiding transmission line bottlenecks.

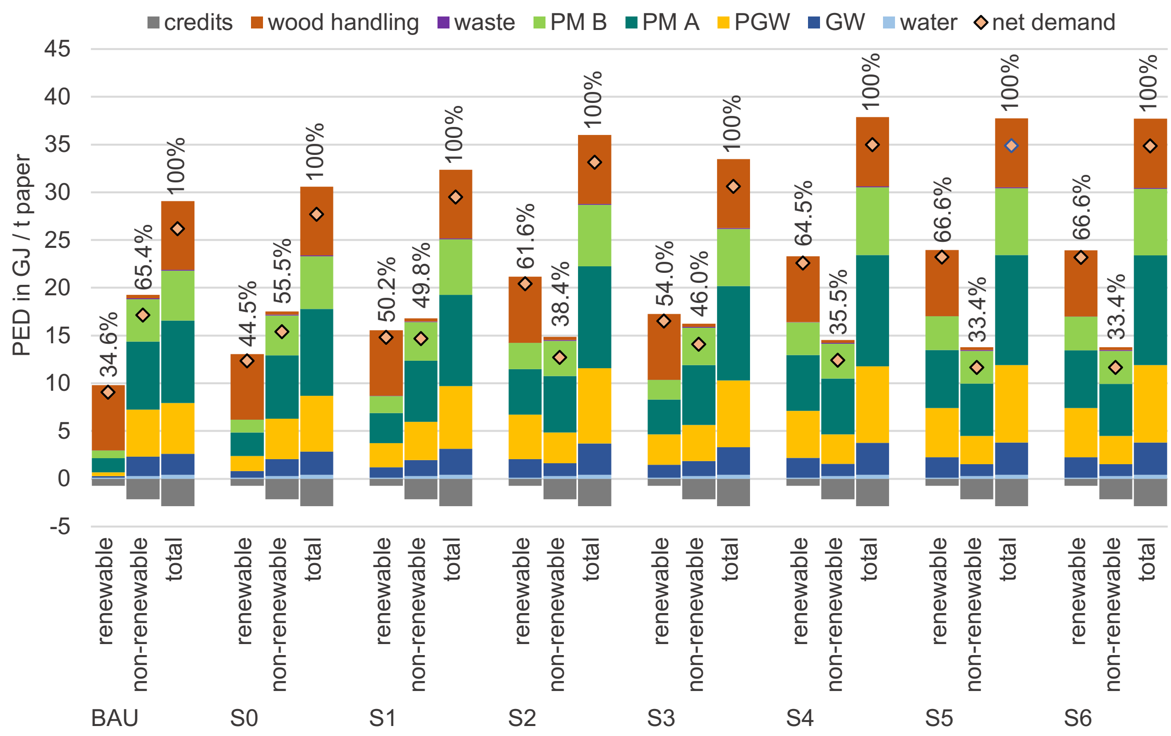

Figure 5-3: Primary energy demand to produce one ton of paper (Source: article A1)

5.1.3 Techno-economic analysis and environmental cost

OPEX and, in the case of new investments, CAPEX, were used to determine the energy supply costs for producing one ton of paper. In scenarios S0 to S3, energy costs were analyzed using the flexibility measures of existing assets and PPAs. To increase the flexibility options, additional investments in heat pumps, electric boilers, and storage were considered in scenarios S4 to S6. Compared to the BAU case with energy costs of 115.6 € per ton of paper, the costs could be reduced by up to 43.8% in the best-case scenario (S3). In scenario S6, which included additional CAPEX, a cost reduction of approximately 19.3% was achieved. If CAPEX in S6 is not considered, there is a reduction potential of up to 44.1%. The specific OPEX cost savings for each scenario are presented in Table 5-2.

Specific CAPEX, ROI, and amortization periods were determined for S4–S6 (Table 5-2). Economic viability could only be achieved in S4 (electric boiler integration) with an amortization period of < 0.27 years. In S5 and S6, where the CAPEX for heat pumps, electric boilers, TES, and electric storage were included, amortization periods of up to six years were determined, and hence they do not meet typical industrial investment requirements of 2–4 years.

Table 5-2: Evaluated economic parameters

Parameter	S0	S1	S2	S3	S4	S5	S6
OPEX cost savings (€/t)	35.5	45.5	45.4	50.6	49.8	50.7	50.9
CAPEX (€/t)	-	-	-	-	13.35	297.1	292.3
ROI	-	-	-	-	3.7	0.17	0.17
amortization period	-	-	-	-	0.27	5.9	5.7

An environmental cost analysis was conducted to determine the cost of preventive measures to avoid environmental impact. The environmental results of the LCA for each impact category were multiplied with the respective cost factors and exposed estimated costs of 80 to 93 € per ton of paper, depending on the scenario. GWP was the most influential factor, followed by MAEP, and HTP. Compared with the BAU case, the decrease in carbon emissions also led to a decrease in the resulting GWP costs, whereas the MAETP increased. This results from the fact that, in the developed scenarios, the purchase of electricity increasingly takes place from the public grid and PPAs, thus leading to increased use of elements and materials needed for electricity transmission and negatively influencing the MAETP.

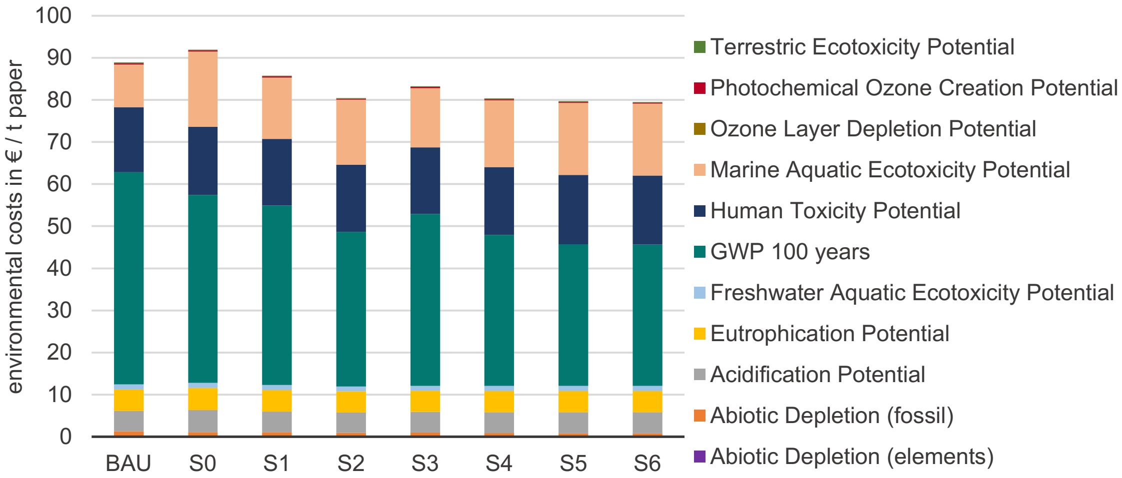

Figure 5-4: Environmental costs for 1 ton of paper divided by impact category (Source: article A1)

5.2 Impact on the chemical and petrochemical industry

Diverse biorefinery set-ups (scenarios) were investigated in article A2, which differ in energy provision and by-product valorization. The aim of this study was to identify the best-case lignocellulosic biorefinery plant for softwood residue-based sustainable aviation fuel (SAF) production from an environmental and energetic perspective. A key objective was to meet the legislated GHG emission reduction targets necessary for product launch. Emphasis was placed on utilizing all products along the value chain, which entails ecological and economic benefits. The specific context to the results of other research studies for biorefineries is discussed in article A2.

Compact scenario description (details in article A2):

- NG-B and LI-B: natural gas or lignin boiler, power from public grid
- NG-B RES and LI-B RES: same as before, but power from renewables
- NG-CHP and LI-CHP: natural gas or lignin CHP plant where 100% of thermal energy demand is covered and only the lack of power is consumed from public grid
- NG-CHP RES and LI-CHP RES: same as before, but lack of power is consumed from renewables

5.2.1 Environmental analysis

The frameworks of the *EU RED 2018/2001/EC*[2] and *CORSIA*[3] require that certain GHG emission savings must be achieved to obtain product certification. The benchmark is a fossil fuel comparator (basically fossil kerosene), but it is defined slightly differently for both frameworks. While the *EU RED 2018/2001/EC* requires ≥65% GHG savings, *CORSIA* has a target of ≥10%. Using LCA, different biorefinery set-ups were investigated and tested for their suitability in reaching these targets. Compared to the black-box biorefinery analysis, an analysis at the process level enables the early identification of hotspots and main emission-causing processes and countermeasures, such as further process adaptations or efficiency increases.

Biorefineries are characterized by energy-intensive processes, considering energy supply a critical factor. Typically, these plants rely on natural gas for boilers or CHP plants to meet their energy demands. In the case of boiler systems, electricity is consumed from the public grid. However, the environmental impact of electricity varies substantially from country to country, as discussed in Section 2.4.3, making it challenging to draw general conclusions for the set-up. Therefore, to derive initial findings, the analysis considers an average electricity mix for the EU-28 and a projected EU RES grid mix for 2050. Additionally, by-products with a calorific value, such as lignin, are considered for on-site energy supply. In cases where lignin is externally valorized for more valuable uses, such as a binder in asphalt production instead of mere incineration, emission allocation is performed based on energy content to proportionally allocate emissions to the SAF product. Energy allocation is also applied to C5 sugars processed into bioethanol. The avoided burden approach is utilized for non-energy-related by-products, such as sludge and biomass streams, providing credits for substituting fertilizer production and soybean imports.

[2] Renewable Energy Directive; Directive (EU) 2018/2001 of the European Parliament and of the Council of 11 December 2018 on the promotion of the use of energy from renewable sources
[3] CORSIA – Carbon Offsetting and Reduction Scheme for International Aviation

The net GWP of the investigated scenarios ranges from 18.7 to 56 gCO_2-eq./MJ, as shown in Figure 5-5. The wood-to-sugar unit and off-site section for auxiliaries have been identified as critical process steps that require improvements due to their high GWP contribution in each scenario. An important consideration for the biorefinery set-up is the utilization of lignin. When lignin is used internally for energy supply, it generally reduces the ecological footprint, but results in increased emissions allocated to the SAF product. The integration of RES has also been identified as driver of achieving lower GWPs. The energy supply through the on-site natural gas CHP plant (NG-CHP RES) is an exception to this trend. Since most of the energy demand can be met on-site, only a small portion of the electricity demand needs to be sourced from RES.

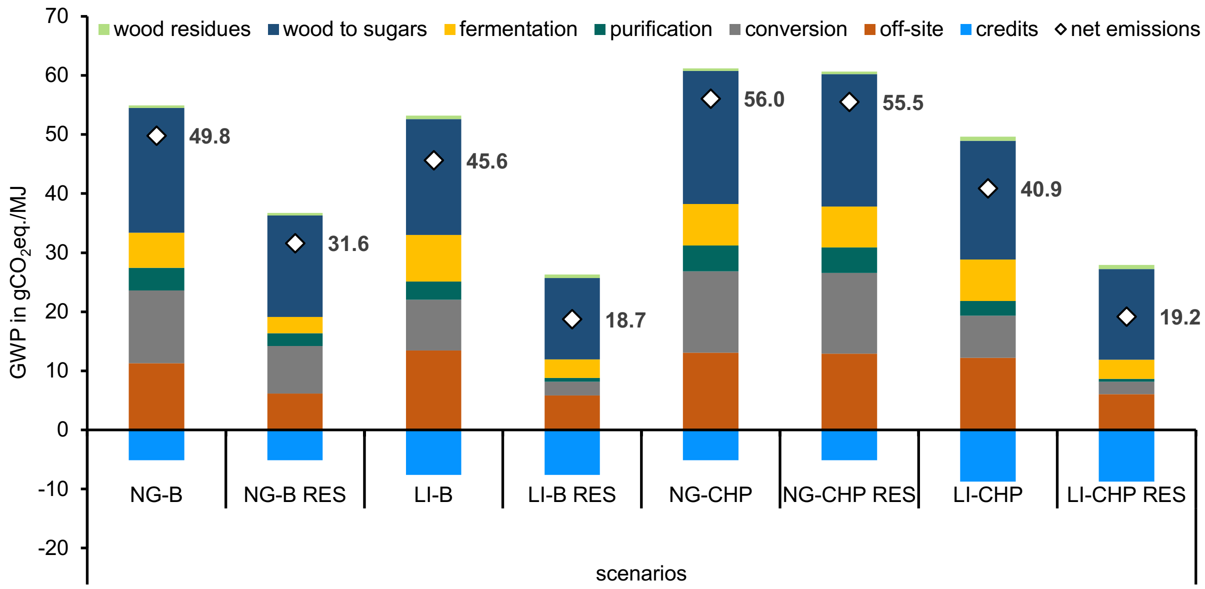

Figure 5-5: Global warming potential of SAF production for various scenarios (Source: article A2)

Based on the determined ecological footprints, the GHG emission reduction potential was calculated as 80% in the best-case scenario (Figure 5-6). However, only the scenarios where RES were integrated for electricity provision could reach the *EU RED 2018/2001/EC* threshold (NG-B RES, LI-B RES, and LI-CHP RES), demonstrating the necessity of future renewable expansion and the shift away from fossil energy sources.

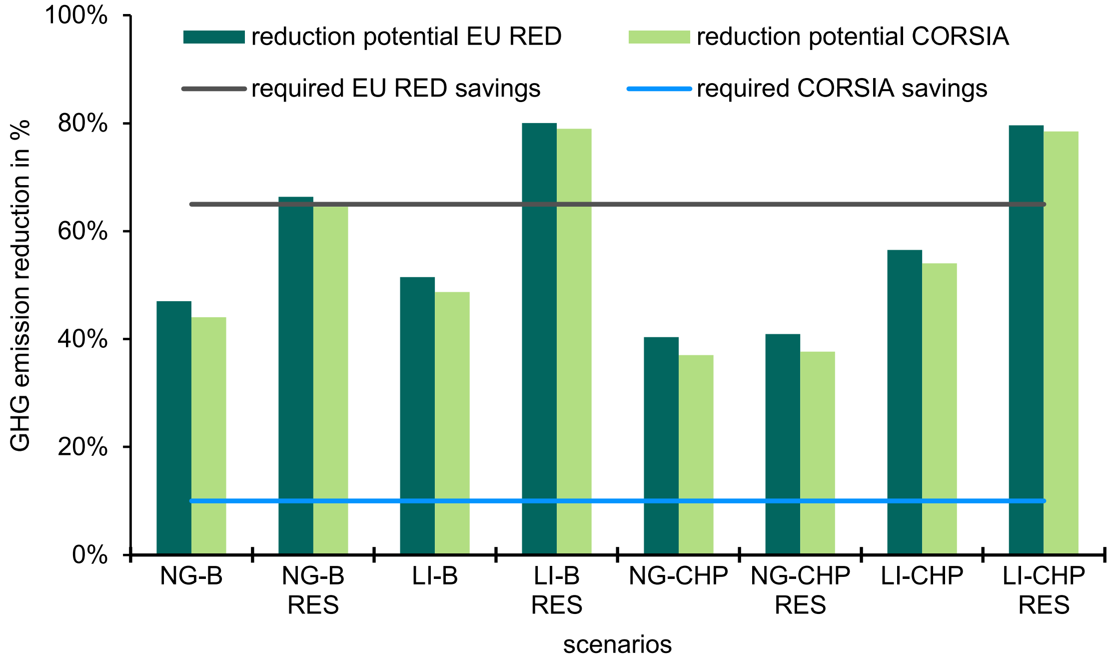

Figure 5-6: Greenhouse gas reduction potential of SAF production against fossil reference by applying ISO 14040/14044 LCA methodology(Source: article A2)

5.2.2 Energetic analysis

The PED evaluation was also conducted at the process unit level, once by considering an allocation (Figure 5-7 a) and once without allocation (Figure 5-7 b), to avoid misinterpretation of the results. The allocated PED for SAF varied between 2.8 and 4.2 MJ, and for the non-allocated PED between 10.7 and 13.1 MJ. The main differences resulted from the valorization of lignin, either internally or externally.

All allocated scenarios, where lignin is internally used as an energy source, had a higher total PED than their fossil counterparts. This results from the fact that, in these cases, the allocation ratio for SAF increased; hence, more PED was attributed to SAF. In such cases, it is important to closely examine the types of PED, i.e., renewable and non-renewable classifications. The fossil PED substantially decreased in each lignin scenario, and in the best-case LI-CHP scenario, up to 82% was covered by renewable energy.

In the non-allocated scenarios, natural-gas-based scenarios reported the highest total PED (NG-B, NG-B RES, NG-CHP, and NG-CHP RES). Owing to the CED method and considering the technical efficiencies for energy generation, natural-gas-based scenarios with a renewable electricity mix had a slightly higher total PED. In principle, the PED of a RES is always higher than that of its fossil fuel counterparts. However, as elaborated in this study, the internal valorization of lignin reduced dependence on fossil fuels, increased the renewable share of energy provision, and supported climate neutrality. In the LI-CHP scenario, approximately 76% of the produced bioproducts were utilized as bioenergy, whereas the share in the NG-CHP scenario was only approximately 35%. Nevertheless, energy efficiency must be addressed in all process units to reduce PED and, hence, environmental implications.

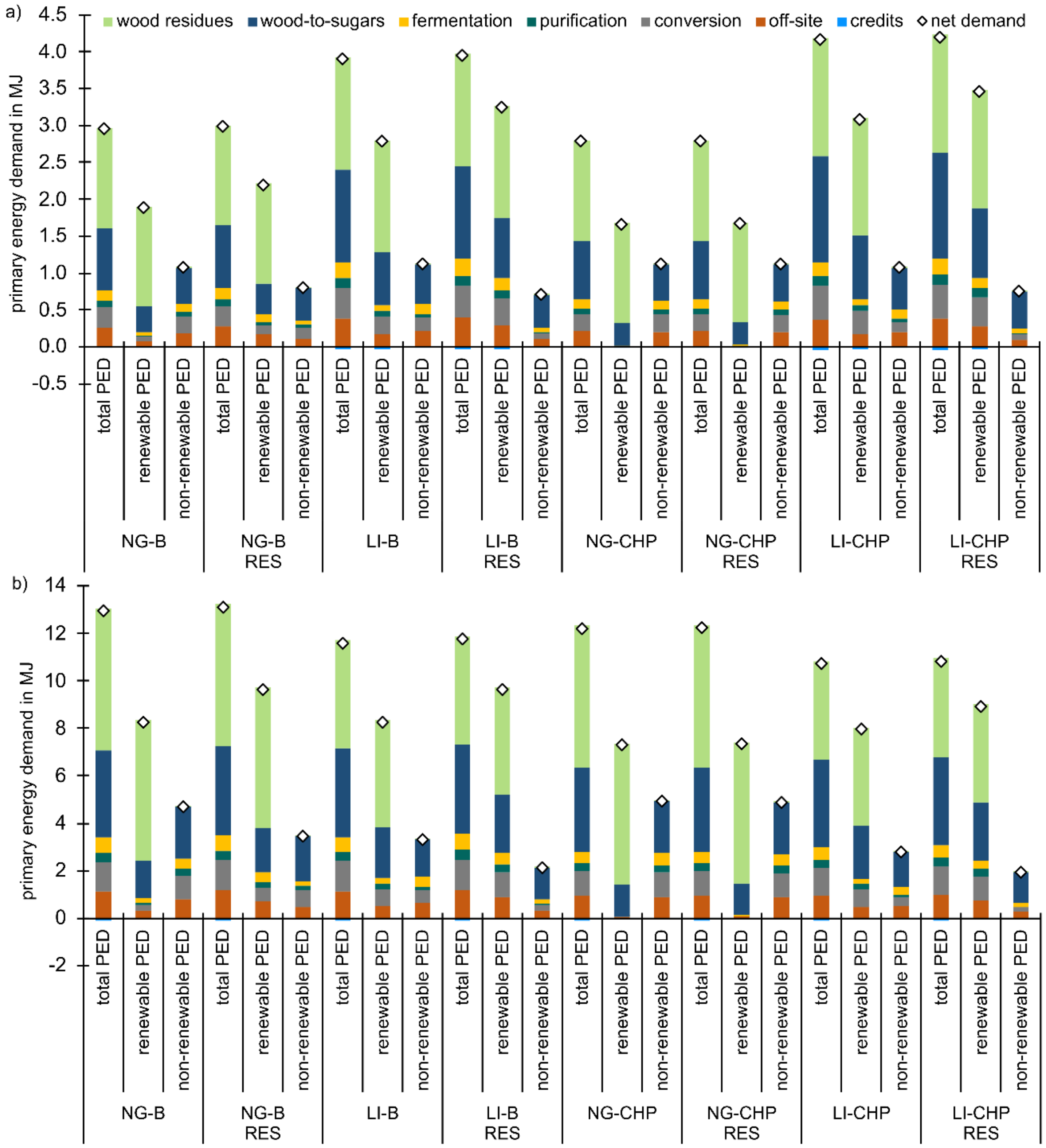

Figure 5-7: a) allocated and b) non-allocated primary energy demand of 1 MJ SAF produced in biorefinery (Source: article A2)

Further energetic and exergetic analyses were conducted to determine the efficiency of each biorefinery set-up. For this purpose, the energetic and exergetic efficiencies were determined for (i) the main product, SAF, and (ii) all biorefinery products. However, the inefficiencies of the upstream processes, such as electricity generation, were not included.

The SAF-based analysis reported energetic and exergetic efficiency of 11.7–14.9% and 11–13.8%, respectively, revealing only marginal differences. However, a system-based analysis of the entire biorefinery highlighted the importance of considering all by-products for biorefinery development. The energetic and exergetic efficiencies increased substantially at the system level to 39.4–50.1% and 40.4–56.9%, respectively.

The exergetic flow rates were visualized using Sankey diagrams, as depicted in Figure 5-8 for NG-B and LI-B scenarios. This enabled differences to be made more obvious and the potential for improvement to be identified more effectively. Softwood residues were identified as the primary exergetic input. It is obvious that with internal lignin utilization for energy provision, the exergy flow of natural gas would no longer be present. However, the exergy output flow of lignin decreased. The high exergy losses in both scenarios became apparent, but they were comparable to those of other biorefinery studies reviewed in article A2. Nevertheless, further developments are needed to increase the specific yields at all process stages along the value chain to increase the SAF and system efficiencies and to be competitive in the market.

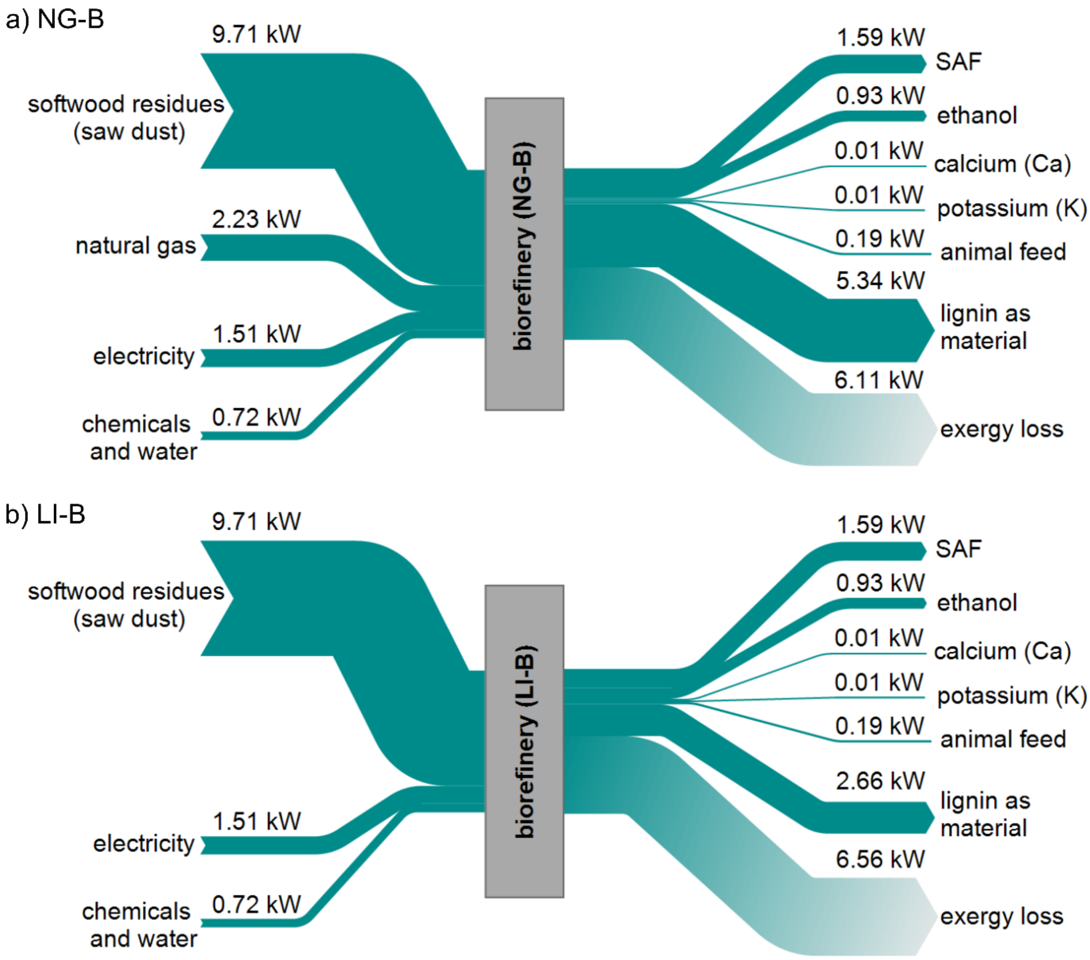

Figure 5-8: Exergy flows of biorefinery to produce 1 t SAF for scenario a) NG-B and b) LI-B (Source: article A2)

5.3 Impact on the cement industry

A preliminary feasibility analysis was conducted to assess the potential for waste heat recovery at a cement plant and its utilization as process heat in a dairy, as described in research article A3 and related conference proceedings [167]. Other forms of waste heat utilization can include preheating of combustion air or use in ORC for electricity generation [168], but were not addressed in this study. The analysis considered both technical and non-technical aspects. Various concepts were examined, which differed in waste heat recovery (approximately 400 °C), transportation, and utilization of high-temperature waste heat. A TEA was performed to evaluate the feasibility of the proposed system, including implementing a TES system with varying capacity for increased flexibility. The benchmark for comparison was an energy system fueled by natural gas for providing process steam.

5.3.1 Environmental and energetic analyses

The cement plant has a theoretical waste heat potential of up to 90 GWh (HHV), with the investigated concepts able to utilize up to 72% of this potential. The higher the utilization rate, the higher the primary energy savings. The analysis determined a theoretical annual reduction potential of up to 22,000 tons of CO_2 emissions.

To address the planned and unplanned interruptions at the cement plant, a TES system is employed to ensure a reliable heat supply to the dairy. An assessment of the interruption data, considering the demand characteristics of the dairy, resulted in the findings presented in Figure 5-9.

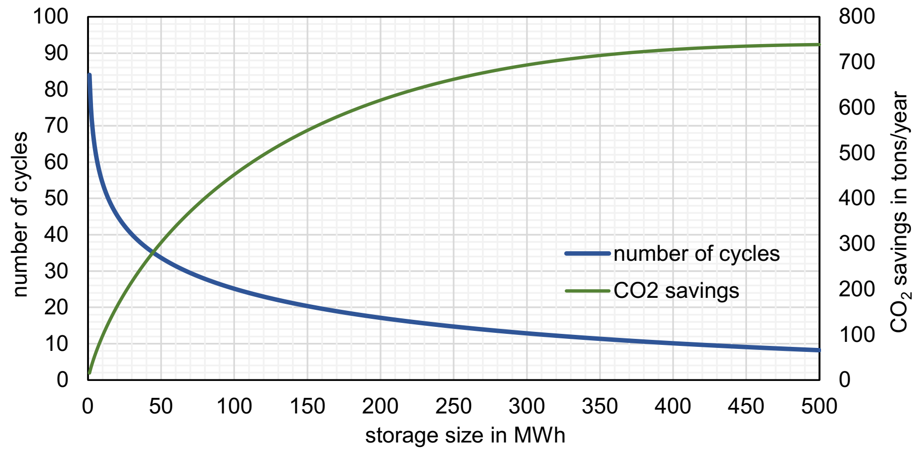

Figure 5-9: Number of achievable cycles depending on the storage size for the cement industry case study (Source: article A3)

A smaller storage capacity allows for more cycles but lowers gas and CO_2 savings. For example, a 30 MWh storage achieves 40 cycles and annual CO_2 savings of 217 tons, while a 300 MWh storage only achieves 13 cycles, resulting in 694 tons of CO_2 savings. However, the selection of an appropriate storage size selection is not only based on ecological aspects, but also on economic aspects, as explained in the next section, and on functional aspects to ensure a continuous heat supply.

5.3.2 Techno-economic analysis

A top-down approach was employed to assess the economic feasibility of waste heat utilization. The maximum acceptable investment cost for the entire system, including waste heat recovery, transportation, and usage, was determined by comparing it to the cost of using gas for energy provision. As depicted in Figure 5-10, the maximum cost without a storage system is up to €10.6 million. The cost decreases with the implementation of a storage system, but it needs to be allocated to the storage system. At this stage, the specific storage technology is not a relevant; instead, the analysis focuses on the cost of the storage technology for economic viability. The maximum specific storage cost was €1.4/kWh for 500 MWh and €14.4/kWh for 1 MWh. The number of cycles achievable by the storage system is crucial in evaluating its economic feasibility. More cycles result in higher cost-effectiveness of the storage. The derived maximum costs can be compared with the current market costs of TES systems to assess their profitability. However, when comparing with available TES cost levels, economic viability was limited, as established sensible TES systems range from €15/kWh to €50/kWh, and lower TRL TES systems using latent, thermochemical, and sorption technologies start at €8/kWh.

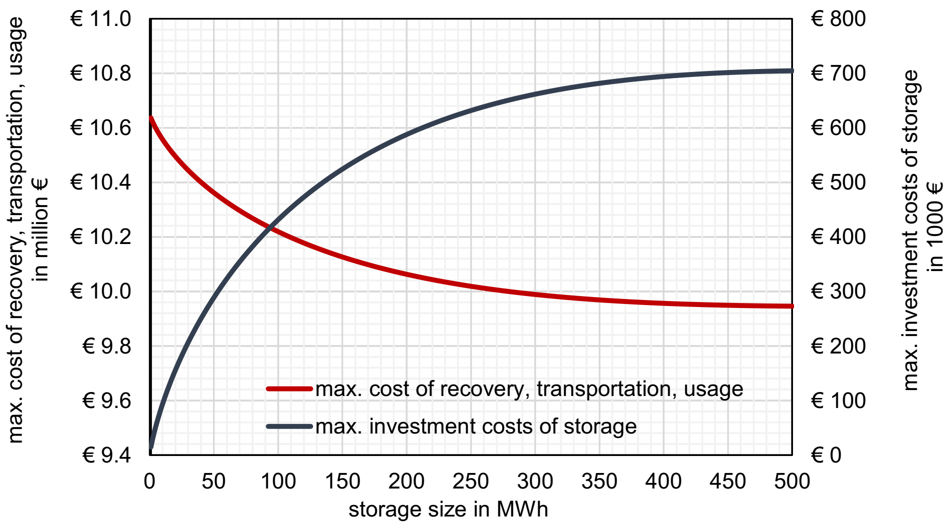

Figure 5-10: Maximum investment costs of storage and the overall system for the cement industry case study (Source: article A3)

A sensitivity analysis was performed to examine the impact of gas prices and CO_2 tariffs on the maximum storage costs. When considering a 100% gas price increase, the maximum storage cost would be 2.8 €/kWh for 500 MWh and 1 MWh. This demonstrates a direct correlation between gas prices and storage costs, as shown in Figure 5-11. Additionally, by varying the

CO_2 price up to 400 €/t, as exemplarily applied in Figure 5-12 for a 300 MWh storage, the maximum storage cost would increase by 6.8 €/kWh, regardless of the gas price.

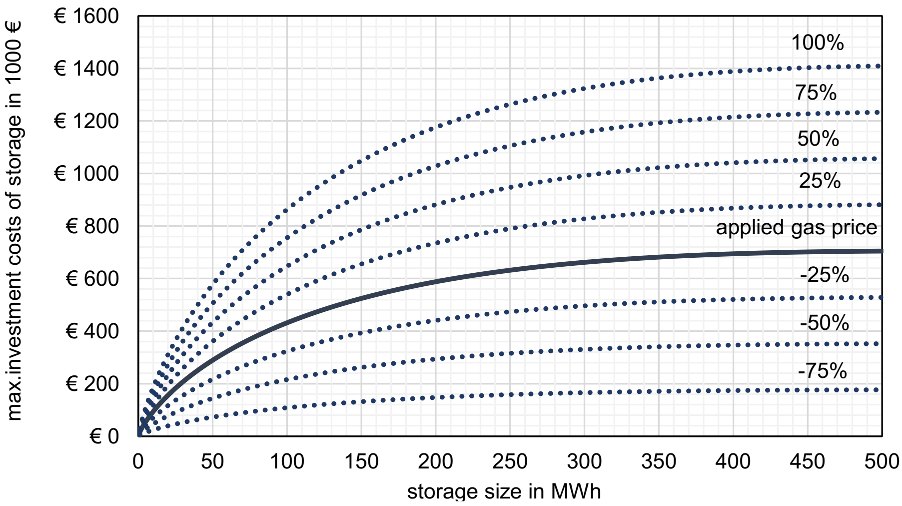

Figure 5-11: Sensitivity analysis of gas price for the cement industry case study (Source: article A3)

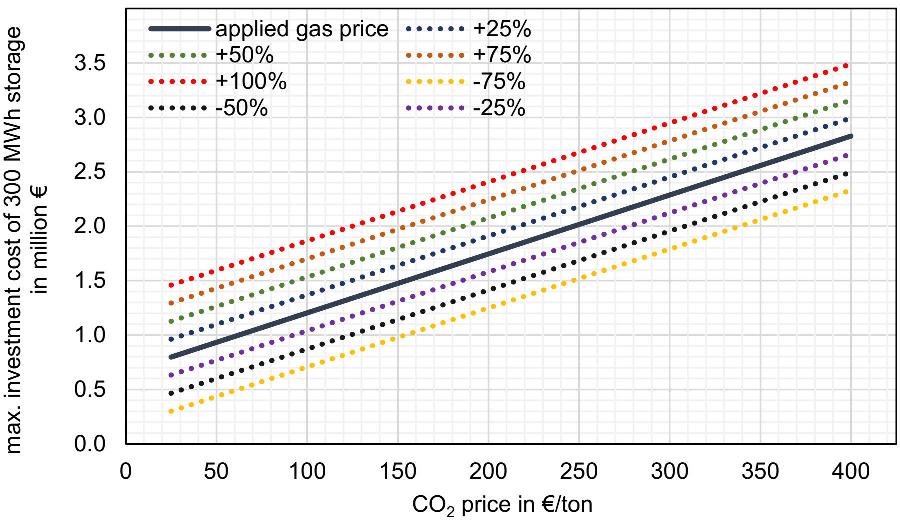

Figure 5-12: Sensitivity analysis of CO_2 tariffs of a 300 MWh storage in the cement industry case study (Source: article A3)

The actual investment costs (CAPEX) for each concept were determined using cost calculation factors and ranged from €23 million to €44 million. The concept with the lowest CAPEX did not include a TES system, resulting in the lowest potential natural gas saving (42 GWh based on the HHV). Contrarily, the concept with the highest CAPEX included a TES system with a capacity of 330 MWh, leading to the highest annual gas savings of 54 GWh (HHV). Considering the price levels of early 2020 for the evaluation, economic viability, in terms of a positive net present value (NPV), could not be achieved, even when assuming a 30% investment subsidy and a CO_2 tariff of €50/t. The high CAPEX costs due to the dust exhaust flow and the low industrial gas prices were identified as the key parameters for future profitability. Subsidies and an increase in CO_2 tariffs contribute positively to economic viability. Gas, and hence, cost savings, cannot compensate for the investment cost.

As discussed in Section 2.1, the energy landscape is currently undergoing a crucial transition. While the initial calculation considered a gas price of €25/MWh, typically for a long period in the past years, the escalation of the Russia-Ukraine War led to a drastic increase in gas prices across Europe. By considering a gas price of €230/MWh (as of August 2022), economic viability of the overall system can be readily attained. However, it is essential to note that future gas price projections entail high uncertainty and pose risks to long-term investments.

5.4 Impact on the magnesia industry

The effects of resource flexibility and energy provision on magnesia production were investigated. Multiple scenarios were analyzed to assess the environmental impact of co-firing alternative renewable fuels (biomass) with pet coke and integrating renewable electricity to produce CCM or DBM. The economic impact is also addressed. The BAU scenario with 100% pet coke usage was defined as a benchmark to determine the savings. Olive kernels (OK), wood sawdust (WSD), and sunflower husk pellets (SHP) were considered as local biomass.

Compact scenario description (details in article A4):

- BAU: 100% of thermal energy demand is covered via pet coke and power supply via Greek grid mix
- ELE: impact of considering 100% of power supply from RES
- CAL scenarios: only the calcination stage with 70% substitution rate for the three local biomass options was considered, power supply from Greek grid mix
- MB scenarios: moderate biomass scenarios with substitution rate of 5% at kiln and 30% at calcination stage for the three biomass options, power from Greek grid mix
- BCB scenarios: best case biomass scenarios with substitution rate of 10% at kiln and 70% at calcination stage for the three biomass options, power supply from RES

5.4.1 Environmental analysis

The main contributors to GHG emissions in magnesia production are the naturally occurring CO_2 released during $MgCO_3$ decomposition and the carbon released during the combustion of pet coke. While GHG emissions from $MgCO_3$ decomposition can be reduced through CCS and/or CCU technologies, substituting pet coke with locally available biomass resources like SHP, WC, and OK offers a promising approach.

In the current BAU scenario, the GWP was calculated to be 2.24 tons for CCM and 2.65 tons of CO_2-eq. for DBM per ton of MgO, which is in the range of other research studies in this field detailed in article A4. The GWP share resulting from $MgCO_3$ decomposition accounts for 45% of CCM and 38% of DBM, respectively. This process is responsible for approximately 1 ton of CO_2 per ton of MgO production, which can be reduced through CCS, but was not investigated in this study. The GWP share resulting from the combustion of pet coke is 50% for CCM and 60% for DBM, respectively. The scenario analysis presented in Figure 5-13 for DBM demonstrates that, in the best case, substituting 10% of the thermal energy demand in the kiln and 70% in the calcination stage with OK leads to a GHG mitigation potential of 38.2%. Only 2.5% of this reduction potential results from the inclusion of renewable electricity. In the best case, the share of pet coke combustion in the GWP decreases to approximately 38% for DBM and 30% for CCM. The GHG reduction potential for CCM is calculated to be 32.5%. Furthermore, implementing a low-NOx burner has reduced NO_x emissions, and additional environmental benefits have been achieved through reductions in SO_x and CO emissions.

In principle, increasing the biomass content of the fuel mixture, ideally achieving a complete substitution of pet coke, can further reduce GHG emissions. However, from a technical perspective, the proportion of biomass implemented is limited. The functionalities and efficiencies of the high-temperature production processes, which reach temperatures of up to 2,000 °C, must remain the same, and integrating biomass is associated with increased ash and moisture content in the production, potentially affecting the longevity of the kilns. The maximum feasible biomass share has not been determined technically and requires further investigations and testing. A first field test at the industrial plant with a 50% substitution of thermal energy demand of pet coke with SHP showed promising results without affecting the quality of the products and harming the kiln.

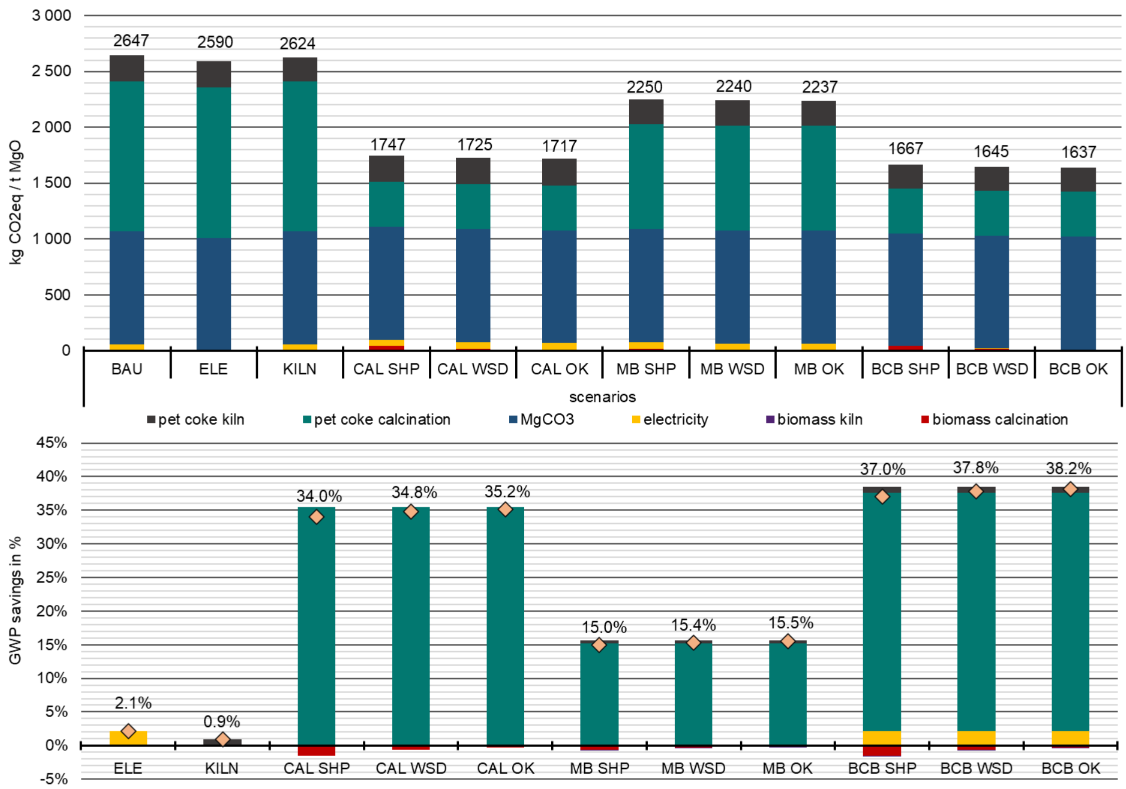

Figure 5-13: Global warming potential of 1 ton dead burnt magnesia (upper figure) and relative global warming potential savings against business-as-usual scenario (lower figure)(Source: article A4)

5.4.2 Techno-economic analysis

The economic analysis focused on assessing the impact of co-firing on production costs. Since raw material prices are market driven, they naturally experience annual fluctuations. Additionally, legal obligations such as CO_2 tariffs can substantially influence production costs.

To calculate the impact on the production costs, a field test was conducted at an industrial plant, considering a 50% substitution of pet coke with SHP. With pet coke priced at 294 €/t, SHP priced at 190 €/t, and a CO_2 tariff of approximately 83 €/t, the annual operational production costs for thermal energy demand were reduced by 9.75% to approximately €11 million. Substituting pet coke with other biomass resources, such as wood chips, WSD, or OK, would also decrease operational production costs. Therefore, using biomass as a substitute for fossil fuels is a promising approach for achieving sustainability, resource flexibility, resilience to future CO_2 tariffs, and cost efficiency, ultimately enhancing competitiveness.

6 SUMMARY

Industrial decarbonization is expected to pose a crucial challenge in the coming decades. Through the *European Green Deal* [5], the EU has presented ambitious decarbonization targets that represent tremendous challenges for energy-intensive industries and require immediate action on the path to climate neutrality. The changing price landscape for energy further reinforces the need for necessary measures to ensure that companies remain competitive in the future. Energy resilience, diversification, and independence are now of central importance.

Industrial energy systems rely heavily on fossil fuels, but alternative green measures must be implemented to achieve climate neutrality. In order to facilitate this energy transition, an integrated LCA method has been developed to thoroughly evaluate various sustainability approaches and assess their potential applications at an early stage. This comprehensive approach considers not only environmental factors but also energetic/exergetic and techno-economic implications. However, economic assessments are always exposed to market price uncertainties, which is why results and conclusions can change. Transparency in the calculation with disclosure of the data used with annual reference is therefore essential. By embedding a scenario analysis, the integrated LCA method identifies key parameters that influence the outcomes and enables optimizing products or systems. One crucial aspect the method addresses is the dynamic nature of energy supply, particularly when purchasing electricity from the public grid. Fluctuations in emissions resulting from different energy generation technologies throughout the day and season are accounted for through an innovative energy modeling approach. This dynamic modeling approach provides a more accurate assessment of environmental footprints compared to static methods. However, the energy modeling approach has its constraints, since it does not account for the dynamics of the energy supply background processes.

The integrated LCA method was developed based on the research findings of specific sustainable measures in four industries: pulp, paper, and print; chemical and petrochemical; cement; and magnesia. Consequently, a comprehensive assessment was not carried out for all industries, but only for specific aspects of industries. The KPI GHG reduction potential was determined for all industrial case studies using CML impact assessment, and is shown for comparison in Table 6-1. To analyze the robustness of the GHG emission results, a comparison was made with other impact assessment methods such as ReCiPe, IPCC, and TRACI applying different time horizons. The investigation was performed for the industrial case study in the pulp, paper, and print industry. For a 100-year time horizon, ReCiPe and IPCC results have slightly higher average GWP at 1.2% and 0.3%, respectively, while TRACI has lower GWP at approximately -0.3%. It can be deduced that for GWP, the impact assessment method has hardly any influence on the results and interpretation. Other evaluation aspects are subsequently summarized according to the industry. Further context to other research studies is elaborated by industry in the research articles A1−A4.

Table 6-1: Summary of greenhouse gas mitigation potential (best-case scenarios)

Industry	Functional unit	GHG mitigation potential
Pulp, paper, and print industry	1 MJ electricity	40%
	1 MJ heat	8%
	1 ton of paper	32.3%
Chemical and petrochemical industry	1 MJ SAF	80.1%
Cement industry	1 GWh waste heat	245 ton of CO_2
Magnesia industry	1 ton of CCM	32.5%
	1 ton of DBM	38.2%

The case study in the pulp, paper, and print industry was analyzed at the process unit level, allowing hotspots to be identified along the production chain. The approach targeted the flexible operation of energy and production assets and the integration of low-emission technologies, such as storage, electric boilers, and PPAs. A detailed environmental analysis was conducted for the energy supply chain and product. A dynamic energy modeling approach was applied. Compared with the BAU case, a GHG reduction potential of up to 32.3% per ton of paper was achievable, independent of applying CML, ReCiPe, or TRACI impact assessment. In this case, the total PED increased by about 33.2% to 34.9 GJ per ton of paper. However, its renewable PED increased by 156% and its non-renewable PED was reduced by 32%. The determined BAU energy costs of 115.6 €/t_{paper} could be reduced by up to 44%. The cost of preventive measures to avoid environmental impacts was determined in the range of 80 to 93 € per ton of paper, revealing that GWP, MAEP, and HTP are the most influential factors.

In the chemical and petrochemical industry, the analysis focused on various biorefinery set-ups for SAF production, aiming to meet mandatory GHG emission reduction targets. Integrating RES and valorizing the by-product lignin for energy supply was essential to achieving the objectives. These measures demonstrated a potential GHG reduction of up to 80% for 1 MJ SAF compared to the fossil benchmark. Although there were increases in PED in scenarios involving lignin and RES, the renewable energy share could meet up to 82% of the PED demand. Energetic and exergetic analyses showed SAF production efficiencies ranging from 11.7% to 14.9% and 11% to 13.8%, respectively, which increased from 39.4% to 50.1% and 40.4% to 56.9% when evaluated at the system level.

In the cement industry case study, several concepts were explored for the recovery of waste heat from cement plant exhaust gases and its utilization as process heat for a dairy. These concepts included TES of various capacities to compensate for different durations of process interruptions. An annual GHG emission reduction potential of up to 22,000 tons was identified, equivalent to 245 tons of CO_2 savings per recovered GWh of waste heat. Using a top-down approach, the maximum acceptable total cost for economic viability was determined based on natural gas savings, amounting to €10.6 million (at the price level in early 2020). However, none of the developed concepts met this cost limit. The concepts' CAPEX ranged from €23 million to €44 million. Including a TES system resulted in maximum storage costs of 1.4 €/kWh for 500 MWh and 14.4 €/kWh for 1 MWh, highlighting the market's scarcity of feasible storage solutions. Nevertheless, the economic feasibility of the concepts may change in the future depending on developments in gas prices and CO_2 tariffs, which are currently in a period of upheaval.

The case study in the magnesia industry focused on integrating various biomass resources as co-firing fuels with pet coke. An environmental analysis was conducted for the CCM and DBM products. By substituting pet coke with olive kernels in the kiln (10% of the thermal energy demand) and calcination stage (70% of the thermal energy demand), GHG reduction potentials of 32.5% for CCM and 38.2% for DBM could be achieved. The integration of electricity from RES played a minor role in the production of magnesia. In addition, a field test demonstrated that the annual operational production cost for thermal energy demand could be reduced by 9.75% to approximately €11 million by co-firing with SHP at a 50% substitution of pet coke.

7 CONCLUSION AND OUTLOOK

Climate neutrality is one of the greatest present challenges facing humankind. Various economic sectors, such as industry, households, and transport, are responsible for harmful GHG emissions and must find climate-neutral paths through suitable measures in their sectors. By ensuing legally binding climate targets, Europe has set its goal of becoming the first continent to become climate-neutral by 2050. In this context, Europe is taking on a pioneering role, followed by other countries and continents. This roadmap is particularly challenging for industries, especially energy-intensive industries that have built their energy systems mainly on fossil fuels and are now being forced to adapt. Time is pressing, and effective decarbonization measures must be taken to avoid future fines while maintaining competitiveness. In this context, LCA plays a crucial role in helping governments and industries in identifying sustainable technologies and transformation pathways at an early stage.

7.1 Originality

The integration of renewable resources, electrification, flexibility options, waste heat recovery, circular economy principles, CCU/CCS, and other efficiency measures are frequently mentioned as key technologies and approaches for the transition towards green industries. While these measures contribute actively and positively to industrial decarbonization and energy efficiency, there is a need for quantifying their specific GHG impact at the site, energy, and product levels. LCA effectively addresses this need by determining GHG savings potential through comprehensive mass and energy balance assessments compared to a business-as-usual (BAU) scenario. Beyond CO_2 emissions, other factors such as acidification and eutrophication are also analyzed, resulting in a holistic ecological assessment. LCA enables the identification of effective measures at an early stage, eliminating the need for costly field trials or plant retrofits. Additionally, it helps identify emission hotspots along the value chain and facilitates targeted actions to improve efficiency. Thus, LCA provides decision-makers with a valuable and cost-effective basis for informed decisions, particularly in a fast-paced environment where decarbonization choices must be made confidently. Furthermore, customers are increasingly concerned about the environmental performance of products and are more willing to accept economic trade-offs if a product is manufactured sustainably.

Scenario and sensitivity analyses broaden the decision-making basis by evaluating and comparing different plant configurations, energy supply options, product focuses, and by-product uses. This enables ecological optimizations and the identification of the best-case set-up and layout for sustainable operations. Sensitivity analyses allow the identification of essential parameters and evaluation of their influence on the main results. Thus, the associated risks can also be minimized in advance when making decisions.

Integrating renewable energy supply technologies with increased capacities will become increasingly important in the coming years and decades. Renewable sources like solar and wind inherently exhibit fluctuations in their generation. To harness the full potential of this energy, it is necessary to integrate new flexible technologies such as electrical, thermal, and chemical storage, as well as heat pumps and electric boilers, to establish a more adaptable manufacturing process. Ensuring uninterrupted supply and avoiding product shortages are fundamental requirements in industrial operations. Matching supply and demand in the power grid is crucial for maintaining grid stability, and industrial plants can contribute positively. Currently, emissions from the energy supply are often considered using static geographically-based average values from previous years, which are then assigned to the product. To accurately represent emissions associated with flexible energy supply and production, a dynamic energy modeling approach has been integrated into the LCA. By using a time-resolved load profile and energy production profile, time-resolved emission profiles are generated, providing a realistic assignment of emissions to the product.

Other factors, such as energetic and economic constraints, must also be considered in conjunction with ecological conditions to remain competitive. A holistic evaluation incorporating multiple criteria allows for identifying the best pathway at an early stage, thus securing a competitive advantage. Techno-economic evaluations, preliminary estimates of economic and environmental impacts, and considering energy quality (exergy) broaden the perspective and enable a systemic view, preventing a narrow focus on a single criterion. The selection of optimization criteria from environmental, techno-economic, and energetic aspects depends on the specific objectives and priorities of the stakeholders involved. Although these criteria may sometimes appear in conflict, it is essential to note that they are not mutually exclusive. For instance, improving energy efficiency can lead to cost savings (economic efficiency) by reducing energy purchases and related expenses.

The developed integrated LCA method provides a comprehensive and early assessment of new technologies and approaches to achieve a transition to a carbon-neutral industry. A structured approach is essential for this purpose so that several criteria can be systematically determined. The entire approach does not always have to be used in the initial analyses and assessments. If ecological objectives cannot be achieved, the profitability calculation becomes obsolete.

7.2 Research limitations

The integrated LCA approach and results are subject to some limitations. A primary limitation is the lack of comprehensive and sophisticated data for holistic assessments of several indicators for informed decision-making. A low TRL is inherent to available data, but which is essential for the accuracy of evaluations. Ex-ante assessments always imply high risks of uncertainty and must never be interpreted as generally valid. Scaling-up laboratory data to final process data can show different results that can lead to different conclusions about the success of technologies. Industries provide usually only limited data to carry out specific assessments. Sensitive production information would allow competitors to draw conclusions about production processes and their efficiency, risking ruining business models. This is especially the case when new technologies are under development and initial analyses should provide insights for further research needs. Another sensitive information is cost data for techno-economic analyses, hardly communicated for research purpose. Costs and results are time dependent, as is currently the case with changes in the energy pricing landscape, and require careful consideration and elaboration. In many cases, literature assumptions must be applied to fill data gaps, leading to non-specific results. This research applied literature and aggregated data in exchange with experts from industrial companies to come up with meaningful results. Scenario development and sensitivity analyses of selected indicators assist in overcoming data limitations and assessing potential impacts. Nevertheless, an initial integrated LCA allows hotspots to be identified at an early stage and dead ends to be avoided from a particular perspective, be it environmental, techno-economic, or energetic. Transparency of assumptions and underlying data is key for communication and interpretation of results.

A further limitation is that the dynamic energy modeling approach does not consider the dynamics of energy background processes, which may influence the results in future. Due to the expected increase of RES in the grids, there will be technological progress for renewable systems, e.g., through higher yields or scale-up of capacities, which potentially can have a positive impact through lower specific emissions for energy supply. However, the applied energy background processes from the LCA database have a valid time representativeness until 2025. Of course, the results can be updated after the validity period to analyze the time-dependent impacts. In addition, future research is needed on how to integrate a temporal behavior of energy background processes into LCA software with suitable interfaces.

7.3 Outlook

Holistic assessments can lead to the development of a carbon-neutral European economy by 2050. There are a variety of innovative low-emission technologies and sustainability approaches, as explained in the study, which have different potentials depending on the industry. Likewise, energy efficiency measures and sufficiency are key to success, as the most environmentally friendly and cost-effective energy sources are those that are not consumed at all. In addition to the environmental objectives, the evolution of the investment costs of renewable energy systems determines the speed of integration. Infrastructural adaptations (for electricity, heat, and gas) are required to operate future renewable energy systems. Electricity is an important factor in energy transition, in parallel with energy imports required to meet the demand cost-effectively. Nevertheless, successful demonstrations and flagship projects of innovative approaches are essential to increasing replication across industries. Replications will increase, particularly when successful field tests are available, without affecting product quality or production targets. For industrial pioneers, availability of sufficient funding can particularly enable the promotion of innovations in a real-world environment and showcasing them in an economically viable manner. These efforts will be the key to achieving a climate-neutral, competitive, and prosperous EU.

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APPENDIX A: PARTICIPATION IN RESEARCH CONFERENCES

(1) Puschnigg, Stefan; Knöttner, Sophie; Lindorfer, Johannes (2022) Development of a virtual battery concept demonstrator: A case study from the pulp and paper industry, 17th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES), 6th to 10th of November 2022, Paphos (Cyprus)

(2) Puschnigg, Stefan; Moser, Simon; Goers, Sebastian (2022) A techno-economic and macro-economic concept study of waste heat utilization of a cement plant, New Energy For Industry (NEFI) conference, 13th to 14th of October 2022, Linz (Austria)

(3) Puschnigg, Stefan; Fazeni-Fraisl, Karin (2022) A life cycle assessment of high characteristics drop-in biofuels from residual soft wood, International Scientific Conference of Environmental and Climate Technologies CONECT, Riga Technical University, 11th of May 2022, Riga (Latvia)

(4) Puschnigg, Stefan; Volkova, Anna; Reuter, Stefan; Kauko, Hanne; Schmidt, Ralf-Roman; Leitner, Benedikt; Moser, Simon; Jauschnik, Gabriela (2021) An analysis of cascaded low-temperature sub-networks in existing district heating networks, 7th International Conference on Smart Energy Systems (SES), 21st to 22nd of September 2021 Copenhagen (Denmark)

(5) Jauschnik, Gabriela; Puschnigg, Stefan; Moser, Simon (2021) Good Practice Examples für Niedertemperatur-Subnetze in bestehenden Fernwärmenetzen, 12. Internationale Energiewirtschaftstagung (IEWT), 8th to 10th September 2021, Vienna (Austria)

(6) Moser, Simon; Puschnigg, Stefan; Rodin, Valerie (2020) Designing the Heat Merit Order to determine the value of industrial waste heat for district heating systems, 14th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES), 1st to 6th of October 2019, Dubrovnik (Croatia)

(7) Puschnigg, Stefan (2019) Talk about EU Horizon project REWOFUEL, Forum Econogy 2019, 25th of September 2019, Linz (Austria)

(8) Puschnigg, Stefan; Fazeni-Fraisl, Karin; Lindorfer, Johannes (2019) Bio-isobutene: Life Cycle Assessment of an emerging technology for bio-based fuels and materials, International Conference on Life Cycle Management (LCM), 1st to 4th of September 2019, Poznan (Poland)

APPENDIX B: PEER-REVIEWED SCIENTIFIC PUBLICATIONS

Article A1

Puschnigg, Stefan; Knöttner, Sophie; Lindorfer, Johannes; Kienberger, Thomas: "Development of the virtual battery concept in the paper industry: Applying a dynamic life cycle assessment approach," Sustainable Production and Consumption, volume 40, 2023, https://doi.org/10.1016/j.spc.2023.07.013

Submitted: 24th of April, 2023

Published: 17th of July, 2023

Table A 1: Author contribution statement for article A1

Activity	Contributing authors
Conceptualization	S. Puschnigg, S. Knöttner
Methodology	S. Puschnigg
Data curation	S. Puschnigg, S. Knöttner
Software development and modeling	S. Puschnigg
Validation	S. Puschnigg, J. Lindorfer, T. Kienberger
Investigation and analysis	S. Puschnigg, S. Knöttner
Visualization	S. Puschnigg
Writing (original draft)	S. Puschnigg, S. Knöttner
Writing (review and editing)	S. Puschnigg, S. Knöttner, J. Lindorfer, T. Kienberger

Johannes Lindorfer was the project manager of the associated project that led to the results of this research article and was responsible for project administration, supervision, and funding acquisition.

Sophie Knöttner was a project partner and contributed to the development of the virtual battery concept, provided simulation data for the dynamic energy modeling approach, and focused on the techno-economic assessment.

Thomas Kienberger validated and reviewed the article prior to submission.

Article A2

Puschnigg, Stefan; Fazeni-Fraisl, Karin; Lindorfer, Johannes; Kienberger, Thomas: "Biorefinery development for the conversion of softwood residues into sustainable aviation fuel: Implications from life cycle assessment and energetic-exergetic analyses," Journal of Cleaner Production, volume 386, 2023, https://doi.org/10.1016/j.jclepro.2022.135815

Submitted: 7th of October, 2022

Published: 29th of December, 2022

Table A 2: Author contribution statement for article A2

Activity	Contributing authors
Conceptualization	S. Puschnigg
Methodology	S. Puschnigg
Data curation	S. Puschnigg
Software development and modeling	S. Puschnigg
Validation	S. Puschnigg, K. Fazeni-Fraisl, J. Lindorfer, T. Kienberger
Investigation and analysis	S. Puschnigg, K. Fazeni-Fraisl
Visualization	S. Puschnigg
Writing (original draft)	S. Puschnigg
Writing (review and editing)	S. Puschnigg, J. Lindorfer, T. Kienberger

Karin Fazeni-Fraisl was the project manager of the associated project that led to the results of this research article and was responsible for project administration, supervision, and funding acquisition.

Johannes Lindorfer and Thomas Kienberger validated and reviewed the article prior to submission.

Article A3

Puschnigg, Stefan; Lindorfer, Johannes; Moser, Simon; Kienberger, Thomas: "Techno-economic aspects of increasing primary energy efficiency in industrial branches using thermal energy storage," Journal of Energy Storage, volume 36, 2021, https://doi.org/10.1016/j.est.2021.102344

Submitted: 20th of November, 2020

Published: 15th of February, 2021

Table A 3: Author contribution statement for article A3

Activity	**Contributing authors**
Conceptualization	S. Puschnigg
Methodology	S. Puschnigg, S. Moser, J. Lindorfer
Data curation	S. Puschnigg
Software development and modeling	S. Puschnigg
Validation	S. Puschnigg, S. Moser, J. Lindorfer, T. Kienberger
Investigation and analysis	S. Puschnigg, S. Moser
Visualization	S. Puschnigg
Writing (original draft)	S. Puschnigg
Writing (review and editing)	S. Puschnigg, S. Moser, J. Lindorfer, T. Kienberger

Simon Moser and Johannes Lindorfer were the project managers of the associated projects that led to the results of this research article and were responsible for project administration, supervision, and funding acquisition.

Simon Moser, Johannes Lindorfer, and Thomas Kienberger validated and reviewed the article prior to submission.

Article A4

Margaritis, Nikolaos; Evaggelou, Christos; Grammelis, Panagiotis; Yiannoulakis, Haris; Papageorgiou, Polykarpos; Puschnigg, Stefan; Lindorfer, Johannes: "Use of biomass as alternative fuel in magnesia sector," Fuels, volume 3, no. 4, 2022, https://doi.org/10.3390/fuels3040039

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Published: 9th of November, 2022

Table A 4: Author contribution statement for article A4

Activity	Contributing authors
Conceptualization	N. Margaritis, C. Evaggelou
Methodology	S. Puschnigg, C. Evaggelou, H. Yiannoulakis
Data curation	S. Puschnigg, N. Margaritis, H. Yiannoulakis, P. Papageorgiou
Software development and modeling	S. Puschnigg, N. Margaritis, P. Papageorgiou, C. Evaggelou
Validation	H. Yiannoulakis, P. Papageorgiou, P. Grammelis, J. Lindorfer
Investigation and analysis	S. Puschnigg, N. Margaritis, H. Yiannoulakis, P. Grammelis, P. Papageorgiou, J. Lindorfer
Visualization	S. Puschnigg, C. Evaggelou
Writing (original draft)	S. Puschnigg, C. Evaggelou, N. Margaritis
Writing (review and editing)	N. Margaritis, H. Yiannoulakis, J. Lindorfer

Haris Yiannoulakis, Nikolaos Margaritis, and Johannes Lindorfer were project managers of the companies involved in the collaborative project that led to the results of this research article and were responsible for project administration, supervision, and funding acquisition. The authors also reviewed the article prior to submission.

Stefan Puschnigg was responsible for the life cycle assessment of this research article and contributed to the respective life cycle assessment sections. This included the life cycle assessment methodology, data curation, software development and modeling, investigation and analysis, visualization, and writing (original draft).

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Development of the virtual battery concept in the paper industry: Applying a dynamic life cycle assessment approach

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ABSTRACT

Energy-intensive industries face the challenge of reducing carbon emissions while remaining competitive. Key measures include fossil fuel substitution, energy efficiency, and integration of renewable energy sources, but their fluctuating production profile makes them difficult to integrate and require industries to adapt their current consumption and production patterns to become more flexible.

In this study, the virtual battery concept (VBC), exemplarily demonstrated for a specific site in the paper industry, is introduced and evaluated from an environmental, energetic, and techno-economic perspective. A mathematical optimization model of the class mixed integer linear programming (MILP) was applied to express the industrial site as VBC and derive the operational data basis for the subsequent life cycle assessment (LCA). A dynamic LCA approach is presented to allow the consideration and assessment of the temporal behavior of energy load profiles and their associated environmental implications.

The results showed that compared to a static LCA, the dynamic approach leads up to 42 % lower greenhouse gas (GHG) emissions for 1 MJ of public electricity. The global warming potential (GWP) of the total energy supply chain was reduced by 40 % for electricity and 8 % for heat, respectively. By means of a scenario analysis, the GWP to produce one ton of paper was reduced up to 33 % compared to the business-as-usual (BAU) case to 672 $kgCO_2eq._r$ in the best case. However, the total primary energy demand (PED) increased by 34 %, but the fossil PED was reduced by 32 % and the renewable PED increased by 157 %. The renewable PED share covered up to 67 % of the total PED. The techno-economic analysis revealed total annual cost savings of up to 44 % to 64.6 € per ton of paper. Environmental costs were estimated to range from 79.6 to 88.9 € per ton of paper.

The VBC is considered a promising approach to utilize regional renewable excess electricity effectively, reduce fossil-based energy generation, increase grid stability, and to avoid costly grid infrastructure investments in future. In principle, the VBC is site-independent and replicable to other industries but needs to be evaluated site specifically according to certain process characteristics and requirements.

1. Introduction

In energy-intensive industries, reducing carbon emissions while remaining competitive is a major challenge. An energy transition from a fossil driven energy system toward renewable energy and increased energy efficiency are key parameters to meet carbon neutrality by 2050 (European Commission, 2019). However, the integration of fluctuating renewables such as solar or wind energy is challenging (Wee et al., 2012), because industries must adapt their current consumption and production patterns (Beier et al., 2017). Consequently, there is a need for new technologies in the industry that allow higher flexibility in power supply and simultaneously reduce consumption and dependence on fossil fuels. Rissman et al. (2020) presents and discusses technologies and policies for decarbonizing the global industry. Waste stream valorization and waste heat recovery are essential toward a decarbonized energy system (European Commission, 2011). If everything has already been optimized internally, industrial symbiosis offers the possibility of external utilization (Rodin and Moser, 2022), and targets the concept of a circular economy (Lieder and Rashid, 2016).

Various initiatives alongside and as part of the *EU Green Deal* (European Commission, 2019) are intended to support overcoming these

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Nomenclature

Abbreviations

ADP elements	abiotic depletion elements
ADP fossil	abiotic depletion fossil
AP	acidification potential
BAU	business-as-usual
CAPEX	capital expenditures
CEPI	Confederation of European Paper Industries
DIP	de-inked pulp
DSM	demand-side management
eq.	equivalent
EB	electric boiler
EP	eutrophication potential
ES	electric storage
EU	European Union
FAETP	freshwater aquatic ecotoxicity potential
GC	grid connection
GHG	greenhouse gas
GW	groundwood
GWP	global warming potential
HOB	heat-only-boiler
HP	heat pump
HTP	human toxicity potential
KPI	key performance indicator
LCA	life cycle assessment
LCI	life cycle inventory
LCIA	life cycle impact assessment
LWC paper	lightweight coated paper
MAEP	marine aquatic ecotoxicity potential
MILP	mixed integer linear programming
NG-CHP	natural gas combined heat and power plant
ODP	ozone layer depletion potential
OPEX	operational expenditures
PED	primary energy demand
PGW	pressurized groundwood
PM A	paper mill A
PM B	paper mill B
POCP	photochemical ozone creation potential
PPA	power purchase agreement
PV	photovoltaic
ROI	return on investment
SC paper	super-calendered paper
TAC	total annual costs
TEA	techno-economic assessment
TES	thermal energy storage
TETP	terrestric ecotoxicity potential
VBC	virtual battery concept

Variables and parameters

a	annuity factor
A	generic coefficient matrix in mathematical optimization
b	generic coefficient vector in mathematical optimization
c	parameter for specific costs of energy for paper production in €/t
c	variable for charging of storages
C	specific prices in €/MWh or €/t
C	consumption matrix
C	continuous operation share of ground wood unit
Cap	capacity of a unit in MW or MWh
$CAPEX$	capital expenditures in M€/a
COP	coefficient of performance
$Cost$	cost in M€/a
d	variable for discharging of storages
D	demand matrix
des	variable for integration of a unit or not (design decision variable)
ΔT	timestep duration in optimization model
e	parameter related to specific energy demand (thermal or electrical)
η	efficiency
f	factor for specific consumption of "subscript" in "superscript"
fun	generic functional expression
I	number of pulper pairs active
i	interest rate
l	generic coefficient vector in mathematical optimization
LB	lower bound
$\dot{m}$	mass flow in t per timestep
m	mass in t/a
n	depreciation period in years
$OPEX$	operational expenditures in M€/a
P	electric power in MW
p	paper production in t
P	production matrix
$payback$	payback period in a
Q	parameter for thermal power
q	variable for thermal power
ROI	return-on-investment
S	variable for state of charge
sd	variable for shut-down decision
su	variable for start-up decision
T	parameter for up and down times as well as start and shut down times
t	running time index
$\tilde{t}$	additional running time index
TAC	total annual costs in M€/a
u	generic coefficient vector in mathematical optimization
UB	upper bound
x	operational decision variable for on- and offline state
y	generic decision variable in mathematical optimization

Subscripts

a	variable is an annualized value
BAU	value or variable related to Business-as-usual scenario
bio	biomass (solid)
CHP	variable related to combined heat and power
CO2	variable related to greenhouse gas specific values
deliv	variable or parameter related to delivery
DIP	variable or parameter related to de-inked pulp
down	parameter related to down time
EB	variable or parameter related to electric boiler
EES	variable or parameter related to electric storage
EH	variable or parameter related to excess heat
ELEC	variable related to electricity specific values
energy	energy related value
ext	variable or parameter related to external consumption
fix	variable or parameter related to fixed costs for investments
FLH	variable related to full load hour specific values
GC	variable or parameter related to specific grid connection point
geo	geothermal
GP	variable or parameter related to ground pulp
GRID	variable related to grid specific values
GW	variable or parameter related to ground wood
HOB	heat only boiler
HP	variable or parameter related to heat pump
holiday	parameter related to national holiday
max	variable or parameter related to upper bound (maximum value)

n.d.	non defined
NG	variable related to natural gas specific values
nuc	nuclear
paper	value related to paper production amount
PM	variable or parameter related to paper machine
PPA	variable related to PPA specific values
pv	photovoltaic
s	variable related to scenario *s*
SG	variable related to steam generation
spec	specific value
STAFF	variable related to staff/employee specific values
TES	variable or parameter related to thermal storage
th	thermal
up	parameter related to up time
wood	variable or parameter related to wood

Superscripts

DIP	variable or parameter related to de-inked pulp
opt	value derived from optimization – can include assumed (lower) cost factors
PM	variable or parameter related to paper machine
price	variable or parameter related to specific costs
real	value derived when considering realistic cost factors
unit	value for a specific unit of the optimization model

Sets

Unit	all units considered in the optimization model
Factor	set of all cost factors

challenges: the *REPowerEU* to save, diversify, and produce clean energy as a response to Russia's invasion in Ukraine (European Commission, 2022), the *Net-Zero Industry Act* to scale-up the manufacturing of clean technologies (European Commission, 2023a), and *The Green Deal Industrial Plan* to increase the competitiveness of Europe's net zero industry (European Commission, 2023b).

This study focuses on increasing flexibility and greenhouse gas (GHG) mitigation measures in the energy-intensive paper industry. In 2021, the pulp and paper sector was accounting for approximately 190 Mt. of CO_2 emissions, corresponding to about 2 % of the total emissions of the industrial sector (IEA, 2022). This sector is responsible for approximately 6 % of global industrial energy consumption (Lipiäinen et al., 2022). China is the largest producer of paper products and energy consumption is the main contributor to carbon emissions (Wang et al., 2016). In Man et al. (2019), a review of energy consumption and energy-saving issues, and hence emission reduction potential, was conducted on a life cycle basis. Owttrim et al. (2022) found that energy efficiency is one of the key elements of a carbon-neutral paper sector. To remain competitive in the market, Laurijssen et al. (2012) pointed out the need for controlled energy costs even as energy prices rise. General insights into the industrial sector and the status of the best available technologies for pulp and paper production are elaborated in Joint Research Centre et al. (2015). The energy flexibility potential in the process industry was generally assessed by Pierri et al. (2020), but with a case-specific analysis of the paper production sector. This research was extended by an impact analysis of integrating fluctuating energy (Pierri et al., 2021).

In Sun et al. (2018), a comprehensive life cycle assessment (LCA) review was conducted for pulp and paper production. The average GHG emissions to produce one ton of paper are estimated to be approximately 950 $kgCO_2eq.$, where energy use is the main influencing parameter, depending on the applied type of pulp and considered country. In 2021, the UPM's environmental product declaration for paper stated 1050 $kgCO_2$ for one ton of SC paper (super-calendered paper) in Germany (UPM, 2021), which was assessed according to the CEPI (Confederation of European Paper Industries) framework. Shang et al. (2022) developed an indicator system to evaluate the transition to a green paper industry on a global level, with the conclusion that developed countries need to promote green technologies. Moosavi et al. (2021) proposed an analytical hierarchy model based on LCA to facilitate decision-makers to move toward greener paper manufacturing.

Dynamic approaches are applied to consider time-dependent parameters in LCA. Dynamic considerations can include expected future technological developments such as for renewables (Pehnt, 2006), operational differences during the lifetime (Negishi et al., 2018), real-time life cycle inventory data (Filleti et al., 2014), temporally differentiated characterization factors (Pinsonnault et al., 2014), and temporally resolved GHG emissions (Sproul et al., 2019). Because the GHG emission reduction potential is widely used in industry to discuss climate impacts, the consideration of GHG variability is recommended for energy technologies in future LCA studies (Lan and Yao, 2022), which was examined in this research. A real-time consumption based carbon accounting approach for European electricity markets was introduced in Tranberg et al. (2019), pointing out the differences between production and consumption carbon intensities, and cross-border flows.

To assess the economic feasibility and environmental implications of new technologies, the combination of LCA and techno-economic assessment (TEA) is considered as a valuable instrument (Ferdous et al., 2023). Especially for emerging green technologies, an environmental and techno-economic assessment framework enables early evaluation of integration potential and derivation of technology improvements (Thomassen et al., 2019).

This study aims to analyze a novel virtual battery concept (VBC) from environmental, energetic, and techno-economic perspectives. The VBC concept enables industries with increased operational flexibility for production and energy provisions aligned with the regional energy demand and supply, thereby potentially supporting the public grid. In addition, a dynamic LCA approach is presented for ecological evaluation, which considers the variability in emissions resulting from energy provision. In principle, static LCAs are typically performed. However, owing to the increased flexibility in energy provision, the need for a dynamic LCA approach was pointed out and its impact was compared to static considerations for energy provision. This approach allows emissions to be realistically assigned to operation modes and products. By understanding the temporal energy emission profiles, operators and energy system planners can make more informed decisions on how to improve the sustainability and efficiency of the analyzed production system as well as for their products. The VBC and dynamic LCA were exemplarily applied for an industrial site in the paper industry, but is replicable to all industrial sectors.

2. Literature

This chapter serves as a basis for the subsequent description in Section 3. This lays the foundation for the structure and objective of the developed VBC and demonstrates the need for dynamic considerations of energy emissions.

2.1. Flexibility in industry

Flexibility in the context of energy systems and the manufacturing industry gains importance due to the necessary integration of fluctuating renewables and set decarbonization targets. To date, there is no uniform definition of flexibility in the energy industry (Beucker et al., 2020). However, a common understanding is seen as a prerequisite for making the best use of flexibility (Degefa et al., 2021). This requirement has also been supported by the creation of a VDI guideline in the subject area of *energy-flexible* factories in the last three years (VDI, 2020, 2021). A property of flexibility is that it typically serves a higher purpose such as incentives or goals to increase the flexibility of a specification (Luo et al., 2022). In Golden and Powell (2000), flexibility is defined as the ability of a system to adapt (capability instead of capacity) and as a polymorphic and multidimensional property of a system, whereby a corresponding definition has a clear meaning only through context and identified dimensions. Degefa et al. (2021) reviewed various definitions and classifications for flexibility and provided a comprehensive definition and taxonomy approach for flexibility resources. From the perspective of the power system, flexibility is often traded as an important factor to succeed in decarbonizing the generation of electric power, including increasing the installed capacity of fluctuating renewable energy carriers. Often, these measures include flexible operation of generation, flexible demands, (electrical) energy storage, expansion of grid infrastructure, or adapted market designs (Alexopoulos et al., 2021; IRENA, 2018; Papaefthymiou et al., 2014). In the manufacturing industry, flexibility is sometimes seen primarily as a competitive advantage to realize economic operations, while helping to reduce GHG emissions (Roesch et al., 2019). Industrial production systems are considered as relevant contributors to the flexibility of the power grid. The industrial demand side as well as the storage and generation side for industrial self-generation can contribute to this. Such measures are often referred to as demand-side management (DSM), where consumer loads are strategically controlled and adjusted to balance supply and demand (Babatunde et al., 2020). Typically, DSM measures include load shifting, peak shaving, and valley filling (Lund et al., 2015). Triggers, or as the introduced incentives, for DSM are price signals or the need for grid stabilization (Roesch et al., 2019).

In contrast to the term flexibility, the term resilience generally defines the ability of a system to return to a stable state after a disruption (Bento et al., 2021). In Di Tommaso et al. (2023), resilience is also considered as a measure to support industrial policy making. Disruptions can arise internally or externally, such as the COVID-19 pandemic or current policies for a green energy transformation, which can be challenging for industries such as the oil and gas by not losing profitability and functional ability (Sindhwani et al., 2022). Flexibility can be considered as one measure to increase resilience (Bento et al., 2021; Sindhwani et al., 2022).

Flexibility can be provided at different levels with different technologies and measures. Thus, flexibility does not necessarily refer exclusively to the use of electricity but also to heat generation and the use of diverse raw materials. An interpretation of flexibility in the context of industrial production can be made as follows:

a) Flexible products and production processes: What is produced and when?
b) Flexible energy supply: How and when energy (electricity and heat) is provided? What energy generation assets are used? How can fluctuating generation from renewables be integrated?
c) Flexible adaption of energy assets: How fast can they adapt to changed circumstances?

In this study, flexibility is understood as a measure of the industrial energy supply and demand system that reacts to (regional) fluctuating renewable electricity. Thus, flexibility in the context of this study supports the integration of renewable energy in a pathway to a decarbonized power system.

Table 1 provides a list of technologies and measures (supply, demand, and organizational) related to flexibility that were considered in this study. The combined heat and power (CHP) plant and heat-only-boilers (HOBs) are established fossil-driven energy assets in industry. Power-to-heat technologies, storage, and power purchase agreements (PPAs) allow for an increased integration of renewables, especially excess renewable electricity, at industrial sites. There is a wide range of options for energy storage, which differ in terms of cost, storage duration, capacity, density, and efficiency. Depending on the case, the appropriate technology must be selected. In the pulp and paper industry, the highest potential for production flexibility is assigned to the pulp and stock preparation processes. Depending on the specific technology, either temporal shutdown or step-wise/continuous load reduction are possible measures (Moser et al., 2018). According to Langrock et al.

Table 1
Industrial energy flexibility technologies and measures considered in this study.

Classification	Technology	Impact on flexibility	Description	Source
Flexible industrial generation asset	CHP (fuel-to-power-and-heat)	With possible substation units and corresponding planning, flexibility provider	Provides the main share of electricity and heat for industrial operation, part-load operation possible under considering technical limitations	(Kahlert and Spliethoff, 2016; Pierri et al., 2020, 2021)
	HOB (fuel-to-heat)	With possible substation units and corresponding planning, flexibility provider	Mostly used as back-up for the CHP, allows for an immediate operation when needed	(Pierri et al., 2020, 2021)
Flexible industrial demand asset	Electric boilers (power-to-heat)	With possible substation units and corresponding planning, flexibility provider	Usually operated in conjunction with a conventional energy supply system as back-up or support measure; frequently used for coupling to short-term energy markets or the secondary control energy market	(Manni et al., 2022)
	High-temperature heat pumps (power-to-heat)	With possible substation units and corresponding planning, flexibility provider	Less (electric) energy and thus less high-exergy energy sources are needed to provide the same amount of heat compared to electric boilers; suitable heat sources: ambient air, groundwater, and industrial waste heat streams; temperatures of up to 160 °C are currently feasible	(IEA, 2023)
	Paper machine	If free production capacities exist with corresponding planning, flexibility provider	Electricity demand depends on amount of paper produced per timestep and thus adaption of product order or shut down of paper machine is technically possible	(Langrock et al., 2015; Pierri et al., 2020)
	Mechanical fibre production	If free production capacities or material storages exist with corresponding planning, flexibility provider	Electricity is used to drive grinders for wood fibre production depending on the technology, either stepwise or continuous consumption adaption above a minimum generation level is possible	(Langrock et al., 2015; Pierri et al., 2021)
Storages	Thermal	Allows temporal decoupling of supply and demand, flexibility provider	Sensible, latent, thermochemical, and sorption storage technologies	(Puschnigg et al., 2021)
	Electrical	Allows temporal decoupling of supply and demand, flexibility provider	Batteries, supercapacitors	(Alexopoulos et al., 2021; Lund et al., 2015)
Contracting	PPAs	Increasing need for flexibility in electricity consumption when integrated	Agreement between an electricity supplier and a consumer such as for solar or wind electricity	(Isaza Cuervo et al., 2021)
Organization	Planning	Providing flexibility	Find optimal operation schedules for economic, ecologic and other frame conditions, e.g. By optimization	(Degefa et al., 2021)

(2015), promising load flexibilities are achieved by (i) pulpers, refiners, and wood grinders that are not continuously in operation, (ii) paper machines, in particular the press section, but also further electrical components, and (iii) coating machines and calenders. In combination with storage for intermediate products such as groundwood, the adaption of energy consumption profiles without a reduction in product quality is possible.

2.2. Power purchase agreements

The integration of renewable energy sources into the industrial sector is key to establishing carbon-neutral energy supply options. To increase the share of renewable electricity in the energy supply chain, on-site renewable assets can be installed or PPAs such as solar or wind can be contracted. A PPA is a long-term agreement between an electricity supplier and a consumer (Isaza Cuervo et al., 2021; Jenkins and Lim, n.d), in which the number of years and price are determined (Gabrielli et al., 2022a). For renewable electricity plant suppliers, long-term PPAs with industries allow them to continue operating after their statutory payment period (Fischer et al., 2019).

Several contractual PPA structures exist that can, in principle, be divided into physical and non-physical PPAs (Gabrielli et al., 2022b; Rövekamp et al., 2021). Physical PPAs are favorable when generation and consumption are in proximity, as costs can be minimized by avoiding the use of public infrastructure. However, a private electricity network must be built (Rövekamp et al., 2021). In non-physical PPAs, also known as virtual PPAs, no direct connection between generation and consumer exists, and a third party often serves as a trading company (Miller and Carriveau, 2018). Whereas traditional PPAs are based on a fixed volume, more flexible PPA contracts such "as produced PPAs" are gaining importance (Jain, 2022), which are generally less expensive, but require a higher degree of flexibility on the demand side. The risks of PPAs are implied by the volatility of renewables, but can be reduced by providing storage functionality to balance supply and demand (Miller and Carriveau, 2018). To optimize future PPA contracts, long-term wind and solar energy generation forecast models were proposed by Mesa-Jiménez et al. (2023).

In this study, photovoltaic PPAs are considered for the development of the virtual battery concept in Section 2.3, since the paper mill under investigation is situated in southern Germany, where PV has a dominant role. There are several PV parks in the vicinity of the plant, which is why a physical connection and an "as produced PPA" contract is foreseen. The intermittent characteristic of PV is integrated in the model by fluctuating available irradiation amounts per timestep, derived from historic irradiation profiles for the region.

2.3. Virtual battery concept

This study introduces the VBC, which is exemplarily demonstrated in the pulp and paper industry, but can basically be replicated in all industries, depending on the specific site process characteristics and requirements. The paper industry is among the energy-intensive industries, along with the steel, non-mineral, and chemical industries. Due to its energy-intensive processes, which usually run continuously and are mostly supplied by on-site energy generation plants, it is ideally suited for the development of the VBC. The VBC unfolds its effects especially in these sectors and industrial sites, where diverse energy generation assets exist already and are available for flexible operation, as it is mostly the case in the paper industry. In addition, the paper industry includes several processes that can produce on stock (as elaborated in Table 1) and can thus be flexibly operated aligned to renewable production and its integration. However, by investing in flexible energy technologies such as storage solutions, the VBC can be in principle implemented in other industries as well, but with reduced flexibility and hence impact.

The aim of the VBC is to operate an industrial plant as a battery that can supply or demand energy, like a normal storage system (Fig. 1). Therefore, the VBC utilizes flexibility options for the production process and for electricity and heat generation assets at the industrial site aligned to the regional electricity supply and demand. In times of high electricity demand in the region, on-site industrial assets support the balancing of demand. In times of low demand, on-site energy generation is reduced and energy is mainly consumed from the public grid. The VBC impacts the energy system by increasing the grid stability, avoiding costly infrastructure investments to prevent bottlenecks in transmission grids, and enabling the integration of volatile renewable energies. In addition, the VBC allows the integration of local renewable electricity surpluses through PPAs.

To fully utilize and analyze the impact of the VBC in the paper industry, two main VBCs were developed:

- **VBC 1:** The power and heat flexibilities of existing energy generation assets are considered. In the production process, the load shifting of grinders and paper machines is executed toward times of high local renewable energy production. The energy flexibility strategy for the industrial site is as follows: in times of high local renewable generation, more electric power from the grid will be used to fulfil the electricity demand of the production process, and CHP generation will be reduced according to technical limitations or even turned off. The reduced heat generation is replaced by the increased heat generation by the HOBs.
- **VBC 2:** Builds on VBC 1, but provides additional flexibility by implementing new energy generation and storage assets. The implementation of further energy flexible assets allows for an increased renewable uptake and a further shift away from a fossil-driven energy system toward a renewable energy system. Sector-coupling power-to-heat technologies such as electric boilers and heat pumps are integrated and operated. Electrical and thermal storage are integrated to enhance temporal flexibility and store the available excess energy.

The integrated PPAs are considered separately for VBC 1 and VBC 2. In this exemplarily VBC study for the paper industry, physical "as produced" PPAs are considered, because of their availability in the region.

To develop a VBC, all production processes with flexibility potential can be considered independently of the industry. Depending on the industrial plant and existing energy generation assets, further energy generation and storage technologies can be integrated according to the needs and requirements of the energy system for enhanced energy flexibility. A list of considered energy technologies is provided in Section 2.1.

A detailed description of the production process and energy supply chain of the analyzed paper mill is presented in Section 3.1.4. The scenario development for each VBC in Section 3.2 discusses the specific energy system setups.

2.4. Consideration of dynamic energy provision and emissions

The electricity provision is subject to seasonal and daily fluctuations. A mix of energy sources is used to balance the supply and demand. The energy supply mix depends on geographic conditions and, thus, on environmental emissions associated with the provision of electricity. In general, static average electricity mixes are used to evaluate the environmental impact of energy supply. However, in this study, the need for a time-resolved consideration of energy provision was highlighted. As a result, a dynamic LCA approach was developed, which is introduced in Section 3.1.

In this study, an analysis of the German public electricity grid is conducted to highlight this need. The aim was to obtain additional insights into the time-resolved electricity consumption profile and thus derive further triggers to reduce environmental impacts. The underlying data were requested and provided by Electricity Map and analyzed with

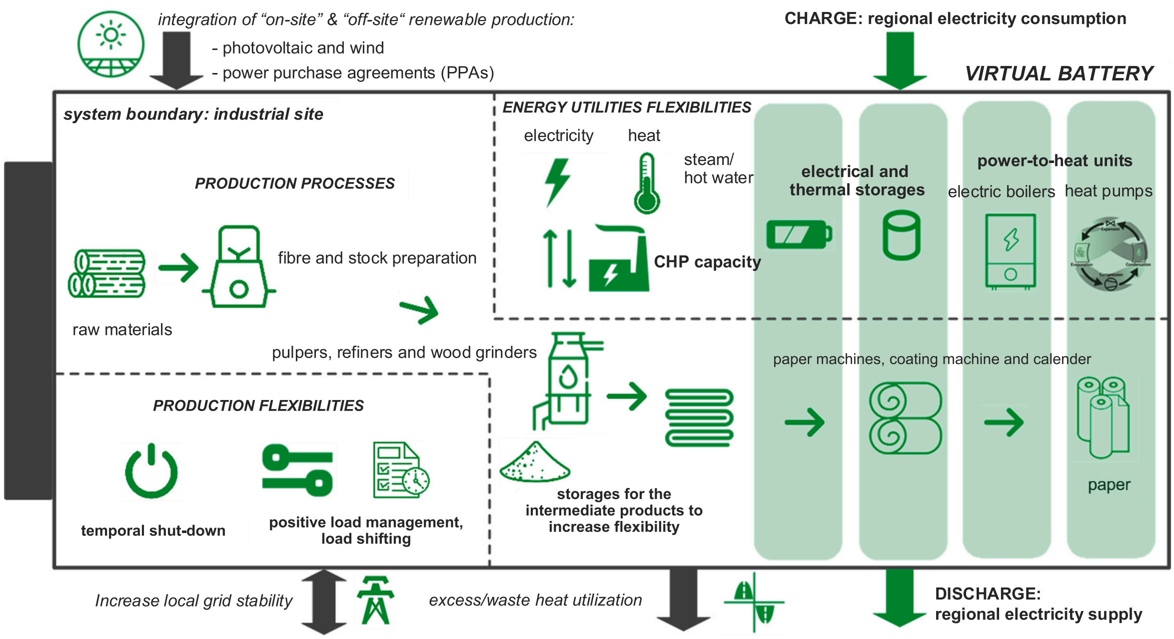

Fig. 1. Description of virtual battery concept.

a time resolution of one hour (Electricity Map, 2023).

A heat map was created to show the temporal occurrence of the most frequently discussed impact category, the carbon emissions (Fig. 2). The carbon intensity refers to how many grams of carbon dioxide (CO_2) are released to produce a kilowatt hour (kWh) of electricity. The heat map shows the carbon intensities plotted over a year, as well as the behavior and change during a day at a one-hour time resolution. Thus, daily and seasonal fluctuations can be revealed and possible future flexibility options for consuming renewable power can be considered in production planning. In times when many renewable technologies are in operation, a low CO_2 footprint is achieved; higher emissions occur when more fossil resources are used to cover the capacity. Through the adapted and more flexible operation of the processes in times of low carbon intensities, the specific ecological footprint per product can be reduced. In view of the decarbonization measures required to achieve a carbon-neutral industry in 2050 (European Commission, 2019), flexibilization measures can provide additional contributions. High-intensity time windows should be avoided for operation in order to reduce the amount of fossil-based electricity generation.

In the context of the German electricity mix in 2021, low carbon intensities have especially occurred during the summer months. In these time windows, renewables and low-carbon-intensive electricity sources can meet the demand. High intensities occurred especially during the night in those time windows, when coal was used to cover the electricity demand. Low-carbon-intensity windows can provide opportunities to consume electricity mainly from the grid and to operate on full load, thereby producing a low-carbon intensive product. The annual evaluation revealed that the CO_2 intensities of electricity generation varied between 123 and 549 gCO_2eq/kWh_{el}. Due to this large bandwidth of carbon emissions, a dynamic LCA approach was developed to represent

Fig. 2. Carbon intensity of German electricity production in 2021.

temporal influences. In addition, other impact categories such as eutrophication and acidification are assessed.

3. Methods

This study applies a dynamic LCA approach and a techno-economic assessment to evaluate the environmental and cost implications of the VBC. A business-as-usual (BAU) case was defined and scenarios were developed to show the impact of selected key performance indicators (KPIs) such as GWP, PED, and energy cost.

3.1. Dynamic life cycle assessment approach

In this study, a LCA was performed according to the ISO 14040/14044 standards by applying the software GaBi 10.6 ts by Sphera (GaBi 10.6 ts by Sphera, 2022). The ISO 14040 standard consists of four steps: definition of the goal and scope, life cycle inventory (LCI), life cycle impact assessment (LCIA), and improvement and interpretation (International Organization for Standardization, 2006b; International Organization for Standardization, 2006a). Owing to the existence of many publications on the standard LCA methodology (Finnveden et al., 2009; Guinee, 2002; Klöpffer, 1997), only the essential aspects are elaborated in the following sub-chapters. Literature on dynamic LCA approaches considering time-dependent parameters exist in several studies (Collinge et al., 2013; Filleti et al., 2014; Lan and Yao, 2022; Pehnt, 2006).

In general, a LCA considers static energy emission profiles by energy carriers available in established LCA databases such as the GaBi ts 10.6 Professional Database (Sphera, 2023) and Ecoinvent v.3.8 database (Ecoinvent, 2023). However, in this study, the static approach was adapted by considering dynamic energy and hence emission profiles resulting from energy provision aligned to the energy consumption at a one-hour time resolution, as shown in Fig. 3. The general energy supply chain is described in Section 3.1.4 and specifically elaborated in the developed scenarios in Section 3.2. All load profiles for energy provision were obtained by mixed-integer linear programming (MILP) optimization for the VBC, which is detailed in Section 3.1.1.

The data merging approach for the public grid is detailed in Section 3.1.2. The dynamic electricity production profiles of the public grid were obtained from the raw data of (Electricity Map, 2023), introduced in Section 2.4.

3.1.1. Load profile: mathematical optimization via mixed-integer linear programming

For the dynamic LCA approach presented in this study, a database that includes temporally resolved operational characteristics of all relevant components in the industrial production system is required. Possible sources for such a database could be the measurement data or the results of simulation studies. For this research, the latter approach of simulation studies was chosen, since by using a mathematical model, a set of scenarios for different parameters and conditions can be derived in a comparably short time, especially compared with collecting measurement data. Furthermore, mathematical models also allow the inclusion of other regulatory settings, different prices, and the analysis of future developments.

The modeling approach chosen in this study was a mathematical optimization method. In general, mathematical optimization aims to find an optimal solution (determine the optimal values of variables) for a defined objective criterion while fulfilling constraints that express, for example, technical or organizational boundaries in mathematical equations. Here, the problem was formulated according to the group of mixed-integer linear programs. A MILP typically consists of a linear objective function, continuous and integer decision variables, and constraints formulated as linear equations, including equality and inequality equations. The general formulation is given by Eq. (1):

$$\begin{aligned}
&\min_{x} \boldsymbol{fun}^T \cdot \boldsymbol{y} \\
&\text{subject to} \\
&\boldsymbol{Ay} \leq \boldsymbol{b} \\
&\boldsymbol{l} \leq \boldsymbol{y} \leq \mathbf{u} \\
&\boldsymbol{y} \in \mathbb{R}^n \\
&y_j \in \mathbb{Z}, j \in S
\end{aligned} \tag{1}$$

The formulation of the optimization model is based on a general tight and compact MILP formulation based on Gentile et al. (2017). The following technical characteristics of the units were considered in the optimization model:

- minimum part-load operation
- efficiencies for full and part load operation
- minimum off- and online times
- storage, charging and discharging efficiencies

Furthermore, regulatory frame conditions and the integration of new power supply possibilities in the form of "as-produced" PPAs are considered in the optimization model.

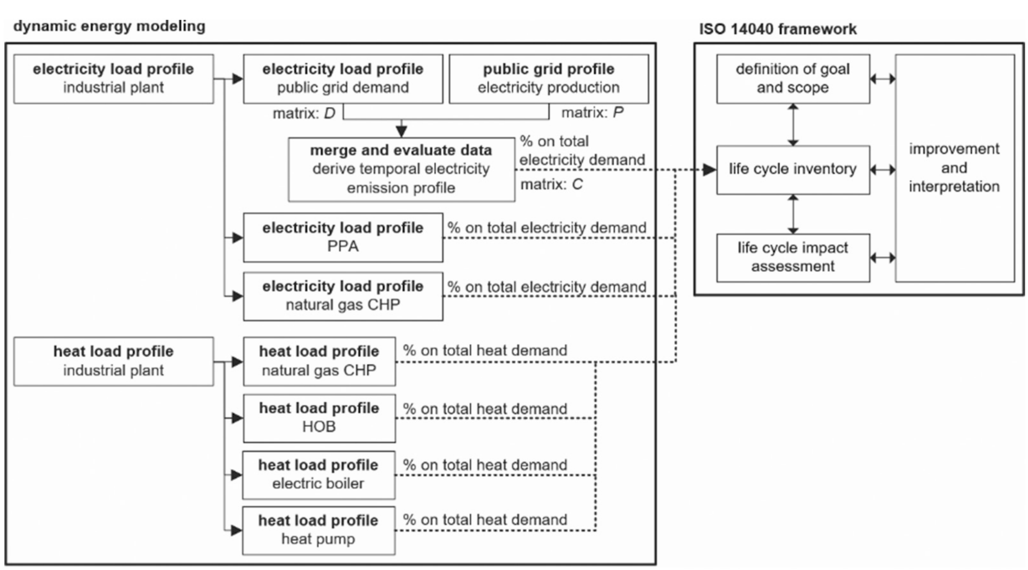

Fig. 3. Overview of dynamic Life Cycle Assessment approach.

For this study, the total costs are defined as the optimization objective. Depending on the scenario, either annual operational costs or the sum of annual operational costs and annualized investment costs are used. The details of the cost calculation are presented in Section 3.4. For the implementation, formulation, and solution of the optimization model, the following settings were chosen for all scenarios: The optimization task was implemented in Python using the Pyomo optimization module (Bynum et al., 2021). The model was set-up to find optimal values for a duration of one year with a timestep size of 6 h resulting in a model with 1460 timesteps. An efficient MILP solver, CPLEX (Cplex and IBM ILOG, 2009), is used. The optimization calculations for the developed scenarios in Section 3.2 had a defined upper time limit of 18 to 48 h.

3.1.2. Dynamic energy and emission modeling

Dynamic energy modeling is used to consider the variability of emissions over time, as well as the influence of external factors such as energy supply mix and energy consumption. To merge the electricity load profile for the public grid with the public electricity production profile into temporal energy consumption profiles, a dynamic modeling approach was used. The load profile was merged with the dynamic electricity production data on a one-hour time resolution in the software R and served as input for the LCA, representing the time-varying behavior of the system. By combining consumption and load profiles with specific energy-related emission, it is possible to create temporal energy emission profiles that provide a detailed picture of the emissions associated with the operation of an industrial plant. Therefore, the approach aims to merge electricity production and the specific industrial load profile to achieve a realistic energy origin emission evaluation.

The yearly public consumption matrix C of the industrial plant by energy carrier is calculated according to Eq. (2):

$$D \times P = C \tag{2}$$

where the public grid demand matrix D is multiplied by the production matrix P. A detailed elaboration of the matrices is given in Eq. (3):

$$\begin{bmatrix} D_1 & D_2 & \cdots & D_{8760} \\ D_1 & D_2 & \vdots & D_{8760} \\ \vdots & \vdots & \vdots & \vdots \\ D_1 & D_2 & \cdots & D_{8760} \end{bmatrix} \times \begin{bmatrix} x_{1,pv} & x_{1,nuc} & \cdots & x_{1,n.d} \\ x_{2,pv} & x_{2,nuc} & \vdots & x_{2,n.d} \\ \vdots & \vdots & \vdots & \vdots \\ x_{8760,pv} & x_{8760,nuc} & \cdots & x_{8760,n.d} \end{bmatrix} = \begin{bmatrix} C_{pv} \\ C_{nuc} \\ C_{bio} \\ C_{coal} \\ C_{hydro} \\ C_{oil} \\ C_{geo} \\ C_{wind} \\ C_{gas} \\ C_{n.d.} \end{bmatrix} \tag{3}$$

where the demand matrix D consists of the hourly load profiles of one year (x = 1 to 8760); the production matrix P of the hourly shares of the public electricity production profiles by energy carrier for PV, nuclear, biomass, coal, hydro, oil, geothermal, wind, natural gas, and a non-defined share; and the calculated yearly consumption matrix C by energy carrier.

The specific inputs for the LCA to determine the public energy mix composition are calculated by defining the specific shares of the energy carriers on yearly consumption according to Eq. (4):

$$E_i = \frac{C_i}{\sum_n C_n} \tag{4}$$

where C_i is the yearly consumption of the energy carrier and $\sum_n C_n$ is the sum of the yearly energy consumption from the public grid.

The energy carrier datasets from the GaBi Professional Database (Sphera, 2023) were used to model the calculated energy mix for each scenario. Because there exists a non-defined share in the data obtained by Electricity Map (2023), the average German electricity mix dataset is considered for this category. For coal, a German-specific assumption for lignite and hard-coal usage was considered at a ratio of 2:1.

3.1.3. Definition of goal and scope

The goal was to analyze the environmental implications of the virtual battery concept and the respective energy supply chains for the developed scenarios to derive the overall GHG emission mitigation potential of the VBC. First, a comparison of the static and dynamic LCA approaches was conducted for electricity provision in Germany. Second, the environmental impacts of the energy supply chains were analyzed for the functional units of 1 MJ of electricity and heat. Third, the emissions to produce one ton of paper were calculated on process unit level and benchmarked against the defined BAU case. The functional unit of one ton of paper was a mix of 66 % of super-calendered paper (SC paper) and 34 % of lightweight coated paper (LWC paper). Although a full LCA was conducted, this study focused on selected KPIs for GWP and PED.

3.1.4. Description of the paper mill and the system boundary

Paper production is a very diverse process that has been described extensively in the literature (Joint Research Centre et al., 2015). Depending on the type of paper produced, it requires its own process. Thus, paper mills and their processes are very different and site-specific. An accurate description of the individual process steps and functionality is omitted; however, the main flow and essential process steps are described in more detail.

The analyzed paper mill shown in Fig. 4 produces SC and LWC paper grades. Depending on the grade, the composition of the virgin fibre, sulfate pulp, recycled paper, and necessary chemicals varies. The detailed composition is listed in the LCI Section 3.1.5. The wood logs are delivered by diesel trucks and trains and then stored on a forecourt. The logs can be debarked as needed, thus providing flexibility. They are then fed to wood grinders, where pressurized groundwood (PGW) and groundwood (GW) are differentiated. Electricity-intensive wood grinders are again a suitable flexibility option, because production can be stocked. Wood pulp is produced on-site, and sulfate pulp is purchased and delivered by train. Recycled paper is collected and delivered by trucks, where it is deinked at the plant. Subsequently, a mixture of raw materials is prepared and bleached before being applied to the papermaking machine. The SC paper is produced at paper mill A (PM A), the LWC paper at paper mill B (PM B). The LWC paper also underwent an additional coating process.

Residual materials are generated along the production chain: bark and wood residues from the grinders, bio-sludge and primary sludge from wastewater treatment, deinked sludge from the deinking process, and waste paper rejects. In addition, low-temperature waste heat is generated, which is made available to external companies such as dairy (steam) and asparagus farmers (hot water).

The energy provision for the industrial plant is as follows: The electricity demand is covered by a mix of the on-site natural gas-fired CHP and/or the public grid, and the heat demand by a mix of the CHP and/or the on-site natural gas heat-only-boilers (HOB) to cover peak demands. In the future, additional energy generation assets will be considered for implementation, which will provide increased energy flexibility. Electricity can be obtained from PPAs and heat produced by an electric boiler and/or heat pumps. Electrical and thermal energy storage provide additional flexibility for electricity and heat provision. The electricity is consumed through four grid connection (GC) points.

The system boundary for the LCA of the analyzed paper production plant is shown in Fig. 4. This LCA follows a “cradle-to-gate” approach according to the LCA framework. In general, a “cradle-to-grave” approach is favorable (Guinee, 2002), but a full end-of-life treatment is not considered due to its complexity. However, the recycling and deinking of paper, as well as end-of-life treatment of bio-sludge residues, were included in the analysis. The geographical system boundary was

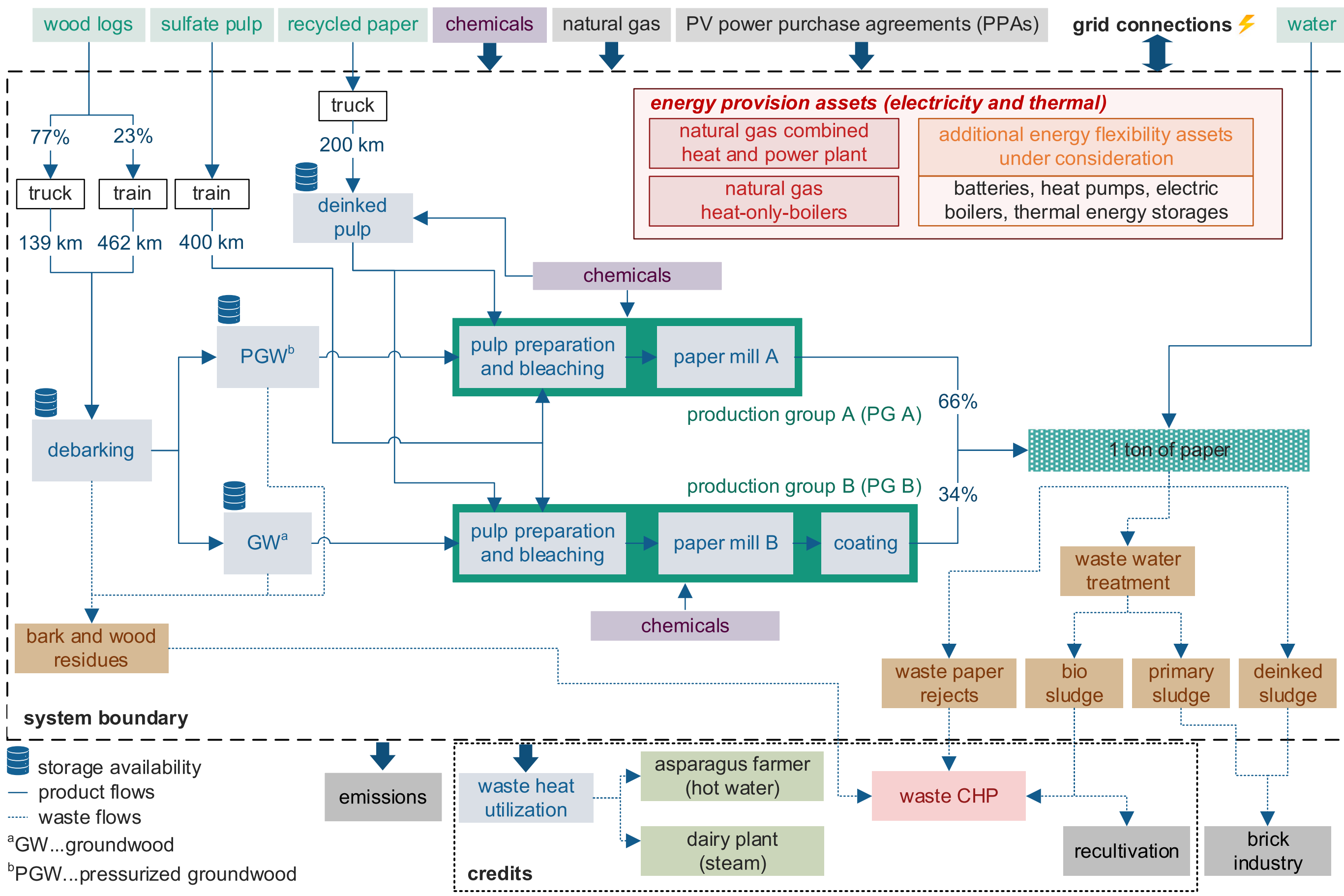

Fig. 4. System boundary of exemplarily analyzed system in the pulp and paper industry.

defined for Germany, as the paper mill is situated in Bavaria, Southern Germany (Pierri et al., 2021). The production and installation phase of the heat pump, electric boiler, electric storage, and thermal storage was not considered in the analysis, but only the operational emissions from the energy source. This is common practice in LCA studies, as it has hardly any influence compared to the amount of energy provided over the lifetime and thus on the functional unit (Bello et al., 2018; Uihlein and Schebek, 2009). A specific research on industrial heat pumps in Zeilerbauer et al. (2023) confirmed, that the environmental implications depend primarily on the operational phase.

3.1.5. Life cycle inventory and data collection

The aim of the life cycle inventory (LCI) is to collect the necessary mass and energy data to conduct the LCA. All relevant data were obtained from the literature and additionally validated by expert insights via meetings and sight visits to the industrial plant. The full LCI is provided in the supplementary material in Table S 1.

The load profiles obtained from the MILP optimization, which served as inputs for the dynamic LCA approach, are provided in Appendix A. The data for electricity production in Germany in 2019, which is also required for this purpose, can be requested and purchased from Electricity Map (2023). The applied background processes, such as for chemicals and energy provision and their associated ecological impact, were obtained from the GaBi ts 10.6 Professional and ecoinvent v.3.8 databases.

3.1.6. Life cycle impact assessment

The Life Cycle Impact Assessment (LCIA) was conducted based on the CML 2016 methodology, which was examined using the LCA software GaBi 10.6 ts by Sphera. Characterization factors were applied to the LCI in Section 3.1.5 and the results were grouped into midpoint categories such as climate change and ecotoxicity. In this study, the focus was placed on selected KPIs mostly relevant to industries: (i) the global warming potential (GWP) calculated in kg CO_2-equivalents, and (ii) the primary energy demand (PED) in MJ structured into total, non-renewable (fossil), and renewable PED according to the cumulative energy demand method (Klöpffer, 1997; VDI, 2012). Several other impact categories were analyzed and are their results provided in the supplementary material, such as abiotic depletion elements (ADP elements) in Fig. S 1, abiotic depletion fossil (ADP fossil) in Fig. S 2, acidification potential (AP) in Fig. S 3, eutrophication potential (EP) in Fig. S 4, freshwater aquatic ecotoxicity potential (FAETP) in Fig. S 5, human toxicity potential (HTP) in Fig. S 6, marine aquatic ecotoxicity potential (MAETP) in Fig. S 7, ozone layer depletion potential (ODP) in Fig. S 8, photochemical ozone creation potential (POCP) in Fig. S 9, and terrestric ecotoxicity potential (TETP) in Fig. S 10.

3.1.7. Avoided burden approach (credits)

The avoided burden approach is part of the framework of the ISO 14040/14044 standards and allows for the use of so-called “credits” to account for auto-generated by-products along the production chain of the main product (International Organization for Standardization, 2006b). A credit substitutes an external resource such as a material and/or energy, which consequently is no longer required to be produced in the corresponding substituted quantity. Other methodologies to assign a specific ecological footprint to by-products are allocations according to mass, energy, or economic value, but were not applied in this study. In general, credit and allocation reduce the ecological impact of the main product (Klöpffer, 1997).

In this research, the waste heat substitutes thermal energy from natural gas for an asparagus farmer and a dairy, which are both located in proximity of the paper mill, with an annual average of 28 MJ and 39.5 MJ per ton of paper, respectively. The bark, wood residues, waste paper rejects, and 40 % of the subsequent dewatered bio-sludge are burned in a residual CHP and substitute electricity and steam from natural gas (Sphera, 2022). The remaining 60 % bio-sludge was used for recultivation and substituted ammonium nitrate, potassium chloride, and phosphate. Substitutions have been chosen according to Turner et al. (2022), where 1 kg of bio sludge substitutes in average 4.4 % ammonium nitrate, 0.039 % potassium, and 1.5 % phosphate. Primary sludge and deinking sludge are frequently used in the brick industry as porosity agents, but no credits have been considered for this (Walter and Tesar, 2009).

3.2. Scenario development and sensitivity

The goal of the scenarios is to evaluate different VBC set-ups and parameters from an ecological, energetic, and economic point of view. The scenarios were developed based on the VBC, technologies, and framework conditions introduced in Section 2 and are described in Table 2. A BAU case, representing a benchmark, is representative of the current operation and energy provision at the paper mill. The scenarios differ in terms of their flexibility potential, implemented technologies, regulatory considerations, capital expenditures (CAPEX), and operational expenditures (OPEX). Price levels for 2019 were considered for each scenario.

Scenarios S0 to S3 are based on the VBC case 1 (Section 2.3) and considers existing flexibilities from the manufacturing process and energy provision assets. Scenarios S4 to S6 are part of the VBC case 2 and includes additional energy assets and hence the use of increased flexibility. The difference between the scenario difference is as follows: S0 includes existing flexibilities and an energy provision via CHP plant, HOB, public grid); S1 is as S0 but with PPAs at 20€/MWh; S2 is as S0 but with PPAs at 0 €/MWh; S3 is as S2 but without grid regulation; S4 is as S1 but with electric boiler as new asset; S5 is as S4 but with heat pump, TES, and electric storage as new assets; and S6 is as S5 but without grid regulation. The structure of the energy supply between the assets and their capacities were determined with the optimization model and are presented as part of the results in Section 4.2.1.

For the LCA, the paper production process is analyzed under the defined system boundary in all scenarios, as shown in Fig. 4. The associated LCI with all the raw materials required and the specific energy demand on process level is listed in the supplementary material in Table S 1. For the new assets of electric boiler, heat pump, electric storage, and thermal storage, only the operational emissions for energy provision were included in the analysis. The external PPAs are considered by using the German specific photovoltaic data set from GaBi Professional database (Sphera, 2019a).

The TEA is based on the same system boundary as the LCA. The corresponding cost parameters for energy, certificates, grid fees, personal and penalties, and investment costs are elaborated in detail in Section 3.4.

A sensitivity analysis is performed for each scenario to evaluate the impact of energy consumption (±10 %, ±20 % and ± 30 % variation) on paper production for the parameters of GWP, total PED, non-renewable PED, and renewable PED. For ±30 % variation, the results are provided in Section 4.3.3, for the other variations in the supplementary material in Table S 2.

3.3. Environmental costs

The so-called "shadow-price" is commonly used to estimate the economic impact resulting from the life cycle environmental impacts. The shadow price is defined as the cost of prevention measures to avoid environmental impact. As a result, shadow-price monetarizes environmental impacts and aims to support the decision-making processes of governments (Amadei et al., 2021; de Bruyn et al., 2010, 2018; Gerloff, 2023; Zeilerbauer et al., 2023).

To determine the environmental costs, the results obtained from the LCA for each impact category are first multiplied by the respective weighting factor of the shadow price for the impact category. The sum of all specific impact categories is then calculated to obtain the environmental costs. The shadow price weighting factors are based on the environmental impact assessment method CML, which was introduced in Section 3.1.6. The weighting factors were defined by Bouwkwaliteit (2019) and applied in this study.

Table 2
Developed virtual battery scenarios for LCA analysis.

Scenario	VBC case	Description	Regulation[a]	PPA	OPEX	CAPEX
BAU	–	Business-as-usual; energy provision: CHP, public grid, HOB	Yes	No	Yes	–
S0	1	Existing flexibilities; energy provision: CHP, public grid, HOB	Yes	No	Yes	–
S1	1	Existing flexibilities; energy provision: CHP, public grid, HOB, PPA: 20 €/MWh	Yes	Yes	Yes	–
S2	1	Existing flexibilities; energy provision: CHP, public grid, HOB, PPA: 0 €/ MWh	Yes	Yes	Yes	–
S3	1	Existing flexibilities, energy provision: CHP, public grid, HOB, PPA: 0 €/ MWh	No	Yes	Yes	–
S4	2	Existing flexibilities and new energy assets; energy provision: CHP, public grid, electric boiler, PPA: 20 €/MWh,	Yes	Yes	Yes	yes
S5	2	Existing flexibilities and new energy assets; energy provision: CHP, public grid, electric boiler, heat pump, electric storage, thermal storage, PPA: 20 €/MWh	Yes	Yes	Yes	no[b]
S6	2	Existing flexibilities and new energy assets; energy provision: CHP, public grid, electric boiler, heat pump, electric storage, thermal storage, PPA: 20 €/MWh	No	Yes	Yes	no[b]

[a] Yes means that the German-specific 7000 h regime for the grid connections is considered to minimize network fees (Bundesministerium der Justiz, 2023).
[b] No means that there are only very low costs (100 €/MW) for S5 and S6 compared to S4 considered.

3.4. Techno-economic assessment

A set of evaluated techno-economic key performance indicators (KPIs) is presented together with relevant equations and parameters to determine the KPIs. The following economic KPIs are derived from the optimization model for each scenario (subindex s):

- annual operational expenditures ($OPEX_{a,s}$),
- annualized investments as capital expenditures ($CAPEX_{a,s}$),
- total summed up annual costs (TAC_s) and the derived specific energy costs (c_{energy}) to produce one ton of paper.

For scenarios, in which additional investments are considered ($CAPEX_{a,s} > 0$), the return on investment (ROI_s) and payback period ($payback_s$) are also evaluated.

The $OPEX_{a,s}$ are calculated according to Eq. (5):

$$OPEX_{a,s} = Cost_{STAFF,s} + Cost_{ELEC,s} + Cost_{GRID,s} + Cost_{FLH,s} + Cost_{PPA,s} + Cost_{NG,s} + Cost_{CO_2,s} \tag{5}$$

where $Cost_{FACTOR,s}$ is the total annual cost for one specific cost group with the sub-index $FACTOR$ for scenario s. The set $FACTOR$ consists of $STAFF$ (for additional personal costs on national holidays), $ELEC$ (for electricity from the public grid), $GRID$ (for power-related grid usage fees), FLH (for penalties in case of violating the 7000 h per year full-load criterion), PPA (for electricity from the PV PPA), NG (for natural gas), and $CO2$ (for certificates required when emissions of CO2 or any other greenhouse gases – here these are caused by natural gas – occur).

For the CAPEX KPI, two values need to be evaluated. $CAPEX_{a,s}^{opt}$ considers the specific cost parameters used in the optimization model, calculated according to Eq. (6). For S5 and S6, specific investment cost parameters lower than in the best estimate of investment costs in S4 are assumed to determine the upper bounds for integrated capacities. Consequently, another value for capital expenditure, $CAPEX_a^{real}$, is determined in Eq. (7) considering the real investment costs.

$$CAPEX_{a,s}^{opt} = a \cdot Cost_{inv,s}^{opt} = \frac{(1+i)^n \cdot i}{(1+i)^n - 1} \left(\sum_{unit} Cost_{inv,s}^{unit,opt} \right) \tag{6}$$

$$CAPEX_a^{real} = a \cdot Cost_{inv,s}^{real} = \frac{(1+i)^n \cdot i}{(1+i)^n - 1} \bullet \left(\sum_{unit} Cost_{inv,s}^{unit,real} \right) \tag{7}$$

where α is the annuity factor, calculated from the interest rate i and depreciation period in years n, and $Cost_{inv}$ is the total investment cost in the corresponding scenario, resulting from investment costs for the set $unit = \{Heat\ pump, Electric\ boiler, Thermal\ Storage, Battery\}$.

To determine the total annual costs (TAC), the OPEX and CAPEX are summed up according to Eq. (8). The specific energy costs (c_{energy}) are calculated based on the annual amount of produced paper ($m_{paper,annual}$) according to Eq. 9.

$$TAC_s = OPEX_{a,s} + CAPEX_{a,s} \tag{8}$$

$$c_{energy} = \frac{TAC_s}{m_{paper,a}} \tag{9}$$

The payback period is calculated based on Eq. (10), and the ROI according to Eq. (11). A comparison of the scenario results for $OPEX_{a,s}$ with the status quo $OPEX_{a,BAU}$, which represents the OPEX in the BAU case, is required to determine savings.

$$payback_s = \frac{\text{investment}}{\text{savings}} = \frac{Cost_{inv,s}^{real}}{OPEX_{a,BAU} - OPEX_{a,s}} \tag{10}$$

$$ROI_s = \frac{OPEX_{a,BAU} - OPEX_{a,s}}{Cost_{inv,s}^{real}} \tag{11}$$

The specific cost parameters in Table 3 and Table 4 were applied to parametrize the optimization model. An interest rate of 3.5 % and a depreciation period of 15 years is assumed based on discussions with the industrial use case operator for the case study presented in this work. The assumption of 15 years depreciation period is oriented at current estimations for technical lifetimes of new assets such as heat pumps and electric boilers. Here, a little lower value than the estimations, often in the range of 20 years) are assumed. The comparably small interest rate of 3.5 % - in industry values of 5 to 7 % are more typical, is chosen, as the authors and the industrial operator are aware of the economic burdens for heat pumps and electric storage feasibility in industry (especially for current price levels). Thus, this parameter is set to a rather low value to promote the integration of new units to a stronger extent.

4. Results and discussion

This section provides the results from the ecological, techno-economic, and energetic evaluation of the energy supply mix and paper production. The results focus on the selected KPIs of GWP, PED and energy cost. In addition, the impact of static versus dynamic LCA modeling is discussed. The results of the other impact categories from the LCA for paper production are provided in Appendix B.

4.1. Comparison of the dynamic vs. static LCA approach for the public grid

The results of the dynamic energy modeling approach were compared against established data sets in LCA for electricity provision for the impact category of GWP (Fig. 5). In principle, the existing country-specific data sets are used in LCA to cover the necessary electricity input flows in the LCA model. In this study, and since the plant to be investigated is in Germany, this would either be the grid mix of 1–60 kV (Sphera, 2019b) or the consumer grid mix of <1 kV (Sphera, 2021). As this study applies the LCA software GaBi, these electricity data sets were extracted from the internal Professional data base, and are valid according to the software provider until 2025. These existing datasets contain the average shares by electricity source and account for factors such as imports and losses in transmission and distribution to determine the GWP. The main electricity sources in Germany are lignite, wind, hard coal, and natural gas. The GWP for the 1–60 kV grid mix is 118.2 gCO_2eq/MJ and slightly higher for the consumer mix <1 kV at 121.9 gCO_2eq/MJ due to greater distribution losses.

The dynamic approach is now applied to determine the influence of the dynamic consideration over these static data sets. It was found that the dynamic GWP could be up to 39.7 gCO_2eq/MJ lower than the static GWP. This reduction is particularly notable in S4, where there is a 32.6 % decrease in GWP compared with the consumer mix. Regardless of the scenario (S0 to S6), lignite, hard coal, and natural gas were mainly responsible for GHG emissions and contributed to approximately 93 % of the GWP. Other energy sources such as renewables energy from wind or photovoltaic, or the often diversely discussed nuclear energy have only a marginal impact.

The analysis showed that a time-resolved analysis for electricity supply reveals substantial differences compared to static considerations and the associated GWP of the plant's electricity supply, which is essential for determining a realistic product carbon footprint. Tranberg et al. (2019) aim in the same direction by claiming the need for time-resolved emissions, which are particularly relevant in the GHG Protocol (WRI and WBCSD, 2015) for determining precise Scope 2 emissions for accurate GHG reporting. The approach was carried out for the system boundary of Germany, but can be transferred and evaluated for other national electricity grids, leading to different country-specific results.

4.2. Ecologic and energetic analysis of the energy supply chain

A detailed analysis of GWP and PED was conducted for the energy

Table 3
Cost parameters for energy, certificates, grid fees, personal and penalties.

Parameter	Symbol	Unit	Specification	Value	Source
Electricity	$C_{el}^{price}(t)$	EUR/MWh		timeseries (spot market Germany 2019) range [−75;101], average ≈ 36.77	(ENTSO-E., 2019)
Grid cost power	$C_{GC\,1}^{price}$	EUR/(MW. a)	GC1	0.2 * 93,290	Based on (Bayernwerk, 2019; Bundesministerium der Justiz, 2023)
	C_{GC2}^{price}		GC2	0.2 * 97,260	
	$C_{GC\,2}^{price}$		GC3	0.2 * 97,260	
	$C_{GC\,2}^{price}$		GC4	0.2 * 97,260	
Grid cost gas	$C_{grid\,3}^{price}$	EUR/(MW. a)		3800	Based on (E-Control., 2019; Energienetze Bayern, 2019)
Natural gas	C_{NG}^{price}	EUR/MWh		22	Assumption based on historical data (Statista, 2019a)
Certificate	C_{CO2}^{price}	EUR/t		25	Assumption based on (Statista, 2019b)
PPA	C_{PPA}^{price}	EUR/MWh		20 to determine max. potential: 0	Assumption aligned to (ENTSO-E., 2019)
Staff cost on holiday	$C_{holiday}^{price}$	EUR/day		60,000[a]	–
Penalty cost for <7000 full load hours	$C_{penalty1}^{price}$	EUR/a	GC1	5,800,000[b]	–
	$C_{penalty2}^{price}$		GC2	3,200,000[b]	

[a] Assumption: 100 EUR/h costs for employer for 24 h and 25 people.
[b] Derived from estimated maximum power consumption in MW, grid cost for power and elimination of discount (80 %).

Table 4
Cost parameters for investments into new assets in the energy supply system with an assumption of equal fixed investment costs factors.

Unit	Scenario	Fixed invest[b]	Specific invest	Source
Electric boiler (EB)	S4 S5, S6[a]	20,000 EUR 100 EUR	120,000 EUR/MW 100 EUR/MW	(Halmschlager et al., 2022)
Heat pump (HP)	S4 S5, S6[a]	20,000 EUR 100 EUR	1,000,000 EUR/MW 100 EUR/MW	(IEA, 2023)
Thermal storage (TES)	S4 S5, S6[a]	20,000 EUR 100 EUR	70,000 EUR/MWh 100 EUR/MWh	(Halmschlager et al., 2022)
Electric storage (ES)	S4 S5, S6[a]	20,000 EUR 100 EUR	550,000 EUR/MWh 100 EUR/MWh	(Halmschlager et al., 2022)

[a] For scenarios S5 and S6, costs were reduced in the optimization with the aim of finding optimal energy cost solutions and determining a technical upper bound for the capacities of the new units. Owing to the characteristics of the optimization problem, a value slightly higher than 0 EUR/MWh for specific and 0 EUR for fixed investment costs were assumed.
[b] The assumption of equal fixed investment costs was done due to the fact that for better estimations a wide range of real offers would be required. Furthermore, the authors aimed at avoiding a preferential integration of a single technology, thus the initial costs were set to comparably small but equal values.

supply chain of the paper mill for each scenario. PED is structured into a total, non-renewable (fossil), and renewable PED share.

4.2.1. Structure and capacities of the energy supply of electricity and process heat

Energy consumption was calculated for each scenario based on the origin of electricity and heat. Table 5 lists the respective shares. The BAU scenario covers the electricity demand to 10 % via the public grid and to 90 % via the on-site CHP. In the subsequent scenarios, the share of electricity from PPAs and the public grid increases, while the share of natural gas-fired CHP decreases. The process heat for scenarios BAU to S3 is produced from natural gas (CHP or HOB). By integrating PPAs and new heat provision assets, additional electricity is applied to electric boilers and heat pumps to cover the heat demand (S4-S6). This will facilitate the decarbonization of the heat supply and reduce dependence on fossil fuels.

PPAs primarily provide electricity when there is a weather favorable supply in the region. By using electricity from PPAs, there is a decrease in the amount of electricity consumed from the public grid, but exactly at those times, when there would be an increased amount of PV electricity in the grid and therefore a lower CO_2 intensity.

The determined capacities by the optimization model for the additional flexibility assets of electric boiler, heat pump, thermal storage, and electric storage are shown in Table 6. These technologies allow the entire energy supply chain to be operated even more flexible, which has a positive effect on increasing the GHG mitigation potential, discussed in more detail in the following chapters. An electric boiler and electricity storage allow for increased integration potential of renewable electricity by PPAs, which is then reused later. In conjunction with the heat pump and thermal storage, sector-coupling effects are achieved.

4.2.2. Global warming potential (GWP)

The primary source of GWP emissions is for both, electricity and heat provision, from the on-site CHP, which uses natural gas as fuel (Fig. 6). As analyzed in Sun et al. (2018), the decisive factor for GWP emissions in paper production is the energy use. In the BAU scenario, the GWP for electricity and heat was 129.3 and 67.9 gCO_2eq/MJ, respectively. However, there is potential for carbon reduction measures in both the electricity and heat supply chains by increasing the share of renewables for energy generation. A comparison of S6 with the BAU scenario revealed a GHG mitigation potential for electricity provision of approximately 40 % and for heat around 8 %, respectively. The positive impacts on the GWP of electricity provision resulted from the substitution of natural gas by lower carbon-intensive electricity consumption via the public grid and PPAs. For heat provision, the positive impacts on the GWP also result from substituting natural gas with new heat assets such as the electric boiler and the heat pump, which utilizes the on-site waste heat potential.

The GWP assessment did not consider the production and installation phase of the electric boiler and heat pump, but only the operational emissions resulting from the electricity consumption. Therefore, this represents a best-case scenario for S4 to S6, revealing the maximum GHG reduction potential. The inclusion of the production and installation phase would lead to a reduction of the maximum GHG savings. However, operational emissions are in general the decisive influencing factor for the GWP in energy supply.

4.2.3. Primary energy demand

A comparison of the electricity and heat PED of the BAU case and the

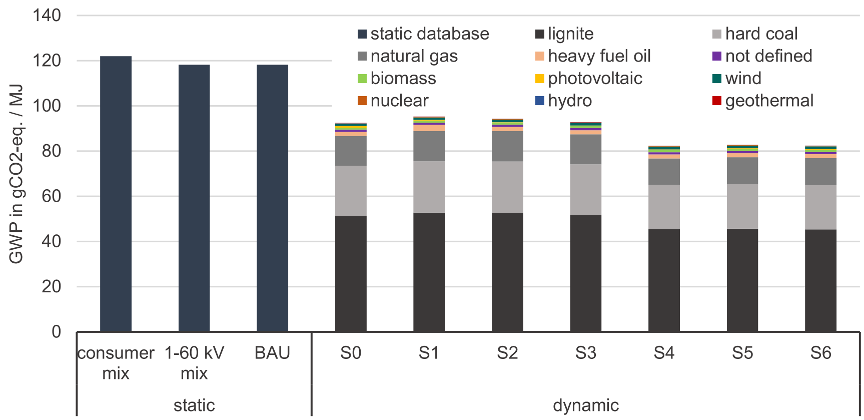

Fig. 5. Comparison of static vs. dynamic electricity LCA approach of GWP impact category for Germany.

Table 5
Structure of energy consumption.

Scenario	Electricity shares in %			Process heat shares in %			
	Public grid	CHP	PPA	CHP	HOB	Heat pump	Electric boiler
BAU	10.0	90.0	0	96.0	4.0	0	0
Scenario 0	47.7	52.3	0	75.5	24.5	0	0
Scenario 1	26.5	60.4	13.1	99.8	0.2	0	0
Scenario 2	28.1	43.4	28.5	72.7	27.3	0	0
Scenario 3	22.8	58.5	18.7	99.7	0.3	0	0
Scenario 4	27.8	42.5	29.6	79.4	0	0	20.6
Scenario 5	33.4	36.5	30.1	68.2	0	20.6	11.2
Scenario 6	32.9	36.8	30.2	68.6	0	21.0	10.4

Table 6
Capacities for new units determined in the optimization calculation.

Technology	Determined capacities		
	S4	S5	S6
Electric boiler	59.9 MW	36.3 MW	36.1 MW
Heat pump	0 MW	32 MW	32 MW
Thermal storage	0 MWh	200 MWh	200 MWh
Electric storage	0 MWh	200 MWh	162.9 MWh

developed scenarios (S0 to S6) revealed substantial changes (Fig. 7). In the electricity supply, the high PED from the public electricity grid and the PPA stands out. This is because in the cumulative energy demand method, the net total PED for 1 MJ of electricity from the natural gas CHP (2.23 MJ) is lower than that of electricity from the public grid (3.21–3.31 MJ) and PV-PPAs (6.05 MJ). Consequently, the more electricity is produced from the natural gas CHP, the lower the total PED. In the heat supply, a high impact on the total PED is detected in the scenarios of applying an electric boiler and heat pump. This results from the fact, that these assets are mainly driven by electricity from the public grid and PPAs, which have again a higher PED compared to the natural gas CHP.

The observations imply that a fossil energy supply is superior to a renewable energy supply in the context of achieving a minimal PED and increased PED efficiency. However, appearances are deceptive, which is why a detailed investigation of the non-renewable and renewable PED is required. In S6, the total PED share for electricity increased by approximately 53 %, but at the same time, the share of the renewable PED increased by remarkable 1272 %, largely due to the purchase of PPAs. Additionally, the share of the non-renewable PED was reduced by approximately 40 %. For heat provision, the total PED share increased by approximately 31 %, but the share of renewable PED increased by astonishing 7350 %, also due to the purchase of PPAs and hence operation of the electric boiler and heat pump. The share of the non-renewable PED was reduced by approximately 8 %.

The results revealed that the purchase of renewable energy under PPAs makes an important contribution to the reduction of non-renewable energy consumption and to the reduction of the energy carbon footprint. PPAs are primarily intended to cover the electricity demand with renewables, but in combination with power-to-heat assets, a renewable heat supply can be achieved. It also makes the energy supply more resilient and reduces dependence on imported fossil fuels.

4.3. Ecologic and energetic analysis of paper production

This chapter provides the results for the KPIs of the VBC for the paper mill at the product level. The results were scaled to the production of one ton of paper. The results for other impact categories are presented in Appendix B. The analysis was structured at the process level into wood handling, GW, PGW, PM A, PM B, waste, water, and credits. As credits were considered within the LCA study, which led to negative values, net emissions were marked.

4.3.1. GHG mitigation potential

The GWP of paper production, excluding the biogenic fraction, can vary clearly, with emissions ranging from 1006 to 681 $kgCO_2eq./t_{paper}$ (Fig. 8). The specific energy supply chain analysis of Section 4.2 was implemented to evaluate the impact per ton of paper. The results are in a similar magnitude as in the literature review of 45 case studies in Sun et al. (2018), with an average of 950 $kgCO_2eq./t_{paper}$. Variations are mainly due to geographical conditions, as for example in China, where carbon-intensive energy sources such as coal are applied for energy provision. The type of pulp and paper produced has also an influence on the results. In the environmental product declaration for SC paper with the geographical system boundary Germany, which thus represents a similar situation as the BAU case in this study, 1050 $kgCO_2/t_{paper}$ were reported (UPM, 2021). In addition, the annual production quantities and energy consumption variations influence the environmental implications per ton of paper, which is why it is discussed in a sensitivity analysis in Section 4.3.3.

The main sources of emissions in this evaluation were the grinders (GW and PGW) and the actual SC and LWC paper production in the production units PM A and PM B. Without considering the credits, these process units are depending on the scenario responsible for 94–96 % of the emissions. The share of the two paper production units makes up the

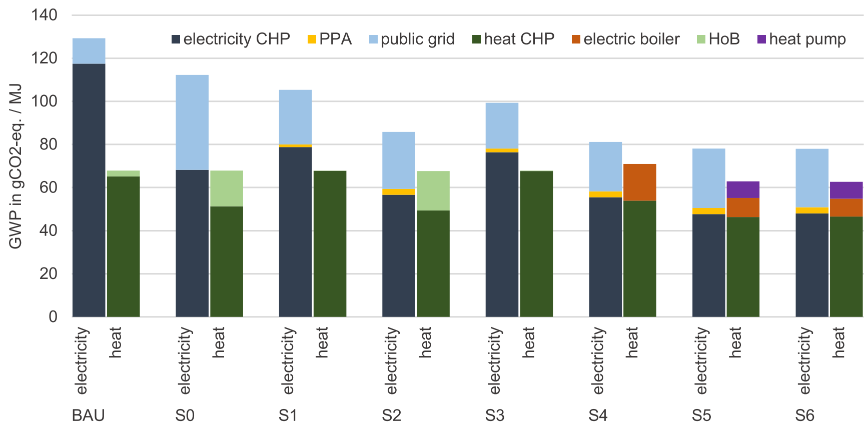

Fig. 6. GWP of 1 MJ of electricity and of 1 MJ of heat.

main part in all scenarios between 59 and 64 %. Grinders account for a share of 30–37 %. Due to the reason that PM A and its SC paper is considered for 66 % of the functional unit, compared to PM B and its LWC paper with only 34 %, PM A and PGW have a larger share of the total emissions.

The GHG mitigation potential was calculated by comparing the scenarios with the BAU case. In the best-case scenario, that is S6, compared to the BAU case, GHG emissions of 325.1 $kgCO_2eq./t_{paper}$ can be saved. In terms of the GHG mitigation potential, this provides a reduction potential of flexibility measures of up to 32.3 % (Fig. 9). The main contributor to the savings is the substitution of fossil-fueled energy generation by the increased integration of renewable energy sources such as PV-PPAs and low-carbon energy systems such as heat pumps in the energy supply chain. At the process unit level, this results in substantial savings in the electricity-intensive grinders of GW and PGW, as well as in energy-intensive paper production in PM A and PM B. The specific case studies in Norway (Ghose and Chinga-Carrasco, 2013) and in Brazil (Mourad et al., 2014) confirm, that a low carbon intensive electricity and thermal energy mix are crucial to achieve a high GHG mitigation potential.

4.3.2. *Primary energy demand analysis for paper production*

The net total PED varies between 26.2 and 34.9 GJ per ton of paper (Fig. 10), using the specific energy supply chain analysis of Section 4.2. This is in the range of an average energy use of 28.3 GJ in 45 reviewed case studies in Sun et al. (2018), where except for Nordic countries no

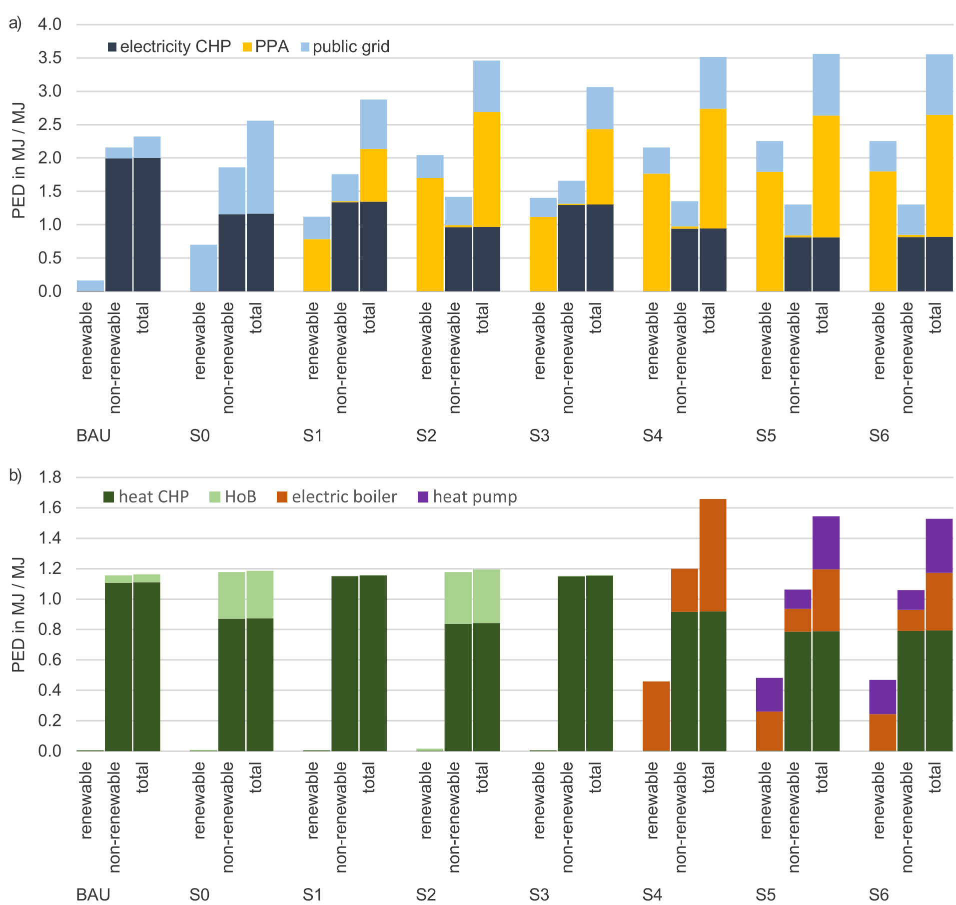

Fig. 7. Total, non-renewable and renewable PED for a) 1 MJ of electricity and b) 1 MJ of heat.

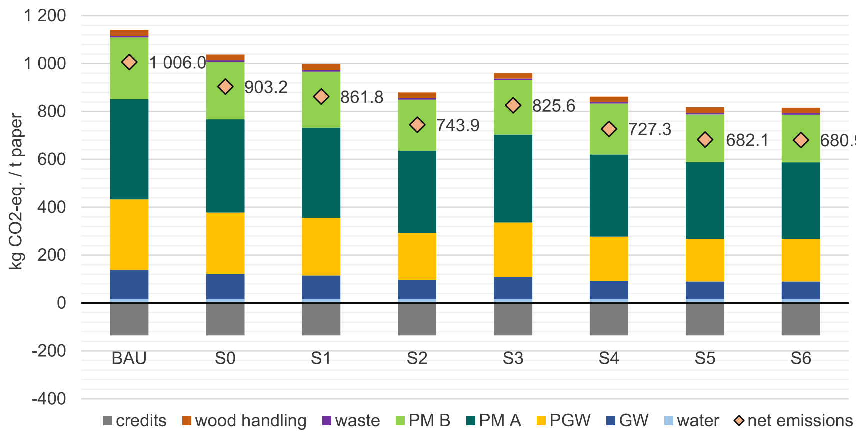

Fig. 8. GWP in kg CO_2-eq. per ton paper (GWP 100 years, excluding biogenic carbon).

correlations between GHG emissions and energy use by geography were identified. Cui et al. (2011) showed that the PED also depends on the pulp production process and if black liquor can be utilized. A higher PED occurs when no black liquor is available for internal energy supply, as it is the case in this research with mechanical pulp. Energy efficiency measures were discussed in Fleiter et al. (2012), with the highest potential for waste heat recovery, which was applied in this study to supply an asparagus farmer and dairy and resulted in credits.

In the BAU case, the PED is the lowest, whereas it increases for scenarios S0 to S6. This is due to the fact, as already elaborated in Section 4.2.3, that in the cumulative energy demand method, the total net demand for 1 MJ of electricity from natural gas CHP is lower than that for public electricity and PV. In scenarios S0 to S6, more electricity from the CHP is substituted by PPAs and from the public grid, which lead to the increased PED. However, the integration of low-carbon-intensive and renewable energy sources has a positive impact on PED. Although the total PED increased by approximately 33 % (S6 compared to BAU), the renewable PED is increased by 156 % and the non-renewable PED was reduced by 32.%.

The specific percentage shares of the renewable and non-renewable PED on total PED are vertically listed in Fig. 10. The share of the renewable PED in the BAU case is 34.6 % on total PED, whereas the remaining share is covered via fossil resources. However, the investigated scenarios revealed that the share of renewable PED increases in all scenarios and can reach a share of up to 67 % in S5 and S6, substantially reducing dependence on fossil fuels and supporting a green industrial transformation.

4.3.3. *Sensitivity analysis*

Fluctuations in annual production cause variations in energy consumption and affect the results to produce one ton of paper. This effect has already been identified in Lipiäinen et al. (2022), where overall inefficiencies occur in production operations due to strikes or economic crises and associated part load operations or shut downs. This phenomenon is transformable to the COVID-19 pandemic, where industrial plants had to produce more inefficiently due to less product demand at partial load. As a result, the specific energy consumption per ton of paper is increased, which is why this correlation was examined more closely in a sensitivity analysis. Conversely, energy efficiency measures can reduce the specific energy consumption.

Fig. 11 shows the impact of a ±30 % variation on energy consumption for the GWP and PED for each scenario, giving a symmetrical behavior. The result for ±20 % and ±10 % variation can be found in the supplementary material in Table S 2. GWP has the largest influence and is rather constant in all scenarios with approximately ±29.4 %, as energy consumption is directly linked to emissions. Carbon emission intensities depends on the scenario and is elaborated in Section 4.2.2. The non-renewable PED (±28.8 % to ±29.1 %) and total PED (±20.1 % to ±22.5 %) are also directly affected by the energy consumption. The higher the share of renewables in the total PED, the higher the impact on the total PED, because electricity provision from renewables (PPAs) has a higher PED compared to fossil fuel electricity production. It is noticeable that in the scenarios with increased renewable integration such as through PPAs (S1 to S6), the renewable PED is essentially impacted. While in BAU the renewable PED impact is ±3.3 %, it is ±19.3 % in S6.

The investigated correlation analysis of annual production fluctuations and the related energy consumption allowed a better understanding of the performance of the system under different conditions and its associated environmental indicators. It revealed valuable insights for decision-making and improvement opportunities for production planning or energy management strategies to optimize the environmental performance.

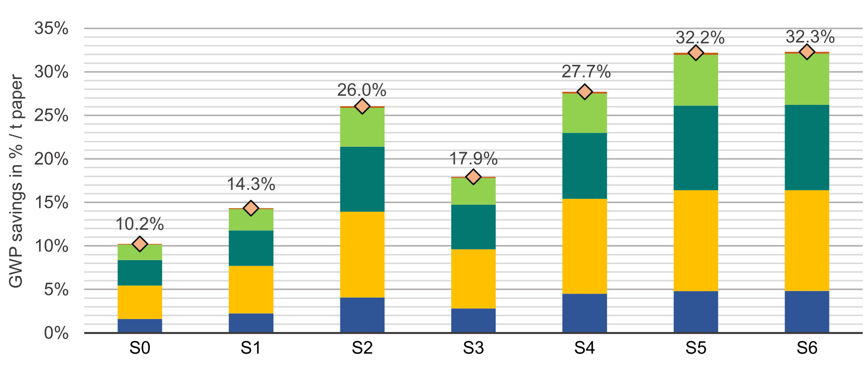

Fig. 9. GWP savings in % per ton of produced paper.

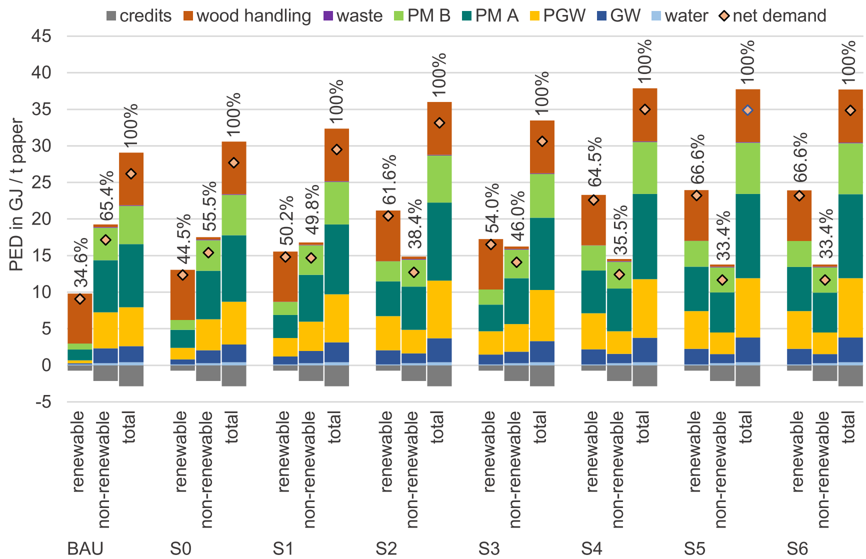

Fig. 10. PED to produce one ton of paper.

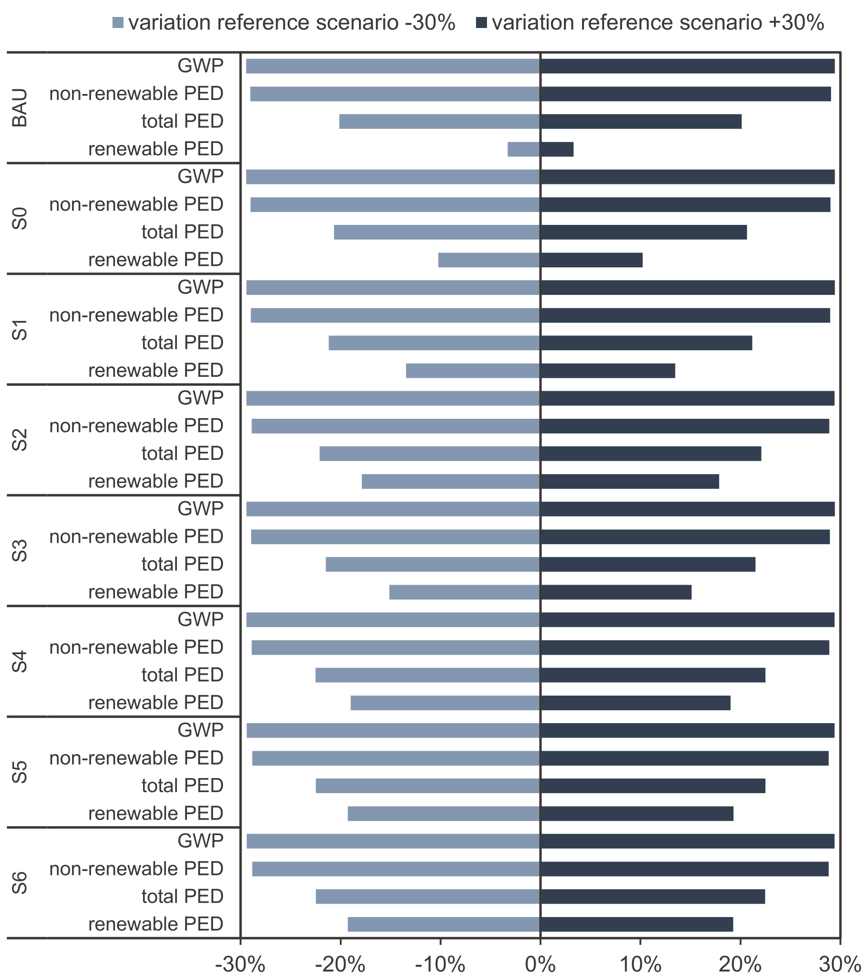

Fig. 11. Sensitivity analysis of varying energy consumption for one ton of paper.

4.4. Environmental costs

The quantification of environmental costs, also known as "shadow costs," refers to the costs of mitigation measures required to avoid environmental impact. In Fig. 12, the environmental costs are calculated divided by impact category to produce one ton of paper. When examining the shadow costs for environmental damage, it becomes clear that there are three defining factors for the developed scenarios: GWP, MAETP, and HTP. In many approaches, only GWP is considered and other impact categories are often overlooked.

The estimated environmental costs associated with the analyzed scenario range from 80 to 93 €/t_{paper}. It can be derived that, compared to the BAU case, the MAETP-associated costs increased in each scenario. This is because more electricity is consumed from the public grid and PPAs, which leads to an increased use of elements and materials required for electricity transmission and negatively affects the MAETP. However, GWP-related costs decreased owing to GHG emission savings. These findings demonstrate the importance of considering environmental costs in decision-making processes to ensure sustainable practices and to avoid negative impacts on ecosystems.

4.5. Techno-economic assessment

The following results were obtained from the optimization model. The results for OPEX and CAPEX for energy provision were defined to produce one ton of paper. The overall Investment costs, the return on investment and payback period were derived for from overall results of the optimization model according to Section 3.4. Compared to the BAU case of 115.6 €/t_{paper}, OPEX savings of 30.7 % (S0) to 44.1 % (S6) were achieved. S6, compared to S0, shows saving of OPEX of about 19.3 %. Detailed results are presented in Fig. 13. The aim of the optimization model was to minimize the costs shown in the first column – sum of annual values for OPEX and optimized CAPEX – for each scenario in Fig. 13. In the second column, the corrected total annual costs are shown; differences occur for scenarios S5 and S6. A research of Laurijssen et al. (2012) showed similar energy costs ranges of 60 to 140 €/t_{paper}, depending on the energy conversion route.

Economic feasible investments were only found for the electric boiler (S4) with a capacity of approximately 60 MW. However, in S5 and S6, with significantly lower investment costs assumed in the optimization model, all technologies (heat pump, electric boiler, steam storage and battery) were included, see Table 6. In a subsequent analysis the real investment costs based on best estimation of specific investments used in S4 were also used for S5 and S6. With these values a corresponding total investment of up to 300 €/t_{paper} was determined. Considering the real investment costs from S4 also rather low values for the ROI (< 0.2), corresponding to high values for the payback period (> 5 years), were derived (Table 7).

When evaluating payback period and ROI with the optimized status quo (S0) as reference instead of the BAU case as reference, even worse results for those indicators can be observed. Payback periods become >18 years in this case for S5 and S6, while the return-on-investment results is approximately 0.05.

5. Conclusion

Energy-intensive industries must reduce their fossil fuel consumption to avoid negative environmental impacts from an increase in emissions. The fossil share can be substituted by low-emission energy technologies such as renewable energy sources like solar or wind, thus paving the way to a decarbonized industry in the future. The integration of renewable energy sources is hence unavoidable but poses challenges due to their volatile energy generation. Industries need to be more flexible in their production processes and energy supply to ensure increased renewable integration and to meet future sustainability requirements. A volatile energy provision also means volatile emissions from energy generation, which need to be considered for a realistic assessment of the environmental impact of a product. With a more flexible plant operation and renewable uptake, the environmental footprint of energy provision and hence for the product can be reduced. Products with a low environmental impact are more important than ever for customers and their selection process, and can make the decisive difference if the quality is the same. Higher product costs are often accepted for more sustainable products.

In this study, a virtual battery concept (VBC) is introduced aiming to utilize the production and energy flexibility potential of industries by operating an industrial plant as a normal storage, aligned to local energy characteristics and requirements. The VBC allows for an increased energy flexibility portfolio and the integration of renewables via PPAs. In addition, the VBC supports increasing local grid stability and avoiding future expensive grid infrastructure investments in the region. The VBC can be replicated in all energy-intensive industries, but a site-specific analysis is essential. Intensive data exchange is required, and interviews and site visits are necessary to understand site-specific challenges.

The use of renewable energy sources can have a substantial impact on reducing GWP and non-renewable primary energy demand. The VBC and the consideration of dynamic energy modeling led to a GHG mitigation potential in the paper industry of up to 33.3 % per ton of paper. By integrating renewables, the carbon energy supply chain of the paper mill can be reduced up to 40 % for electricity and 8 % for heat, respectively, and support toward reaching the climate targets of industries. However, the total PED increased by approximately 34 % through increased electricity consumption via PPAs and the public grid, but the non-renewable was reduced by 32 %, and the renewable increased by 157 %. It was also found that through the VBC, there was a decrease in photovoltaic electricity consumed from the public grid due to an increased reliance on PPAs. PPAs are consumed when the public grid has a high PV share.

Besides the environmental aspects, other criteria such as competitiveness and economic viability play a decisive role for industry. Of course, it then becomes difficult to balance potential GHG savings with

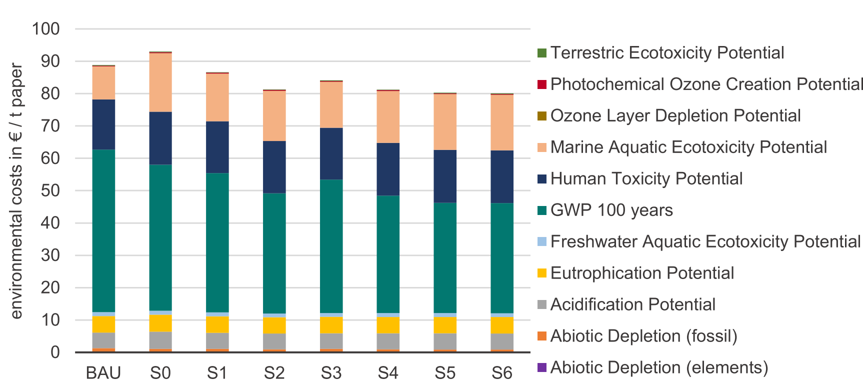

Fig. 12. Environmental costs for one ton of paper divided by impact category.

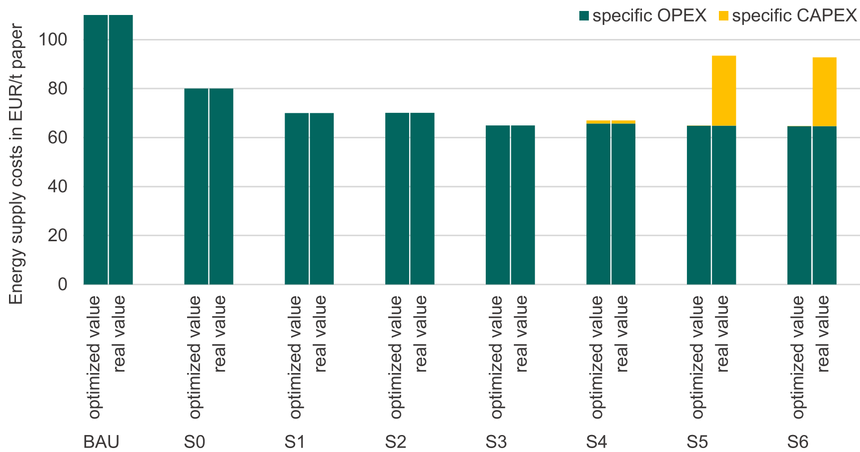

Fig. 13. Specific energy costs (OPEX and CAPEX) to produce one ton of paper.

Table 7
Summary of specific savings and specific investment costs compared to the BAU case for all scenarios.[a]

	S0	S1	S2	S3	S4	S5	S6
	VBC 1				VBC2		
Savings compared to BAU (EUR/t)	35.50	45.52	45.43	50.59	49.81	50.70	50.93
Invest (EUR/t)	0.00	0.00	0.00	0.00	13.35	297.11	292.26
ROI	–	–	–	–	3.73	0.17	0.17
Payback period	–	–	–	–	0.27	5.86	5.74

[a] For scenarios with invest >0, also payback period and return on investment are shown. For S5 and S6, the real investment costs are determined for the row "invest (EUR/t)", using the same specific investment factors as in S4, instead of the reduced investment factors and costs determined by the optimization model.

optional investments for a more sustainable energy supply and product. The quantification of environmental and energetic impacts, as well as the determination of environmental costs and total annual operation cost, highlight the importance of considering several aspects in decision-making processes to ensure sustainable practices and avoid negative impacts on ecosystems. Multi-criteria decision-making methods can be used to take all these aspects into account.

In the future, the integration of low-emission technologies supplied by renewables will depend on the development of their investment cost and associated levelized cost of energy. In order to exploit the full flexibility potential of industries, a change in regulation is needed to allow flexibility in the consumption of electricity from the public grid and to avoid the transport of excess electricity over long distances with new infrastructure to be built.

CRediT authorship contribution statement

Stefan Puschnigg: conceptualization, methodology, investigation, data curation, formal analysis, visualization, writing (original draft), writing (review and editing); **Sophie Knöttner:** conceptualization, data curation, formal analysis, writing (original draft), writing (review and editing); **Johannes Lindorfer:** project administration, supervision, funding acquisition, writing (review and editing); **Thomas Kienberger:** validation and writing (review and editing).

Declaration of competing interest

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

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Appendix A. Supplementary data

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Biorefinery development for the conversion of softwood residues into sustainable aviation fuel: Implications from life cycle assessment and energetic-exergetic analyses

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Aviation

ABSTRACT

Biofuels present a strong potential to support the rapid decarbonization of the mobility sector and substitution for fossil fuels. In the aviation sector, sustainable aviation fuels (SAF) are currently produced from various feedstocks and conversion pathways to achieve sustainability targets. A new SAF production pathway has been recently developed, which is based on enzymatic hydrolysis of softwood residues (saw dust), fermentation of wood sugars into isobutene, and subsequent conversion to SAF isoparaffins by oligomerization and hydrogenation. This pathway is currently under consideration for inclusion as an additional annex to ASTM standard D7566.

In this study, several biorefinery set-up scenarios including various process energy provisions and co products valorization were considered in order to assess the environmental impact of SAF production. First, a life cycle assessment (LCA) was conducted to estimate the greenhouse gas (GHG) emissions of the conversion pathway. Second, the GHG reduction potential was evaluated according to the frameworks of EU RED 2018/2001/EC and CORSIA. Third, energetic and exergetic analyses were performed to evaluate the efficiency of the biorefinery. Inefficiencies of upstream processes, such as for electricity provision, were not considered.

Depending on the plant layout, the GHG emissions vary between 18.7 and 56 gCO2eq/MJ. Thus, compared to the fossil reference, GHG emission reductions of up to 80.1% and 79% can be achieved for both frameworks, respectively. Plant set-up comparisons revealed that the highest reduction in GHG emissions can be achieved when using the by-product lignin for thermal energy provision and renewable energy sources (RES) to cover electricity demand.

The energetic and exergetic efficiency analyses of SAF as a single product were 11.7%–14.9% and 11%–13.8%, respectively. A lignin-CHP plant set-up revealed the highest efficiencies and has the additional benefit of covering up to 82.3% of the total primary energy demand (PED) via RES. Taking all by-products into account, the energetic system efficiency ranged from 39.4% to 50.1% and the exergetic system efficiency from 40.4% to 56.9%, respectively. The highest efficiencies were achieved with the natural gas boiler set-up and electricity consumption from the public grid. The analysis revealed the importance of utilizing all biorefinery products (main and by-products) to increase the system efficiency of the biorefinery.

1. Introduction

Aviation has been a growing trend over the past few decades. Except for the COVID-19 pandemic IEA, 2020 and 2021, the global number of flights increased to 38.9 million in 2019 (Statista, 2021). The International Air Transport Association (IATA) expects a full recovery of the aviation sector by 2024. Air passenger numbers are expected to increase at an average annual rate of 3.3% between 2019 and 2040 to 7.8 billion (IATA, 2022a). However, this will depend on airlines and their actions to provide a safe flying experience in the future (Lamb et al., 2020).

Carbon emissions from global aviation accounted for approximately 2.8% of the global emissions in 2019. Emissions have increased by 2% annually since 2000 (IEA, 2020). In Europe, 3.7% of carbon emissions result from aviation (European Environment Agency, 2019). In 2015, the share of European emissions in global aviation was approximately 20% (European Aviation Safety Agency. and EAA., 2019). In this

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context, the aviation industry aims to reduce CO_2 emissions by up to 50% by 2050 compared to the levels in 2005 (Yang et al., 2019).

The initiatives impacting the environmental footprint of the aviation industry are structured at the EU and global levels. At the European level,policies such as Flightpath 2050, EU Low Carbon Roadmap, Renewable Energy Targets, EU ETS, and Biofuel Flightpath 2020 are applicable to emission savings (de Jong et al., 2018; Deane and Pye, 2018). The Carbon Offset and Reduction Scheme for International Aviation (CORSIA) and the carbon-neutral growth strategy are considered globally (Prussi et al., 2021). Although the policy awareness of bio jets remains low, it would positively impact the uptake of sustainable aviation fuels (SAF) (Deane and Pye, 2018).

Prospects for achieving carbon neutrality in aviation by 2050 rely primarily on the renewal of engine technologies adaptive to sustainable fuels. This is predominantly based on the utilization of drop-in SAF, hydrogen powered engine technology, hybrid kerosene, and electric-powered engine technologies, as well as improved Air Traffic Management (ATM) and carbon removal projects (Sman et al., 2021). SAF carbon emissions are up to 80% lower than those of fossil fuels (ATAG, 2022). Current trends in road transport and the aviation sector facilitate the establishment of a biorefinery value chain that produces renewable fuels and SAF (Yilmaz and Atmanli, 2017). Road transport is slowly transitioning toward electrification, either with battery electric or fuel cell vehicles (Rosenfeld et al., 2019). However, the aviation sector is likely to demand for SAF, as electrification is difficult in his sector. Yet, the development of hybrid and electric aircraft is ongoing (European Aviation Safety Agency. and EAA., 2019); notably, long-haul flights will rely more on SAF as there is a lack of alternatives (IATA, 2022b). The attitude of communities toward biorefinery facilities was assessed in (Lee et al., 2017).

In 2019, <1% of the global jet fuel usage (approximately 40 million liters) was covered by SAFs (ATAG, 2022). Owing to the low-profit margins of airlines and the higher costs of SAF production compared to that of fossil-based jet fuel, policy measures to promote SAF consumption are required to drive demand growth (IEA, 2020). The RefuelEU mandate of the European Commission aims to boost the supply and demand of SAF. The anticipated blending targets are 5% in 2030, 32% in 2040, and 63% in 2050 (European Commission, 2021). Targeting support for more conversion pathways was achieved by evaluating sustainable feedstock availability to meet the proposed SAFdeployment goals (O'Malley, 2021). Currently, high production costs, policy uncertainty, and the low SAF awareness are the main barriers (Deane and Pye, 2018). Economies of scale and learning effects of production technologies in biorefineries can help to decrease SAF production costs (Valentim Bastos et al., 2022). A techno-economic analysis by (Zeilerbauer et al., 2022) revealed that both, biorefinery scale up and by-product utilization into valuable products, are critical to achieve economic feasibility. By 2050, power-to-liquid and alcohol-to-jet technologies are expected to have a substantial share in the EU SAF supply (SkyNrg, 2021).

To meet future SAF blending targets and demand, the utilization of various feedstocks and the construction of respective biorefinery capacities is required. Technical and economic challenges as well as future prospects of biorefineries for lignocellulose is discussed in (Chandel et al., 2018). In this study, SAF is produced in a lignocellulosic biorefinery based on softwood residues (saw dust) and is thus a second-generation (2G) biofuel. Compared to first-generation (1G) biofuels, which are seen as critical owing to the conflict of food security (Ayodele et al., 2020), 2G biofuels demonstrate a high potential for market acceptance (Mohr and Raman, 2013). First, the obtained sugars are derived via pretreatment of sustainable softwood residue feedstock, followed by enzymatic hydrolysis. Second, the wood hydrolysate is fermented to produce the chemical intermediate bio-isobutene. Finally, the bio-isobutene is converted to SAF isoparaffins by oligomerization and hydrogenation. Along the value chain, generated by-product streams are valorized.

Existing studies focused on the development and conversion of 1G sugars and 2G agricultural residues. Compared to the heterogenous and complex 2G lignocellulosic sugars (Ashokkumar et al., 2022), 1G sugars have a single sugar species and are thus easier efficiently processable. A review on latest advances of biofuels production from diverse lignocellulosic biomass was conducted by (Saravanan et al., 2022). The usage of largely available wood residues as feedstock followed by deconstruction and direct fermentation to gaseous bio-isobutene is an innovative approach and not yet considered in comprehensive ecological and energetic analyses. In contrast, biomass fractionation can also be achieved with technologies such as gasification (Akbarian et al., 2022; Heidenreich et al., 2016) and subsequent bio-syngas conversion (Shahabuddin et al., 2020), or pyrolysis (Lahijani et al., 2022). However, the 2G wood residues SAF conversion is expected to provide additional benefits with the utilization and hence value creation of the various by-product streams.

This study aims to demonstrate, if the environmental sustainability of the proposed SAF conversion pathway can be met. Life Cycle Assessment (LCA) was applied to evaluate greenhouse gas (GHG) emissions at the process unit level. The estimated GHG emission reduction potential was calculated based on the certification requirement and framework of the EU RED 2018/2001/EC (European Commission, 2018) and CORSIA (ICAO, 2021a), respectively. An interpretation of the LCA results toward the GHG protocol was made. The SAF conversion pathway further aims to be approved as an additional annex to ASTM D7566, the American Society for Testing and Materials. To identify suitable biorefinery locations, we included a review on sawn-wood residues potentials in EU-28. We also conducted a scenario analysis for various biorefinery set-ups by varying energy provision and by-product utilization. The study investigates how the on-site usage of the by-product lignin and the integration of renewable energy resources (RES) influences fossil primary energy demand (PED) substitution and hence the ecological footprint. To allow a comprehensive analysis of the biorefinery, energetic and exergetic analyses are included for evaluating efficiencies for SAF production and for all biorefinery products, respectively.

2. Materials and methods

The methodological structure of this study is shown in Fig. 1. LCA was applied to analyze environmental impacts. Software GaBi 10.6 ts by Sphera was used (GaBi 10.6 ts by Sphera, 2022), following the ISO 14040 standards consisting of four steps: definition of goal and scope, life cycle inventory (LCI), life cycle impact assessment (LCIA), and improvement and interpretation (International Organization for Standardization, 2006). Detailed material regarding LCA methodology can be found in the literature (Finnveden et al., 2009; Guinee, 2002; Klöpffer, 1997; Reap et al., 2008) and has been omitted in this text; we have elaborated the relevant information to this study. Energetic and exergetic analyses were conducted to evaluate the efficiency of the biorefinery. Exergetic analyses of specific materials have been extensively examined in the literature (Liu et al., 2017; Szargut, 2005, 2007). Therefore, we have only elucidated the calculation approach and applied material references.

2.1. Definition of goal and scope

The goal was to produce of SAF and analyze the environmental impacts resulting from the production. In addition, the obtained by-products were valorized and considered in the analysis. A crucial part of LCA is the definition of a functional unit, as this allows comparability with other studies (Cooper, 2003; Lagerstedt et al., 2003). To produce SAF, the functional unit was defined as 1 MJ of SAF following the methodology of EU RED 2018/2001/EC of GHG emission calculation (European Commission, 2018).

The biorefinery concept is elaborated in detail in chapter 3.1, and the

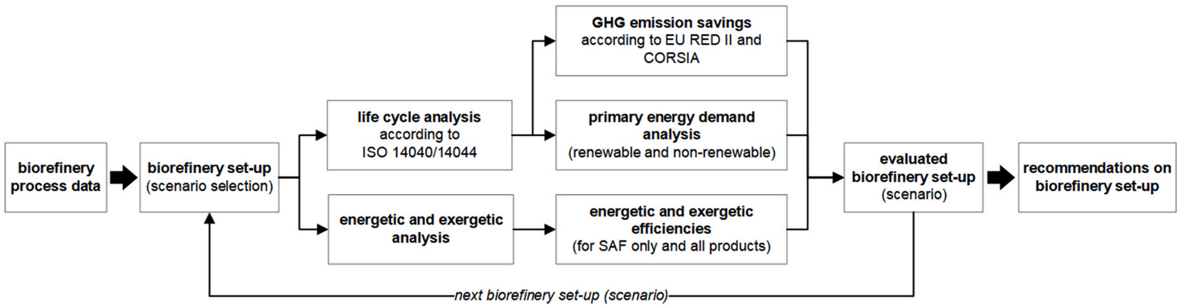

Fig. 1. Methodological structure of assessment.

system boundary for the LCA is shown in Fig. 3. The LCA applied for SAF production follows a "cradle-to-gate" approach according to the LCA framework and the EU RED 2018/2001/EC methodology. Generally, a "cradle-to-grave" approach is favorable (Guinee, 2002). An interpretation toward the GHG protocol methodology can be found in chapter 3.4. The geographical system boundary is defined for EU-28 countries, because electricity and thermal energy mixes vary significantly between single countries and would strongly influence the results.

2.2. Life cycle inventory and data collection of SAF biorefinery

The life cycle inventory (LCI) collects the data for conducting the LCA and quantifies the inputs and outputs of the biorefinery (Suh et al., 2004). For innovative process technologies, data gaps can occur and must be filled with valid literature values and assumptions. In this study, LCI was compiled based on the evaluations and results of the REWOFUEL project (REWOFUEL, 2022). In addition, background processes and their environmental impacts, such as electricity generation or the production of diverse materials, were obtained from the GaBi ts 10.6 Professional and ecoinvent v.3.8 databases (Ecoinvent, 2022; GaBi 10.6 ts by Sphera, 2022).

Mass and energy balances are the basis of LCA. The main input and output parameters for producing SAF are listed in Table 1. The additional energy and material demand of downstream processing of the by-products was out of the scope of the analysis and hence not considered. Details on the energy demand of processing the by-product C5 sugars to ethanol depends on the mass concentration and is elaborated in (Leitner and Lindorfer, 2016). Saw dust as input for the biorefinery is assumed in the REWOFUEL project to be locally available (REWOFUEL, 2022). On average, a transportation distance of 50 km was estimated. Generally, biomass upstream GHG emissions have only a relatively small impact compared to the conversion process itself (Vera et al., 2020). According to the Joint Research Center (JRC) of the European Commission on solid and gaseous bioenergy pathways (Giuntoli et al., 2017), the transportation of wood chips is a 40-ton diesel truck with a payload of 27 tons by default. This type of transportation was also assumed anticipated for saw dust in this study.

Saw dust is considered an agricultural residue. Thus, no ecological footprint of upstream production emissions is considered; only emissions from the transportation. This is in line with the EU RED 2018/2001/EC methodology Annex V C 18 (European Commission, 2018). Only emissions for the transportation of the saw dust are considered.

The by-product lignin in Table 1 is listed as absolute value. However, the specific ratios change depending on its use as (i) energy vector on-site in the combined heat and power (CHP) or in the boiler of the biorefinery and/or as (ii) material to substitute bitumen in the asphalt industry. To meet the heat demand of the biorefinery, 3.5 t/t_{SAF} is required in the case of using lignin as an energy vector for CHP, and 2.74 t/t_{SAF} lignin is required in the case of a lignin-fired boiler. The remaining lignin is used as a material for bitumen substitution in the asphalt industry.

The fermentation unit delivers sludge applicable as an organic fertilizer, which substitute calcium and potassium. In addition, the fermentation unit provides a biomass stream applicable as an animal feed, which substitutes the soybean import from Brazil. The substitution of conventional calcium and potassium fertilizer with sludge and soybean with spent biomass protein resulted in specific emission credits (refer to chapter 2.4.2).

Table 2 lists the demand for chemicals and water as well as for the produced waste water. The data were structured based on the process-unit level.

2.3. Life cycle impact assessment

The Life Cycle Impact Assessment (LCIA) follows the LCI by applying the CML 2001 methodology in the LCA software GaBi 10.6 ts by Sphera to demonstrate the impact on environmental impact categories. Quantified mass and energy flows are assigned to impact categories by applying characterizations factors (Guinee, 2002). The results are

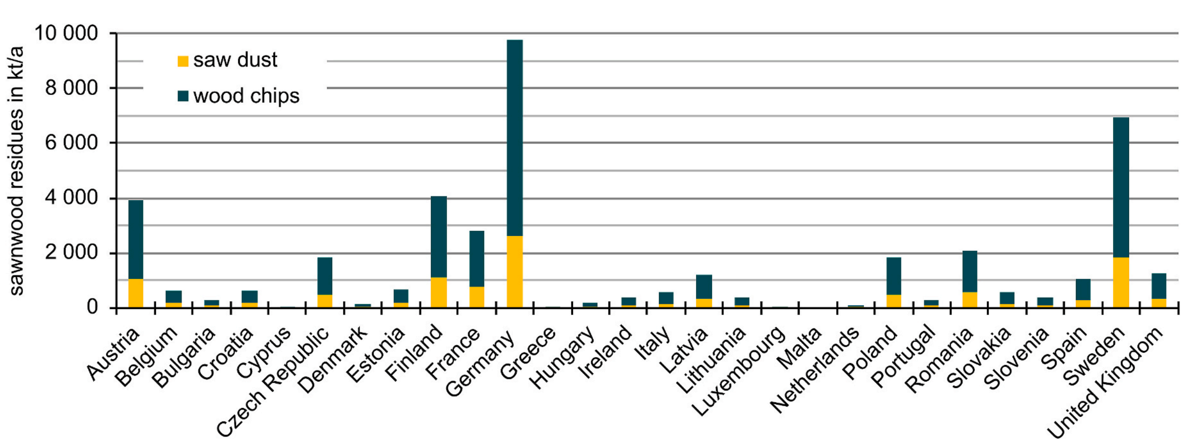

Fig. 2. Sawn-wood production residues in EU-28 IEA (2020) based on FAO (2022).

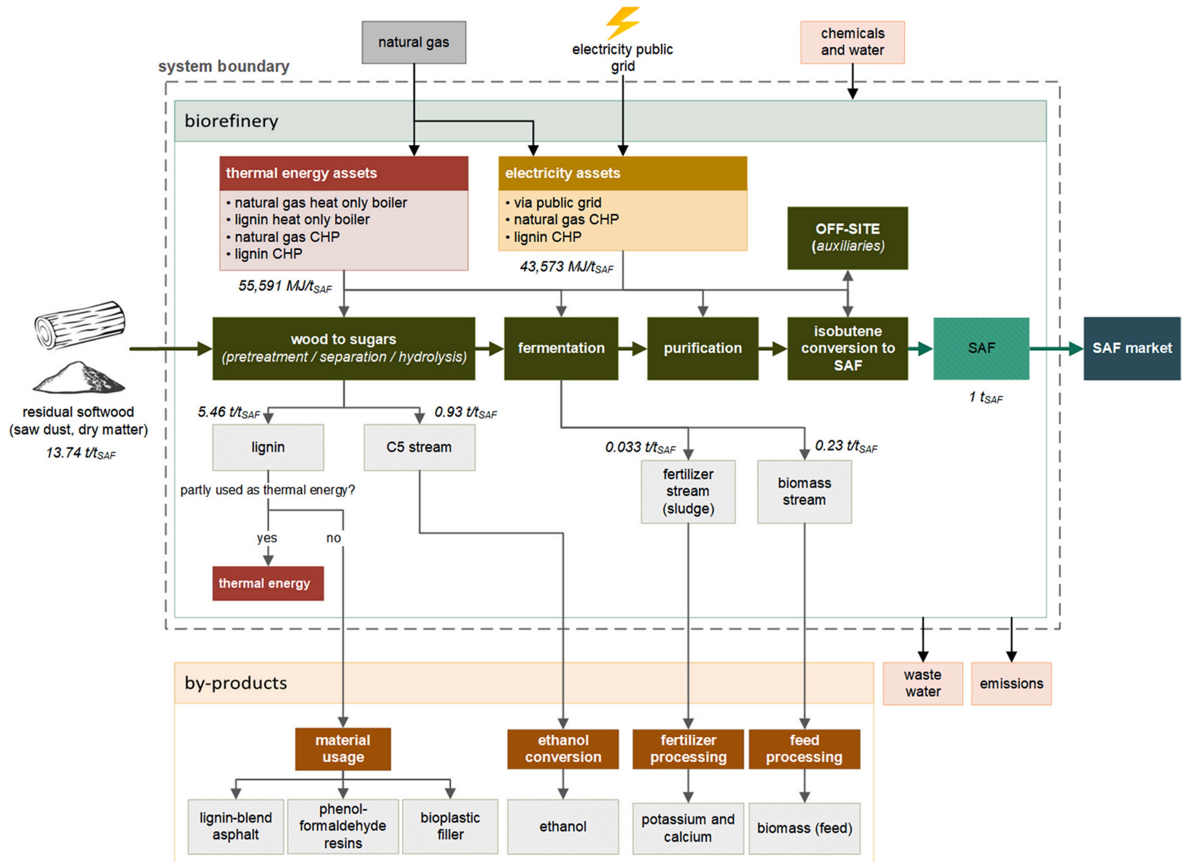

Fig. 3. Biorefinery concept and system boundary to produce SAF.

Table 1
Main inputs and outputs for SAF production based on (REWOFUEL, 2022).

Main and by-products	LHV in MJ/kg	t/t_{SAF}	MJ/ t_{SAF}	chemical exergy in MJ/kg
Inputs				
softwood residues dry matter (saw dust)	19	13.74	261,09	20.35[a]
electricity demand	–	–	43,573	–
thermal energy demand[b]	–	–	55,591	–
Outputs				
SAF	43.9	1.00	43,90	45.7[c]
Lignin	22.8	5.46	124,57	28.16[d]
biomass (feed, protein)	15	0.23	3,38	24.5[d]
calcium (Ca) as fertilizer	n.c.[a]	0.014	n.c.	18.2[e]
potassium (K) as fertilizer	n.c	0.019	n.c	9.375[e]
C5 sugars (as ethanol equivalent)	26.8	0.93	24,85	29.45[e]

*n.c., not considered.
[a] Based on (Liu et al., 2017) with a chemical exergy of cellulose (18.81 MJ/kg), hemicellulose (14.6 MJ/kg) and lignin (28.16 MJ/kg) and assumed softwood composition of 40%-30%-30%.
[b] Aggregated average value based on different pressure levels of 41, 23, 11, 7.5 and 3 barg
[c] Based on (Yildiz and Caliskan, 2020).
[d] Based on (Liu et al., 2017).
[e] Based on (Szargut, 2005, 2007).

grouped into midpoint categories according to common mechanisms (e.g., climate change) or commonly accepted groupings (e.g., ecotoxicity). A key performance indicator (KPI) for SAF production is the global warming potential (GWP), calculated in kg CO_2-equivalents, as the savings in GHG emissions compared to fossil fuels are benchmarked using this KPI. Additionally, the primary energy demand (PED) in MJ as an indicator of energy performance (total, renewable, non-renewable) of SAF production and the biorefinery was evaluated as KPI. Besides evaluating and analyzing the GWP and PED, other environmental impacts such as acidification and eutrophication were assessed and provided in Appendix A. Supplementary data.

2.4. *Allocation procedures*

If the main product and one or more by-products are produced as part of an LCA of a biorefinery system, allocation rules can be applied to account for the product-specific emissions (Ahlgren et al., 2015). A multi-product biorefinery system not only have a positive impact on the environmental performance, but also on the economic feasibility as it utilizes the complete feedstock (Liu et al., 2021). In this study, the main product is SAF, and by-products are ethanol, fertilizer, lignin and animal feed. In principle, ISO 14040/14,044 prioritizes system expansion and not allocation; however, this would result in a hardly manageable effort in terms of system expansion and data collection. Therefore, allocation methods frequently applied according to the ISO 14040/14,044 framework, such as allocations according to mass, energy, or economic value, are used (Klöpffer, 1997).

2.4.1. *Energy allocation*

The EU RED 2018/2001/EC methodology (European Commission, 2018) obliges the application of the lower heating value based energy allocation to determine the environmental burden of the biofuel. As this methodology must be used to certify biofuels in Europe, this study applies an energy allocation for the ISO 14040/14,044 LCA as well. Since the purpose of the main product, SAF, is to be used as a biofuel in energy generation units, energy allocation is the most reasonable method for this study. Consequently, an energy allocation is applied between the energy-related products (SAF, C5 sugars and lignin) to determine the

Table 2
Mass balances for chemicals and water demand on process unit level for SAF based on (REWOFUEL, 2022).

chemicals and water in kg/t_{SAF}	wood to sugars	fermentation	SAF conversion	off-site	chemical exergy MJ/kg
sulfur dioxide, SO_2	137.75	–	–	–	4.889[a]
enzyme mixture	569.54	–	–	–	12.168[b]
sodium hydroxide (NaOH)	443.13	0.38	–	173.67	1.873[a]
sulphuric acid (H_2SO_4)	11.52	–	–	21.57	1.666[b]
Antifoam	0.53	0.53	–	–	n.c.
Yeast	–	34.44	–	–	11.38[b]
phosphoric acid (H_3PO_4)	–	1.01	–	1.81	0.914[a]
sodium chloride (salts)	–	56.69	–	–	0.245[a]
ammonia (NH_3)	–	40.05	–	–	19.841[a]
hydrogen (H_2)	–	–	0.38	–	328.68[a]
Isobutane	–	–	0.88	–	48.245[a]
nitrogen (N_2)	–	–	–	63.84	0.025[b]
cation polymer	–	–	–	0.41	n.c.
iron chloride ($FeCl_3$)	–	–	–	2.46	1.406[a]
calcium oxide (CaO)	–	–	–	118.54	2.27[a]
water (H_2O)	47,470.2	12,960.74	0.11	84,198.33	0.05[a]
Wastewater	30,463.58	19,271.52	–	–	0.05[a]

*n.c., not considered.
[a] Based on (Szargut, 2005, 2007).
[b] Based on (Liu et al., 2017).

environmental burden of SAF. This has the benefit that the results for biofuels are comparable between the EU RED 2018/2001/EC and ISO 14040/14,044 methods. An allocation by economic value implies the risk of price fluctuations and thus provides uncertain results; allocation by mass can lead to unfairly distributed emissions due to high mass flows of by-products (Ahlgren et al., 2015). Therefore, these allocation methods were not applied in this study.

2.4.2. Avoided burden approach – substitution

The ISO 14040/14,044 framework provides the opportunity to use "credits" (system expansion or substitution method) for by-products. The aim of a credit is to replace an external resource or material with an automatically produced by-product. Consequently, the external resource/material must no longer be produced in the respective substituted quantities. As a result, the credit reduces the total environmental burden (Klöpffer, 1997).

In this study, an extended allocation to the applied energy allocation elaborated in chapter 2.4.1 is conducted based on a hybrid allocation approach introduced in (Cherubini et al., 2011; Njakou Djomo et al., 2017; Sandin et al., 2015). The hybrid allocation approach uses both credits and partitioning in form of energy, mass or economic allocation. The supplementary credit is calculated for the by-product streams of sludge and biomass and is visualized separately in the results chapter 4. It allows to show the additional environmental burden reduction potential of the non-energy related by-products, which would otherwise not be considered. The sludge from the fermentation unit can be used as a fertilizer and substitute for production of potassium and calcium (due to data availability, German production is assumed within the LCA model in GaBi software). The biomass stream (animal feed) from the fermentation unit substitutes for soybean imported from Brazil and hence increases the feed efficiency (Global Bioenergies, 2022; Sturm et al., 2022). In addition, it reduces the dependence on soybean imports to the European Union, which has a positive impact on land use change and deforestation (Sturm et al., 2022). The biomass stream is assumed to provide the same protein as soybeans.

2.5. Impact of country-specific electricity emissions

The country selected for a biorefinery is an essential factor for calculating GHG emissions. Average electricity generation emissions of the public grid vary significantly between countries, which can lead to misinterpreted results in terms of GHG emissions. The higher the country-specific ecological electricity footprint, the higher the GHG emissions of SAF production, and thus the lower the savings. For example, the Estonian carbon footprint of the public grid is 264 gCO_2eq/MJ, the Austrian one is 81 gCO_2eq/MJ and the French one is 21 gCO_2eq/MJ. Therefore, an EU-28 electricity mix of 102 gCO_2eq/MJ was applied in this study (carbon footprints are from (GaBi 10.6 ts by Sphera, 2022)).

To evaluate the impact of RES on GHG emission savings, a forecast of electricity fuel types by share for EU-28 in 2050 of the (European Commission et al., 2021) is used to build an RES model in the LCA software GaBi. The environmental footprints of the respective fuels were calculated based on their carbon footprint. The average EU-28 RES electricity carbon footprint for 2050 was 21 gCO_2eq/MJ. Although not all forecasted fuel types are renewable by 2050, it is still assumed to be an RES scenario in this study. The aim was to demonstrate the potential of integrating renewable electricity (especially from wind and solar) and thus find an additional trigger for reducing GHG emissions to produce biofuels.

2.6. Scenario development

The aim of the scenarios is to support the identification of the best plant layout from an LCA perspective. A plant design was engineered and elaborated in (REWOFUEL, 2022), which serves as a reference for the developed scenarios. In the engineered plant design, the required thermal energy is covered by a natural gas boiler, the electricity demand via the public grid.

The developed scenarios in Table 3 differ in terms of process energy provision and by-product valorization. Thermal energy can either be provided by either a natural gas or a lignin boiler. In this case, electricity is obtained from the public grid. If a CHP plant is integrated (either natural gas or lignin fired), it would provide in addition to the thermal energy electricity; only the lack of electricity is consumed via the public grid. In the best case, an electricity surplus is available for sale (not the case in this study). However, technologically developments and efficiency improvements in production units may lead to such a case in the future. According to the EU RED 2018/2001/EC methodology (European Commission, 2018) Annex V C 16 (b), the size of the CHP is determined by the justifiable economical heat demand, which is assumed to be the thermal energy demand of the biorefinery. The on-site usage of the by-product lignin for thermal and electricity production would result in less lignin available for external usage (i.e. in the asphalt industry as bitumen substitution). Nevertheless, the on-site usage of lignin leads to less dependency on external energy suppliers. Other by-products such as ethanol, fertilizer and animal feed are not varied.

To demonstrate the impact of the carbon footprint from electricity on the environment, the scenarios were evaluated with the present and

Table 3
Developed scenarios for LCA analysis for SAF.

scenario	Description	by-products	lignin usage
NG-B	Natural gas boiler[a], EU-28 grid mix	lignin, fertilizer, ethanol, animal feed	off-site
NG-B RES	Natural gas boiler, RES grid mix EU scenario 2050	lignin, fertilizer, ethanol, animal feed	off-site
LI-B	Lignin boiler[b], EU-28 grid mix	lignin, fertilizer, ethanol, animal feed	off- and on-site
LI-B RES	Lignin boiler, RES grid mix EU scenario 2050	lignin, fertilizer, ethanol, animal feed	off- and on-site
NG-CHP	Natural gas CHP[c], EU-28 grid mix	lignin, fertilizer, ethanol, animal feed	off-site
NG-CHP RES	Natural gas CHP, RES grid mix EU scenario 2050	lignin, fertilizer, ethanol, animal feed	off-site
LI-CHP	Lignin CHP[d], EU-28 grid mix	lignin, fertilizer, ethanol, animal feed	off- and on-site
LI-CHP RES	Lignin CHP, RES grid mix EU scenario 2050	lignin, fertilizer, ethanol, animal feed	off- and on-site

[a] Based on (BIOGRACE I calculation tool, 2012) η_{th} is 90% (LHV).
[b] Based on (Giuntoli et al., 2017) η_{th} is 89% (LHV).
[c] Based on (BIOGRACE I calculation tool, 2012) η_{th} is 53.6% and η_{el} is 16.3% (LHV).
[d] Based on (Giuntoli et al., 2017) η_{th} is 69.6% and η_{el} is 16.3% (LHV).

predicted EU-28 electricity mix for 2050 (European Commission et al., 2021). The EU-28 electricity mix for 2050 was considered as a renewable energy source (RES) mix in the scenarios.

2.7. Biorefinery efficiency analysis

Energetic and exergetic efficiency analyses were conducted for the biorefinery. The system boundary for the analysis is defined in Fig. 3, considering only the input and output streams to and from the biorefinery, but not at a process unit level. The mass and energy balances listed in the LCI of the LCA were used to examine the energetic and exergetic analyses. For both analyses, the efficiencies were calculated i) in relation to the main product SAF and ii) considering all biorefinery products (SAF, ethanol, lignin, fertilizer such as calcium and potassium, and animal feed). The full load hours of the biorefinery are 8000 h. The inefficiencies resulting from upstream processes, such as for electricity provision, were not considered.

2.7.1. Energetic analysis

The energetic efficiency of a biorefinery can be calculated in various ways, which challenges the development of a general approach for all types of biorefineries. Calculations can be performed only for the biorefinery and the corresponding inputs and outputs, can include upstream processes for heat and electricity provision, can be calculated only for the main or all resulting products at the system level. In this context, the definition of system boundaries and assumptions is crucial and necessary for comparability (Lind et al., 2022).

In this study, the energetic balance was written for the biorefinery according to Equation (1):

$$\sum_{in}\dot{E}_{en,i} + \sum_{in}\dot{E}^{Q}_{en,j} + \sum_{in}\dot{E}^{W}_{en,k} = \sum_{out}\dot{E}_{en,pr} + \dot{E}_{I.,en,l} \tag{1}$$

where the input energy flow rates are $\sum_{in}\dot{E}_{en,i}$ for materials, $\sum_{in}\dot{E}^{Q}_{en,j}$ for thermal energy, $\sum_{in}\dot{E}^{W}_{en,k}$ for work, and output energy flow rates are $\sum_{out}\dot{E}_{en,pr}$ of products and $\dot{E}_{I,en,l}$ are the energetic losses.

The ratio of useful energetic outputs to inputs reveals energetic efficiency (Lind et al., 2022; Rauch and Koroveshi, 2021). The energetic efficiency to produce SAF can be calculated according to Equation (2):

$$\eta_{en,SAF} = \left(\frac{\dot{E}_{en,SAF}}{\sum_{in}\dot{E}_{en,i} + \sum_{in}\dot{E}^{Q}_{en,j} + \sum_{in}\dot{E}^{W}_{en,k}}\right) \times 100 \tag{2}$$

where $\dot{E}_{en,SAF}$ is the SAF energy flow rate. The denominator $\sum_{in}\dot{E}_{en,i} + \sum_{in}\dot{E}^{Q}_{en,j} + \sum_{in}\dot{E}^{W}_{en,k}$ represents the energy balance of Equation (1) with the defined inputs.

To calculate the energetic system efficiency of the biorefinery, the SAF and by-products were considered according to Equation (3):

$$\eta_{en,sys} = \left(\frac{\dot{E}_{en,SAF} + \dot{E}_{en,et} + \dot{E}_{en,af} + \dot{E}_{en,li}}{\sum_{in}\dot{E}_{en,i} + \sum_{in}\dot{E}^{Q}_{en,j} + \sum_{in}\dot{E}^{W}_{en,k}}\right) \times 100 \tag{3}$$

where the numerator is extended by the energetic flow rates of ethanol $\dot{E}_{en,et}$, animal feed $\dot{E}_{en,af}$, and lignin $\dot{E}_{en,li}$. Non-energetic outputs such as calcium and potassium were not considered.

2.7.2. Exergetic analysis

Exergetic evaluation is frequently used to assess the thermochemical efficiency of biorefineries. In particular, the process sections with high exergy losses can be identified and improved (van der Heijden and Ptasinski, 2012).

The exergy determines the maximum useful work of a system interacting with a reference environment with T_0 and p_0. For material streams, a classification into physical, chemical, kinetic and potential exergy can be made (Liu et al., 2017). The kinetic and potential exergy are often neglected in stream analyses due to their small magnitude (Bösch et al., 2012).

We did not calculate the exergy of various materials and streams as part of this study, as it has already been extensively described in the literature (Bösch et al., 2012; Liu et al., 2017; Lythcke-Jørgensen et al., 2014). Therefore, the applied standard chemical exergy values were obtained from literature, mainly from (Szargut, 2005, 2007) with a reference environment of T = 298.15 K and p = 101.325 kPa. The respective values are listed in Tables 1 and 2.

Detailed exergetic efficiency analysis of biorefineries and the process unit level has been reported in numerous studies (Aghbashlo et al., 2018, 2016; e Silva and Miranda, 2021; Hepbasli, 2008; Liu et al., 2017; Modarresi, 2012; Patiño-Ruiz et al., 2021; van der Heijden and Ptasinski, 2012; Zhang et al., 2022). In this study, the exergy balance is applied at the biorefinery level and evaluated according to Equation (4) (van der Heijden and Ptasinski, 2012):

$$\sum_{in}\dot{E}_{ex,i} + \sum_{in}\dot{E}^{Q}_{ex,j} + \sum_{in}\dot{E}^{W}_{ex,k} = \sum_{out}\dot{E}_{ex,pr} + \dot{E}_{I,ex,l} \tag{4}$$

where the input exergy flow rates are $\sum_{in}\dot{E}_{ex,i}$ for materials, $\sum_{in}\dot{E}^{Q}_{ex,j}$ for thermal exergy, $\sum_{in}\dot{E}^{W}_{ex,k}$ for work, and output exergy flow rates are $\sum_{out}\dot{E}_{ex,pr}$ of products and $\dot{E}_{I,ex,l}$ are the exergy losses.

Exergetic efficiency is calculated as the ratio of useful exergetic outputs to all exergetic inputs. Considering SAF as the only product, the exergetic efficiency can be calculated using Equation (5):

$$\eta_{ex,SAF} = \left(\frac{\dot{E}_{ex,SAF}}{\sum_{in}\dot{E}_{ex,i} + \sum_{in}\dot{E}^{Q}_{ex,j} + \sum_{in}\dot{E}^{W}_{ex,k}}\right) \times 100 \tag{5}$$

where $\dot{E}_{ex,SAF}$ is the exergy flow rate of the SAF and the denominator of $\sum_{in}\dot{E}_{ex,i} + \sum_{in}\dot{E}^{Q}_{ex,j} + \sum_{in}\dot{E}^{W}_{ex,k}$ represents the inputs defined in the exergy balance in Equation (4).

If the by-products of the biorefinery are considered, the exergetic efficiency is calculated according to Equation (6):

$$\eta_{ex,sys} = \left(\frac{\dot{E}_{ex,SAF} + \dot{E}_{ex,et} + \dot{E}_{ex,af} + \dot{E}_{ex,li} + \dot{E}_{ex,ca} + \dot{E}_{ex,pot}}{\sum_{in} \dot{E}_{ex,i} + \sum_{in} \dot{E}^{Q}_{ex,j} + \sum_{in} \dot{E}^{W}_{ex,k}} \right) \times 100 \tag{6}$$

where the numerator was adjusted by the exergy flow rates of ethanol $\dot{E}_{ex,et}$, animal feed $\dot{E}_{ex,af}$, lignin $\dot{E}_{ex,li}$, calcium $\dot{E}_{ex,ca}$ and potassium $\dot{E}_{ex,pot}$.

3. Theory and calculation

This section describes the conversion process from saw dust to SAF via enzymatic hydrolysis and fermentation. Moreover, the SAF evaluation standards, existing SAF conversion processes and the requirements for SAF approval and certification are elaborated. The GHG Protocol is included and put in relation to the LCA of ISO 14040/14,044.

3.1. Description of SAF conversion pathway

The lignocellulosic biorefinery converts residual softwood (saw dust from saw mills) into a high-performance drop-in biofuel (SAF) for the aviation sector (Fig. 3). The resulting by-products along the value chain (lignin, C5 sugars, sludge as organic fertilizer, and microbial biomass as animal feed) are valorized in various branches. The biorefinery was developed by combining the knowledge and technologies of several technology providers during the REWOFUEL project (REWOFUEL, 2022).

Softwood residues are applied as a 2G feedstock. IEA, 2020, saw dust and wood chips in EU-28 revealed residue potentials of 11,232 kt/a and 30,633 kt/a, respectively. Saw dust and wood chips is mainly available in Austria, Finland, Germany, and Sweden (Fig. 2); making these countries for feedstock provision suitable locations for the biorefinery to limit transport distances. These countries account for approximately 59% of the total EU-28 potential.

SAF is produced in several process units: wood-to-sugars, fermentation, purification and conversion. Saw dust is transported by trucks to the biorefinery. In the first step, the sugars (C6 and C5) contained in the cellulose and hemicellulose of saw dust are degraded via pretreatment an enzymatic hydrolysis in the wood-to-sugars unit into residual wood hydrolysate. The obtained C5 sugars are separated and converted to bioethanol. In contrast, the other by-product, lignin, can be used on-site to produce energy and/or as a material substitution, which are currently under investigation. Lignin can be applied as substitute for bitumen in the asphalt industry as a binder (Moretti et al., 2021). analyzed the environmental implications of lignin-based asphalt. Lignin can also be applied in end-use applications such as phenol-formaldehyde resins and bioplastics filler. The obtained residual wood hydrolysate (C6 sugars) is fermented to bio-isobutene, a gaseous hydrocarbon and a well-known commodity chemical usually derived from fossil resources (Olah and Molnár, 2011). Modified bacterial Escherichia coli (E.coli) strains are applied and the fermentation protocol adapted and optimized (REWOFUEL, 2022). Metabolic routes and an isobutene market overview are discussed in (van Leeuwen et al., 2012). The usage of genetically engineered E.coli strains to produce bio-isobutene from 2G feedstocks is elaborated in (Fazeni-Fraisl and Lindorfer, 2022) for cereal straw, and in (Lopes et al., 2019) for corn stover and wheat straw as feedstock. The production of bio-isobutene from residual wood hydrolysate is an innovative process and currently in development to further increase the process performance and yield (Delcourt, 2018; Global Bioenergies, 2014, 2019). Several patents of the company Global Bioenergies are available on their fundamental research (Marliere, 2010, 2011). The by-products of fermentation include sludge and microbial biomass, which may be used as fertilizer and animal feed, respectively. The obtained microbial biomass (amino acids) can be used as protein feed (Dalibard et al., 2014; Linder, 2019), such as in broiler and piglet feed. In general, there is a long history of using amino acids as animal feed (Food and Agriculture Organization of the United Nations, 2004). However, the feed contains inactivated genetically modified organisms, which is why the permission of the European Food Safety Authority is required before usage. Respective experimental trials are still ongoing and a final decision on use and nutrient composition is still pending at the time of manuscript preparation. The obtained sludge can substitute potassium and calcium mineral fertilizers. After fermentation, the obtained bio-isobutene is purified with adsorption/desorption column principle. In the last step, bio-isobutene is converted into SAF isoparaffins by oligomerization and hydrogenation. Generally, the bio-isobutene conversion unit can be adapted to other modes to produce bio-isooctane and bio ethyl tert-butyl ether (bio-ETBE) for the automotive sector.

The "off-site (auxiliaries)" section is an essential process unit within the biorefinery. This section includes components for storage and logistics such as conveyor belts for raw material transport, pumps for various fluids, storages, agitators, blowers, and heat exchangers, which are necessary for operation.

The thermal energy demand can be met (depending on the scenario) with an on-site natural gas or lignin boiler, a natural gas CHP or with a lignin CHP plant. Depending on the thermal energy generation unit, the electricity demand can be entirely covered by the public grid and/or to a certain share with an on-site CHP unit to increase self-sufficiency.

The aim of the described conversion pathway is to obtain approval as an additional annex to ASTM D7566 (Section 3.2) and meet the sustainability criteria for certification (Section 3.2).

3.2. SAF and approved conversion processes

Jet fuels must meet the standard specifications before they can be used in aviation. Two standard options are mostly used to obtain the approval of jet fuel. The most widely used standard globally is the ASTM D1655 standard by the American Society for Testing and Materials in the US. The second standard is the DEF STAN 91-91 by the British Ministry of Defence in the UK (Yang et al., 2019).

The ASTM community, a large group of industry stakeholders, is responsible for SAF usage in aviation. SAF is subject to strict specifications and must comply with the ASTM D1655 standard, which ensures a safe use phase in aviation. SAF is always blended with conventional jet fuel and the blending ratios depend on the conversion process (ASTM, 2021a, 2021b). The conversion processes that have already been approved and included in the Annexes of ASTM D1655 and ASTM D7566 are listed in Table 4. A list of the corresponding feedstocks is described by (Prussi et al., 2021). Feedstocks can include agricultural and forestry residues, used cooking oil, soybean oil, rapeseed oil, corn grain, sugar beet, sugarcane, and many more. Several tests and analyses are required to certify a new technological SAF pathway (such as that elaborated in this study) and are described in ASTM D4054 (ASTM, 2021c).

3.3. Frameworks and requirements for biofuel certification

Specific GHG emission savings must be achieved to obtain a certification for a produced biofuel. Generally, biofuels are certified according to the EU RED 2018/2001/EC methodology. For the aviation sector and thus SAF, CORSIA provides an additional framework for calculating GHG emission savings. Both frameworks have specific and independent methodologies for calculating GHG emissions. However, in this study, ISO 14040 standards were applied to evaluate the expected GHG emission savings for both frameworks.

3.3.1. EU RED 2018/2001/EC eligible

The EU RED 2018/2001/EC provides a methodology to be strictly followed for evaluating the GHG emissions of biofuels. The GHG emis-

Table 4
Approved conversion processes by the ASTM (ASTM, 2021b, 2021a; ICAO, 2022).

ASTM	conversion process	abbreviation	max blending ratio [%-vol]
ASTM D7566 Annex 1	Fischer-Tropsch hydroprocessed synthesized paraffinic kerosene	FT-SPK	50
ASTM D7566 Annex 2	Synthesized paraffinic kerosene from hydroprocessed esters and fatty acids	SPK-HEFA	50
ASTM D7566 Annex 3	Synthesized iso-paraffins from hydroprocessed fermented sugars	SIP	10
ASTM D7566 Annex 4	Synthesized kerosene with aromatics derived by alkylation of light aromatics from non-petroleum sources	FT-SKA	50
ASTM D7566 Annex 5	Alcohol to jet synthetic paraffinic kerosene	ATJ-SPK	50
ASTM D7566 Annex 6	Catalytic hydrothermolysis jet fuel	CHJ	50
ASTM D7566 Annex 7	Synthesized paraffinic kerosene from hydrocarbon-hydroprocessed esters and fatty acids	HC-HEFA-SPK	10
ASTM D1655 Annex A1	Co-hydroprocessing of esters and fatty acids in a conventional petroleum refinery	co-processed HEFA	5
ASTM D1655 Annex A2	Co-hydroprocessing of Fischer-Tropsch hydrocarbons in a conventional petroleum refinery	co-processed FT	5

sion reduction potential of biofuels is calculated using a fossil fuel comparator. According to the EU RED 2018/2001/EC Annex V C 19, the fossil fuel comparator has emissions of 94 gCO_2eq/MJ. The required default savings for installations operating after January 1, 2021, must be at least 65% (European Commission, 2018). The GHG emission savings are calculated according to Equation (7):

$$\%_{RED,savings} = 1 - \frac{Calculated\ GHG\ Emissions}{Fossil\ Fuel\ Comparator_{RED}} \geq 65\% \tag{7}$$

3.3.2. CORSIA eligible

CORSIA has developed a framework to evaluate the GHG emissions of SAF elaborated in (Prussi et al., 2021). However, the CORSIA framework has a structured similar to that of the EU RED 2018/2001/EC (European Commission, 2018). GHG emission reductions for SAF are calculated using a conventional fossil jet fuel comparator. According to the CORSIA sustainability criteria for CORSIA eligible fuels, the fossil fuel comparator is 89 gCO2eq/MJ (ICAO, 2021b). To be eligible as a CORSIA sustainable fuel, at least a 10% reduction compared to the baseline comparator must be achieved (ICAO, 2021a). The GHG emission savings are calculated according to Equation (8):

$$\%_{CORSIA,savings} = 1 - \frac{Calculated\ GHG\ Emissions}{Fossil\ Fuel\ Comparator_{CORSIA}} \geq 10\% \tag{8}$$

3.4. Interpretation of LCA ISO 14040/14,044 results toward GHG protocol

The GHG Protocol framework is a global standard to estimate GHG emissions. Emissions are structured in scope 1, 2 and 3 emissions. Scope 1 includes direct emissions of company facilities; scope 2 indirect emission from the purchase of electricity, steam, heating and cooling; and scope 3 indirect emissions of upstream and downstream processes such as purchased goods or end-of-life treatment. The GHG protocol is well described in the literature, so a detailed elaboration has been omitted (Green, 2010; Patchell, 2018; WRI and WBCSD, 2015).

The "cradle-to-gate" LCA based on the ISO14040/14,044 framework includes the emissions from the company facilities such as from natural gas combustion (linkable to scope 1), from purchased energy such as electricity from the public grid (scope 2), and from the production of purchased goods like chemicals (linkable to scope 3 upstream). The residual soft wood transport belongs also to scope 3 upstream. Emissions from the distribution of SAF are not included in the LCA, but would be classified into scope 3 downstream emissions (Bhatia et al., 2011). Scope 3 upstream emissions such as the required chemicals listed in Table 2 are considered by the databases of GaBi ts 10.6 Professional and ecoinvent v.3.8. Consequently, the estimated GHG emissions shown in Fig. 4 are consisting of scope 1, scope 2 and scope 3 upstream emissions.

4. Results and discussion

This section presents the environmental assessment results (GWP and PED) and the energetic and exergetic efficiency evaluation of the biorefinery plant set-up for SAF production and the developed scenarios. Furthermore, GHG emission savings compared to the fossil fuel reference were calculated based on the frameworks of EU RED 2018/2001/EC and CORSIA.

4.1. GHG mitigation potential

LCA was conducted at process unit level to better understand where emissions occur along the value chain of the biorefinery. Therefore, emissions were calculated and structured according to the main process unit sections of saw dust (wood residues) transport, wood-to-sugars, fermentation, purification, conversion to SAF, and off-site (auxiliary). Compared to an LCA only at the biorefinery level, this process unit approach allows for an emission hot-spot analysis and provides detailed and important insights for process development. The assessment supports the detection of these process units, where the environmental footprint can be further improved through efficiency increases and/or technology developments.

The GWP of various SAF scenarios is shown in Fig. 4. Based on the applied energy system and by-product usage, net emissions of the biorefinery vary in a broad range of 18.7–56 gCO_2eq/MJ. Net emissions are calculated, as credits are applied for fertilizer and animal feed substitution, which decreases the total emissions. The allocation share changes if part of the lignin is used as energy on-site. Consequently, more emissions were attributed to SAF. The SAF share increased for the LI-B and LI-CHP scenarios to 33.6% and 38.7%, respectively. Lignin utilized as energy for the LI-B and LI-CHP amounts to 2.74 t/t_{SAF} and to 3.5 t/t_{SAF}, respectively. The energy-intensive wood-to-sugar unit and off-site section have an essential share of the total emissions in each scenario.

A change in the present EU-28 electricity mix to an RES mix (EU-28 mix in 2050) leads to significantly reductions of the GWP, except for the scenario applying an NG-CHP. Comparing the NG-B and NG-B RES scenarios revealed, that 18.2 gCO_2eq/MJ can be avoided by applying an RES mix as an electricity source. The impact of an RES mix for the NG-CHP scenarios is hardly noticeable (56 vs. 55.5 gCO_2eq/MJ), as almost 100% of the electricity demand is already covered on-site.

The best-case scenario from an environmental perspective is the LI-B RES, which utilizes part of the lignin on-site and consumes renewable electricity. The emissions amount to 18.7 gCO_2eq/MJ.

The calculated GHG reductions against fossil references are shown in Fig. 5. Only NG-B RES, LI-B RES and LI-CHP RES scenarios met the EU RED 2018/2001/EC requirement of 65% emission reduction. The 10% requirement for a CORSIA eligible fuel was met with all scenarios. LI-B RES was the best-case scenario in terms of the lowest emissions and highest GHG reduction potential. With this scenario, GHG emission reductions of up to 80.1% and 79% can be achieved. However, the LI-CHP

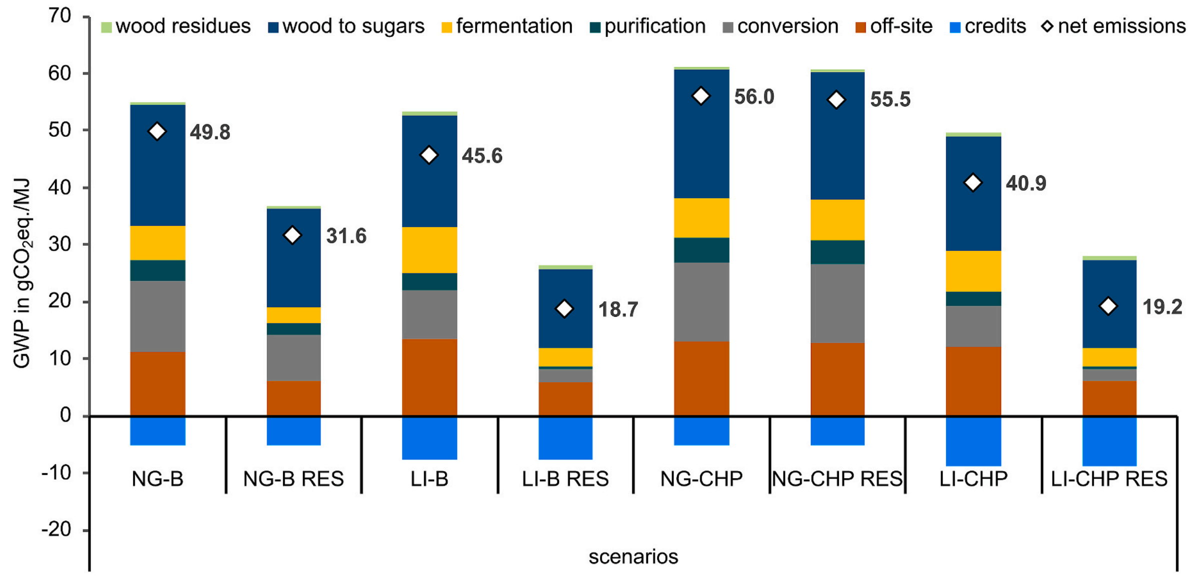

Fig. 4. Global Warming Potential of SAF production for various scenarios.

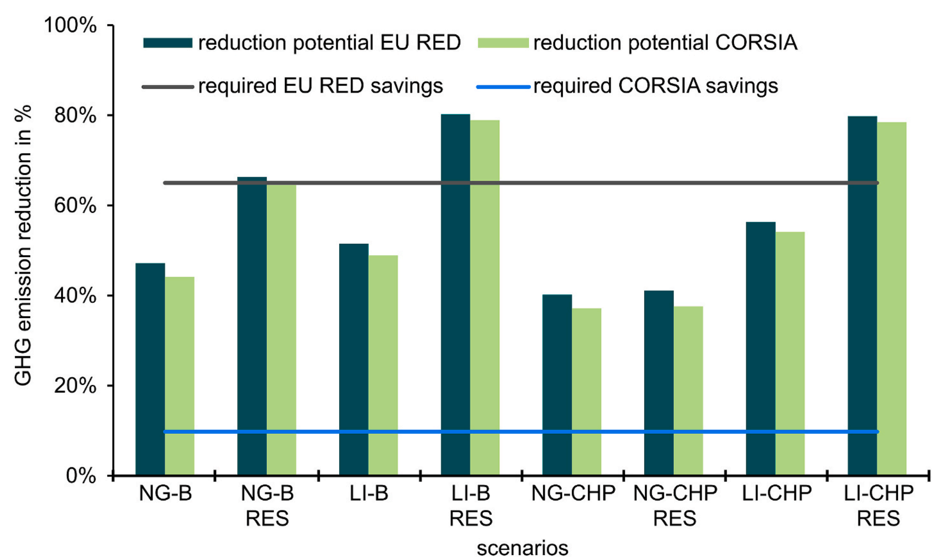

Fig. 5. Relative greenhouse gas reduction of SAF production scenarios against fossil reference elaborated applying ISO 14040/1404444 LCA methodology.

RES led to GHG reduction potentials of 79.6% and 78.5%, respectively, with similar results.

4.2. Primary energy demand

The analysis of PED was conducted for 1 MJ SAF output of the biorefinery, where (i) an allocation on SAF was applied (Fig. 6a) and (ii) no allocation was considered (Fig. 6b). Discussing only the allocated results can lead to misleading interpretations. The PED is structured into total, renewable and non-renewable PED.

As shown in (Fig. 6a), the allocated PED revealed that all scenarios that applied lignin on-site for energy provision had a higher PED. Because of use of lignin as an energy source, the allocation ratio increases compared to the non-lignin energy supply scenarios, and more PED and emissions are attributed to SAF. However, renewable PED uptake resulting from lignin usage was evident. The fossil PED is reduced by substituting natural gas and consuming electricity from the grid. In the best-case LI-CHP scenario, up to 82.3% of the total PED can be covered with renewable primary energy. The allocated PED ranges from 2.8 to 4.2 MJ.

The non-allocated biorefinery PED varies between 10.7 and 13.1 MJ (Fig. 6b). The maximum results from the NG-B RES scenario, the minimum from the LI-CHP. Generally, the use of biogenic raw materials results in a higher PED than that of fossil resources. Wood residues (saw dust), however, are classified as residues and only the PED for transport to the biorefinery is considered. If the lignin produced as a by-product from saw dust is utilized for energy purposes, no additional PED resulting from natural gas and partly from the public electricity grid is considered. Hence, the total PED in the lignin scenarios is lower than that in the fossil scenarios, as saw dust is always required as a material for the SAF conversion pathway.

More detailed results on the process unit level for the allocated and non-allocated PED can be found in Appendix A. Supplementary data.

4.3. Biorefinery efficiency analysis

An energetic and exergetic efficiency analysis was conducted once each, considering SAF as the main product and for the entire system,

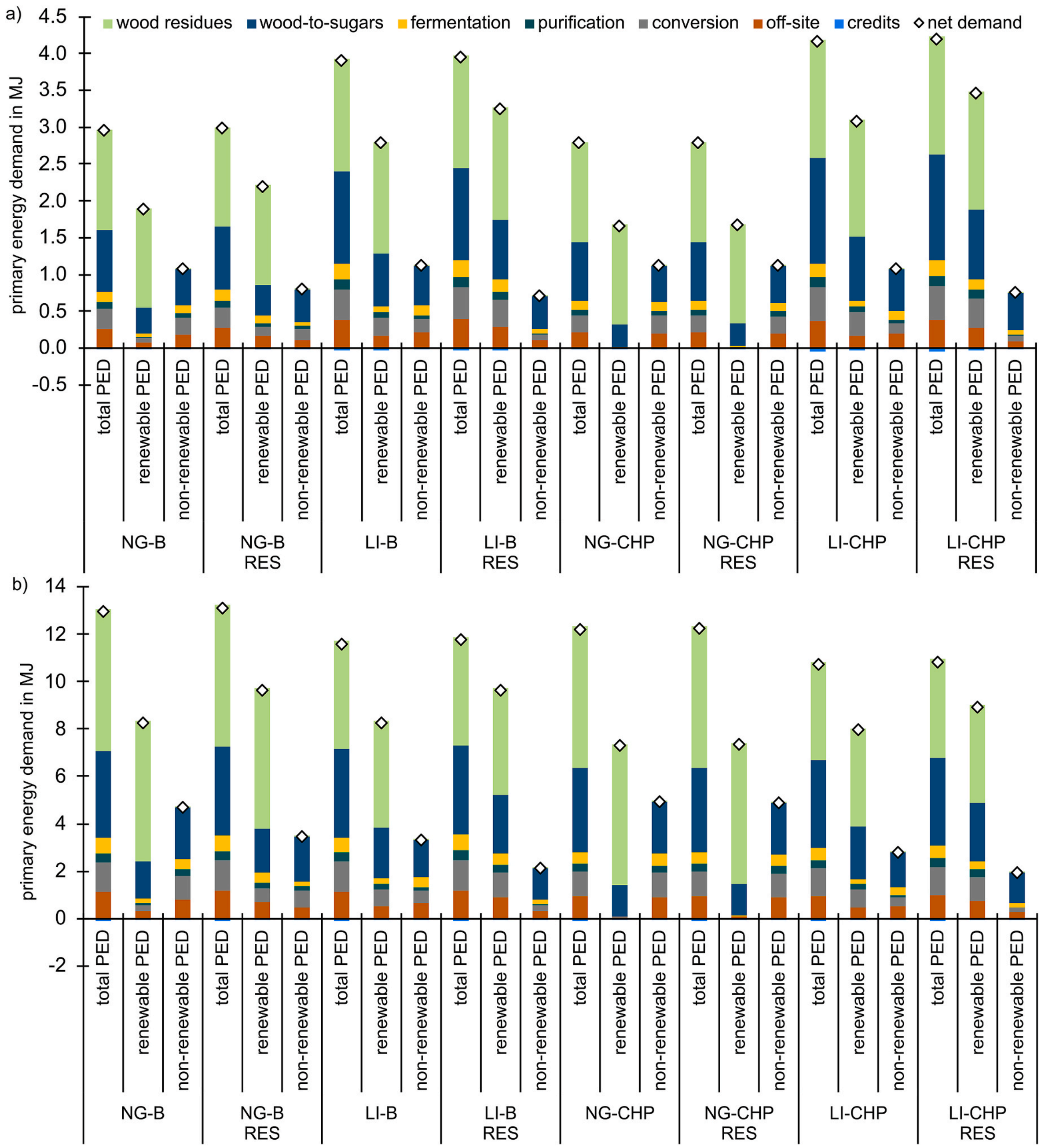

Fig. 6. a) allocated and b) non-allocated PED of 1 MJ SAF produced in biorefinery.

including all by-products (Fig. 7). The evaluation revealed that the energetic and exergetic SAF efficiencies varied slightly between scenarios. The energetic and exergetic efficiency ranged between 11.7%–14.9% and 11%–13.8%, respectively. Substantially efficiency improvements were observed for the entire system. The energetic and exergetic system efficiency ranges between 39.4%–50.1% and 40.4%–56.9%, respectively. This confirms the necessity of utilizing all by-products in addition to the main product to increase the system efficiency of the biorefinery. Detailed results for the energetic and exergetic efficiency evaluation of the scenarios can be found in Appendix A. Supplementary data.

A Sankey diagram illustrates the exergetic flow calculations (Fig. 8). The NG-B and LI-B scenarios were compared. Saw dust is evidently the primary exergetic input for both scenarios. In the case of the LI-B scenario, natural gas is not required, because thermal energy is provided by the by-product lignin extracted from the saw dust. Consequently, the exergetic output flow of lignin as a material decreased compared with the NG-B scenario. Fertilizers, such as calcium and potassium, and animal feed play a minor role in the exergetic output flow. In both scenarios, a notably exergy loss is detected, which can be compared to exergy loss in other lignocellulosic biomass studies.

The exergetic efficiencies of the analyzed pathway under different plant set-ups can be compared with previous published results showing exergetic efficiencies between 22% and 52.71% for biofuel production. When exergetic results are compared with other lignocellulosic biomass studies, system boundaries, especially the considered products, must be observed carefully. The bio-jet fuel production in (Zhang et al., 2022) has an efficiency η_{ex} of 22%, and $\eta_{ex,sys}$ of 43.5% considering the system. In (Liu et al., 2017), bio-ethanol, xylose and power were produced at an η_{ex} of 36.6%. In (Bösch et al., 2012), η_{ex} of 29.9% was achieved considering bio-ethanol and power as products (Modarresi, 2012). calculated η_{ex} of 44.1% considering bio-ethanol, bio-gas and power as main outcomes. The biorefinery analyzed by (Aghbashlo et al., 2018) for

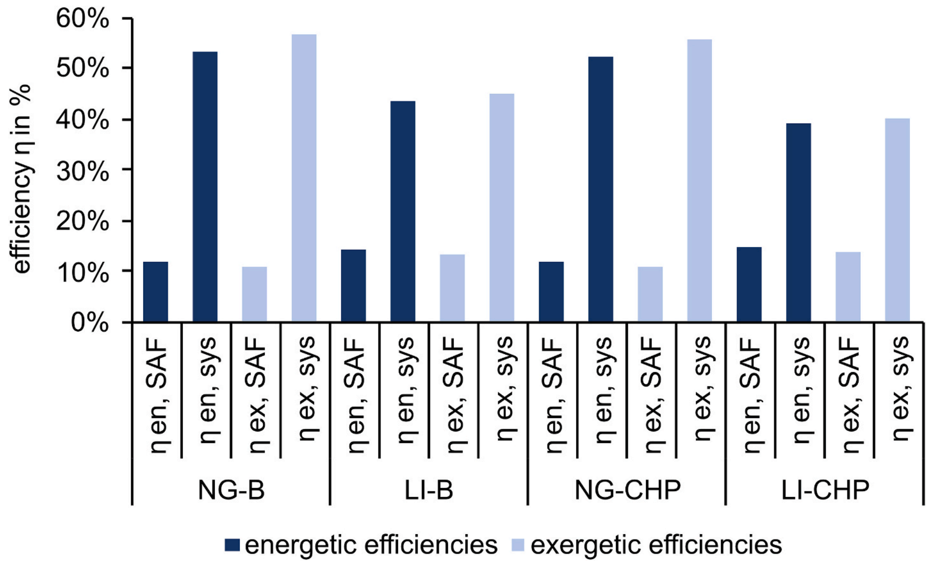

Fig. 7. Energetic and exergetic efficiencies of biorefinery.

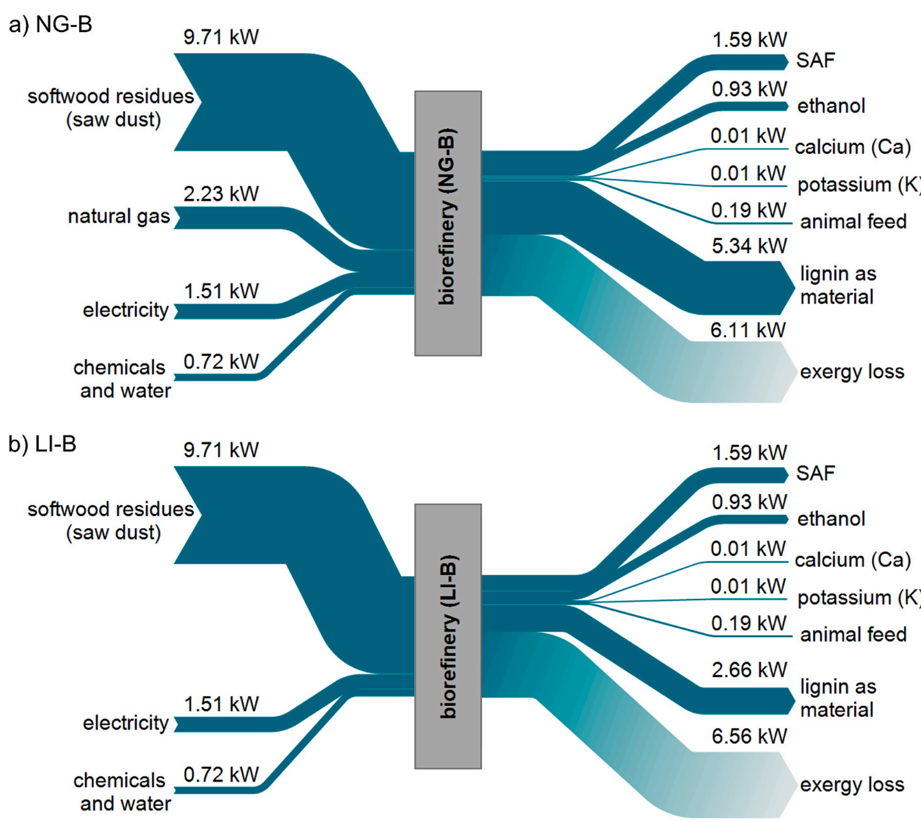

Fig. 8. Exergy flows of biorefinery to produce 1 t_{SAF} for scenario a) NG-B and b) LI-B.

the production of lactic acid and electricity had an universal η_{ex} of 52.71% and a functional η_{ex} of 44.73%.

We further examined the application rate of the produced bio-products as bioenergy. LI-CHP utilizes 75.56% of the produced bio-products as bioenergy, followed by LI-B (66.72%), NG-B (34.95%) and NG-CHP (34.95%).

5. Conclusion and outlook

The under-development biorefinery can be a promising pathway for producing SAF or biofuels. Softwood residues (saw dust) are used as the raw materials. Consequently, a 2G biofuel is produced and there exists compared to 1G biofuels no concerns on food issues. In EU-28, a wood residues potential of 41,864 kt/a was estimated. In energy-intensive processes such as pretreatment and enzymatic hydrolysis, valuable sugars (C6 and C5) are derived from cellulose and hemicellulose and treated in subsequent processes. The hydrolysate is fermented into the chemical intermediate bio-isobutene, which is eventually converted to SAF by oligomerization and hydrogenation. By-products from the SAF value chain are utilized. Lignin is used as a substitute for bitumen in the asphalt industry and thus reduces the ecological footprint of production, or in end-use applications such as phenol-formaldehyde resins and bioplastics filler. Separated C5 sugars from the wood-to-sugar unit are converted to ethanol. The sludge from the fermentation process is used as fertilizer, which substitutes potassium and calcium. The produced microbial biomass contains valuable nutrients that can be used as animal feed and thus as a substitute for imported soybeans.

This research analyzed the environmental sustainability of the SAF conversion pathway according to the LCA standard ISO 14040/14,044. The GWP and PED (renewable and non-renewable) were evaluated. In addition, energetic and exergetic efficiency analyses were conducted. The initial plant design was engineered within the REWOFUEL project (REWOFUEL, 2022). However, scenarios have been developed to identify the best plant set-up from an environmental perspective. The scenarios differ in terms of energy provision and by-product utilization.

The GHG emission calculation was conducted for the production of 1 MJ of SAF and revealed a GWP between 18.7 and 56 gCO_2eq/MJ. These results can be interpreted in the GHG Protocol framework as emissions of scope 1, scope 2 and scope 3 upstream. The best biorefinery plant set-up is the LI-B RES scenario, where the thermal energy is provided by a lignin boiler, and the electricity demand is covered with an RES. The biorefinery PED ranged between 10.7 and 13.1 MJ, when no allocation on SAF was applied. On-site lignin utilization and the integration of RES increased the renewable PED share up to 82.3%.

To obtain a certification for the produced SAF, sustainability requirements must be met. The EU RED 2018/2001/EC requires default savings of at least 65% compared to a fossil reference. The CORSIA framework requires at least a 10% reduction compared with the baseline comparator. According to the EU RED 2018/2001/EC benchmark, only three scenarios meet the sustainability requirements (NG-B RES, LI-B RES and LI-CHP RES). However, these requirements are not met without a renewable energy source mix to meet the electricity demand. Therefore, the carbon intensity of the electricity mix is a crucial factor affecting the GWP calculation. In the CORSIA framework, all scenarios meet the requirements. The best plant layout (scenario LI-B RES) revealed GHG emissions reductions of up to 80.1% and 79% for both. However, up to 50% of the available lignin is required for energy provision instead of its use in the asphalt industry.

An energetic and exergetic efficiency analysis was conducted for the main product, SAF, and the biorefinery system. Inefficiencies of upstream process such as for electricity provision were not considered. For SAF, the energetic efficiency was between 11.7% and 14.9%, and the system efficiency ranged between 39.4% and 50.1%. The SAF exergetic efficiency was between 11% and 13.8%, and the exergetic system efficiency between 40.4% and 56.9%.

The yield of specific process units under development must be further improved to increase efficiency and reduce environmental implications. Moreover, energy efficiency considerations must be addressed in all process design units to limit utility consumption.

In general, EU RED 2018/2001/EC and CORSIA provide independent GHG assessment methods, which must be applied to a country specific biorefinery evaluation. In this study, an universal calculation was conducted for the EU-28 following a cradle-to-gate system boundary. Therefore, the hub distribution of SAF is not considered, but is required in the EU RED 2018/2001/EC and CORSIA methods.

In this study, we have only discussed the environmental impacts and energetic/exergetic efficiency of producing SAF and biofuels. A more comprehensive review from other perspectives on SAF must be conducted. Economic, social and public acceptance aspects are crucial conditions for the development of new processes, technologies, and products.

CRediT authorship contribution statement

Stefan Puschnigg: Conceptualization, Methodology, Data curation, Formal analysis, Visualization, Writing – original draft. **Karin Fazeni-Fraisl:** Project administration, Supervision, Funding acquisition, Validation. **Johannes Lindorfer:** Validation, Writing – review & editing. **Thomas Kienberger:** Validation, Writing – review & editing.

Declaration of competing interest

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

Data availability

The authors do not have permission to share data.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2022.135815.

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Techno-economic aspects of increasing primary energy efficiency in industrial branches using thermal energy storage

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ABSTRACT

Thermal energy storage (TES) can play a key role in increasing primary energy efficiency in the industrial sector. Differences in location-specific conditions lead to differences in TES requirements across companies and to a lack of techno-economic knowhow regarding standardized implementation. This study provides a techno-economic overview of potential TES technologies (sensible, latent, thermochemical, and sorption) based on key performance indicators (KPI) and performs a qualitative pre-selection of the TES to be used in specific industrial branches at specific temperature levels. The outcome is a TES application matrix for industrial branches based on the quantified energetic and exergetic heat demand per temperature level and branch. This matrix is expected to facilitate and support the selection of future TES projects. The study demonstrates its methodology of estimating the energetic and exergetic heat demand of a country by applying it to Austria. In this case, the estimated energetic industrial heat demand is about 88 TWh/year, and the exergetic industrial heat demand is about 50 TWh/year. In the application matrix, 2,470 variants of industrial energetic heat demand and potential TES applications are evaluated. The results show that there is only a 6% match between a TES priority field of application and the fields with the greatest energetic heat demand. As the costs of a TES system influence its industrial use, an economic top–down method of determining the maximum costs (and thus economic viability) of a TES system is presented. The generic approach is demonstrated by conducting a case study of a cement plant. The acceptable storage costs are derived by determining the energy and cost savings relative to a conventional gas-driven energy supply system. Depending on the size of the TES, the acceptable costs are found to vary between 1.4 and 14.4 €/kWh for a capacity of 500 MWh and 1 MWh, respectively. A sensitivity analysis is also conducted to show how gas and CO_2 emission allowance prices affect the acceptability of storage costs. The study also discusses the main considerations and factors in efficient TES selection and successful system integration. Finally, the development and innovation required to increase industrial use are outlined. The study's economic analysis of TES integration in a cement plant shows that TES implementation is not feasible under the present conditions unless appropriate measures and incentives are applied.

1. Introduction

Combating climate change by creating a sustainable and renewable energy supply is one of the largest challenges humanity is facing [1]. In future energy systems [2], energy from fossil energy sources will be replaced by renewable energy. This will reduce the use of fossil fuels and, in the best-case scenario, eliminate them. Various approaches — such as the utilization of solar and geothermal energy, wind energy, hydro energy, and biofuels — combined with an efficient use of energy and waste stream valorization will play a decisive role in cross-sectorial solutions for shaping the energy supply of the future. According to Aydin et al. [3], developing renewable energy systems is as important as improving energy storage systems for tackling mismatches between supply and demand.

One key task is lowering primary energy demand by exploiting available thermal energy sources. The Association of German Engineers

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[4] conducted a general strength-weakness-opportunity-threat analysis on several thermal energy storage (TES) options. Shkatulov et al. [5] considered TES as a way to utilize waste heat and renewable energy sources. Gasia et al. [6] regarded TES as a key factor in improving energy efficiency in different energy systems. The International Energy Agency [7], the International Renewable Energy Agency [8], and Hauer et al. [9] all recognized a high potential for TES as a way to balance energy supply and demand and, thus, reduce energy consumption. The heat demand of industrial processes and their potential waste heat supply can vary daily, weekly, or even seasonally. This variation is caused by the dynamics of thermal energy demand in industries, such as day and night variations (shift operation), seasonal dependencies (summer/winter), and performance fluctuations in process heat demand (which is usually required only for 3 or 4 days a week) [10]. To avoid peak loads in the heat network and partial load operation in heat generation plants, TES supports load management via an optimized and economical heat supply [11]. TES can also serve as a backup during unplanned shutdowns and power outages. Moreover, TES increases the flexibility of heat supply through diverse energy sources and can be used, if supplied with electricity, in the control energy market for grid stabilization and the generation of additional revenues [12]. In the heat sector, excess energy from renewables in the form of electricity can be converted through sector coupling (e.g., via power-to-heat) [13]. Ultimately, TES can help reduce primary energy consumption, CO_2 emissions, and costs.

A few approaches already exist for TES integration, but a common and complete methodology is not known. Rathgeber et al. [14] use an economical method by calculating the maximum acceptable costs for a TES dependent on the underlying energy costs, the number of cycles, and the annuity factor. Gibb et al. [15] developed a multi-step approach for TES process integration by analyzing and characterizing the process and accompanying requirements, the storage system and its performance, and the benefits of TES integration within an application via chosen key performance indicators (KPIs). Cabeza et al. [16] and van Helden et al. [17] also state the importance of using KPIs to assess and to compare TES systems and to demonstrate their application potential. In this context, Kapila et al. [18] points out the need of clearly defined TES system boundaries to be comparable at all. Beck and Hofmann [19] use a sequential approach including a mathematical model and pinch analysis to come up with cost efficient TES systems.

In the EU-28, heat is the most important secondary energy and comprises 51% of the final energy demand [20,21]. Industrial heat consumption is about 1821 TWh/year, from which a waste heat potential of 300 TWh/year can be derived [22]. Naegler et al. [23] conducted a more detailed study on the EU-28 industrial heat demand according to industry branch and temperature level. In Austria, about 50% of the final energy is consumed as heat. Thermal energy is used for space heating, hot water supply, and process heat at various temperature levels [24]. The industrial sector, with its many energy-intensive processes, consumes a particularly enormous amount of energy, implying a huge potential for increasing primary energy efficiency [12]. The industrial sector is responsible for almost 30% of the final energy consumption [25]. Several countries are introducing policies and measures for waste heat utilization in order to enhance the attractiveness of industrial companies while making them more competitive and increasing primary energy efficiency [26,27]. Industrial waste heat utilization is already common among companies. Moser et al. [28] analyzed external waste heat implementation projects in Austria and found that about 93% of them were used to supply district heating networks.

This study shows the potential for TES use in industries depending on their energetic and exergetic heat demand and the temperature at which it is consumed. First, it provides a practical overview of theoretical TES based on selected KPIs. TES technologies have typically been reviewed in scientific papers and reports (refer to Section 3.1), and there is little comprehensive understanding of TES technologies in terms of their main techno-economic characteristics and potential use. Second, the study pre-selects which TES is useful and theoretically applicable in which industrial branch and temperature profile, and discusses the main influencing factors that should be considered in a purposive selection of TES projects.

As the costs of a TES are a key aspect of its industrial use, this study also provides an economic top–down method of determining the maximum costs at which TES is economically viable. Energy and cost savings are used as the benchmarks for the maximum acceptable storage costs. We evaluate TES integration in a cement plant as a case study. Finally, we describe the development and innovation required to increase its industrial use based on an economic evaluation and comparison to currently available TES.

Although the study's industrial heat demand analysis is conducted for Austria, its methodology is independent of region and can be applied to other countries. Similarly, the study's economic top–down method of determining the maximum TES costs depending on energy savings can be applied to any industry.

2. Materials and methods

As shown in Fig. 1, this study unfolds on four layers. Layer 1 elaborates a catalogue of TES, layer 2 assesses the industrial branches, layer 3 creates an application matrix by matching layers 1 and 2, and layer 4 conducts a case study of a TES integration in a cement plant, along with a basic economic and ecological assessment.

2.1. Layer 1: elaborate a catalogue of TES

TES can be classified into sensible, latent, thermochemical, and sorption technologies [3,29]. This study clusters and reviews the main TES technologies discussed in the literature and provides an overview of their main techno-economic characteristics relevant for practical implementation. We analyze the following KPIs: temperature level and application range, technology readiness level (TRL) [30], specific TES costs, specific storage density, and storage capacity. We also compare among TES type-specific characteristics, such as conductivity, specific latent heat, melting point, and reaction enthalpy. Moreover, we identify the main design and factor requirements that influence successful TES integration.

2.2. Layer 2: assessment of industrial branches

This layer is applicable for every country, but is exemplarily applied to Austria, as it has an energy-intensive business landscape that encompasses sectors of various sizes. This includes industries such as an iron and steel and non-metallic mineral processing sector with a high final energy consumption for industrial furnaces, a paper and pulp industry with high energy consumption for process steam, and a mechanical engineering and automotive industry with heat requirements for hot water and the space heating of production halls [31,32].

The Austrian Energy and Climate Strategy (#mission2030) has set the goal of increasing the share of renewable energies in the electricity sector to 100% and increasing the share in final energy consumption to 45–50% by 2030. Primary energy intensity is also to be improved by 25–30% by 2030 [25]. One way of increasing primary energy efficiency in Austria's industrial sectors is to use waste heat optimally within the framework of the given requirements (examples of waste heat utilization are listed in Moser et al. [28]). Integrating TES can also help achieve this energy-saving objective and reduce carbon emissions.

In addition to the energy and heat intensity of the industrial branches, the temperature levels of the heat used should also be identified. We used data from Statistics Austria [31,33] (energy balance and useful energy [UE] analysis of 2018) and the Austrian Economic Chamber [32,34] (categorization and number of Austrian companies) for this purpose. Naegler et al.'s [23] study on EU-28 heat demand quantification used outdated final energy consumption data for 2012. We apply our approach only to Austria, but our method goes further

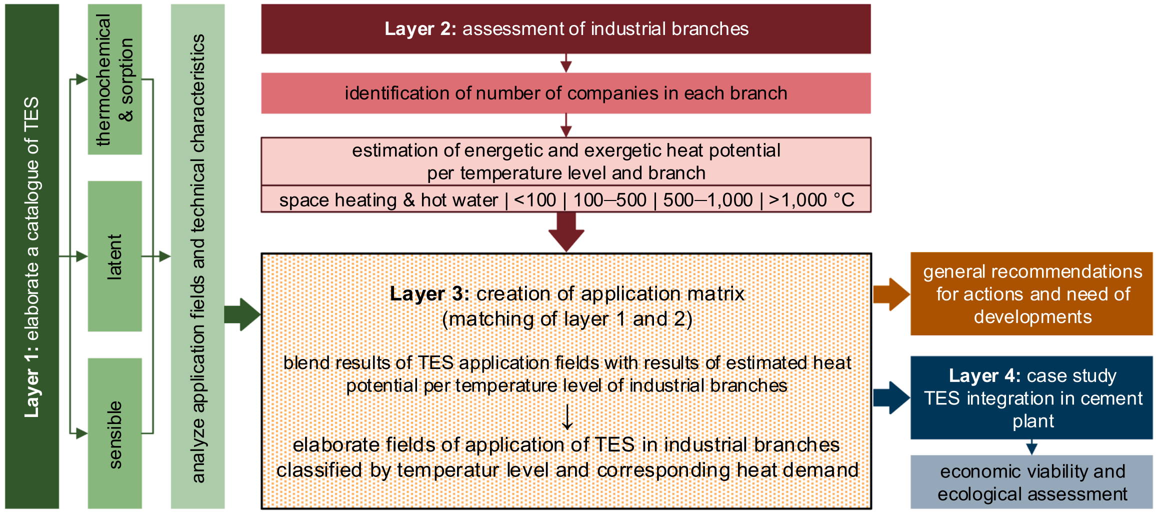

Fig. 1. Methodology and structure of assessment.

than prior attempts by analyzing and quantifying the energetic (en) industrial heat demand (HD) per branch (b) and temperature level (T_{level}) and including the energy of conversion processes (CE), as well (see Eq. (1)). The amount of CE is especially high in the iron and steel industry (where the yearly CE of 18 GWh is around twice the UE of 10 GWh). Omitting CE would neglect a major part of the energy required for conversion processes within cookeries and blast furnaces, as it is not considered within the UE demand. Geyer et al. [35] also pointed out the importance of the non-negligible CE in their study on gross industrial energy demand in Austria. Since the overall heat demand (UE+CE) provides no information about the temperature level of the consumed heat, the heat demand quantity per temperature level and branch is calculated using the guideline values of characteristic temperature distributions ($T_{\%,b}$) drawn from the literature [23,36,37]. The temperature levels are classified into space heating + hot water (SH+HW), <100, 100–500, 500–1000, and >1000 °C (Fig. 4).

$$HD_{en,\ b}(T_{level}) = (UE_b + CE_b)\cdot T_{\%,b}(T_{level}) \tag{1}$$

Moreover, we analyze the exergetic (ex) industrial heat demand in the industry branches per temperature level, expressed in Eq. (2). The Carnot factor η_C links thermal energy and exergy, whereby T_S is the surrounding temperature and T is the supplied temperature [38]. T_s and T are chosen following Sejkora et al. [39]. Furthermore, the industrial landscape is analyzed in detail to identify which and how many companies across the industry branches are responsible for the estimated heat demand. The number of companies is given to illustrate the energy intensity in each branch.

$$HD_{ex,\ b}(T_{level}) = HD_{en,\ b}(T_{level})\cdot\left(1 - \frac{T_S}{T(T_{level})}\right) = HD_{en,b}(T_{level})\cdot\eta_C(T_{level}) \tag{2}$$

2.3. Layer 3: creation of application matrix (matching of layers 1 and 2)

We match the results of the TES characterization (Section 2.1, layer 1) and the results of the industrial analysis regarding the energetic and exergetic heat demand of each branch and temperature level (Section 2.2, layer 2) to create an application matrix of TES and conduct a preselection to identify potential fields of application for several industrial branches (Fig. 6).

This analysis is conducted using traffic-light logic (with green, yellow, and red colors), in which a blank traffic light denotes no demand, a green symbol signifies that the TES operating temperature matches ideally with the temperature level of the branch, and a yellow symbol indicates that the TES operating temperature and planned industrial application temperature are theoretically overlapping, but may not lead to a reasonable practical application. In such cases, this has to be evaluated case specifically.

Heat demand is expressed on a colored scale to visualize the intensity of energetic heat demand at the different temperature levels of each branch. The darker the coloring, the higher the energetic heat demand at that temperature level. If there is no coloring (blank), there is no significant heat demand assigned to that level.

The highest application potential is observed in cases where a green symbol (priority field of TES application) meets a dark-colored heat demand (largest heat demand per temperature level within an industrial branch). However, other promising combinations are possible, including a yellow symbol with a medium-colored heat demand intensity field. Such fields should not be excluded but should be evaluated on a case-specific basis. This analysis aims to identify suitable storage technologies for each industrial branch at their respective temperature levels. An analysis aiming to provide an industrial temporal resolution regarding heat demand and supply would be interesting, but we do not attempt this due to a lack of available data.

2.4. Layer 4: case study of TES integration in cement plant

The non-metallic mineral processing sector belongs to the most energy-intensive industry in Austria (Fig. 5). Within this branch, there is a high potential for reducing gross industrial energy demand through energy-efficiency measures, by recovering waste heat, and by integrating TES.

The cement plant in Gmunden (Austria) [40,41] belongs to this industry. It has a waste heat potential of 10 MW_{th} at 400 °C. We analyze this plant in order to find a way to recover the waste heat and transport it 1.5 km away to a dairy plant, which requires process heat in the form of saturated low-temperature steam (Fig. 2). Though the cement plant is in continuous operation, both planned and unplanned process interruptions occur. The dairy plant operates in general continuously, but sees demand fluctuations, why it needs a TES and/or a gas boiler as a backup system in case of process interruption at the cement plant. Moreover, the cement plant shuts down in winter for several weeks; a gas boiler system is required to provide steam during these weeks. The integration of a TES is analyzed from a technical perspective (e.g., the time taken until the gas boiler is operational) and from economic and environmental points of view (e.g., the avoidance of gas input). The analysis is based on real-life confidential interruption data covering 2 years. These data show more than 100 process interruptions lasting

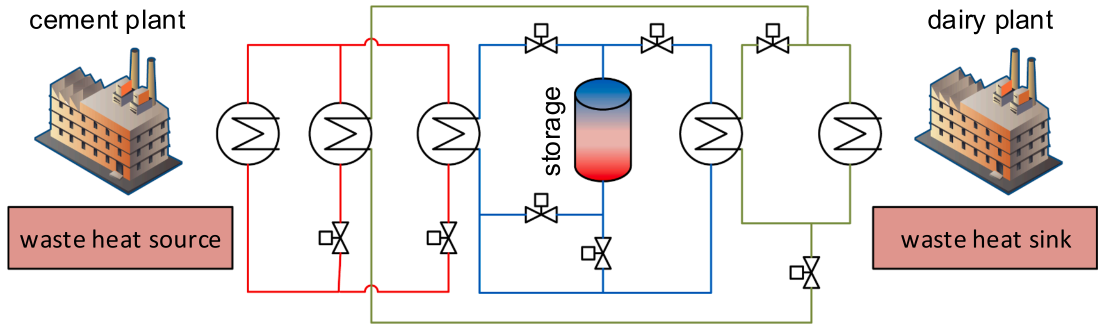

Fig. 2. Flow sheet showing waste heat recovery (red), storage (blue), and transportation (green), based on [40].

anywhere between a few minutes to several days, the average being a few hours. The capacity of the TES is an essential parameter for ensuring continuous supply to the dairy plant in case of cement plant process interruption. The higher the capacity, the longer each interruption can be without requiring the use of the gas boiler backup system. Gas savings are dependent on storage capacity. The number of storage cycles is an essential parameter of economic viability (see [42]).

This study examines only the cost-effectiveness of the TES and does not discuss the technologies for heat extraction and recovery, transportation via a steam pipe, or the operational and business model aspects of waste heat sources and sinks.

2.4.1. Economic assessment

Storage systems must be capable of operating economically under all business conditions. Subsidies are sometimes necessary to attain economic viability. If the storage system is essential for the functionality of the overall system, it is important to include the storage cost in the overall system cost assessment. However, if the storage is not systemically relevant but serves only to avoid further energy input, the costs of the storage system should be compared to the costs of the energy consumed.

For the economic assessment of such a storage integration, capacities from 1 to 500 MWh are considered at a capacity of 8.5 MW. The aim is to investigate the maximum storage costs, which can then be competitively compared to a benchmark system (i.e., the existing gas boiler). An economic top–down method is used to identify maximum investment costs, instead of calculating elusive component costs. Based on energy and cost savings, the maximum TES costs are derived. Moser et al. [43] developed this method to determine the value of waste heat for designing a heat merit order in district heating systens. The analysis measures only the saved energy costs and does not consider the technical requirements. The costs are calculated using the capital value method [44]. The investment modeling data are presented in Table 1.

2.4.2. Sensitivity analysis

A sensitivity analysis is conducted for two essential parameters: gas and CO_2 prices. The analysis shows how varying the gas price for all storage sizes impacts the maximum storage investment cost. The gas price is varied by ±25%, ±50%, ±75%, and +100%. The price of one ton of CO_2 emissions is varied for the 300 MWh storage size, which covers nearly all (96%) interruptions to demonstrate the impact of the CO_2 emissions allowance price on storage costs. Following Król and Ocłoń [48] and the European Energy Exchange AG [49], the CO_2 price is assumed to start at 25 €/ton and is increased sixteen fold.

Table 1
Data for investment modeling.

	Unit	value	reference
assumed gas price[1] (HHV)	€/MWh	22	[45]
payback period	years	10	[40]
discount rate	%	6	[40]
possible storage usage	months/year	10	[40]
dairy plant consumption	MW	8.5	[40]
storage size (x)	MWh	1–500	[40]
number of cycles (y)	-	see Eq. (8)	[40]
CO_2 emissions gas boiler	tons/MWh	0.18	[46,47]

[1] Average prices in 2018 and 2019 are used in the case study (including cost of the network but not taxes and duties).

3. Theory and calculation

3.1. Thermal energy storage (layer 1)

Gil et al. [50] and the International Renewable Energy Agency [8] define a TES as equipment employed to increase the use of thermal energy. The aim of a TES is to store the energy and use it later. A TES helps balancing the mismatch between supply and demand, thus reducing peak demand, energy consumption, and CO_2 emissions and costs. According to Hasnain et al. [51], a storage process occurs through three steps — charging, storing, and discharging — which can take place simultaneously. This study discusses the techno-economic characteristics of TES systems and materials and the design criteria that must be considered.

3.1.1. Design criteria and influencing factors

TES system selection is based on several criteria and depends on many cost-benefit considerations as well as technical and environmental criteria [50]. Sensible storage systems are usually selected in combination with single-phase working media, whereas latent systems are often used in systems with two-phase working media. A successful economic storage selection requires an optimal system integration. Thus, it is crucial that the TES must be well-adapted to the plant in terms of charging and discharging processes, necessary temperature levels, mass flows, and other factors. Therefore, design factors and characteristic values can be determined only through a concrete application, and general information on the costs of TES systems are, in principle, available only to a very limited extent [52].

According to Gil et al. [50], Alva et al. [53], the International Renewable Energy Agency [8], and Steinmann [52], the most important factors in economic assessments are storage and power capacity; performance during charging and discharging; temperature and pressure levels; heat transfer between heat transfer fluid and TES; number of cycles (charging and discharging), including for the lifetime span (to evaluate reversibility); start-up time; mechanical and chemical stability of storage material; compatibility between heat transfer fluid-heat exchanger-storage medium (for safety issues); efficiency and thermal losses of TES and overall system; and difficulty level of system control. Other key factors in TES design and selection include the operation strategy, maximum load, specific enthalpy drop, and integration issues in the overall system.

TES is also classified and designed according to time, space, and economic aspects. The discharge duration of TES is an important time factor. This is divided into short-term storage (seconds, minutes, hours, and days) and long-term storage (weeks, months, and seasons). Regarding the spatial aspects, a distinction is made between large/centralized and smaller/decentralized storage facilities. Spatial storage systems can also be fixed (bound to one location) or mobile. The economic aspects concern the essential cost structure. This includes capital costs (investment costs), operating costs, the amortization period, and the planned useful life. It is common to relate capital costs to the installed power capacity in €/kW or installed storage capacity in €/kWh and to relate operating costs to the generated energy in €/kWh [29]. The cost of a TES depends mainly on the storage material, heat exchanger for the charging and discharging processes, enclosure, and space needed for the storage [50]. Sterner et al. [29] and the Association of German Engineers [4] provide a more detailed list of TES parameters according to power, energy, time, and efficiency. Alva et al. [54] conducted research on the thermophysical properties of storage materials. According to their findings, materials should have a favorable melting point, high energy storage density, high latent heat of fusion, high specific heat, high thermal conductivity, minimal super cooling, minimal volume change, low price, high availability, and high thermal and chemical stability; they should also be non-toxic, non-corrosive, non-flammable, and non-explosive, and feature congruent melting and low vapor pressure.

We consider the following KPIs to assess the TES: temperature level and application range, TRL, specific TES costs, specific storage density, and storage capacity.

3.1.2. Classification of thermal energy storage

According to Sterner et al. [29], TES can be classified as follows: a) as high-, medium-, or low-temperature storage (>500 °C, 500–120 °C, <120 °C, respectively); b) as short- or long-term storage (from a few hours to a few days or from a few weeks to a year, respectively); and c) based on their thermodynamic principle. This study classifies TES according to their thermodynamic principle, dividing them into sensible, latent, thermochemical, and sorption storage types [3,29].

Fig. 3 provides an overview of TES and their theoretical operating temperature ranges. An additional sub classification according to their physical state and type of reaction is included. Sections 3.1.2.1–3.1.2.3 describe TES technologies and their specific characteristics in detail.

3.1.2.1. Sensible heat storage. Sensible storage stores thermal energy within its specific heat capacity, wherein there is no phase change. The total stored thermal energy is determined via Eq. (3), where m is mass in kg, c_p is specific heat capacity in kJ/kgK, and dT is the temperature difference in K.

$$Q = \int_{T_1}^{T_2} m\, c_p\, dT \tag{3}$$

The relation between stored thermal energy and the key parameters is proportional [53,55,56]. When heat is absorbed or dissipated, the sensible heat storage experiences a noticeable change in temperature. Since the temperature difference between the storage medium and the environment is usually higher than in other storage technologies, thermal insulation is an essential parameter. Many storage systems are operated with water, because water has a high specific heat capacity, low costs, environmental compatibility, and high availability [29].

The expectable investment cost of sensible storage vary between 0.1 and 50 €/kWh and have a power capacity between 0.001 and 10 MW [2,8,57,58]. The specific energy storage density is 70 to 200 kWh/m^3, and

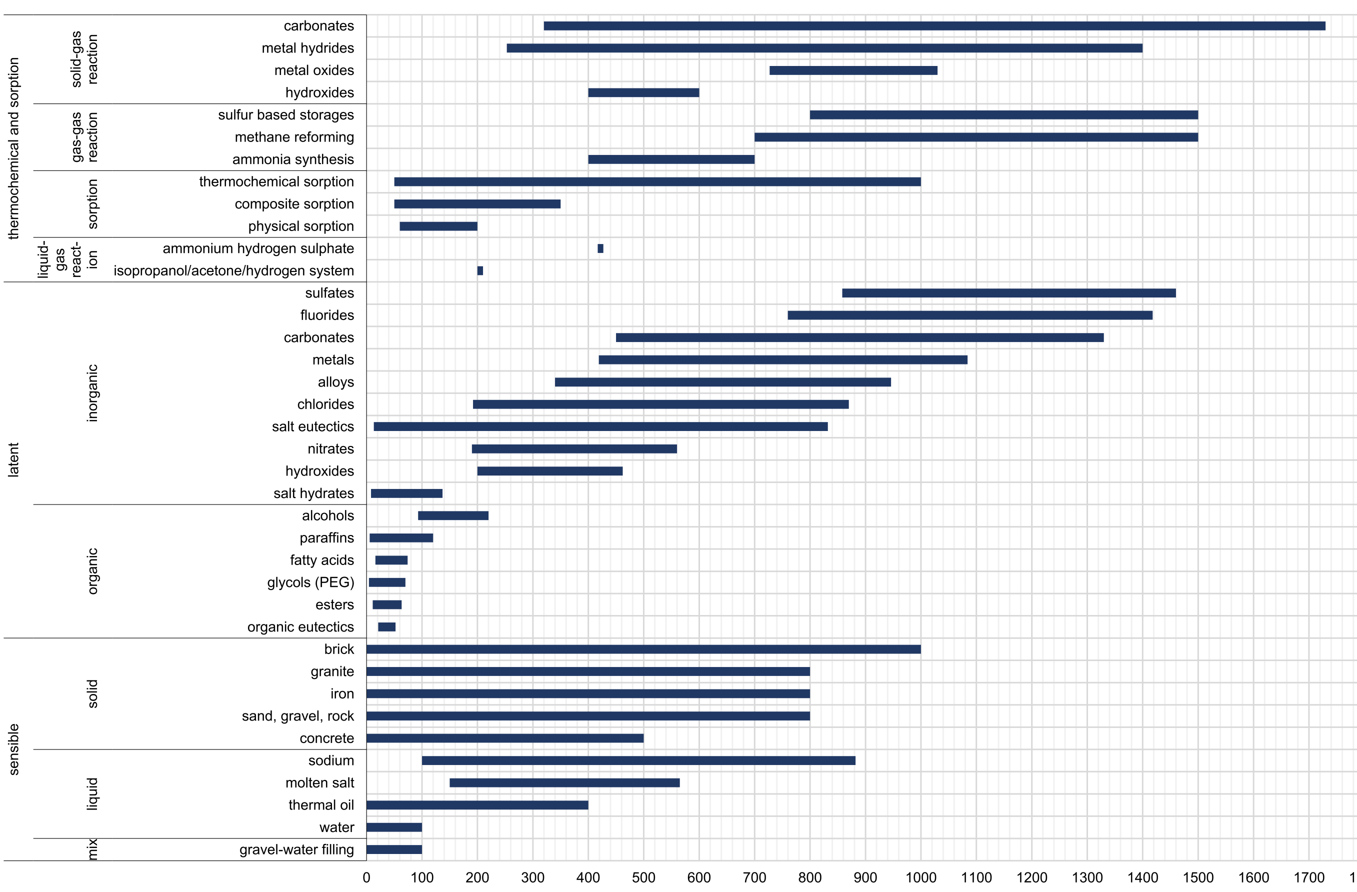

Fig. 3. Theoretical storage operating temperatures of thermal energy storage types.

typical storage sizes range between 1 and 5000 MWh. There is no limit on the specific power capacity density in liquid storage, whereas the limit is 20 to 40 kW/m^3 for solid storage [2]. Prototypes of high temperature solid storage above 500 °C can achieve a capacity of up to 100 MW. Storage of up to 200 GWh is yet to be developed, but capacities of up to 500 MW can be achieved [58].

According to Alva et al. [53], sensible heat storage is the most commonly used TES, because of its thermal stability and low-cost materials. However, during the discharge process, the temperature becomes unstable and decreases gradually. Seitz et al. [2] claimed that water storage has a TRL of 9, whereas the TRL of other liquid and solid storage types range between 4 and 9. They are used in commercial applications as regenerators for the steel and non-metallic mineral processing industry and as molten salt storage for solar power plants with a TRL of 9. However, other uses in power plants and the process industry have proven economical only at the laboratory stage and, hence, have a TRL of 4–5. The storage initiative undertaken by Austria [58] estimates high-temperature solid storage such as ceramic storage as having a TRL of 6–7 (or 70–80% efficiency). Liquid storage is estimated to have a TRL of 2–9, but water storage (with a TRL of 8–9) is included in this general evaluation.

Table 2 shows the temperature ranges and characteristics of sensible storage materials as reported in the literature. A distinction is made based on the physical state of aggregation in liquid, solid, and liquid–solid storage.

3.1.2.2. Latent heat storage. The storage capacity of latent heat storage systems is greater than that of sensible storage systems due to melting or evaporation enthalpy during the phase transition of so-called “phase change materials” (PCMs). To determine the stored energy of a latent storage system using Eq. (4), Eq. (3)—for sensible storage—is extended by considering the share of latent heat in Eq. (5) during the phase change, where m is mass in kg and L is the specific latent heat in kJ/kg. By using this physical effect, latent heat storage can store more heat at lower temperature changes than sensible heat storage. One prerequisite is that a phase change that occurs in the material must take place at a constant temperature while charging and discharging [29,53].

$$Q = \int_{T_1}^{T_2} m\, c_p\, dT + Q_{lat} \tag{4}$$

$$Q_{lat} = m \cdot L \tag{5}$$

The expectable storage investment cost vary between 10 and 80 €/kWh and have a power capacity of 0.001 to 1 MW [2,8,57,58]. Demonstration projects are currently in development that have a power capacity of up to 6 MW. The specific energy storage density is at about 100 kWh/m^3, the specific power capacity density is from 15 to 80 kW/m^3, and the realizable storage sizes range from 0.1 to 500 MWh [2]. According to Cárdenas et al. [63], the solid–liquid phase change is typically used. The solid–solid phase change is also used, but it has less specific latent heat; however, it also has advantages, such as no leakage and no need for encapsulation. The liquid–gas phase change has the highest specific latent heat, but it is rarely used due to large volume changes and the evaporation of the storage material, which make a TES system complex. Latent heat storage are typically more compact than sensible storage. However, its usually low thermal conductivity is a main disadvantage.

Latent heat storage systems are structured into inorganic and organic storage materials. Inorganic PCM include metals, salts, and other compounds, and carbon is not bonded to hydrogen. In general, inorganic PCM have a sharp melting point, high heat of fusion, high latent heat storage capacity per unit mass, and a high thermal conductivity. Organic PCMs have a congruent melting and a lower heat of fusion than inorganic PCM [55]. Additionally, organic PCM are not storable or transportable in plastic containers, as plastic is lipophilic, while inorganic PCM display corrosive behavior in metal containers [64]. As a result, PCMs have a poor long-term stability, as the capacity of the storage material decreases after several cycles because of chemical reactions with the storage containers. Therefore, the selection and design of storage containers based on their physical and thermal characteristics as well as the selection of PCM, which can provide multiple cycles without changing properties, are essential factors in a successful TES system [55].

According to Seitz et al. [2], the commercially available latent heat storage systems (TRL 9) in the low-temperature range are ice storage and passive storage for air conditioning in buildings, whereas PCMs in active storage have a TRL of 7–8. For high-temperature latent heat storage, passive storage for steam processes have a TRL of 6, but practical uses have been demonstrated only in the laboratory (with a TRL of 4). The Austrian storage initiative [58] assesses inorganic salt hydrate storage as having a TRL of 6, whereas organic storage with paraffin or alcohol is still in development (with a TRL of 2–5).

Table 3 shows the melting temperature and heat of fusion of several materials reported in the literature. Inorganic materials are theoretically capable of covering temperatures of up to 1460 °C, while organic materials are limited to up to 220 °C.

3.1.2.3. Thermochemical and sorption heat storage. Thermochemical heat storage systems use the reaction energy of reversible chemical processes or physical surface reactions (adsorption or absorption) to achieve high energy densities, increased storage time, and lower thermal losses. The energy is not stored as heat but as reaction energy, which implies that, theoretically, no thermal losses occur during storage and a long storage period is possible. As shown in Eq. (6), an endothermic charging process allows the absorption of heat (+Q) and dissociates a chemical reactant AB into products A and B. During the discharging process, an exothermic reaction releases the stored energy in the form of heat and produces AB again (-Q) [5,29,53,54]. The stored thermal energy is determined via Eq. (7), where n is the mol number of AB and ΔH

Table 2
Sensible heat storages.

Medium	T-range [°C]	c_p [kJ/kg K]	c_p [kJ/m^3 K]	density [kg/m^3]	λ [W/mK]	Reference
Liquid						
water	0–100	4.19	4175	998–1000	0.58–0.6	[24,48,49,54]
thermal oil	0–400	1.6–2.1	1360–1620	850–900	0.06–0.12	[29,53,56]
molten salt	150–565	1.3–1.5	1350–3900	500–2243	0.2–2	[29,50,53,56,59,60]
sodium	100–882	1.3	750–968	975–1203	64.9–71	[29,50,53,56,59]
solid						
sand, gravel, rock	0–800	0.83–0.96	1278–1420	1555–2560	0.48	[3,29,53,54,61,62]
granite	0–800	0.6–0.95	2062	2640–2750	2.6–3.1	[29,53,60]
concrete	0–500	0.75–1.13	1672–3005	1900–2700	0.9–2.0	[3,29,50,53,54,60]
brick	0–1000	0,84–1	1176–1596	1400–1900	1.5–1.8	[3,29,50,60,62]
iron	0–800	0.47–0.84	3348–6612	7200–7860	29.3–73	[29,50,60]
liquid-solid						
gravel-water filling	0–100	1.32	2904	2200	-	[29]

Table 3
Latent heat storages.

medium	melting-T [°C]	specific latent heat [kJ/kg]	reference
Inorganic			
salt hydrates	8–137	68–296	[29,53,55,65–73]
hydroxides	200–462	165–873	[29,53,65]
nitrates	190–560	172–370	[29,51,53,65,74]
carbonates	450–1330	142–509	[29,53,65,74]
sulfates	858–1460	84–212	[53,65]
fluorides	760–1418	391–1044	[29,51,53,65]
chlorides	192–870	75–452	[29,51,53,65,74]
metals	419–1084	113–397	[53,54,75,76]
alloys	340–946	92–757	[53,54,75,76]
salt eutectics	13–832	74–790	[53,65,70,77,78]
organic			
paraffins	5.5–120	148–269	[29,53,55,65,70,72, 79–81]
alcohols	93–220	110–344	[29,53,65,82]
fatty acids	16–74	141–227	[29,53,55,65,79,80, 83–91]
esters	11–63.2	100–215.8	[53,65,69,79,92–94]
glycols (PEG[2])	4.2–70	117.6–175.8	[29,53,65,70,95,96]
organic eutectics	21–52.3	143–182.7	[53,65]

[2] PEG is polyethylene glycol.

is the reaction enthalpy in kJ/mol [54].

$$AB \underset{-Q}{\overset{+Q}{\longleftrightarrow}} A + B \tag{6}$$

$$Q = n \cdot \Delta H \tag{7}$$

The expectable storage investment cost vary between 8 and 100 €/kWh, the power capacity varies between 0.01 and 1 MW, and the specific energy storage density varies between 150 and 500 kWh/m^3 [2, 8,57]. The specific storage power capacity is about 20–40 kW/kg [58]. Thermochemical storage has higher storage density, a longer storage duration, and less heat loss than sensible and latent storage systems and is, therefore, a promising alternative. Its ability to conserve stored energy at ambient temperatures without heat loss makes it an interesting seasonal storage option. However, its charging and discharging processes face technical challenges. Thermochemical storage remains an immature technology, and further research is needed for its commercial use [3,53].

According to Seitz et al. [2], thermochemical storage has a TRL of 3–4 (solid–gas reactions), while sorption technologies have a TRL of 5–7. The research and development foci on sorption and chemical reaction systems have been considerable. Several prototypes have been developed through national and European research projects, with a focus on specific use cases with the appropriate reactor systems. An efficient integration in real systems and an appropriate scaling still needs to be developed, and the risks must be minimized. A similar assessment was made by the storage initiative undertaken by Austria [58], which estimated thermochemical storage as having a TRL of 1–4. Friedl et al. [12] estimated adsorption and absorption storage as having a TRL of 1–4 and storage with gas–solid reactions as having a TRL of 3.

Thermochemical storage systems enable very high energy densities but are rarely used as the technology is still largely nascent [53]. Table 4 shows the temperature ranges and characteristics of thermochemical and sorption materials, organized according to their basic reaction (solid–gas, liquid–gas, gas–gas, and sorption).

3.2. Heat demand in industrial branches (layer 2)

Layer 2 conducts an analysis for Austria, where primary energy demand in 2018 was about 373 TWh, and final energy consumption was about 312 TWh. The transport sector was responsible for 35.8% of the total, the manufacturing sector was responsible for 29.1%, and the remainder was consumed by households, services, and agriculture [25]. The manufacturing sector is composed of 13 branches, four of which (iron and steel, paper and pulp, non-metallic mineral processing, and chemicals and petrochemicals) account for 61% of the final energy demand [25]. Statistics Austria [31] establishes heat-consuming useful energy categories in space heating and air conditioning, steam generation, and industrial furnaces. The remaining categories involve electrical process energy supply.

Table 4
Thermochemical and sorption based heat storages.

medium	T [°C]	p range [bar]	reaction enthalpy [kJ/mol]	reference
solid–gas reaction				
carbonates	320–1730	0.1–10	88–273	[97–104]
hydroxides	400–600	0.1–10	101.4	[97,102, 104,105]
metal hydrides	253–1400	0–60	74–186	[97,102, 106–112]
metal oxides	727–1030	0.11–1	32–200	[97,104, 113,114]
liquid–gas reaction				
ammonium hydrogen sulphate	417	1.48	336	[97,102, 104]
isopropanol/acetone/ hydrogen system	200	-	-	[104]
gas–gas reaction				
ammonia synthesis	400–700	100–300	66.9	[97,104, 115]
methane reforming	700–1500	3.5–150	247–250	[97,104, 116]
sulfur based storages	800–1500	1–5	197.9	[97,102, 104,116]
Sorption				
physical sorption	60–200	-	-	[117]
thermochemical sorption	50–1000	-	-	[104,117]
composite sorption	50–350	-	-	[117]

The heat-relevant shares of useful energy demand and conversion energy are considered in an in-depth analysis of energetic and exergetic heat demand in the industry branches. Since the use categories provide no explicit information about the temperature levels at which the heat is consumed, the heat quantities per temperature level are calculated for each branch using guideline values of characteristic temperature distributions drawn from the literature. Fig. 4 shows the temperature shares from space heating to temperatures above 1000 °C of the heat demand for various industries. The heat-demand calculation is based on the useful energy demand and energy statistics for 2018 provided by Statistics Austria [31,33]. The energetic heat demand per temperature level $HD_{en,b}$ is determined through Eq. (1), and the exergetic demand $HD_{ex,b}$ is determined through Eq. (2). The use categories of space heating and hot water are merged.

Fig. 5 shows the energetic and exergetic heat demand calculated for Austrian industry. The number of enterprises causing this heat consumption are also identified [32,34]. The estimated energetic industrial heat demand for Austria is about 88 GWh/a, and the exergetic demand is about 50 GWh/a. The greatest energetic share of 36% is used for temperatures above 1000 °C, followed by 21% for 100–500 °C, and 18% for 500–1000 °C. Space heating and hot water as well as heat <100 °C represent just 11% and 13%, respectively. The specific heat utilization varies across industries. For example, in the iron and steel, non-mineral processing, and non-ferrous metal industries, the largest share of heat demand is used for operating the industrial furnaces, whereas the largest share is used for steam generation in branches such as the paper and pulp industry, the chemicals and petrochemicals sector, and the food and beverage industry.

The most energy-intensive branches, such as the iron and steel and paper and pulp industries, are represented by only 32 and 23 companies,

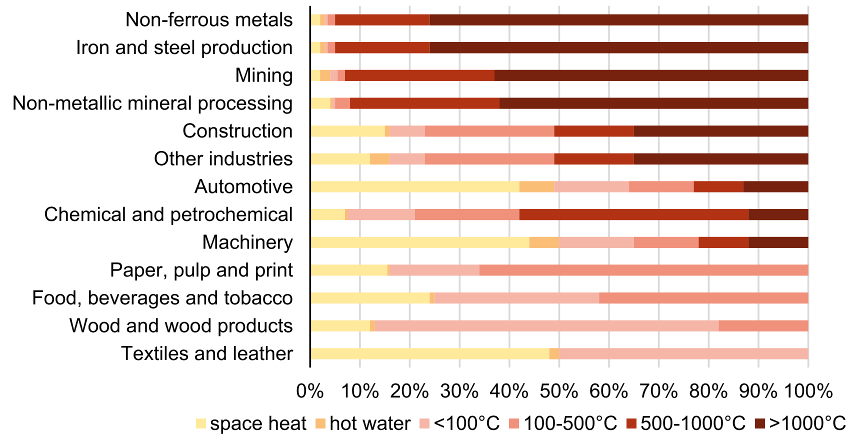

Fig. 4. Temperature shares of heat levels in various industries [23,36,37].

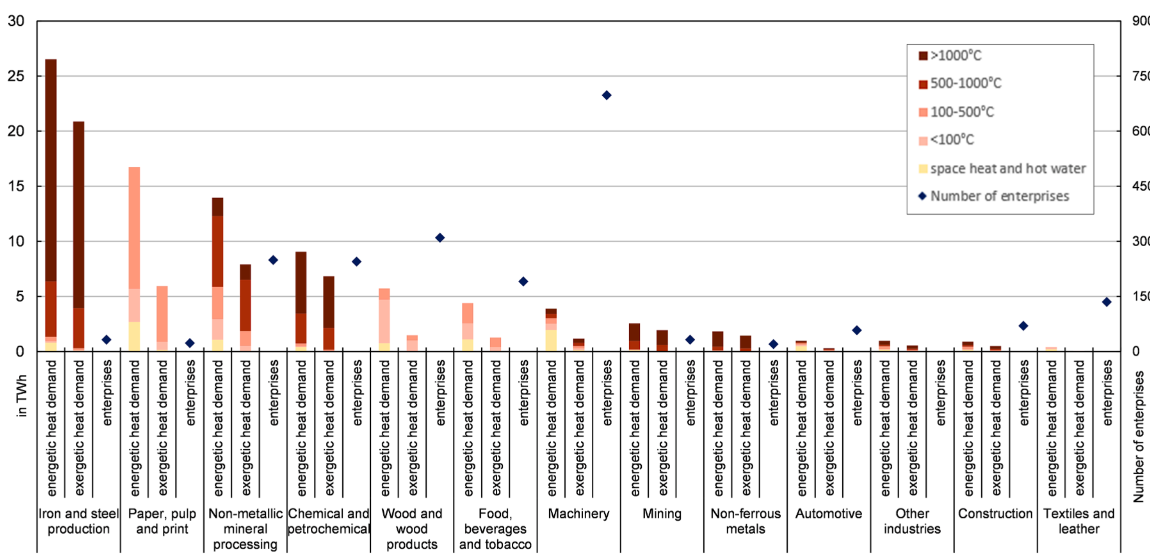

Fig. 5. Estimated heat potential and number of enterprises per industrial branch.

respectively. The chemical and petrochemical and non-metallic mineral processing sectors, which are also energy-intensive, have 249 and 245 companies, respectively. By contrast, the machinery industry—with a total heat demand of only about 4 GWh—consists of 698 companies.

The branches also differ in terms of the temperature levels at which heat is consumed. While the iron and steel industry consumes about 76% of its heat at temperatures higher than 1000 °C, the paper and pulp industry consumes about 42% of its heat at temperatures between 100 and 500 °C. In the non-metallic mineral processing industry, more than 90% of the heat is consumed at temperatures higher than 500 °C. Regarding the supply of space heat and hot water, the share ranges up to 50% of the heat demand in branches such as the food and beverage, mechanical engineering, and automotive industries. Comparing energetic heat demand between the iron and steel industry and other sectors in absolute values reveals the enormous heat consumption and size of this industry. The paper and pulp industry consumes about 63%, the chemical and petrochemical industry about 53%, the non-metallic mineral processing sector about 33%, and the wood and wood products industry about 22% of the heat consumed by the iron and steel industry.

The following findings are derived from the results shown in Fig. 5:

- Heat is required at the highest temperature levels (>1000 °C) in the iron and steel, chemical and petrochemical, non-metallic mineral processing, and non-ferrous industries due to their melting, firing, and sintering processes.
- Heat at temperatures between 500 and 1000 °C is in particularly high demand in the chemical and petrochemical, iron and steel production, non-metallic mineral processing, and non-ferrous industries. It is typically used for thermal refinery, steel hardening, and ceramic glazing and baking.
- Usage in the 100–500 °C range includes many processes that require a steam supply, especially in the paper and pulp and food and tobacco industries.
- Heat in the temperature range below 100 °C is mainly used in paper and pulp production as well as in cooking and thickening processes and drying processes. The food, paper, wood, and chemical industries are the main users.
- Space heat and hot water are in demand in all branches. However, demand is highest in industries that have large production areas such as halls and that have less waste heat potential from production processes, such as in the mechanical and automotive industries.

4. Results and discussion

This section describes the application potential of TES in various industrial branches as expressed in layer 3. Layer 4 conducts a case study in the non-metallic mineral processing industry, analyzing the economic and ecologic viability of TES storage integration. A sensitivity analysis also considers factors such as the gas and CO_2 emission allowance prices.

4.1. Application potential of TES in industrial branches (layer 3)

Fig. 6 presents an application matrix (matching the results of layers 1 and 2) along with the derived fields of TES use in Austria's industrial branches. The information used for Fig. 6 can be found in Section 3. Temperature ranges in °C, associated storage densities in kWh/m^3, power capacity in MW, TRL, and specific investment costs in €/kWh are vertically listed for the specific TES. The analysis of the industrial branches in terms of number of firms, energetic and exergetic heat demand in GWh/year according to different temperature levels (space heating + hot water, <100, 100–500, 500–1000, and >1000 °C) are provided horizontally. As described in Section 2.2 (layer 2), the variants in which a green symbol is matched with the largest heat demand indicate a significant application potential for the TES type considered. In these variants, the application of the storage technology corresponds well with the heat demand intensity for the respective temperature level of the branch. However, other combinations, such as a yellow symbol matched with a medium heat demand, also show a potential field of application; these should not be excluded but must be analyzed on a case-specific basis. The number of firms per branch is also essential. The more firms that are available, the more likely it will be to increase replication among firms within the branch. Thus, a new standard could be established rather than developing case-specific solutions.

Fig. 6 clearly shows the potential application fields of the respective storage technologies in various branches and for each temperature level. Sensible storage systems are mostly used in the lower temperature segments (<500 °C), especially for space heating and hot water, because of their mature technology and low investment costs. Their theoretical application potential reaches up to 1000 °C. Latent storage is suitable for all temperature levels. For temperatures up to 100 °C (including space heating and hot water), organic resources are applied. For temperatures above that, inorganic resources are suitable. The main application range for thermochemical storage is theoretically between 200 °C and 1700 °C. However, immature storage technologies (low TRLs) and the related high specific investment costs hamper their application. Nevertheless, thermochemical storage is characterized by high storage density. Sorption technologies are applicable for temperatures <100 °C.

A total of 2470 variants of the application matrix are evaluated in terms of potential TES application and energetic heat demand. The results show that there is only a 6% match between a TES priority field of application (green symbol) and the largest heat demand. Extending the evaluation by comparing a TES priority field of application with a medium heat demand produces only a further 10% match. Attempts to match potential fields of TES application and the largest and medium heat demand produce a 12% match. The TES priority fields should be favored for implementation more highly than the TES potential fields, which are technically feasible but require an ongoing TES integration assessment for specific applications.

4.2. TES integration: case study of a cement plant (layer 4)

The cement plant in Gmunden has a waste heat potential of 10 MW_{th} at 400 °C (as described in Section 2.4). An analysis is conducted to recover the waste heat and transport it to a dairy plant, which has a fluctuating operating mode. A consideration of TES integration is therefore an essential part of the case study. A solution for continuous supply to the dairy plant without a TES is also conceivable, and process interruptions could be overcome with alternatives such as a gas boiler system.

As shown in Fig. 3, at least one TES of each type (sensible, latent, thermochemical, and sorption) has the capability to store the cement plants' waste heat potential of 400 °C. However, we also observe from Fig. 6 that there is only a 16% match of a TES priority field of application

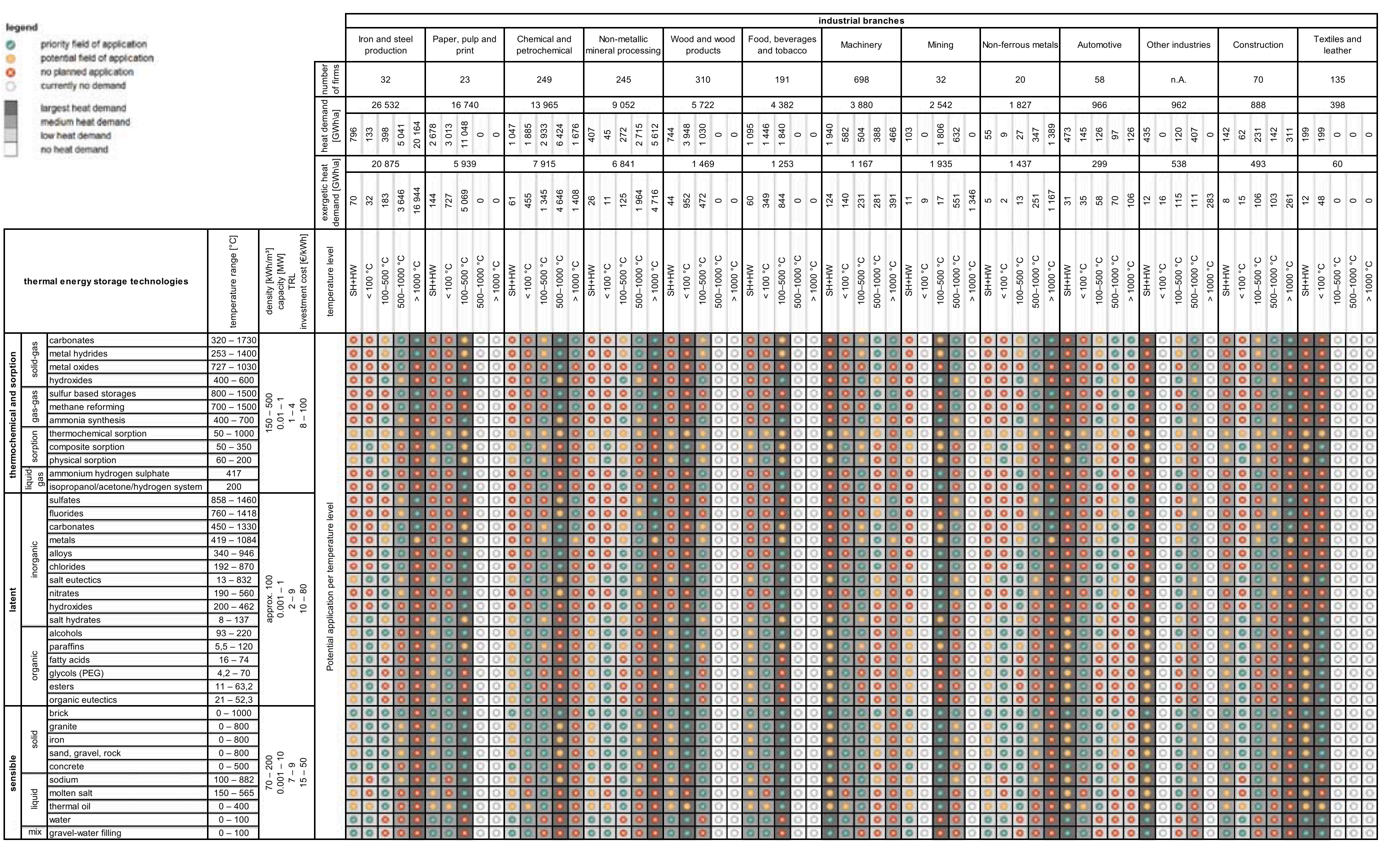

Fig. 6. Qualitative evaluation of fields of TES application in various industrial branches.

with the largest and medium heat demand. For sensible TES, only sodium and molten salt and solid materials fulfill the temperature requirement. For latent TES, organic materials are not applicable, but some of the inorganic materials are — such as chlorides, salt eutectics, nitrates, hydroxides, and alloys that meet the 400 °C storage prerequisite. Carbonates, metal hydrides, hydroxides, and thermochemical sorption fulfill the necessary precondition for thermochemical and sorption TES.

The TES has to be implemented at either the cement plant or the dairy plant. Thus, the TES has to fit within an existing infrastructure. Spatial aspects in terms of storage size and storage density therefore play an important role. Additionally, its performance during the discharging process is crucial for guaranteeing a continuous and stable energy supply to the dairy plant. Further relevant design criteria can be found in Section 3.1.1.

This section evaluates the impact of TES of different sizes in terms of economic and ecological factors; the environmental benefits resulting from reduced CO_2 emissions are not discussed.

4.2.1. Storage cycle analysis, energy, and CO_2 savings

The process interruptions at the cement plant at Gmunden [40] are analyzed over a period of 2 years. In an interruption, no waste heat can be recovered. The analysis makes the following assumptions: a) if there is more than one interruption per day, the duration of all the interruptions is cumulated and is counted as one long-lasting interruption; b) if a longer interruption occurs in a day, it is counted together with an interruption on the following day as one interruption; and c) it is assumed that there is sufficient time between the remaining interruptions to fully reload the storage. The study uses confidential data on interruptions. A fitting curve, expressed in Eq. (8), is derived using Matlab software from the original data. The exact number and duration of interruptions are veiled, but we can describe the achievable number of cycles *(y)* depending on the storage size *(x)* from this real-world example.

$$y(x) = -13\ln x + 0.01x + 84 \tag{8}$$

The fitting curve is sufficiently accurate in an interval from 1 to 500 MWh. The average dairy plant heat consumption is 8.5 MW. The 2-month winter shutdown is not included in this analysis. A cycle is defined as the amount of energy released, which corresponds to the storage capacity. A TES with lower capacity will convert more energy, so the income per investment (capacity) will be higher. A TES with a higher capacity will become more inexpensive per MWh capacity; however, each additional MWh capacity will be used less.

As shown in Fig. 7, the case study data show that the smaller the storage size, the higher the number of achievable cycles per year. However, the overall amount of energy saved increases along with storage size, though the number of cycles decreases. With a storage size of only 30 MWh, 40 cycles can be achieved, 1200 MWh/year can be saved, and 217 tons of CO_2/year can be avoided. Compared with a 300 MWh storage, wherein only about 13 cycles are feasible, 3900 MWh/year can be avoided in gas boiler energy savings, and 694 tons of CO_2/year can be saved.

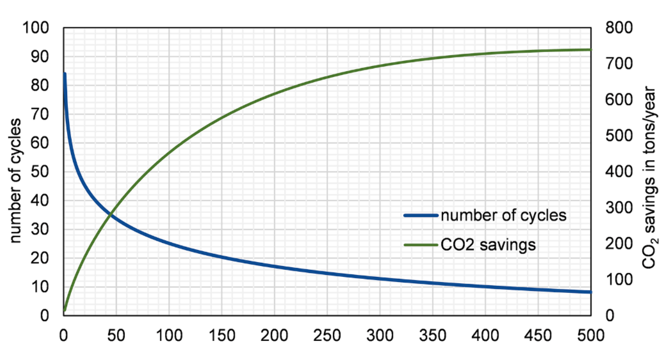

Fig. 7. Number of achievable cycles depending on the storage size for cement industry case study.

4.2.2. Economic assessment

Fig. 8 presents the maximum total investment cost for the project, including costs for functionalities such as the actual waste heat recovery at the cement plant, the heat transportation to the dairy plant, and the installation process required to use the heat provided there (a TES is not included in this curve). To be competitive, the sum of these costs must be compared with the costs of the energy otherwise consumed in the form of gas. For the TES to be economically viable, the total investment cost without considering a TES must not exceed €10.6 million.

Fig. 8 also presents the maximum storage costs. If no storage is included, the total investment cost is calculated as the costs of recovery, transportation, and use. In storage integration, fewer costs can be allocated to these other essential functionalities. The larger the storage capacity foreseen for overcoming longer interruptions without starting the gas boiler backup system, the more the maximum cost for the other functionalities decreases. The maximum specific storage investment cost is dependent on the storage size and varies between 1.4 and 14.4 €/kWh for 500 MWh and 1 MWh, respectively. Comparison of the specific maximum investment costs with the results shown in Fig. 6 indicates that economic viability can hardly be reached in the current circumstances. Even for sensible storage systems, where there are mature and proven storage solutions and economies of scale, investment costs start at 15 €/kWh and reach 50 €/kWh. Latent, thermochemical, and sorption TES tend to have lower investments costs, starting at 8 €/kWh. However, their TRL levels are quite low, and their costs can go up to 100 €/kWh.

This economic assessment is based on the condition that the gas boiler infrastructure and the gas boiler itself are already available and that only energy costs are to be considered. This condition is established because the gas boiler is needed as a backup system and a continuous supply must be guaranteed during the cement plant shutdown in the winter.

4.2.3. Sensitivity analysis

We conducted a sensitivity analysis to investigate how cost factors, such as gas and CO_2 prices, affect the maximum storage costs.

4.2.3.1. Gas price.

As shown in Fig. 9, there is sensitivity in the form of a direct dependency between the maximum storage costs and gas prices. In the +100% gas price scenario (when gas prices double and have a positive impact on the maximum economical investment), the maximum feasible storage costs would increase up to 2.8 and 28.8 €/kWh for 500 MWh and 1 MWh, respectively. The -75% case scenario for investment would involve a decrease in gas prices. Regarding sensitivity, therefore,

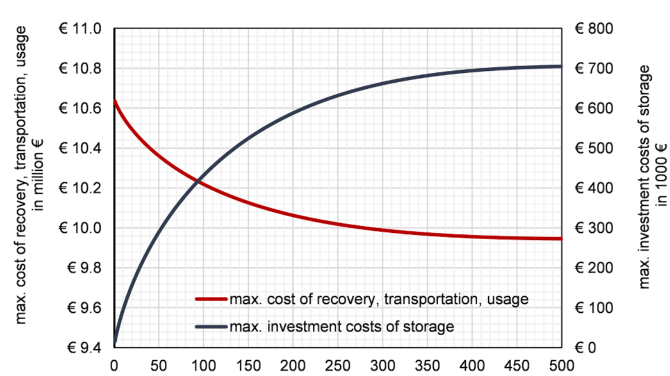

Fig. 8. Maximum investment costs of storage and overall system for cement industry case study.

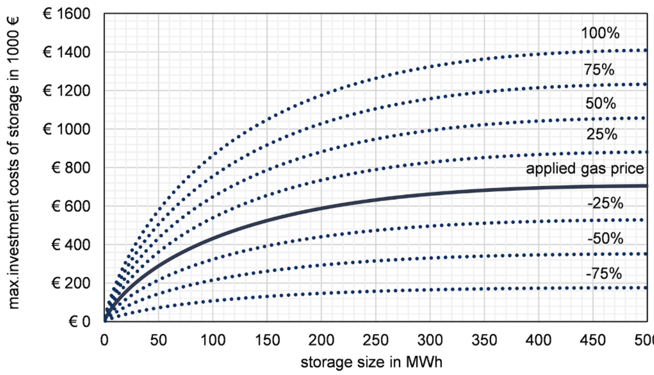

Fig. 9. Sensitivity analysis of gas price for cement industry case study.

gas prices and their expected variation within the amortization period represents a key factor in TES implementation.

4.2.3.2. CO_2 price. Fig. 10 shows the impact of gas and CO_2 emissions allowance prices on the maximum storage costs for a capacity of 300 MWh. The CO_2 price is included in the investment cost for different gas prices. An increase in the CO_2 price enhances economic viability. Independent of gas prices, an increase in the CO_2 price from 25 to 400 €/t would increase the maximum feasible storage costs up to 6.8 €/kWh. For the applied gas price case, the maximum feasible storage costs of 2.7 €/kWh would increase to 9.4 €/kWh. The gas price alternation leads to a variation of only +2.2 €/kWh and −1.7 €/kWh. However, an increase in CO_2 prices of this magnitude is unlikely. Nevertheless, this analysis shows the power of such an instrument to achieve primary energy saving.

5. Conclusion and outlook

Integrating a TES could enable industries to move toward a more sustainable energy system, as it can increase primary energy efficiency and reduce carbon emissions. TES systems (sensible, latent, thermochemical and sorption) are used to balance the differences between heat supply and demand. This implies that waste heat and volatile renewable energy sources can be more strongly valorized, and fluctuations in heat demand profiles (whether dependent on the day, season, or application) can be better compensated. A TES can serve multiple functions in diverse fields, such as for waste heat utilization, waste heat electricity generation, sector coupling, and system services. In waste heat utilization, the resulting process heat is temporarily stored for use in batch processes or to decouple the supply of electricity and heat in combined heat and power plants to achieve a demand-oriented heat supply (i.e., district heating). Waste heat can also be used to generate electricity via thermal process cycles. Sector coupling is another way to integrate heat storage; this allows excess energy to be moved from one sector (heat, electricity, gas) to another. A typical example is power-to-heat technology (the conversion of electricity into heat by, for example, electrode boilers), which occupies a special position in the control energy market for system services. This can help stabilize the power grid and generate additional revenue from the surplus energy. The aim is to create long-term load balancing, a flexible heat supply, and optimized waste heat utilization via the use of TES.

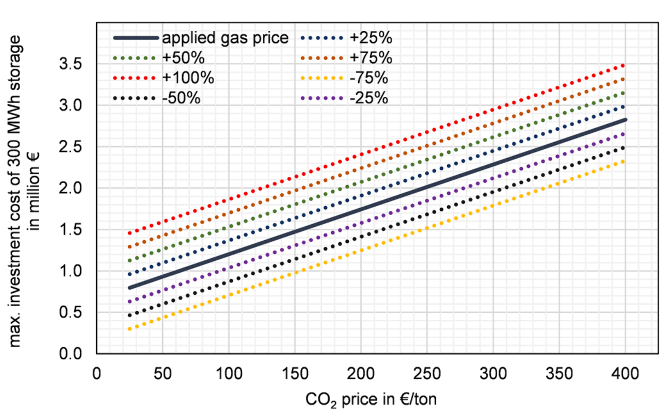

Fig. 10. Sensitivity analysis of CO_2 emission allowance price of a 300 MWh storage in the cement industry case study.

We conducted a qualitative evaluation of TES use in various industrial branches at different temperature levels (space heating and hot water, <100, 100–500, 500–1000 and >1000 °C) to describe the capability of TES and its characteristics and to facilitate the selection of potential TES projects. We considered the temperature level and application range, TRL, specific TES costs, storage density, and storage capacity as the key KPIs. Our analysis shows that a TES is theoretically available at all the evaluated temperature ranges and for all industrial branches. Sensible storage systems are the ones used most often, as they are already established and have a TRL of up to 9. Water is most commonly used due to its low cost, relatively high specific storage capacity, environmental compatibility, and high availability. Thermochemical storage is too costly and needs further development; it has great potential, however, due to its high storage density and compact size. Based on its characteristic properties, latent storage is positioned between sensible and thermochemical TES. Sensible storage is mostly used at lower temperature segments (<500 °C), but it can theoretically be used up to 1000 °C. Latent storage with an organic medium can cover temperatures up to 100 °C; anything above has to be completed with inorganic resources. Thermochemical storage is theoretically possible between 200 °C and 1700 °C. Appropriate storage selection requires a knowledge of the site-specific properties (e.g., existing temperature level, mass flow, required storage duration, available space, required storage capacity, number of charging and discharging cycles) and the specific requirements of the potential use. Suitable storage concepts can be developed according to the boundary conditions and requirements of the planned field of application.

Another criterion for TES integration is provided by the economic top–down approach used in this study. The approach is exemplarily applied in form of a case study by a TES integration at a cement plant. The results show that a TES integration in industrial branches is dependent on the fossil fuel prices related to existing energy supply prices. The saved energy and costs must compensate for the cost of TES system integration in order for TES to be economically viable. The amount of energy saved is dependent on the number of potential cycles: The higher the number, the more energy will be saved. Storage size is another important factor, from both the economic and functional points of view, as unforeseen process interruptions must be addressed without needing to start the backup system. Another factor is the potential increase in CO_2 prices on fossil fuels, which also makes a TES more competitive. Moreover, technological innovations and maturity will decrease the specific storage costs. The crucial cost factors for waste heat use are not only the TES costs but also the costs of recovering, transportation, and re-use. Beyond improvements to the primary energy efficiency of the overall system, changes in regulations and markets (e.g., an emission trading system) can also increase the economic feasibility of a TES. The environmental benefits of CO_2 emissions reduction are obvious, which increases the attractiveness of a TES. However, our economic analysis of TES integration at a cement plant shows that TES integration is not feasible under current conditions unless the appropriate measures and incentives are used.

In the future, companies should be encouraged to recognize that the heat potential of their operations can be used and to increase their primary energy efficiency. First, this requires identifying the primary energy saving measures in the form of a TES. The lack of knowhow regarding the use of heat potential is a major obstacle. This information gap could be closed by employing energy consultants who, together with the companies in tailor-made consulting programs, could identify heat potential and develop suitable storage concepts. Second, subsidies should be introduced for the efficient use of TES. High specific investment costs for TES systems and immature storage technologies are hampering their integration and increased use by companies. Third, TES demonstration projects for waste heat or surplus electricity should be created in the form of power-to-heat plants. Such research and development projects are necessary to test TES systems in practice and convince companies to make storage investments.

CRediT authorship contribution statement

Stefan Puschnigg: Conceptualization, Methodology, Data curtion, Formal analysis, Writing – original draft, Visualization. **Johannes Lindorfer:** Project administration, Supervision, Funding acquisition, Validation, Writing – review & editing. **Simon Moser:** Project administration, Funding acquisition, Methodology, Writing – review & editing. **Thomas Kienberger:** Validation, Writing – review & editing.

Declaration of Competing Interest

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

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fuels

Article

Use of Biomass as Alternative Fuel in Magnesia Sector

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Abstract: The European Union has started a progressive decarbonization pathway with the aim to become carbon neutral by 2050. Energy-intensive industries (EEIs) are expected to play an important role in this transition as they represent 24% of the final energy consumption. To stay competitive as EEI, a clear and consistent long-term strategy is required. In the magnesia sector, an essential portion of CO_2 emissions result from solid fossil fuels ($MgCO_3$, pet coke) during the production process. This study concerns the partial substitution of fossil fuels with biomass to reduce carbon emissions. An experimental campaign is conducted by implementing a new low-NO_x burner at the magnesia plant of Grecian Magnesite (GM). Life cycle assessment (LCA) is performed to quantify the carbon reduction potential of various biomass mixtures. The experimental analysis revealed that even with a 100% pet coke feed of the new NO_x burner, NO_x emissions are decreased by 41%, while the emissions of CO and SO_x increase slightly. By applying a biomass/pet coke mixture as fuel input, where 50% of the required energy input results from biomass, a further 21% of NO_x emission reduction is achieved. In this case, SO_x and CO emissions are additionally reduced by 50% and 13%, respectively. LCA results confirmed the sustainable impact of applying biomass. Carbon emissions could be significantly decreased by 32.5% for CCM products to 1.51 ton of CO_2eq and by 38.2% for DBM products to 1.64 ton of CO_2eq per ton of MgO in a best case scenario. Since the calcination of $MgCO_3$ releases an essential and unavoidable amount of CO_2 naturally bound in the mineral, biomass usage as a fuel is a promising way to become sustainable and resilient against future increased CO_2 prices.

Keywords: co-firing; NO_x emissions; low NO_x burner; CCM; DBM; LCA; CO_2 emissions; biomass; fuel analysis

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1. Introduction

In the last decades, there has been an alarming increase in energy consumption worldwide. Within only the 20 years from 1995 to 2015 the increase exceeded 50%, from 8588.9 million tons oil equivalent (Mtoe) in 1995 to 13,147.3 Mtoe [1] in 2015. Energy-intensive industries (EIIs) are one of the top energy consumers with a global share of 24%. Of this, up to 80% is met with fossil fuels and their associated energy systems. Current energy systems rely in general on burning fossil fuels, which are not renewable; they are distributed worldwide and are critically unsustainable to deliver [2]. Most of the CO_2 emissions that cause global warming derive from solid fuel combustion [3]. In 2016, 32.3 Gtn of CO_2 emissions resulted from solid fuel combustion. The industrial sector is responsible for 19% of these emissions [4,5]. A study from the International Energy Agency (IEA) [6] showed that fossil fuels that can cause environmental issues when combusted, such as air pollution and climate change, still play a major role in energy sources globally. CO_2 emissions increased from 20.9 Gtn in 1990 to 28.8 Gtn in 2007 and are expected to rise to 40.2 Gtn in 2030, with an average yearly increase rate of 1.5% over the projection period [5].

It is believed that replacing fossil fuels with biomass fractions in the fuel feed for combustion will lower the overall unwanted major emissions from power facilities as biomass fuels present lower amounts of some elements, such as sulfur. The European Union (EU) has started a progressive decarbonization with the aim to become carbon neutral by 2050. EIIs are expected to play an important role in this transition. Biomass will continue to have an important role in the EU energy mix as it is important among renewable sources, covering approximately 5% of the primary energy supply of the EU-27 [4]. Emissions of complete combustion in biomass applications include CO_2, NO_x, N_2O, SO_x, HCl, and heavy metals, while emissions of incomplete combustion include CO and unwanted organic compounds, among others; particle emissions can be the result of both complete and incomplete combustion [7]. Combustion of most biomass materials is known to result in lower emissions of SO_x, and NO_x, as biomass sulfur and nitrogen contents are low compared to fossil fuels; alkali-based compounds also have a retention effect on sulfur, resulting in an additional incremental reduction [8]. On the other hand, co-firing of different biomass fuels and fossil fuel usually does not lead to reduced sulfur emissions because inherently existing potassium chloride has a higher reactivity with aluminum silicates than sulfur compounds [9]. In most biomass materials, a significant amount of submicron fumes and vapor material can be formed in the flame that can pose a challenge to particulate emissions abatement equipment. This may lead to lower collection efficiencies and increased particulate emissions from the stack, which is likely a highly site-specific occurrence of interest in retrofit projects.

A very interesting study by Monika Zajemska et al. [10] presents the emissions of gaseous pollutants from the co-firing of sunflower husk pellets according to metrological processes but also through a simulation program. The calculated concentration of sulfur dioxide in the flue gas was higher by about 200 ppm from measured concentration (355 ppm) and reached a value of 588 ppm. Higher levels were also observed for nitric oxide although not as large as in the case of SO_2; namely, the calculated concentration reached a value of 192 ppm, and the measured concentration was equal to 162 ppm.

It is noted that there is renewed interest in many industrial countries in biomass combustion as a result of environmental and climate change concerns and because of energy security supplies in a world where fossil fuels are concentrated in a few countries and resources are finite. In addition, biomass combustion leads to reduction of net carbon dioxide (CO_2) and to better waste management, mainly due to the CO_2 neutrality and large availability of biomass [11]. Biomass combustion or co-combustion with fossil fuels can significantly reduce CO_2 emissions from energy production. It is asserted that although biomass has the advantage of CO_2 neutrality, or nearly so, there are potential problems concerning the environment, such as NO_x and CO emissions, noted as the most considerable gaseous pollutants during biomass combustion [12,13].

The several economic and environmental advantages of biomass combustion are offset by its major disadvantage, which is its low energy potential, especially compared to fossil fuels [14]. It is therefore quite difficult to meet the large amounts of energy required, mainly in industry, by biomass combustion. This is the main reason why biomass/fossil fuel co-firing technology has been developed and largely implemented worldwide. The co-firing of biomass with fossil fuels is a flexible and easily applicable treatment. No specialized burners are required as the biomass can be burned in all types of kilns without creating technical problems, while, depending on the energy requirements, the percentage of fossil fuels that the biomass replaces may vary. The technology of co-firing has been tested in various sectors for several years, but a great growth has been presented in the field of electricity generation, where it is now an extremely efficient process. At the beginning of the second decade of the 21st century, more than 220 power plants were put into operation with biomass co-firing technology. The majority of these power plants are located in Europe and mainly in the Nordic countries, where in Finland alone there are more than 70 units and in Sweden 15 units [15].

In the United Kingdom, co-firing was not commercially productive until 2002. Producing 286 GWh in 2002, co-firing only accounted for 2.57% of the renewable electricity generation. However, co-firing rates nearly doubled every year until 2005. Producing 2533 GW h in 2005, co-firing accounted for 14.95% of the renewable electricity generation in the UK. Co-firing production remained level in 2006, but in the following years (2007–2009) co-firing production decreased steadily to 1625 GWh. However, in 2010 and 2011, co-firing production increased to a high of 2964 GWh. [16] Another example is the city of Aarhus in Denmark, where there are two stations with a production of 150 and 350 MWe [17]. The main fuel used is pulverized coal, and straw replaces 20%. At the same time, in the Netherlands, a wider effort has been made to develop the technology as several units operate in different cities with a capacity of 400 to 600 MWe [13,14]. The substitution rate varies; however, it moves at low levels between 4% and 8%. An important element is the type of biomass used; in addition to solid biomass, pellets, husk, and wood biomass are used. Finally, Poland is a country where biomass co-firing has been greatly developed [13,14]. There are three large plants, of which two have a capacity of 1800 MWe and a third has a capacity of 590 MWe. The replacement rate is 10%, and they mainly use sawdust, chips, and coffee shells.

Outside of Europe, there is a great growth in North America as well, with the most characteristic example being the city of Ontario in Canada, where there are seven power plants with a capacity of 150 to 500 MWe, where different types of biomass are used, mainly wood pellets, agricultural residues, and grain screening [18].

As already mentioned, various types of biomass have been tested in co-firing applications. Forest and agricultural residues, wood biomass, solid and waste biomass, and wood pellets are the most common types of biomass used in co-firing applications. In addition, husk, grains, plant biomass, wood chips, and olive kernels are combustible biomass materials that are tested and can be more efficient if they first undergo upgrade processes such as torrefaction [19]. It should be noted that there are other biomass materials such as hazelnut shells [20], fruit pellets [21], lignocellulosic plants, and algae biomass that are most effective when used in gasification processes [22,23].The main criteria for selecting a type of biomass is its price and its availability. For example, the Nordic countries use forest biomass as large areas of forest cover their spatial boundaries, while in many industrial areas, waste biomass is used as there are large amounts of industrial waste. Low availability and high costs are the main reasons that sunflower husk pellets are not widely used. However, they have been tested in the laboratory mainly to test their effectiveness and possible problems that their use as a fuel can create [24–26].

It is well known that cement industries are using waste-based biomass (RDF, used tires, sludge, etc.) as alternative fuels in rotary kilns, mostly for clinker production. In Heidelberg cement, the waste-based biomass used, which accounted for around 42% of the alternative fuel mix in 2021, makes a special contribution as it is considered climate-neutral under European legislation [27]. Additionally, LafargeHolcim [28], through a circular approach, wants to reduce the carbon intensity of its cement by substituting fossil fuels with pretreated non-recyclable and biomass waste fuels to operate its cement kilns. Currently they aim to increase thermal substitution of biomass from 20.9% to 37% by 2030.

Of course, co-firing conditions found in the cement or lime industry cannot be compared to the conditions realized in GM and in magnesia sector in general due to the type of fuels (usually in the cement industry are preferred low cost fuels such as RDF, sludge, and others) and level of temperatures (lower temperatures are anticipated in comparison with GMs in cases where a range from 1100 to 1900 °C or higher is expected).

The emissions from life cycle assessment (LCA) for the production of MgO vary depending on the production route and fuel. Depending on the characteristics of the production process, total emissions can vary up to $+/-1.17$ tons of CO_2 per ton of MgO. The company RHI-AG in Austria produces MgO based on $MgCO_3$ with a rotary kiln and natural gas with emission of 1.34 CO_2 per ton of MgO. In comparison, the production using a shaft kiln and hard coal as fuel leads to emissions up to 2.51 tons of CO_2 per ton of MgO [29]. A comparison focusing only on the applied process fuel (e.g., pet coke, natural gas, and others) shows that fuel emissions can vary between 0.4 and 1.3 tons of CO_2 per ton of MgO [30]. This means that the greatest prospects, as well as requirements in terms of reducing emissions, are in the types of fuels used to produce the required energy.

In this paper, an experimental campaign is presented with the main characteristic being the co-firing of a sunflower husk pellets/pet coke mixture in the new low-NO_x burner of the Yerakini Mine site calcination plant of Grecian Magnesite (GM) [31]. An LCA is performed to assess the GHG reduction potential of various biomass feedstocks and mixtures with pet coke. Co-firing of fossil and biomass fuel is expected to lower greenhouse gas (GHG) emissions in the magnesia sector, hence playing a major role in sustainable MgO production. This research, both experimentally and theoretically, builds the foundation of future co-firing developments and improvements in the magnesia sector. The novelty of the paper lies in the fact that for the first time, the application of a fossil fuel/biomass co-firing process (with 50% energy substitution), in combination with the operation of an LNB burner, is being tested on a practical level in magnesia sector in order to reduce emissions and associated costs in a production process that has special requirements, such as large quantities of energy, extremely high temperatures (up to 1900 °C or higher), and specific strict properties for its final products (CCM, DBM).

2. Materials and Methods

2.1. Description of GMs Facilities and Use of Biomass

GM is a private company established in 1959 as a mining and industrial company that produces and trades CCM (caustic calcined magnesia), DBM (dead-burned magnesia), carbonate magnesium ($MgCO_3$ –raw magnesite), and basic monolithic refractories. GM is listed as one of the top magnesia producers and exporters worldwide. Especially for CCM, the company is a leading producer in terms of volume and applications. The produced MgO (magnesia) is well known for its bright white color (whiteness) resulting from the low percentage in iron and its low levels of heavy metals and trace elements. In addition, the magnesia product is low in lime and has a microcrystalline structure. The ore is mined via open pit method. It is then transformed into the final product through the following four stages:

i. Pre-beneficiation, where different types of impurities are sorted out from the ore;
ii. Main-beneficiation, where the material enters the main beneficiation stage, in which it either passes through camera sorting or a combination of dense media and magnetic separation stages depending on the desired chemistry of the kiln-feed magnesite;
iii. Calcination and sintering in which the magnesite is fired in the kiln to produce CCM or DBM. During calcination, $MgCO_3$ is decomposes to MgO. In sintering, the decomposed material is fired up to 2000 °C;
iv. Final processing, where the product is crushed and classified in different sizes.

Figure 1 gives an overview of the calcination plant in Yerakini, while in Figure 2, GM's production flowsheet is presented.

There are three (3) rotary kilns (RK) with a calcination capacity of 550 tpd and one shaft kiln (Figure 1). Kiln-feed magnesite is fired in the kilns to produce either caustic calcined magnesia (CCM, at about 900 °C) or dead-burned magnesia (DBM, at about 1900 °C), using mostly pet coke as fuel. During calcination, magnesite ($MgCO_3$) is decomposed to magnesia by release of carbon dioxide according to the following reaction.

$$MgCO_3 \underset{HEAT}{\rightarrow} MgO + CO_2$$

Figure 1. GMs calcination plant.

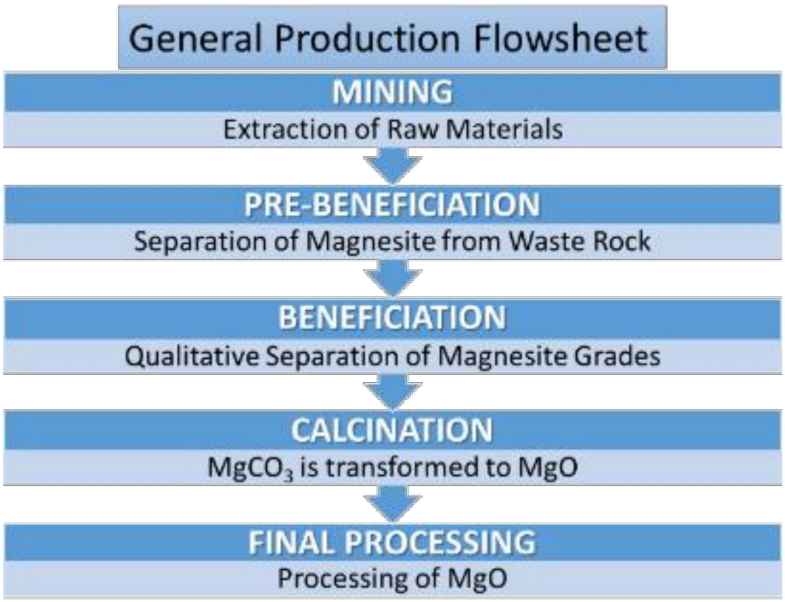


Figure 2. GM's general production flowsheet.

In the GM production process, petroleum coke (pet coke), heavy oil, and biomass are used as fuel. The firing process of magnesite into CCM/DBM produces large amounts of CO_2 and nitrogen oxides (NO_x) deriving from fuel combustion. There are two types of CO_2 emissions that are produced during this process: CO_2 produced from $MgCO_3$ decomposition, which is inevitable, and CO_2 emissions produced from fuel combustion. NO_x emissions produced during DBM production, where a 2000 °C temperature is needed, are also inevitable. In order to reduce the CO_2 emissions produced from fuel combustion, GM is substituted for a percentage of pet-coke energy with pulverized biomass (Figure 3) in the form of sunflower husk pellets, olive cake, or sawdust, according to their seasonal availability and prices. In the BAMBOO project [32], a novel and versatile low NO_x burner (LNB) was implemented by GM in order to reduce the respective emissions for temperatures up to 1600 °C but also to be able to reproduce high enough temperatures for the production of DBM. The required versatility is related to the fact that the new burner (~20 MWth) must have the ability to combust mixtures of pulverized biomass and pet coke and that it must have adjustable swirl to operate as an LNB for temperatures up to 1600 °C and in normal operation mode for DBM production (above 1600 °C). To optimize the combustion conditions of the raw material (raw magnesite), a small amount of wood chips (about 2–4% of pet coke) is also fired along with raw magnesite.

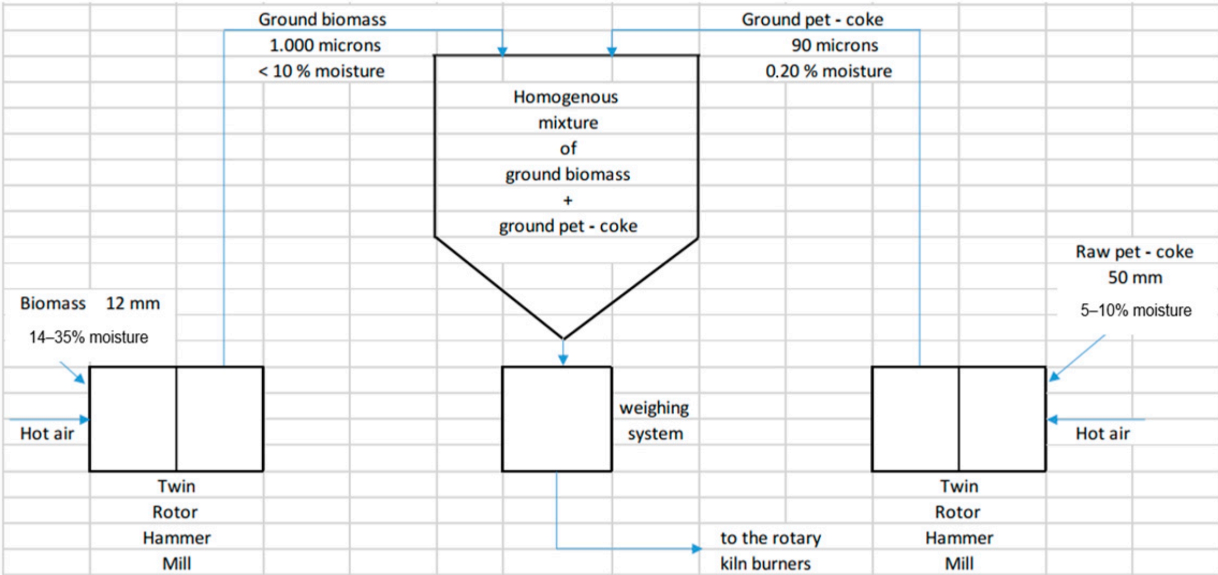


Figure 3. Biomass at GM: Co-firing mode.

The potential of use wood chips as a feedstock in parallel with the magnesite gives the advantage of in situ and simultaneously De-NO_x and De-SO_x procedure. Feeding of wood chips along with raw magnesite (Figure 4) can reduce NO_x emissions due to NO_2 reaction with the carbon (C) from wood chips and production of CO_2 and N_2 ($2C+2NO_2 \rightarrow 2CO_2+N_2\uparrow$). The overall benefits of the wood chip feedstock are expected to be: (a) NO_x (mainly NO_2) reduction, (b) SO_x reduction, and (c) preparation of the material.

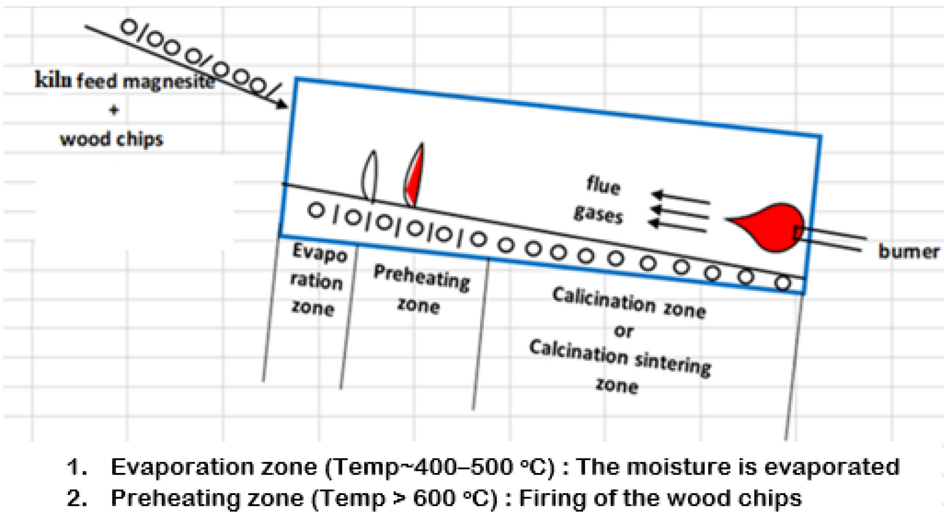


Figure 4. Biomass at GM: Co-feeding with raw magnesite.

2.2. Experimental Campaign in GM

After the installation of the new LNB in Rotary Kiln No.3 and the successful initial operation trials with 100% pet coke as fuel, GM conducted preliminary biomass/pet coke co-feeding trials with its initial preparation and feeding system (April–June 2021). Results were promising, but due to feeding system limitations, the trials faced problems caused by feeding instabilities. GM went on to design and construct a new system able to handle the new fuel mixture and conducted a successful experimental campaign in February of 2022.

Figure 5 describes the new fuel mix preparation and feed process designed and constructed by GM for the purposes of this trial. Biomass and pet coke are fed from the fuel temporary storage square adjacent to the calcination department facilities to two separate twin rotor hammer mills, and after size comminution, they are transported pneumatically to the solid fuel silo. From there they are conveyed by a screw feeder to a smaller buffer silo which assures further homogenization of the mixture and enables control of the mass feed rate of the mix to the new burner.

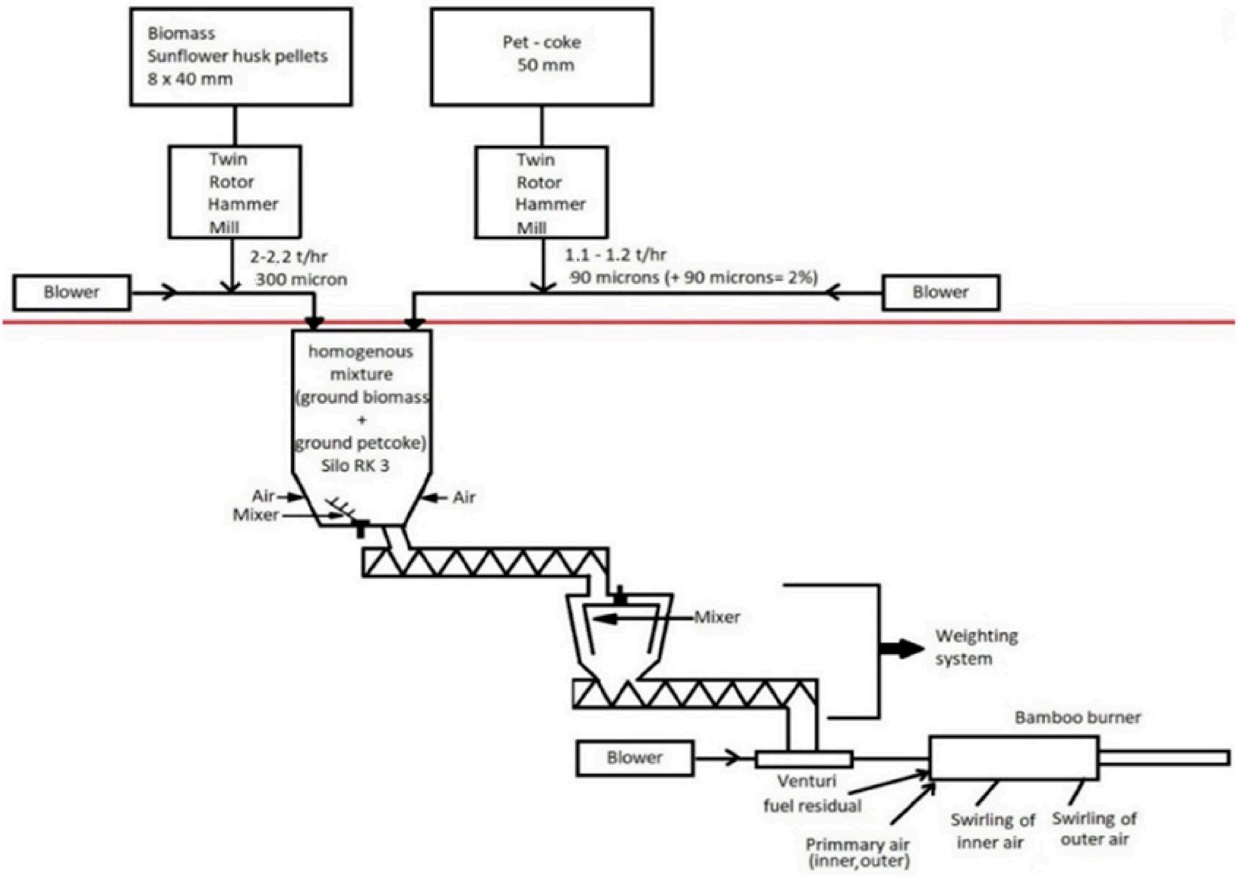


Figure 5. The new fuel mix preparation and feed system for Rotary Kiln No. 3. The part under the red line refers to the new installation.

GM conducted initially a 4-day trial (100% pet coke) to validate the NO_x reduction accomplished with the installation of the new burner that earlier shorter trials had indicated. Pet coke feed rate was 2000 kg/h with production of the base-case DBM product. Burner swirl was adjusted to the maximum levels for both inlet and outlet air.

After the 100% pet coke trial, without changing the kiln's product and productivity, GM conducted a 5-day trial (co-firing with biomass) using a biomass/pet coke fuel mixture. The biomass used was sunflower husk pellet comprising 2/3 of the mixture by weight, or around 50% of the energy requirement. Burner swirls were kept at the maximum levels as before.

2.3. Description of Metering Equipment Used in Campaign

A dedicated control set-up, with the use of SCADA system, controls the operation of the feeding unit. Set point is a given mass flow rate (kg/h), which is achieved by adjusting screw speed. What is actually measured is the buffer silo weight with respect to time. A series of kiln parameters are controlled and monitored, the most important of which are the raw magnesite feed rate, rotation speed (as % of maximum), and temperature profile.

Flue gas composition is monitored by a SICK's MCS100FT FTIR analyzer system (located in the stack of desulfurization unit) coupled with a flame ionization detector, a zirconium dioxide sensor, and backward light scattering systems able to monitor SO_2, NO_2, CO, HCl, HF, H_2O and TOC, O_2, and dust.

Spot measurements at various points for SO_2, NO_2, CO, and O_2 are made with a portable, heavy-duty Varioplus Industrial by MRU, suitable for industrial applications by means of infrared technology (combination of NDIR technology with electrochemical sensors).

2.4. Description of Laboratory Equipment Used for Fuel Analysis

Several tests were conducted on pet coke and sunflower husk fuels and wood chips, including proximate analysis, ultimate analysis, determination of major and minor elements, bulk density and determination of ash melting temperature and calorific value.

Total moisture was measured using a furnace type Heraeus Thermo Scientific T-12 (temperature temporal deviation of ± 5 °C). The measurement of moisture, ash, and volatiles was carried out in a Thermo Gravimetric Analysis (TGA ELTRA Thermostep, temperature control precision of 2% or ± 2 °C).

The calorific values of the fuels were determined using a Parr 6400CL Calorimeter (relative standard deviation below or equal to 0.10%). The elemental analysis (CHN) was conducted using a Perkin Elmer Series II instrument (accuracy below 0.3%).

The concentration of major elements and selected heavy metals was determined by means of Flame and Graphite Furnace Atomic Absorption Spectrometry (AAS, Shimatzu AA-6300, relative standard deviation below 0.5%) after the complete digestion of samples with an acid mixture of $HNO_3/H_2O/HF$ in a microwave oven (Berghof SW-2).

Ash fusion temperatures were measured in an oxidizing environment in a SYLAB IF2000G analyzer (precision better than ± 20 °C on specific points). Fusion of ash is characterized by the physical state of the ash, which occurs during the heating process under well-defined conditions in the furnace. During ash fusion, the following temperatures were monitored:

1. Shrinkage temperature (ST): the temperature at which shrinking of the test piece occurs. This temperature is defined as when the area of the test piece falls below 95% of the original test piece area.
2. Deformation temperature (DT): the temperature at which the first signs of rounding of the edge of the test piece occurs due to melting.
3. Hemisphere temperature (HT): the temperature at which the test piece forms approximately a hemisphere, i.e., when the height becomes equal to half of the base diameter.
4. Flow temperature (FT): the temperature at which the ash is spread out over the supporting tile in a layer, the height of which is held of the height of the test piece at the hemisphere temperature.

During the laboratory analyses, the measurement processes and standards were strictly followed. Table 1 records the processes as well as the standards that were followed in the laboratory facilities both during the analysis of the fuel (pet coke) and during the analysis of the different types of biomass. More information on the measuring instruments is presented in Appendix A.

2.5. Description of LCA Methodology and Developed LCA Model

The environmental impacts are examined using the LCA software GaBi 10.6 ts by Sphera, following the ISO 14040 standards for LCA. This framework consists of four steps: definition of goal and scope, life cycle inventory (LCI), life cycle impact assessment (LCIA), and, finally, improvement and interpretation [33]. As the LCA methodology is already extensively described in the literature [34–36], only the relevant definitions to conduct the LCA are described.

Table 1. Laboratory tests and standards.

Laboratory Tests and Standards for Fuel Analysis		Laboratory Tests and Standards for Biomass Analysis	
Testing	**Standard**	**Testing**	**Standard**
Collection and preparation of samples	ASTM D346/D346M-11	Collection and preparation of samples	ISO 14780
Test method for total moisture	ASTM D 3302, ASTM D 7582	Test method for total moisture	ISO 18134-1
Moisture/ash volatiles	ASTM D 7582, ASTM D 3174	Moisture/ash volatiles	ISO 18134-3, ISO 18122, ISO 18123
Elemental analysis (CHN)	ASTM D 5373	Elemental analysis (CHN)	ISO 16948
Sulfur analysis	ASTM D 3177	Sulfur and chlorine analysis	ISO 16994, ASTM D 516
Chlorine analysis	ASTM D 4208	Gross calorific value	ISO/DIS 18125
Gross calorific value	ASTM D 5865	Ash fusibility	CEN/TS 15370-1
Ash fusibility	ASTM D 1857-03	Mechanical durability	ISO 17831-1
		Bulk density	ISO 17828
		Major elements	ISO 16967
		Minor elements	ISO 16968

2.5.1. Definition of Goal and Scope

The goal is to analyze the environmental impacts resulting from the use of biomass as alternative fuel compared to a business-as-usual (BAU) case. As elaborated previously [37], the definition of a functional unit is crucial to guarantee comparability of alternatives. In this study, the functional unit is the production of 1 ton of MgO, either CCM or DBM. A cradle-to-gate system boundary for the MgO production plant is chosen according to the LCA framework. This means that the transport of the resources (pet coke, $MgCO_3$, biomass resources, etc.) and the production of MgO is considered within the analysis, but the utilization and transport of MgO is not part of the analysis.

The reference system is defined as the BAU system. The BAU case uses fossil pet coke for the kiln and calcination stage as fuel for thermal process energy provision and an electricity consumption mix for Greece as electricity supply. As the thermal energy demand is different for CCM and DBM, the LCA is conducted for CCM and DBM separately concerning the representative input data but is analogously related to applied methods.

2.5.2. Life Cycle Inventory and data collection

The life cycle inventory (LCI) phase focuses on data collection and quantifies the inputs and outputs of the production system. The mass and energy balance data for MgO production are collected based on [33] (Tables 2 and 3), and data gaps are filled using valid literature data. For the evaluation of the environmental impacts of the $MgCO_3$ mining process, representative literature values for open mining are applied [38]. As the transportation of the $MgCO_3$ to the MgO production plant is not considered in the literature, this is included separately.

Table 2. Main LCI parameters of MgO production plant [33].

Parameter	CCM	DBM	Unit
inputs			
$MgCO_3$	147	104	kt/a
electricity demand	288	288	MJ/t_{MgO}
thermal energy kiln zone	2.04	2.04	GJ/t_{MgO}
thermal energy calcination zone	8.1	11.6	GJ/t_{MgO}
substitution of thermal energy in kiln zone with biomass	0–10	0–10	%
substitution of thermal energy in calcination zone with biomass	0–70	0–70	%
outputs			
MgO	62	43.8	kt/a

Table 3. Transportation routes and LHV of MgO production plant inputs [33].

Resource	Ship [km]	Ship Payload [t]	Truck [km]	Truck Payload [t]	Truck [km]	Truck Payload [t]	LHVGJ/t
magnesium carbonate ($MgCO_3$)	-	-	2	40.6	2.3	22	-
pet coke	370	3000	20	22	-	-	31.4
sunflower husk pellets (SHP)	1750	3000	20	22	-	-	16.56
wood saw dust (WSD)	-	-	180	22	-	-	11.33
olive kernels (OK)	-	-	20	22	-	-	17.64
wood chips (WC)	-	-	280	24.7	-	-	9.68
pruning (PRU)	-	-	280	24.7	-	-	15.00

In contrast, the background processes, such as electricity generation or material production, were taken from acknowledged LCA databases, such as GaBi ts 10.6 Professional Database and ecoinvent v.3.8 database.

The electricity used for the production process of MgO is consumed from the public grid of Greece. In addition, a future renewable energy (RES) mix for Greece is composed using Greek data from GaBi LCA software. The production of 1 MJ electricity consists equally of hydro power, wind, and photovoltaic power in this RES mix.

The applied biomass resources can be mostly considered as agricultural residues and thus no ecological footprint is allocated. This is in line with the renewable energy directive (RED) of the European Parliament and Council [39]. However, energy and emissions resulting from the collection, clustering, chipping, and pelletizing of biomass have to be considered. The respective data reported by the Joint Research Center (JRC) of the European Commission is applied [40].

The calcination of $MgCO_3$ releases an essential amount of CO_2 naturally bound in the mineral complexes. The production of 1 ton of MgO from pure $MgCO_3$ generates 1.09 tons of CO_2 (assuming a stoichiometric reaction), which is considered within the LCA. In addition, the combustion of 1 ton of carbon (C) generates 3.66 tons of CO_2 (assuming again a stoichiometric reaction). Within the LCA model, 1 ton of pet coke is considered with a carbon content of 88% and is taken into account for emissions from fuel combustion.

2.5.3. Life Cycle Impact Assessment

LCI compilation follows by setting up the MgO production process as an LCA model in GaBits 10.6 software and conducting the LCIA, applying CML 2001 methodology. In general, the LCA analyzes the environmental impacts of the MgO production in several categories. The most discussed and crucial one in this study is the global warming potential (GWP). The GWP indicator is calculated in kg CO_2-equivalents for the impact category climate change.

2.5.4. Scenario Development for CCM and DBM MgO LCA Analysis

Scenarios support identifying the impacts of various parameters. Table 4 gives an overview of the defined scenarios for the LCA analysis valid for CCM and DBM. The scenarios differ into following issues:

- The electricity supply is changed for a best case scenario from the Greek electricity consumption mix to a renewable energy sources (RES) mix for Greece.
- At the kiln process stage, biomass resources substitute pet coke as fuel based on their LHV for thermal process energy supply. Applied biomass resources are wood chips (WC) and pruning (PRU).
- At the calcination process stage, biomass resources substitute pet coke as fuel. Applied biomass resources are sunflower husk pellets (SHP), wood saw dust (WSD), and olive kernels (OK).

Table 4. Scenario description for CCM and DBM MgO LCA analysis.

Abbreviation	Scenario	Description
BAU	business as usual	fossil fuel supplied process, thermal energy from pet coke and electricity from GR electricity mix
ELE	only electricity	100% use of renewable electricity sources, thermal energy from pet coke
KILN	only kiln	10% WC biomass share at kiln, GR electricity mix
CAL SHP	only calcination SHP	70% SHP biomass share at calcination, GR electricity mix
CAL WSD	only calcination WSD	70% WSD biomass share at calcination, GR electricity mix
CAL OK	only calcination OK	70% OK biomass share at calcination, GR electricity mix
MB SHP	moderate biomass SHP	biomass share: at kiln WC 5%, at calcination SHP 30%; GR electricity mix
MB WSD	moderate biomass WSD	biomass share: at kiln WC 5%, at calcination WSD 30%; GR electricity mix
MB OK	moderate biomass OK	biomass share: at kiln WC 5%, at calcination OK 30%; GR electricity mix
BCB SHP	best case biomass SHP	biomass share: at kiln WC 10%, at calcination SHP 70%; RES electricity mix
BCB WSD	best case biomass WSD	biomass share: at kiln WC 10%, at calcination WSD 70%; RES electricity mix
BCB OK	best case biomass OK	biomass share: at kiln WC 10%, at calcination OK 70%; RES electricity mix

3. Results and Discussion

3.1. 100% Pet Coke

The installation and operation of a new LNB had as its main purpose the reduction of NO_x emissions. During the experimental process where the fuel composition consists of 100% pet coke, NO_x emissions were measured over a period of 120 h and values ranged between 500 and 1600 mg/Nm^3. Figure 6 presents the fluctuation of NO_2 values throughout a 102 h period.

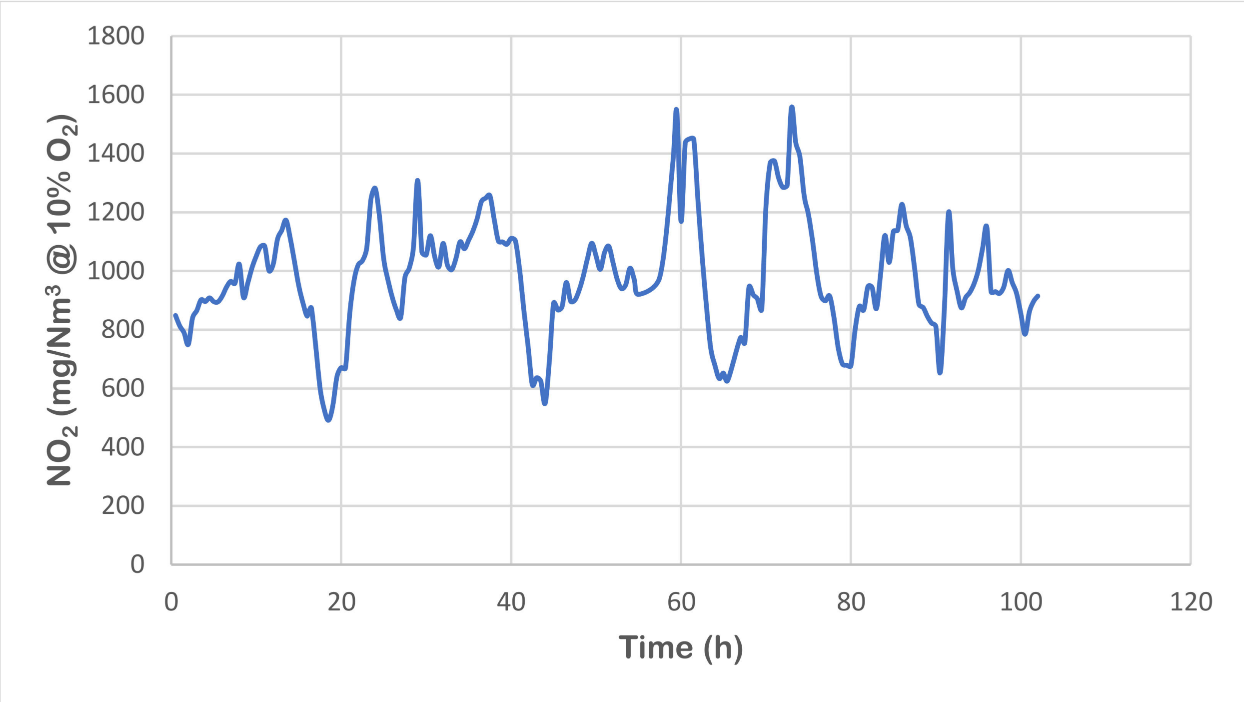


Figure 6. NO_2 pollutant concentration in flue gases during 100% pet-coke trial. NO_x trial average is 980 mg/Nm^3 at 10% O_2.

Table 5 summarizes the key pollutant levels and provides comparison with the old-conventional burner. It is observed that NO_x emissions are reduced by more than 40%, as has already been suggested. CO emissions increased during these trials, but such values are not associated with the new burner but with the operational conditions. It should be noted that the CO average values were high during the trials due to CO trips associated with inadequate fuel/air ratio control.

Table 5. Old vs. new burner.

Averages	New Burner	Old Burner
Data range (days)	4.3	65
NO_2 (mg/Nm^3)	980 (−41%)	1670
CO (mg/Nm^3)	2000	1180
SO_2, pre FGD * (mg/Nm^3)	4780	4560
Exit temperature (°C)	450	450–500

* FGD: Flue gas desulfurization.

3.2. Biomass and Pet-Coke Fuel Mixture

Table 6 summarizes the average key pollutant levels and provides comparison with the 100% pet coke case and the April–June 2021 initial trial that was conducted before replacing the fuel feeding system.

Figure 7 gives the SO_2 and NO_2 variation during the biomass/pet coke fuel mixture trial. Comparison of the biomass utilization with the 100% pet coke utilization demonstrates significant merits: reduction of SO_2 concentration by 47% and a further NO_2 reduction of 21%.

Table 6. Fuel mix main trail compared with 100% pet-coke.

Case	Bulk Density of Product	Raw Kiln Feed	Pet Coke	Sunflower Husk Pellet	Residual Fuel	Wood Chips	Biomass Energy Contribution	Swirl Out	Swirl In	Sintering Temperature	SO_2 Pre FGD	NO_2	CO
	g/cm³	tph	kg/h	kg/h	kg/h	kg/h	%			◦ C	mg/Nm³	mg/Nm³	mg/Nm³
100% Pet coke	3.07–3.18	14	2000	0	0	0	0	0.9	0.9	1580	4780	980	2000
SHP/Pet coke	3.16–3.20	13.7	1090	2210	0	0	50	0.9	0.9	~1600	2530	770	1740
Initial April–June Trials	3.18–3.31	4–12.6	0–900	1170–1600	300–400	400	40–76	0.9	0.9	1630–1850	322–1600	115–872	590–1700

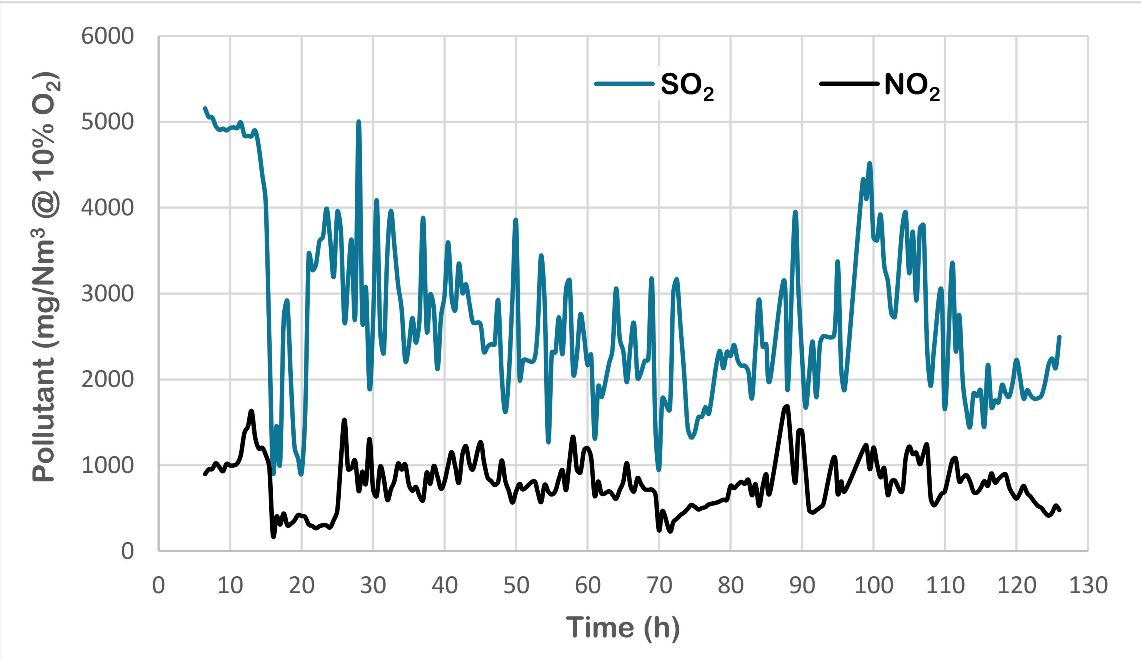


Figure 7. SO_2 and NO_2 concentration of the flue gases at kiln exit during the 5-day trial (February 2022).

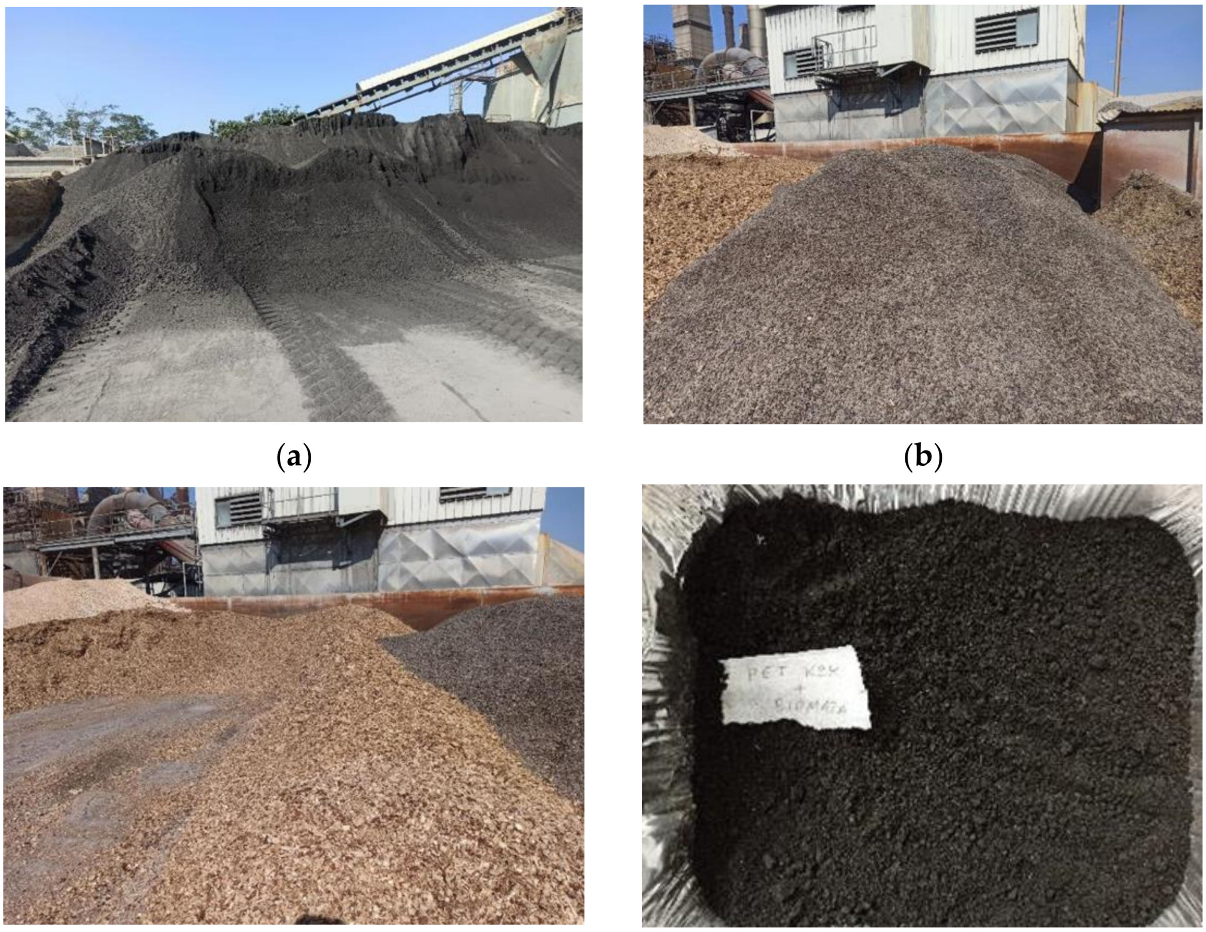
This reduction comes on top of the reduction achieved by the LNB (in total 61%). Note that the significant SO_2 reduction reduces the load of the desulfurization unit and the associated processing costs, while the further NO_2 reduction enables operation without $deNO_x$ requirements (max allowable NO_x emissions <1500 mg/Nm³, Table 7). The CO emissions are reduced but are still high, as reported for 100% pet coke. The issue can be remedied with typical CO trip prevention measures and poses no risk to the application of the proposed solution.

Table 7. Emission limit values according to BAT-AEL [41] for magnesia industry.

Polluting Substance	Emission Limit (mg/Nm^3)
Dust	<20–35
NO_x stated as NO_2	<500–1500
CO	<50–1000
SO_x expressed as SO_2	<50–400 mg/Nm^3 (<1500 mg/Nm^3 in absence of wet scrubber)

3.3. Fuel Analysis Results

As already mentioned, GM uses pet coke as fuel while adding small amounts of wood chips to some processes. The type of biomass chosen to substitute part of the fossil fuel is the sunflower husk pellets. The following figure shows the fuel storage silos (8a for petcoke, 8b for sunflower husk pellets and 8c for mixed fuel) and a sample of the mixture of pet coke and biomass (Figure 8d) that is used as the final fuel in the current co-firing trials.



(**a**) (**b**) (**c**) (**d**)

Figure 8. Pictures of fuels used during experimental campaign (**a**) pet coke, (**b**) sunflower husk pellets, (**c**) wood chips, and (**d**) sample of mixed fuel (sunflower husk pellets and pet coke).

3.3.1. Pet Coke Analysis

Thorough analysis of pet coke proved that it is a fuel with high-energy content and low percentages of moisture, ash, and volatile matter. Its composition contains a large percentage of carbon (C), while the percentages of nitrogen (N) and sulfur (S) content are relatively high. Table 8 summarizes the results of the laboratory pet coke analysis. Methods and standards that were followed for the correct and effective laboratory analysis have been previously presented in Table 1.

Regarding pet coke used in the experimental process, its humidity was measured at 0.37%, ash at 0.5%, and volatiles at 13.77%. Carbon (C) was measured at 83.57%, and hydrogen (H) at 5.05%. The Higher Heating Value (HHV) was 8479.5 cal/g (35.48 MJ/kg) as received. Pet coke is a type of fuel with properties that can vary depending on the raw materials and the production process.

Table 8. Pet coke analysis.

Type	Value
Proximate Analysis	
Moisture (%w.b.)	0.37
Ash (%d.b.)	0.5
V.M. (%d.b.)	13.77
Ultimate analysis and Cl	
C (%d.b.)	83.57
H (%d.b.)	5.05
N (%d.b.)	1.52
S (%d.b.)	3.12
Cl (ppm d.b.)	<400
Energy Content	
HHV (cal/g d.b.)	8603.4
HHV (cal/g a.r.)	8479.5
LHV (cal/g d.b.)	8345.9
LHV (cal/g a.r.)	8217.4
Ash Melting Behavior	
ST (°C)	1127
DT (°C)	1169
HT (°C)	1178
FT (°C)	1187

However, in order to estimate the values' fluctuation for important properties, some recently published studies, where thermogravimetric analysis was conducted, were accessed. The analyzed studies refer to different scientific fields and have different backgrounds so that the results could be considered more objective. The following Table 9 lists the studies used and presents the respective properties of the fuels used in each case.

Table 9. Studies from literature review on the properties of pet coke.

C (%)	H (%)	O (%)	S (%)	N (%)	VM (%)	Ash Content (%)	Moisture (%)	HHV (kj/kg)	Reference
84.7	3.5	1.3	5	1.9	11.8	2.7	0.9	33.2	[42]
86	3.74	1.4	3.98	1.62	10.6	0.58	1.58	34.81	[43]
81.57	3.49	4.01	10.25	0.68		6.24	0.73	35.25	[44]
91.63	3.46		2.78	1.68	7.99	2.03	0.71		[45]
82.51	6.02	0.49	5.65	1.71	10.8	2.99		35.72	[46]
90	3	1.2	2.75	1.45	8.8	0.75	1.15		[47]
88.97	3.61	2.85	3.43	1.14	9.8	0.8	0.67	35.72	[48]
82.21	3.11	7.02	5.5	1.9	13	0.26			[49]

According to the above references, the moisture content of pet coke ranges between 0.67% and 1.58%, while that of ash ranges between 0.26% and 6.24%, and the volatile matter ranges between 7.99% and 13%. Regarding the chemical composition of the fuel, the literature states that carbon (C) has values between 81.57% and 91.63%, and hydrogen (H) has values between 3% and 6.02%. Finally, the Higher Heating Value (HHV) ranges between 33.2 and 35.72 MJ/kg.

3.3.2. Sunflower Husk Pellets Analysis

For sunflower husk pellets, a very detailed analysis was performed where energy content was evaluated, the percentages of moisture, ash, and volatile matter were identified, and the content of carbon, nitrogen, sulfur, and other minor and major elements were determined. Finally, the ash melting behavior was examined. Table 10 represents the results of the laboratory analysis.

Table 10. Sunflower husk pellet analysis.

Type	Value	Type	Value
Proximate Analysis		**Major and Minor Elements Analysis**	
Moisture (%w.b.)	5.5	Al (ppm d.b.)	222.92
Ash (%d.b.)	3.5	Ca (ppm d.b.)	4701.3
V.M. (%d.b.)	75.4	Fe (ppm d.b.)	231.44
Ultimate analysis and Cl		K (ppm d.b.)	7905.75
C (%d.b.)	50.58	Mg (ppm d.b.)	2811.59
H (%d.b.)	6.74	Na (ppm d.b.)	97.3
N (%d.b.)	0.54	Si (ppm d.b.)	720
S (%d.b.)	0.12	Cd (ppm d.b.)	0
Cl (%d.b.)	0.12	Co (ppm d.b.)	7.16
Energy Content		Cr (ppm d.b.)	3.03
HHV (cal/g d.b.)	4770.8	Cu (ppm d.b.)	14.4
HHV (cal/g a.r.)	4421.8	Ni (ppm d.b.)	4.28
LHV (cal/g d.b.)	4329.5	Pb (ppm d.b.)	1
LHV (cal/g a.r.)	3958.8	Zn (ppm d.b.)	17.17
Ash Melting Behavior			
ST (°C)		707	
DT (°C)		928	
HT (°C)		>1550	
FT (°C)		>1550	

Sunflower husk pellets, used to substitute a part of the fuel, had a moisture content of 5.5%, an ash content of 3.5%, and volatile matter of 75.4%. According to the international literature [50], the humidity of sunflower husk pellets corresponds to about 8.5%, the ash content is close to 2.8%, and the volatile matter is estimated at about 80%. Regarding the chemical composition of sunflower husk pellets, it was measured that carbon (C) rises to 50.58% and hydrogen (H) to 6.74%. Similar values are found in the literature [31], where carbon (C) is estimated at 50.90% and hydrogen (H) at 5.60%. The Higher Heating Value (HHV) was measured in the laboratory at 4421.8 cal/gr (18.50 MJ/kg) as received and 4770.8 cal/gr (19.96 MJ/kg) on a dry basis. The corresponding values, according to the literature [31], are 18.14 MJ/kg and 19.85 MJ/kg.

3.3.3. Wood Chip Analysis

A corresponding thorough analysis with the one that was performed for sunflower husk pellets was also carried out for the wood chips. Table 11 represents the results of the laboratory analysis.

The woodchips, used to contribute to the process of decomposition, had a moisture content of 3.7%, an ash content of 1.5%, and volatile matter equal to 79.3%. According to the international literature [51], the humidity of woodchips corresponds to about 3%, the ash content is close to 0.9%, and the volatile matter is estimated at about 83%. Regarding the chemical composition of woodchips, it was measured that carbon (C) rises to 51.13% and hydrogen (H) to 5.86%. Similar values are found in the literature [32], where carbon (C) is estimated at 49.60% and hydrogen (H) at 6%. The Higher Heating Value (HHV) was measured in the laboratory at 4690.1 cal/gr (19.62 MJ/kg) as received and 2733.4 cal/gr (11.44 MJ/kg) on a dry basis. The corresponding value, according to the literature [32], is 19.04 MJ/kg a.r.

3.3.4. Mixed Fuel Analysis

The homogenized fuel mixture (pet coke and SHP) used at the second period of the experimental process in the co-firing process, quantitatively, consists of 32.26% pet coke and 67.74% biomass per weight. Biomass, as has been clarified before, consists exclusively of sunflower husk pellets. It should also be noted that despite the fact that the ratio of masses of pet coke and biomass is 1 to 2, in terms of energy contribution the ratio is 1 to 1. The following Table 12 presents the results of the laboratory analysis for mixed fuel.

Table 11. Wood chip analysis.

Type	Value	Type	Value
Proximate Analysis		**Major and Minor Elements Analysis**	
Moisture (%w.b.)	3.7	Al (ppm d.b.)	274.27
Ash (%d.b.)	1.5	Ca (ppm d.b.)	5465.96
V.M. (%d.b.)	79.3	Fe (ppm d.b.)	198.85
Ultimate analysis and Cl		K (ppm d.b.)	7905.75
C (%d.b.)	51.13	Mg (ppm d.b.)	1226.28
H (%d.b.)	5.86	Na (ppm d.b.)	87.68
N (%d.b.)	0.26	Si (ppm d.b.)	793.53
S (%d.b.)	0.05	Cd (ppm d.b.)	0.11
Cl (%d.b.)	0.08	Co (ppm d.b.)	7.16
Energy Content		Cr (ppm d.b.)	3.03
HHV (cal/g d.b.)	4690.1	Cu (ppm d.b.)	2.62
HHV (cal/g a.r.)	2733.4	Ni (ppm d.b.)	1.63
LHV (cal/g d.b.)	4385.2	Pb (ppm d.b.)	0.24
LHV (cal/g a.r.)	2312.2	Zn (ppm d.b.)	26.01
Ash Melting Behavior			
ST (°C)	1078.0		
DT (°C)	1357.0		
HT (°C)	1497.0		
FT (°C)	1514.0		

Table 12. Mixed fuel analysis.

Type	Value
Proximate Analysis	
Moisture (%w.b.)	4.2
Ash (%d.b.)	5.1
V.M. (%d.b.)	38.6
Ultimate analysis and Cl	
C (%d.b.)	70.66
H (%d.b.)	4.61
N (%d.b.)	1.48
S (%d.b.)	2.11
Cl (ppm d.b.)	0.04
Energy Content	
HHV (cal/g d.b.)	6701.2
HHV (cal/g a.r.)	6419.1
LHV (cal/g d.b.)	6464.2
LHV (cal/g a.r.)	6167.5
Ash Melting Behavior	
ST (°C)	810
DT (°C)	1266
HT (°C)	1340
FT (°C)	1361

The mixed fuel (sunflower husk pellets and pet coke) was analyzed for its main properties. Humidity was measured at 4.2%, ash at 5.1%, and volatiles at 38.6%. Carbon

(C) was estimated at 70.66% and hydrogen (H) at 4.61%. The Higher Heating Value (HHV) reached 6419.1 cal/g as received.

The substitution of part of the fuel with sunflower husk pellets, although it did not affect the regular and efficient operation of the production process, greatly affected the characteristics of the final fuel fed into the LNB. Obviously, its calorific value decreased because of the reduction of the percentage of carbon content (C) from 83.57% to 70.66%. In addition, humidity, ash percentage, and volatile matter increased without creating any problems. Finally, the percentage of sulfur (S) and chlorine (Cl) content is significantly reduced, while to the lowest extent, the percentage of nitrogen (N) is also reduced, which is also reflected in the reduction of the corresponding NO_x and SO_x emissions.

3.3.5. Ash Index Calculation

The behavior of ash and its tendency to form deposits during combustion is estimated using empirical indicators. Empirical indicators, despite the limitations in their application due to the complex process of combustion chamber simulation, are very widespread and are the most common way, along with testing in pilot units, in taking decisions regarding the potential of fuel utilization. The slagging index Rs takes into account the ash melting temperatures (measured according to CEN/TS 15370-1 or ASTM D 1857-03) and indicates the ash behavior within the boilers during combustion. This index is calculated as a weighted average of hemisphere (*HT*) and deformation temperature (*DT*) through the following formula proposed by Gray and Moore [52]:

$$Rs = \frac{4 \times DT + HT}{5}$$

The above index directly correlates the slagging tendency of (mostly lignitic type) ash with experimental measurements, for example, the characteristic temperatures measured during the ash fusibility analysis. The above ash fusibility index was proposed in order to take the temperature range into account. This index is considered as one of the most promising indices for biomass, with a close correspondence to the real ash melting behavior of fuels [53–56]. The higher the Rs index, the less the tendency to form deposits that are difficult to remove. Typically, the limit values for this index are as follows:

Rs > 1340 °C, → low trend for deposit formulation
1250 °C < Rs <1340 °C → medium trend for deposit formulation
1150 °C < Rs <1250 °C → high trend for deposit formulation
Rs < 1150 °C → very high trend for deposit formulation

The results of the ash index calculation for sunflower husk pellets, wood chips, and the mixture of sunflower husk pellets and pet coke are presented in Table 13.

Table 13. Ash melting temperatures and deposit formulation trends.

Sample	Ash Melting Temperatures (°C)				
	Shrinkage (ST)	Deformation (DT)	Hemisphere (HT)	Flow (FT)	Rs Index
Pet coke	1127	1169	1178	1187	1170.8 (high trend)
Sunflower husk pellets	707	928	>1550	>1550	>1052.4 (very high trend)
Wood chips	1078	1357	1497	1514	1385 (low trend)
Mixture of SHP and pet coke	810	1266	1340	1361	1280.8 (medium trend)

According to the measured ash melting temperatures and calculation of the Rs index, the mixture of sunflower husk pellets with pet coke, used during the experimental campaign of GM, presents a medium trend for deposit formulation, a fact that needs to be considered carefully by the company in combination with the assessment of actual deposit formulation after a long time of kiln operation.

3.4. Life Cycle Assessment Results

This section provides the ecological results and life cycle impacts quantified for the production of 1 ton of MgO for CCM as well as for DBM. First, the BAU case is evaluated. Second, the developed scenarios by implementing diverse biomass resources and integrating renewable power sources are calculated and presented. Finally, the relative savings compared to the BAU case are outlined.

3.4.1. Environmental Assessment for CCM Production

The GWP for the BAU CCM case amounts to 2.24 tons of CO_2eq per ton MgO (Figure 9). The most influencing factors are the decomposition of $MgCO_3$ and the carbon released by the combustion of pet coke. The GWP induced by the electricity consumption plays only a minor role. In comparison, the GWP of the best case scenario (BCB OK scenario) amounts only to 1.51 tons of CO_2eq. It becomes obvious that the GWP resulting from the $MgCO_3$ decompositions stays the same and cannot be avoided based on technical measures except carbon capture, whereas the GWP of the kiln, and especially of the calcination zone, decreases enormously by using carbon-neutral biomass instead of carbon-rich pet coke. The low GWP resulting from the use of biomass results from the clustering, collection, chipping, pelletizing, and transportation steps. The higher the substitution rate in the kiln and calcination zone, the more it becomes relevant, but, overall, it still plays a minor role compared to the other more essential factors. For the kiln zone, the GWP from biomass is hardly noticeable in the figure based on its low contribution.

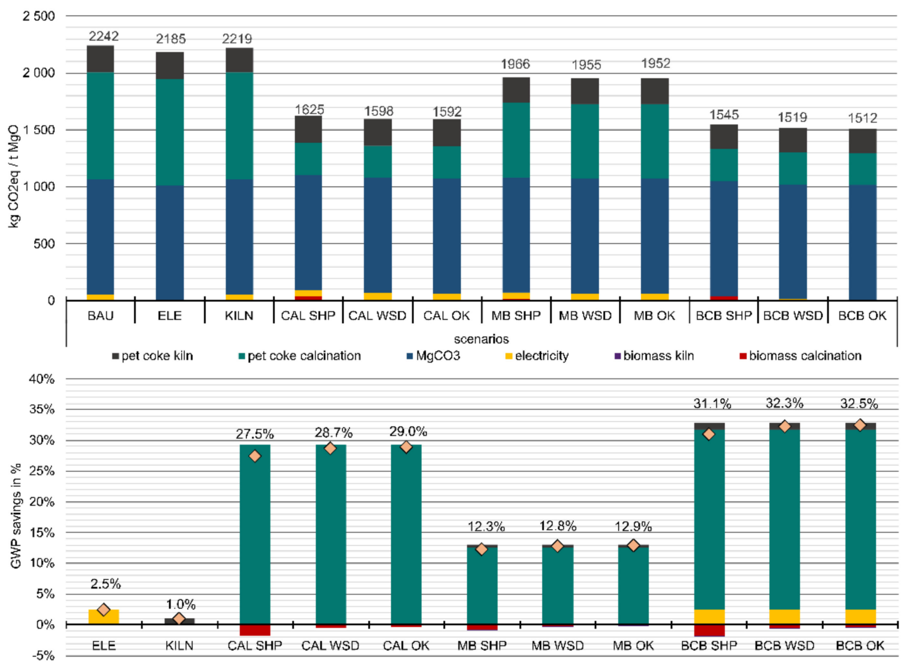


Figure 9. GWP of 1 ton of CCM MgO (**upper** figure) and relative GWP savings against business-as-usual scenario (**lower** figure) based on scenario description of Table 4.

The GWP savings in the different scenarios, compared to the BAU case, are a result of using biomass in the kiln and calcination zone or/and integrating renewable electricity sources to cover electricity demand. The integration of RES electricity only leads to GWP savings of 2.5%. However, the integration of biomass resources, in a best case scenario (BCB

OK), can lead to savings up to 32.5%. The negative values, thus meaning that there is an increase in emissions, results from the fact that in the BAU case no biomass is considered.

Due to the fact that the $MgCO_3$ decomposition and pet coke combustion release a high share on CO_2 emissions in all scenarios, the implementation of carbon capture storage (CCS) and carbon capture utilization (CCU) technologies can be a further solution to reduce the ecological footprint of MgO production [57]. Whereas the emissions from pet coke combustion can be reduced by substituting it with biomass, the decomposition of $MgCO_3$ is still and will remain responsible for around 1 ton of CO_2 per ton of MgO production. However, the implementation of CCS or CCU technologies is not considered within the LCA of CCM.

3.4.2. Environmental Assessment for DBM Production

The GWP for the BAU DBM case amounts to 2.65 tons of CO_2eq per ton MgO (Figure 10). The most influencing factors are again the decomposition of $MgCO_3$ and the carbon released by the combustion of pet coke. The GWP induced by the electricity consumption plays again only a minor role. In comparison, the GWP of the best scenario (BCB OK scenario) amounts only to 1.64 tons of CO_2eq. It becomes again obvious that the GWP resulting from the $MgCO_3$ decompositions stays the same, whereas the GWP of the kiln, and especially of the calcination zone, decreases enormously by using carbon-neutral biomass instead of carbon-rich pet coke.

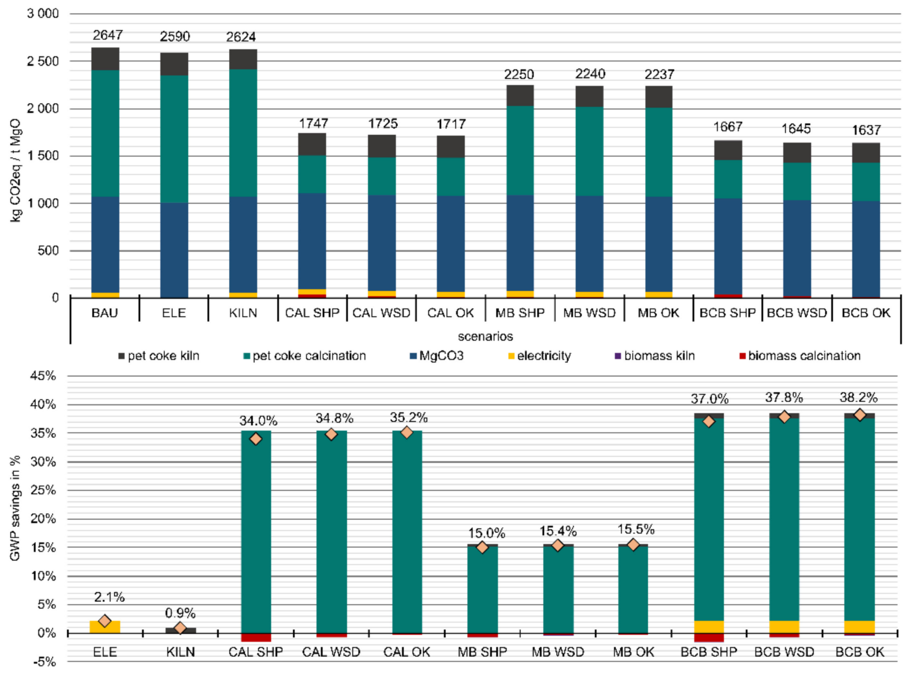


Figure 10. GWP of 1 ton of DBM MgO (**upper** figure) and relative GWP savings against business-as-usual scenario (**lower** figure) based on scenario description of Table 4.

The comparison with the BAU case shows again that the electricity mix leads only to 2.1% savings in GWP emissions. An additional substitution of pet coke with biomass in the kiln and calcination can lead in a best case scenario (BCB OK) up to 38.2%. This is substantial considering the fact that a high proportion of non-reducible emissions results from the mineral-bound CO_2. Analogously for CCM, the integration of CCS and CCU is not considered within the LCA of DBM.

3.4.3. Cost Analysis

Estimating production cost is a difficult process as it involves many variables, such as the prices of raw materials, CO_2 tariffs, and other factors. Considering all this and choosing to use the current prices (Pet-coke = EUR 294/ton, CO_2 tariff = EUR 82.37/ton and SHP = EUR 190/ton), a brief economic analysis was made regarding the practical application of the pet coke and biomass co-firing technology at the GM demo site. The production cost for the operation of the unit with the exclusive use of fossil fuels amounts up to EUR 12 million. The substitution of 50% with SHP reduces this cost down to EUR 11 million. In conclusion, the substitution of 50% of pet coke with SHP reduces the production cost by 9.75%.

In addition, based on evaluated local biomass sources such as wood chips (approximately EUR 86/t; 9.7 GJ/t), sunflower husk pellets (approximately EUR 190/t; 16.6 GJ/t), olive kernels (approximately EUR 57/t; 17.6 GJ/t), and wood saw dust (approximately EUR 86/t; 11.3 GJ/t), production cost could be lowered with biomass substitution of pet coke fuel (approximately EUR 294/t; 34.4 GJ/t) already at current CO_2 price. The higher the substitution at low fuel costs, the higher the profit for both emissions and cost reduction. A scenario based evaluation provided evidence for encouraged biomass fuel use in the production process to become sustainable and resilient against future increased CO_2 prices.

4. Conclusions

The implementation of new, innovative processes that contribute to the reduction of emitted pollutants is a requirement for every industry. GM, with the implementation of the LNB system, drastically reduced (over 40%) NO_x emissions. At the same time, by substituting part of the fuel (pet coke) with biomass (SHP), NO_x emissions were further reduced by 21%, while SO_x and CO were reduced by 20% and 13%, respectively. The ratio of substitution was 2 to 1 by weight, which corresponds to a contribution of biomass to the energy potential of the final fuel that reaches 50%. Mixing the fuel with biomass varied its characteristics, reducing its calorific value and increasing the percentage of moisture and ash, which, however, did not create any problems in the operation and efficiency of the burner. However, the calculation of an empirical ash fusibility index (Rs) showed that mixture of pet coke with sunflower husk pellets presents a medium trend for deposit formulation, a fact that needs to be considered carefully by the company in combination with the assessment of actual deposit formulation after a long time of kiln operation.

The conducted comparison via life cycle assessment for 1 ton of MgO revealed that for both CCM (2.24 ton of CO_2eq) and DBM (2.65 ton of CO_2eq), the most influencing GWP factors are the decomposition of $MgCO_3$ and the carbon released by the combustion of pet coke. It turned out that the substitution of the fuel by biomass and the use of renewable electricity can significantly reduce both the emissions of gaseous pollutants and the general environmental footprint of the MgO production. In a best case scenario, emissions can be decreased by 32.5% for CCM to 1.51 ton of CO_2 and by 38.2% for DBM to 1.64 ton of CO_2 per ton of MgO. The $MgCO_3$ decomposition process releases an essential and unavoidable amount of CO_2 naturally bound in the mineral complexes. In addition, the combustion of pet coke still releases a high share on total CO_2 emissions. However, the scenario-based evaluation of different biomass mixtures and resources provided evidence for encouraging biomass fuel use in the production process to become sustainable and resilient against future increased CO_2 prices. The implementation of CCS and CCU technologies can be an additional option to lower the ecological footprint of produced MgO to reduce the actual significant environmental impact of global magnesium production [58].

The effective application of co-firing technologies, especially in such operating conditions, is a big step towards reducing the emissions of industry sector while at the same time proving that the use of fossil fuels can be reduced without altering the functionality and efficiency of processes that require large amounts of energy, extremely high temperatures, and high quality of final products. The further substitution of pet coke with biomass (perhaps the complete substitution) as well as the development of more environmentally friendly burners are a subject of further study but also an attractive target for GM and corresponding industries in the magnesia sector.

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Appendix A

Table A1. Information about lab instrumentation.

Equipment	Model/Type	Applications	Manual/Information
110 litre furnace, with natural air circulation Tmax = 250 °C	Heraeus Thermo Scientific T-12 drying oven with natural convection	Drying of solids, evaporation of liquids (Proximate Analysis of solid fuels: % moisture)	https://www.pi.infn.it/wp-content/uploads/2021/07/productPDF_31123.pdf (accessed on 22 February 2022).
Shell Calorimeter	PARR 6400CL isoperibol calorimeter	Isoperibol calorimeter for finding higher calorific value of fuels	https://www.parrinst.com/products/oxygen-bomb-calorimeters/6400-automatic-isoperibol-calorimeter/ (accessed on 22 February 2022).
Elementary Analyser (C, H, N, S)	Perkin Elmer Series II CHNS/O Analyzer	Elementary analysis (% C, H, N, S) in solid and liquid fuels	https://resources.perkinelmer.com/corporate/cmsresources/images/44-74656prd_2400seriesiichnsoanalyzer.pdf (accessed on 22 February 2022).
Atomic Absorption	Shimadzu AA-6300 Atomic Absorption Spectrophotometer with GFA-EX7i Graphite Furnace Atomizer.	Measurement of major and trace elements (heavy toxic metals: Sb, As, Cd, Cr, Co, Cu, Pb, Mn, Hg, Ni, Tl, V) in liquid and solid samples	https://uotechnology.edu.iq/NTRC/root/PDF/equipments/AA-6300.pdf (accessed on 22 February 2022).

Table A1. *Cont.*

Equipment	Model/Type	Applications	Manual/Information
Microwave digester	Berghof SW-2	Digestion of samples before measurement of metals in atomic absorption	https://www.somatco.com/MWS-2_Digestion.pdf (accessed on 22 February 2022).
Ash Fusing	Ash fusing analyser SYLAB IF2000	Automatic instrument for determination of ash fusion points by image analysis	http://www.jjexotranoz.com/sylab/if2000.php (accessed on 22 February 2022).
Flue gas analyzer	SICK's MCS100FT FTIR analyzer system	Monitoring of SO_2, NO_2, CO, HCl, HF, H_2O and TOC, O_2, and dust.	https://cdn.sick.com/media/docs/4/74/674/Product_information_MCS100FT_FTIR_Analysis_System_en_IM0018674.PDF (accessed on 22 February 2022).
Flue gas analyzer	Varioplus Industrial by MRU	Simultaneous measurement of up to 9 gas components	https://www.instrumart.com/assets/VARIO-Plus-Datasheet.pdf (accessed on 22 February 2022).

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