Master's Thesis

Evaluating environmental impacts of H_2 application using hourly consumption based LCA emissions factors

In partial fulfillment of the requirements for the degree
Master of Science
at the department Electrical and Computer Engineering
of the Technical University of Munich.

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Abstract

Global climate change is heavily influenced by greenhouse gas (GHG) emissions released into the atmosphere. Emission accounting is used to determine the amount of GHG emissions emitted into the atmosphere. Emission accounting is required to be as accurate as possible. Climate change mitigation strategies are based on the quantified amount of GHG emissions. Strategies based on erroneous information have the potential to cause detrimental effects.

The goal of the thesis is to evaluate the environmental impact of hydrogen (H_2) produced from electrolysis. A methodology is developed to determine hourly emission factors (EMF) of energy carriers (EC) occurring within energy systems. Emissions are accounted to the region of EC consumption to consider emissions arising along the holistic production process of consumed ECs. Flow tracing methodologies are implemented to allocate emission occurring from EC production to EC consumption. Life Cycle assessment (LCA) methodologies are applied to integrate upstream emissions from EC production processes. The environmental impact evaluation of H_2 produced from electrolysis is based on the calculated hourly consumption based LCA-EMFs. H_2 is defined as green according to international regulatory framework. Frameworks differ in methodologies applied to determine H_2's carbon footprint, as well as different threshold values for the definition of green H_2. Differences between regulatory frameworks are evaluated.

Hourly consumption based LCA-EMFs have been calculated and evaluated. The amount of H_2 produced from electrolysis defined as green has been evaluated. Differences between regulatory frameworks have been evaluated. A loophole in the definition of green H_2 has been detected and examined. Equivalent H_2 may simultaneously be defined as green and not as green, depending on the methodology used to calculate H_2's carbon footprint.

Keywords: greenhouse gases; emission accounting; flow tracing; life cycle assessment; electrolysis; green hydrogen.

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List of Abbreviations

AEC	Alkaline Electrolyser Cell
DA	Delegated Act of Renewable Energy Directive
EC	Energy Carrier
ECT	Energy Carrier Track
EI	Ecoinvent
EMF	Emission Factor
ENTSO-E	European Network of Transmission System Operators for Electricity
ESM	Energy System Modelling
FECS	Final Energy Consumption Sector
FfE	Forschungsstelle für Energiewirtschaft e.V.
GEA	German Environmental Agency
GHG	Greenhouse Gas
GWP	Global Warming Potential
H2	Hydrogen
IPCC	Intergovernmental Panel on Climate Change
IRA	Inflation Reduction Act
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
P2X	Power-to-X
PEM	Polymer Electrolyte Membrane Cell
pLCA	Prospective Life Cycle Assessment
PSEMF	Process Specific Emission Factor
RE	Renewable Energy
SMR	Steam Methane Reforming
SOEC	Solid Oxide Electrolyser Cell
UEC	Upstream Emissions from Facility Construction
UEF	Upstream Emissions from Fuel Supply
UNFCCC	United Nations Framework Convention on Climate Change

Contents

Chapter 1

Introduction

As of today global energy demand is served almost entirely from fossil fuels [1]. The usage of fossil fuels as the world's major energy source comes with the side effect of fossil fuels being the largest contributor to global climate change [2]. The global energy system is required to significantly be defossilized to keep global warming well below 2 °C, as defined within the Paris agreement. H_2 and fuel cell technologies have significant potential to enable this transition towards a low-carbon energy system [3]. H_2's potential in energy system transition can be attributed to two of its main properties: [4]

- H_2 is emission-free at the point of final use
- H_2 can be produced from a range of low-carbon energy sources

As a versatile and safe EC H_2 can be used as feedstock, as fuel or as storage medium within the energy system. H_2 can be used to enable large-scale RE deployment, to distribute energy across sectors and regions or to act as a buffer to increase system reliance. H_2 enables the decarbonization of existing processes when used as a fuel for combustion [3]. H_2 produced from locally available primary energy sources can reduce a country's dependence on external energy suppliers [5]. The use of H_2 solely from a climate policy perspective is difficult to be justified. Any environmental benefit from using H_2 as a fuel depends on how the H_2 has been produced [6]. Since H_2 is a secondary EC its environmental impact is defined by the primary energy source's. Methodologies to assess ECs' environmental impacts often lack in accuracy. Interlinkages between ECs or between regions are commonly neglected in environmental impact assessment. The energy system's environmental performance often is not assessed in a highly resoluted manner. Environmental impact assessment has to be performed with the upmost accuracy to holistically assess an energy system's GHG mitigation process .

Hourly consumption based EMFs are calculated and evaluated in the context of this thesis. LCA methodologies are implemented to integrate emissions occurring in all stages of EC production. The EMF-calculation is performed ex-post based on data obtained from FfE's[1] energy system model ISAaR [7]. The EMF-calculation is performed in hourly resolution with the upmost accuracy. Interlinkages between ECs and regions are considered within the EMF-calculation. A GHG accounting methodology is developed to fulfil the calculation's requirements. A H_2 application's environmental impact is evaluated once the LCA based EMFs are calculated. H_2 production from electrolysis is evaluated with regards to internationally published regulatory framework defining green H_2 production.

[1] FfE: Forschungsstelle für Energiewirtschaft e.V.

The goal of this thesis is to perform an environmental impact evaluation of H_2 produced from electrolysis based on hourly consumption based LCA-EMFs. The following research questions should be answered:

- What are the hourly consumption based LCA-EMFs of distinct ECs, based on scenarios of FfE´s energy system model ISAaR?
- Which amount of H_2 produced from electrolysis is considered green according to international regulatory framework?
- What are the differences in the amount of H_2 considered green in between international regulatory frameworks?

The theoretical framework is described in *Chapter 2* with the introduction of relevant terms and methodologies required to achieve this thesis' objectives. The methodological framework to calculate and evaluate hourly consumption based LCA-EMFs is described in detail in *Chapter 3*. Calculation results are displayed and interpreted in *Chapter 4*. *Chapter 5* conflates the findings of this thesis, outlines the contribution and the limitations and gives suggestions for future research.

Chapter 2

Theoretical Framework

2.1 Greenhouse Gas Accounting

Greenhouse gas (GHG) emissions are the main driver of global climate change [8]. Understanding and mitigating GHG emissions has become a major issue for organizations and political entities around the globe. GHG accounting is the process of quantifying and reporting GHG emissions emitted directly or indirectly due to an entity's activities. GHG accounting is an essential tool in understanding an entity's carbon footprint and progress towards reducing GHG emissions. [9]

The goal of GHG accounting is to provide a clear and accurate picture of an entity's carbon footprint. This information is used to support decision making processes, set emissions reduction targets and track mitigation progress. In addition to meeting legal requirements, GHG accounting is frequently conducted to address social responsibility concerns and identify potential cost savings. According to the United Nations Framework Convention on Climate Change (UNFCCC) the foundation of GHG accounting is rooted in the development of national GHG inventories. [10]

2.1.1 National GHG Inventories

GHG inventories are reports about an entity's annual GHG emissions. GHG inventories provide a detailed breakdown of an entity's GHG emissions. GHG inventories support entities in identifying opportunities to reduce their carbon footprint and contribute to global efforts in mitigating climate change. Emission removals, i.e. carbon sinks, might be considered within GHG inventories. The most common environmental impact category to measure an entity's GHG inventory is global warming potential (GWP). GWP describes a GHG's ability to trap heat in the atmosphere. GWP was developed to allow comparisons of different GHGs' global warming impacts. GWP is an index that relates the impact of a GHG's emissions to the impact of emitting the equivalent amount of CO_2. GWP is measured in CO_2-equivalents (CO_2e). GWP is measured over a specified time horizon. GWP is often determined over a time period of 100 years, i.e. GWP100. The Intergovernmental Panel on Climate Change provided 100-year GWPs in its Fourth Assessment Report [11]. [12]

At the national level, the UNFCCC requires all Annex I countries, i.e. developed countries and economies in transition, to annually submit their national GHG inventories. The inventories must follow specific guidelines outlined in the UNFCCC and are subject to regular quality assurance and control checks. Non-Annex I countries, i.e. developing countries, are encouraged to prepare national GHG inventories voluntarily. [13] [14]

The development of German national GHG inventories is displayed in *Figure 1*.

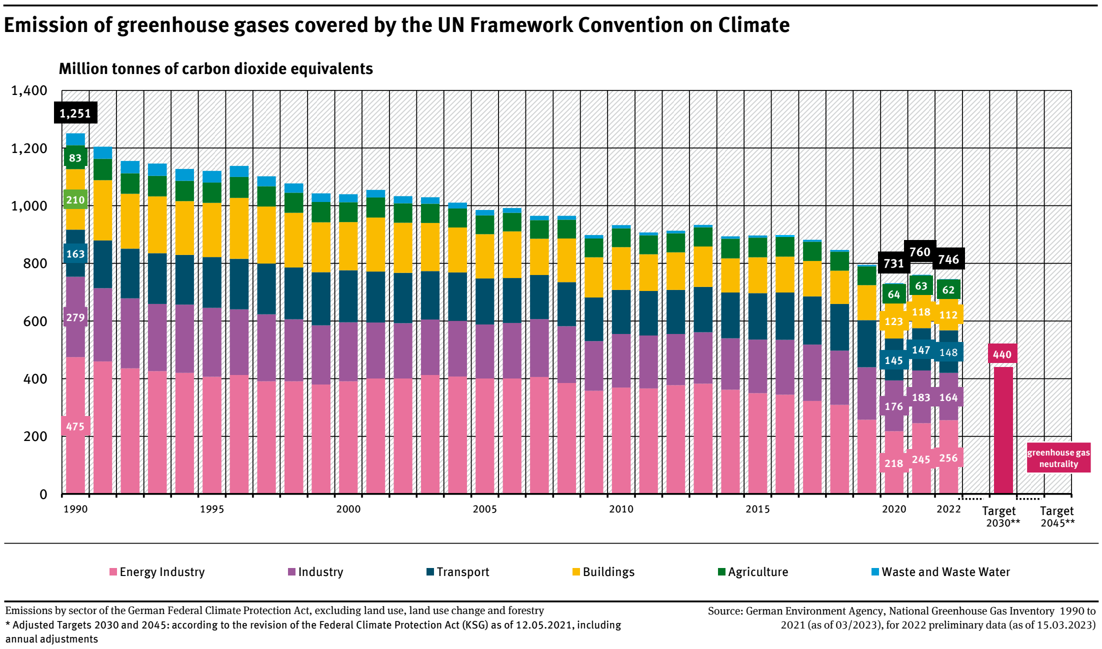

Figure 1: National GHG Inventories - Germany [15]

At the organizational level, companies, non-governmental organizations and other entities may determine GHG inventories as part of their sustainability initiatives or to comply with regulatory requirements. Investors and financial institutions may require companies within their portfolios to report on GHG emissions. An integrated set of tools introduced for measuring, quantifying and reducing GHG emissions is provided in ISO 14064. These globally recognised standards allow organisations to take part in emissions trading schemes. [16]

2.1.2 GHG Protocol

The GHG Protocol is a globally recognized standard for accounting and reporting GHG emissions. It was developed by the World Resources Institute and the World Business Council for Sustainable Development in 1998 [17]. It has been updated several times to reflect changes in the scientific knowledge about climate change, as well as changes in business practices and policies. The GHG protocol is the most common standard in emission accounting. Different regulatory is built upon the GHG protocol's standards, e.g. ISO 14064. [18]

The GHG Protocol provides a consistent and transparent framework to measure and report GHG emissions occurring along an entity's entire value chain. The GHG Protocol differentiates between different types of emissions an entity is responsible for. Emissions occurring from sources owned or controlled by the reporting entity are referred to as direct emissions. Direct emissions typically result from the combustion of fossil fuels in on-site equipment, such as boilers, generators or vehicles. Emissions occurring along the reporting entity's value chain, emitted from facilities controlled or owned by other entities are called indirect emissions. Indirect emissions are more difficult to measure and track than direct emissions. The GHG protocol divides direct and indirect emissions into different scopes. Scope 1 emissions refer to emissions from sources owned or controlled by the reporting entity, such as emissions from fuel combustion or industrial processes. Scope 1 emissions are equivalent to direct emissions. Indirect emissions are divided into scope 2 and scope 3 emissions. Scope 2 emissions refer to emissions associated with the generation of purchases electricity, steam, heat or cooling. Scope 3 emissions include all other indirect emissions occurring along the reporting entity's value chain, such as emissions from the production of purchased goods and services, transportation of products and end-of-life treatment of products. Scope 3 emissions commonly are the largest part of an entity's total GHG emissions. Emission scopes in addition to their respective emission sources are displayed in *Figure 2*. [19]

The GHG Protocol provides guidelines for emission accounting in each of the three scopes. Specific guidance for different sectors has been published, such as emissions from land use and forestry or from the use of refrigerants. Entities are recommended to have their emission inventories independently verified to ensure accuracy and transparency. [19]

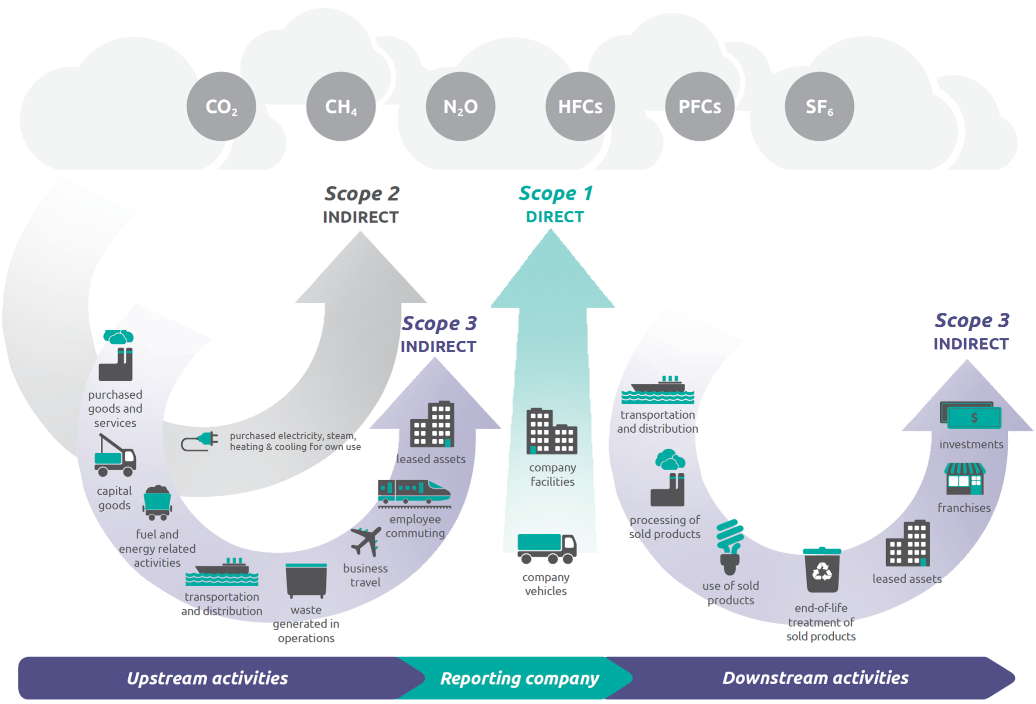

Figure 2: Emission Scopes [19]

2.1.3 Emission Accounting Methodologies

Production- and consumption based emission accounting are the two most common methodologies to set up national GHG inventories [20] [21]. Production based emissions are defined as emissions occurring *"within national territory and offshore areas over which the country has jurisdiction"* [14]. GHG emissions occurring during the production of goods and services are accounted to the region where they are emitted into the atmosphere. In the context of consumption based emission accounting, GHG emissions arising from a region's consumption of goods and services are attributed to the region where the consumption takes place. The entire supply chain of a good or service is considered. Consumption based emission accounting enables countries to take responsibility for emissions resulting from the consumption of goods and services within their borders, regardless of where they were produced. [14] [22]

Consumption based emission accounting considers the impact of trade, encompassing both emissions resulting from domestic final consumption and emissions associated with the production of imported goods. Production based emission accounting considers emissions from exported products while excluding emissions from imported goods. The choice of accounting method holds significant implications for policymaking, as each approach can yield vastly different outcomes [23]. Deviating values for national GHG inventories can result in different mitigation strategies. Decisions based on erroneous information have the potential to cause detrimental effects. The Kyoto Protocol and its follow up agreements, including the Paris Agreement, requires countries to annually submit their national GHG inventories based on the production based methodology. As of today production based emission accounting is the favoured methodology despite the methodology's weaknesses in the consideration of international trade [20]. Due to the growth of emissions embodied in interregional trade the consumption based approach has gained interest within the scientific community. Consumption based emission accounting is often considered to be the more accurate way of accounting GHG emissions. GHG emissions occurring along a product's entire supply chain are considered when using consumption based emission accounting. Production based accounting is more easily executable since a product's supply chain is not considered holistically. Due to better data availability and the neglection of trade production based accounting is the less complex but more transparent methodology. [24] [21]

A detailed comparison of the production- and consumption based emission accounting methodology is displayed in *Table 1*.

	Production based Emission Accounting	Consumption based Emission Accounting
Emissions considered	Administered territory	Global
Allocation	Domestic production	Domestic consumption
Allocation of trade	Exports included, Imports not included	Imports included, Exports not included
Mitigation focus	Domestic activities and exports	Domestic activities and imports
Comparability	Consistent with GDP	Consistent with national consumption
Consistent with trade policy	No	Yes
Complexity	Low	High
Transparency	High	Low
Uncertainty	Lower	Higher
Current country coverage	Relatively high	Low with current data
Mitigation analysis	Domestic mitigation only	Global mitigation

Table 1: Production vs. Consumption based Emission Accounting, based on [24]

2.2 Flow Tracing Methodology

Today's energy system is a complex interwoven network integrating a multitude of different generation, distribution, storage, transformation and load technologies. Competition thrives best if all market participants are convinced that the market is operating fairly. Transparency in the operation of the transmission system is a vital point in establishing this confidence. The knowledge of power flows throughout an energy system is of major importance. [25]

Consumption based emission accounting methodologies, described in *Chapter 2.1.3*, are based on the concept of flow tracing. Flow tracing was originally introduced to allocate network transmission losses to the responsible load [26]. Flow tracing has been used as a transmission-usage allocation methodology [27] [28] [29]. The idea of flow tracing is to follow energy flows throughout the energy system from the generating unit to the respective load unit. This process enables the allocation of a unit's energy production to different consumers within the energy system. Important use-cases of flow tracing are the development of fair grid usage fees and public discussions concerning the benefit of new infrastructure [30] [31].

The flow tracing methodology is based on the proportional sharing principle. The proportional sharing principle is explained based on the network displayed in *Figure 3*. The network is assumed to be without transmission losses. Node x acts as a mixer of its income flows since electrical energy is indistinguishable by nature. Node $x's$ outgoing flows are proportionally composed of node $x's$ income flows and result to: [26]

$$P_{x\to d_j,g_i} = \frac{P_{in,g_i\to x}}{\sum_{g_i} P_{in,x}} * P_{out,x\to d_j} \tag{1}$$

g_i	*Net-generation node i*
d_j	*Net-demand node j*
$P_{x\to d_j,g_i}$	*Energetic flow from x to d_j, supplied from g_i*

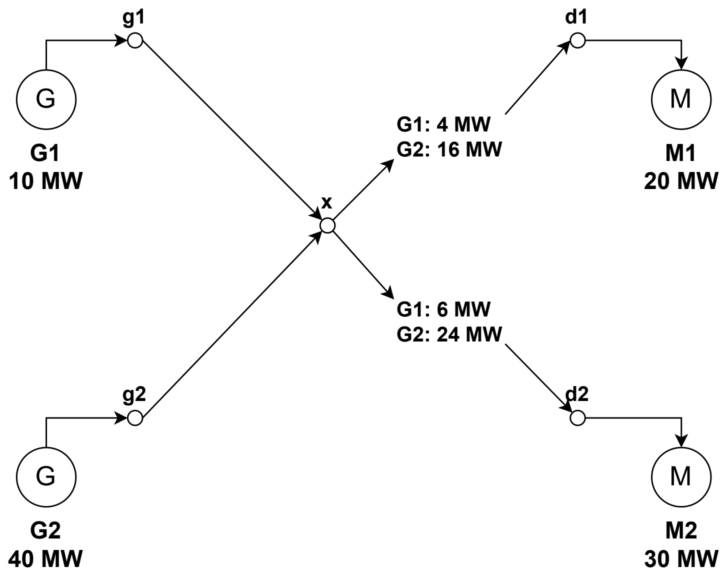

Figure 3: Proportional Sharing Principle, based on [26]

2.3 Life Cycle Assessment

2.3.1 Methodology

Life Cycle Assessment (LCA) is a methodology used to evaluate environmental impacts of a product or service throughout its life cycle, i.e. from the extraction of raw materials to the disposal of the product. The goal of LCA is to identify and quantify environmental impacts associated with each stage of a product's life cycle. LCA is used in process development and policy making. As of today LCA methodologies have not been standardized yet. Results might vary between different LCAs depending on the used methodology. A common methodology to conduct LCAs is published in ISO series 14000. ISO 14040 describes the principles and the framework for conducting LCAs. Requirements and guidelines for conducting LCAs are described in ISO 14044. [32] [33] [34]

Prior to assessing a product's life cycle, the life cycle itself has to be defined. Certain phases of a product's life cycle can be excluded from the LCA depending on life cycle phases of particular interest or data availability. A multitude of life cycle models is established in LCA, some of whom are displayed in *Figure 4*.

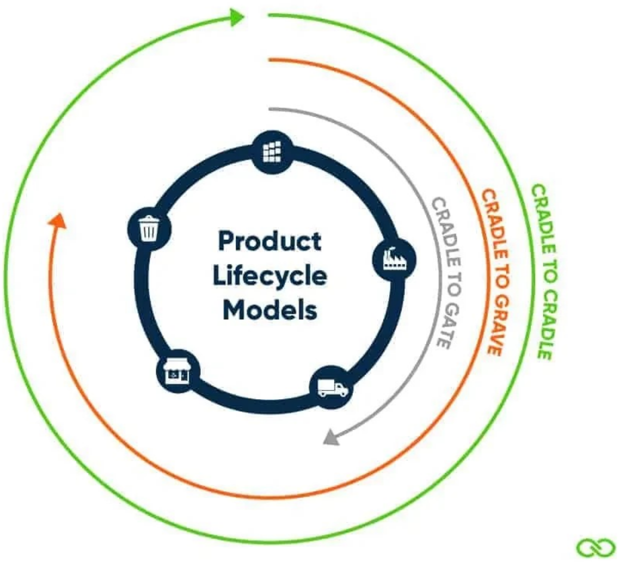

Figure 4: Life Cycle Models [35]

Cradle-to-Grave is a widely used life cycle model. A product's life cycle is defined from the point of raw material extraction to the disposal the product. Environmental impacts at each stage of the product's life cycle, including energy use, resource depletion, emissions and waste generation are considered. The life cycle model Cradle-to-Gate defines a product's life cycle up to the point of supplying the product, i.e. the product leaves the manufacturing facility. Environmental impacts linked with product usage, transportation or disposal are not considered within this model. The Cradle-to-Cradle model aims to create a closed-loop system wherein products are designed for reuse or recycling when they reach the end of their life cycle. Environmental impacts of a product's life cycle from the point of raw material extraction to the end of its useful life are considered. A product's potential for reuse or recycling is considered within this model. The life cycle model Well-to-Wheel often is used to evaluate environmental impacts of transportation systems. The entire life cycle of the fuel used to power a vehicle, from the extraction of raw materials to the combustion of the fuel inside the engine, is considered. [32] [33] [34]

According to the standards defined in ISO 14040 and ISO 14044 an LCA involves four distinct phases:

– Goal and Scope definition
– Life Cycle Inventory (LCI)
– Life Cycle Impact Assessment (LCIA)
– Interpretation

The first step of conducting LCA is the definition of the assessment's purpose and the scope of the study. The assessment's goal defines the context of the study and to whom the results are communicated. The scope of the study is defined by outlining qualitative and quantitative information included within the study. According to the standards defined in ISO 14040 and ISO 14044 a multitude of parameters have to be defined in the scope of the study. The product system defines a set of all processes that are required to perform the specified function, e.g. the production of a product or service. The functional unit describes a quantifiable measure of a product system's performance. It is used as a reference unit to which a processes' in- and outputs are related to. The functional unit is an essential part in LCA and needs to be defined exactly, as it provides the basis for comparing alternative goods and services within an LCA. System boundaries are a delineation of the processes being in- or excluded in the LCA study. They define the scope of the analysis and determine which inputs, outputs and environmental impacts are considered. Boundaries may be defined by geographic, temporal or technological limits, depending on the goal and purpose of the LCA study. Impact categories describe a set of environmental issues that are used to categorize and describe a product's environmental impacts. Impact categories are used to transform Life Cycle Inventory (LCI) data into environmental impact scores. Commonly used impact categories are GWP, eutrophication potential and human toxicity potential. [32] [33] [34]

The second step of performing a LCA study is the identification and quantification of environmental in- and outputs associated with each stage of a product's life cycle. All data needed for the quantification of in- and outputs into and out of the product system is collected and analysed. This includes the usage of raw materials, the consumption of energy and waste generated during the production, usage, and disposal phases of the product's life cycle. [32] [33] [34]

The third step of performing a LCA study is the evaluation of environmental impacts associated with a product's in- and outputs identified in the LCI using the defined impact categories.

The LCA study is concluded with an interpretation of the LCIA results and drawing conclusions about the environmental performance of the product or service. This step involves analysing strengths and weaknesses within a product's life cycle and identifying opportunities for improvement. The accuracy of the LCIA results has to be examined and ensured that the goals of the study are met. Elements significantly contributing to each impact category have to be identified, their sensitivities have to be evaluated and the consistency and completeness of the study has to be assessed. Conclusions and recommendations can be drawn based on a clear understanding on how the LCA was conducted. [32] [33] [34]

2.3.2 LCA database

LCA data is globally accessible from a multitude of databases. Ecoinvent's (EI) database is a widely used LCI database providing data on the environmental impacts of various products and services. It is a comprehensive database containing data on a multitude of processes, e.g. the extraction of raw materials, energy production, transportation, manufacturing and waste management processes. Data is organized into various modules, such as agriculture, energy and transportation. Each module contains data on the in- and outputs of each process, as well as the environmental impacts associated with each process. The data is based on a combination of primary data collection, secondary data sources and modelling. Each process is attributed to a geographic location within the database. Geographic coverage is dependent on data quality and availability. Most processes feature a dataset representing the process on a global scale. LCIA scores based on different impact assessment methodologies, e.g. IPCC2013, and corresponding impact categories, e.g. GWP100, are available for each process. The database's structure enables users to trace impacts of their products throughout the supply chain. [36]

Transparency and traceability were two main points of motivation for the implementation of the database in 2003. One of the main advantages of the database is its comprehensiveness. Data is provided on a wide range of processes and activities, enabling accurate and comprehensive environmental impact assessments of a multitude of products and services. The database is regularly updated and revised, ensuring that data is up-to-date and reflective of current practices. Despite the database being a valuable resource for LCA practitioners, there are some limitations when working with the database. One limitation is that data is based on European and North American conditions and may not be applicable to other regions. Additionally, databases are never completed. Missing data on processes and activities may be supplemented by data from additional sources. [36] [37] [38]

2.3.3 Prospective LCA

Databases used to perform LCA often contain outdated data. The usage of an outdated background database is especially problematic when performing LCA on future technologies [39]. The methodology of prospective LCA (pLCA) was developed to evaluate environmental impacts of emerging technologies at an early stage of development. pLCA is used to study future scenarios with currently emerging technologies [40]. The growing importance of adjusting background processes in LCA when assessing future energy system is described in several studies [41] [42] [43]. The adjustment of LCI background databases is a common approach in executing pLCA. The open-source python library $premise$[1] increases the extent of prospective scenario integration in LCA across multiple models, as well as different versions of the Ecoinvent database [44]. [39]

[1]The library $premise$ is described in detail in its *documentation*

2.4 Energy System Modelling

Energy system modelling (ESM) is a tool used for analysing and optimizing the energy system. It involves the creation of a computer based model of an energy system. Municipal, national or international polities are often used as geographical scopes. Models' horizons vary from single-year models with hourly resolution to long-range models, typically modelling a couple of decades. [45]

Holistic energy systems consider all energy processing units within the system's boundaries. ESM employs scenario analysis to investigate assumptions about technical and economic conditions at play. Models are optimized to a multitude of output variables, e.g. GHG emissions, total system costs or the use of natural resources. Optimization constraints are considered during the optimization of the energy system, e.g. GHG neutrality by year 2050. ESM results are used for energy policy development, since the energy supply sector is the largest contributor to global GHG emissions [8]. Energy system models represent a simplified picture of the real energy system and the real economy. A large diversity of modelling approaches has been developed depending on their target group, intended use (data analysis, ex post evaluation, forecasting, simulation, optimization, etc.), regional coverage (regional, national, international), conceptual framework (top-down, bottom-up) and data availability. [46]

Top-down models are macroeconomic models simulating sector-specific energy demand and energy supply, while including impacts on economic growth, employment and foreign trade. They strongly rely on energy price changes and financial policies. Top-down models are not well suited to describe the development of specific technologies or sectoral policies and related changes in energy demand, emissions and investments at a detailed level. Top-down models may also violate fundamental physical restrictions such as the conservation of matter and energy. Bottom-up models use a business economics approach for the economic evaluation of the modelled technologies. The main characteristic of bottom-up models is their comparatively high degree of technological detail used to assess future energy demand and supply. Macroeconomic impacts of energy or climate policies are not considered. Transaction costs, implicitly considered by top-down models, are not considered. Due to the high degree of modelling detail bottom-up models heavily depend on data availability and credibility. Bottom-up models regularly are used by engineers and energy supply companies, whereas top-down models are favoured by economists and public administrations. Combining the advantages of both model types into a hybrid model more adequately describes and projects the changes of the energy system. The quality of discussions on future energy perspectives will improve by being able to differentiate among technologies and sectors and to analyse macroeconomic implications of large policy portfolios in a consistent and transparent manner. [46] [47] [48]

2.4.1 ISAaR

The EMF-calculation performed in the context of this thesis is based on optimization results of FfE's energy system model ISAaR. The name „ISAaR“ results as an abbreviation from its German name „Integriertes Simulationsmodell zur Anlageneinsatz- und Ausbauplanung mit Regionalisierung“. Linear optimization is used to mathematically describe the European energy system. ISAaR is a linear programming model optimizing plant deployment and expansion in terms of minimizing total system cost. ISAaR is a holistic energy system model. All energy-related processes within the energy system's boundaries are modelled. The conventional power plant fleet, RE units, energy consumption from the final energy sectors (FECSs) as well as network infrastructure, e.g. transmission grids and storage units are modelled. The six ECs electrical energy, district heating, methane, liquid hydrocarbons, H_2 and biomass are modelled. Liquid hydrocarbons are referred to as SynFuels within ISAaR. The ECs are balanced on their respective energy carrier tracks (ECTs). Generation, consumption and storage processes are assigned to each ECT. Conversion technologies serve as connections between the ECTs. A graphical overview of the ISAaR's modelled energy system is displayed in *Figure 5*. [7]

2.4.2 Scenario description

The scenario analysed in the context of this thesis is called $solidEU$. $solidEU$ is a quantitative scenario framework implemented in FfE's research project eXtremOS. It is a European climate protection scenario with a GHG emission reduction target of 95% up to 2050 w.r.t. 1990 [49]. A detailed look into $solidEU$ can be found in ***FfE's ISAaR Dashboard***, which is a tool to visualize the modelled energy systems of different ISAaR scenarios. [50]

In $solidEU$ the energy system of the European Network of Transmission System Operators for Electricity (ENTSO-E) is modelled with national resolution. All of ENTSO-E's regions are modelled separately in addition to the aggregated ENTSO-E region. ECTs' modelled temporal resolutions vary between ECs. The energy carriers electrical energy and district heating are modelled with hourly resolution. Methane is modelled with daily resolution, while biomass, H_2 and liquid SynFuels are modelled with yearly resolution. The energy system is modelled from 2020 to 2050 with 5-year intervals between modelled years. Optimization runs are performed with hourly resolution within ISAaR. The temporal resolution of ISAaR processes is of hourly nature, i.e. each process is assigned with hourly time series. ECTs' temporal resolutions can deviate from the hourly resolution of the optimization run. An ECT's EC balance must be fulfilled with regards to the ECT's temporal resolution (optimization constraint).

Due to the fact that ISAaR's optimization results are modelled with hourly resolution the terms power and energy are used interchangeably. Within this thesis the term $P(ec)$ is regularly used to describe an energetic flow of EC ec. [7]

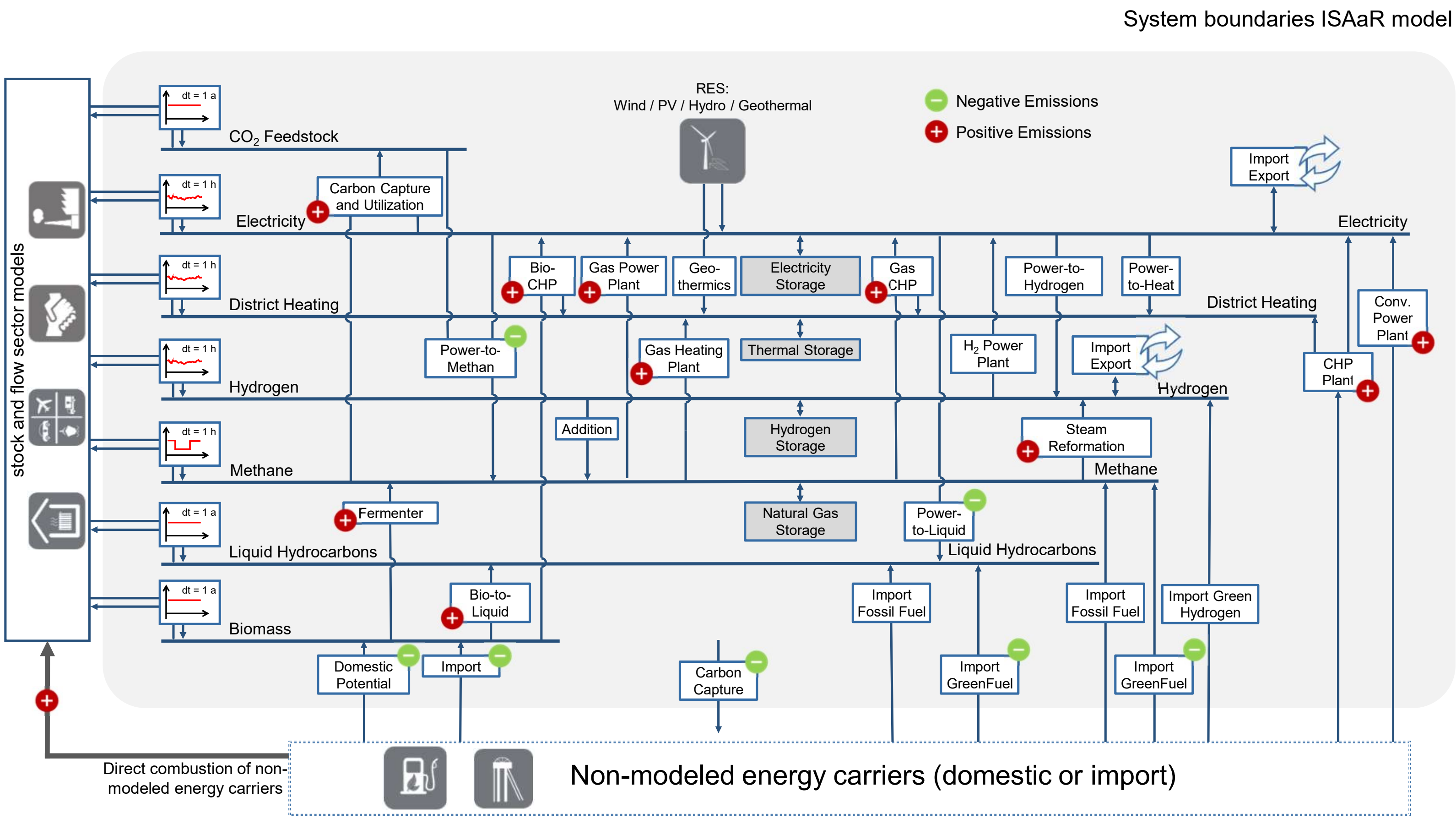

Figure 5: System Boundaries ISAaR [7]

2.5 LCA in Energy System Modelling

ESM most often determines an energy system's cost-optimized development based on assumptions made within different scenarios [51]. Most models exclusively consider emissions occurring during the operational phase of energy production, e.g. from fuel combustion. Emissions linked to up- and downstream processes are neglected in most energy system models. Upstream emissions compose of emissions occurring during the construction of technical facilities (UEC) and emissions occurring from the supply of fuel to be used within different processes (UEF), e.g. mining processes. Downstream emissions derive from a product's end-of-life treatment. Climate mitigation policies particularly rely on RE based energy systems. An increasing deployment of RE generation leads to a growing importance of considering UEC. Holistic models of future energy systems require the inclusion of LCA methodologies in ESM. [52] [53]

A wide range of approaches for incorporating LCA into ESM has been developed and utilized. The integration of LCA into ESM can be performed by four different methodological approaches. In case of ex-post assessment the energy system is optimized to minimized total system costs. Environmental impacts are not considered within the optimization function itself. GHG emission reduction targets are integrated as optimization constraints. An LCA is performed ex-post based on the cost-optimized results. The other three approaches can be aggregated to the term integrated assessment. Environmental impacts are integrated in the ESM's optimization problem. Environmental impacts directly influence the optimization problem and technology mix when applying integrated assessment methodologies. In case of the monetization approach emissions are integrated to the optimization function as additional costs of energy system components. In case of the multi-objective optimization approach the environmental dimension is considered as a separate objective. The uncertainty associated with the monetization of externalities is decreased by considering trade-offs between impact categories. Multi-criteria decision analysis is an extension of multi-objective optimization approach. Qualitative aspects, such as risk, resource, social and political drivers are included in the optimization problem. [52]

2.6 H_2 Production

H_2 is an essential element within the energy system, currently mainly used in the chemical and refining industry [54]. H_2 applications are gaining in importance on the path towards a carbon neutral energy system . H_2 is a promising substitute for fuels in transportation since the usage of H_2 in fuel cells or combustion engines is not causing GHG emissions or other pollutants [55]. Electrolysis is a promising solution for the integration of surplus energy, which indirectly reinforces the deployment of RE. [3]

2.6.1 Production technologies

In 2021 global H_2 demand was almost entirely covered by production from unabated fossil fuels. As of today the three major fuels used in the commercial production of H_2 are natural gas, oil and coal. More than 80% of global H_2 production is sourced by these fossil fuels. A significant share of global H_2 production comes as a by-product of naphtha reforming at refineries. As of today, electrolysis is not yet established as a H_2 production technology in commercial production. Electrolysis is gaining importance in H_2 production when transforming towards a RE based energy system. [54]

H_2 is either provided from Steam Methane Reforming (SMR), electrolysis or H_2 import within $solidEU$. SMR is an advanced and mature H_2 production process building upon existing natural gas pipeline infrastructure. In 2021 more than 60% of global H_2 production derived from natural gas reforming processes. Natural gas is a mixture of different gases containing methane, which can be used for H_2 production from thermal processes. High temperature steam (700℃ – 1100℃) pressurized to 3–25 bar reacts with methane in the presence of a catalyst to produce H_2, carbon monoxide and a small amount of carbon dioxide. SMR is an endothermic process. Process heat has to be supplied externally for the reaction to proceed. SMR processes yield an efficiency in H_2 production of up to 85%, among the highest of current commercially available H_2 production methodologies. The SMR reaction is displayed in *Equation 2*. [56] [57]

$$CH_4 + H_2O \rightarrow CO_2 + 3H_2 \tag{2}$$

Electrolysis is a H_2 production process using the process of water splitting. Electrical energy is used to split the water molecule H_2O into its components O_2 and H_2. On a commercial scale electrolysis is often referred to as power-to-gas. The process itself does not produce any by-products or emissions other than H_2 and O_2. The environmental impact of H_2 produced from electrolysis mainly derives from the used electrical energy's carbon footprint. The electrolysis reaction is displayed in *Equation 3*.

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2 \tag{3}$$

As of today H_2 production from electrolysis yields a system efficiency of 60–80% [58]. H_2 production from electrolysis is more expensive compared to by fossil based production methodologies. This is due to lower system efficiencies in addition to higher prices of primary energy sources. The system efficiency of electrolysis is expected to reach up to 85% by 2030 [59]. The three main types of electrolytic cells are solid oxide electrolyser cells (SOECs), polymer electrolyte membrane cells (PEM) and alkaline electrolyser cells (AECs). AECs are a well-established technology that offers cost-effective investment, long lifetimes and reasonable system efficiencies of up to 80% in the long term. AECs are sensitive to impurities in product gases and they do have a long cold start time. PEM electrolysers are more expensive in investment while producing H_2 of higher purity. They have the advantage of lower requirements to the electrical energy source, making them ideal for the integration of RE into electrolysis. PEM electrolysers operate at high current densities, which enables cheap H_2 production on a commercial scale. SOECs are a promising technology, which are currently at the Research Development stage. They are the most expensive technology considering investment costs while having the highest starting time from cold. SOECs yield the highest system efficiencies compared to AECs and PEM. They operate at high temperatures (around 800 °C) requiring a significant amount of thermal energy, which has to be provided externally. SOECs have the potential to reduce overall system cost of H_2 production by reducing the amount of electrical energy required for electrolysis. [60] [61]

PEM is the only technology considered within ISAaR's process electrolysis. All H_2 from electrolysis derives from PEM electrolysers.

2.6.2 H_2 Colours

H_2 is produced from different primary energy sources by a multitude of production processes as described in *Chapter 2.6.1*. Emissions related to the produced H_2 vary significantly depending on the production process and the used primary energy source. Colour codes have been implemented to categorize H_2 based on its environmental impact during production. As of today there is no standardized naming and colour convention. Definitions may change over time or between countries. Common H_2 colours in addition to their respective production process are displayed in *Figure 6* Colours. [62]

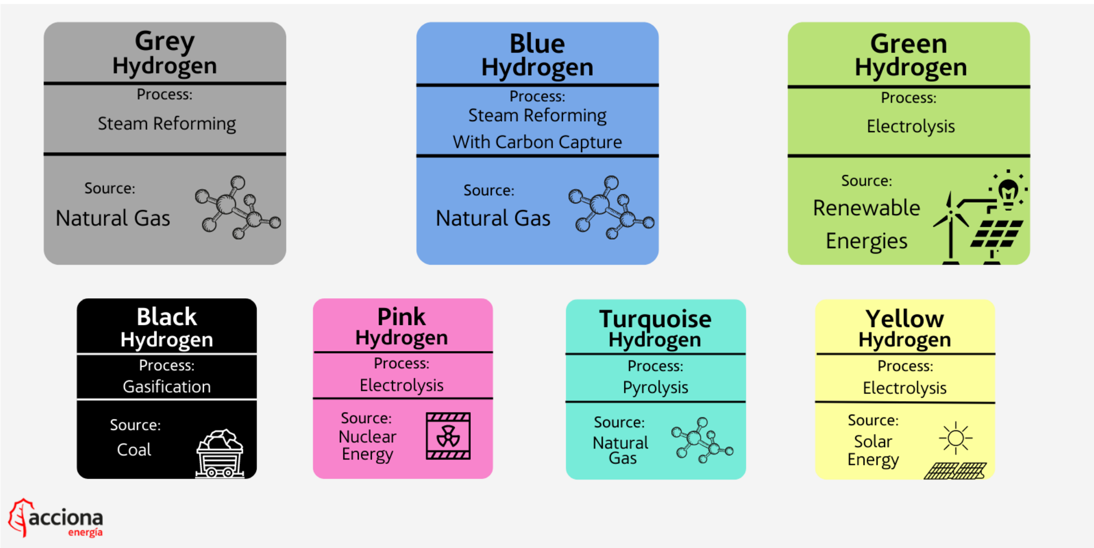

Figure 6: H_2 Colours and Production Processes [63]

2.6.3 Green H_2 Classification

As of today there is no standardized definition for the term “green” H_2. H_2 is referred to as “low carbon”, “sustainable” or “green” within different regulatory framework. In the context of this thesis green H_2 is exclusively defined by its carbon footprint. The regulatory framework for the definition of green H_2 is still evolving, with several stakeholders having developed private standards. The overall carbon footprint or GHG emission savings can be subject to regulatory requirements in addition to rules regulating the renewable electricity source, e.g. additionality principle. A threshold value for the carbon footprint of H_2 ensures a reduction of GHG emissions compared to a fossil reference. [64]

Many countries are currently developing a regulatory framework for H_2. In 2022 the Inflation Reduction Act (IRA) was signed into law in the United States of America. Green H_2 production is promoted with tax benefits graded on the H_2’s carbon footprint [65]. In the European Union green H_2 production is defined by two different regulations, leading to less clarity in regulation. The Renewable Energy Directive regulates H_2 in the context of transportation and is complemented by a delegated act (DA) [66]. The EU-Taxonomy is a classification system used for sustainability reporting and sustainable financial products [67]. Key differences in the definition of green H_2 between the regulatory frameworks are displayed in *Table 2*. The threshold value for the definition of green H_2 is displayed in the unit $\frac{kg\ CO_2e}{kg\ H_2}$.

	DA	EU-Taxonomy		IRA
Threshold value Green H_2	3.4	3	3	4
Methodology	DA	DA	LCA	LCA
System Boundaries	Cradle-to-Gate	Cradle-to-Gate	Cradle-to-Gate	Well-to-Gate
Plant Construction	✗	✗	✓	✓
Renewable Electricity	0	0	LCA-EMF	LCA-EMF
EMF grid electricity	Country-specific or Marginal Appr.	Country-specific or Marginal Appr.	Country-specific	Country-specific
Inputs	Rigid / Elastic	Rigid / Elastic	✗	✗

Table 2: Green H_2 Classification - Regulatory Framework

The two emission accounting methodologies defined in DA, EU-Taxonomy and IRA are referred to as DA- and LCA-methodology in the context of this thesis. Both methodologies in principle follow an LCA based approach. The functional unit is defined as 1 kg of produced H_2. The impact category is defined as GWP100 using the impact assessment methodology from the IPCC2013 [68]. System boundaries are defined as Cradle-to-Gate. System boundaries are described as “Well-to-Gate” within IRA. Whilst this is not a standardized term in LCA it can be explained as a product’s life cycle from the point of raw material extraction, i.e. well, to the point of supply of produced H_2, i.e. gate. Hence, there is no difference in system boundaries between the methodology provided by IRA compared to methodologies from DA or EU-Taxonomy.

DA- and LCA-methodology differ in three key aspects:

1. UEC are not considered by the DA-methodology.
2. The neglect of UEC leads to renewable electricity being accounted with net-zero emissions when applying the DA-methodology. Grid electricity is either accounted with a country-specific EMF, provided within the DA, or by a marginal power plant approach. Renewable electricity is accounted with an LCA based EMF according to LCA-methodology. Grid electricity is accounted with a country-specific LCA based EMF. Grid electricity's LCA based EMFs are not provided within EU-Taxonomy. In case of Germany annual LCA based EMFs of the national electricity mix are annually published by the German Environmental Agency (GEA).
3. The DA divides inputs into elastic and rigid inputs. This is especially relevant for recycled carbon fuels, as by definition captured carbon is classified as a rigid input.

H_2 is defined as green according to EU-Taxonomy if the environmental impact during H_2 production is max. $3\ \frac{kg\ CO_2e}{kg\ H_2}$. The threshold values for green H_2 production defined in DA and IRA are $3.4\ \frac{kg\ CO_2e}{kg\ H_2}$ and $4\ \frac{kg\ CO_2e}{kg\ H_2}$. EU-Taxonomy allows the emission accounting methodology to be chosen. The carbon footprint of H_2 production is lower when applying the DA-methodology compared to the LCA-methodology. This is due to the fact that UEC are not considered within the DA-methodology. H_2 might be defined as green when applying the DA-methodology but might not defined be as green when applying the LCA-methodology. This regulatory loophole is referred to as Green H_2 Gap in the context of this thesis. [64]

Chapter 3

Methodology

The first research question asks for the calculation of hourly consumption based LCA-EMFs of distinct ECs based on scenarios of FfE's energy system model ISAaR. Emissions occurring during the holistic production process of EC supply are considered within the EMF-calculation. The inclusion of lifetime emissions is based on LCA theory described in *Chapter 2.3*.

3.1 Emission Flow Tracing

The EMF-calculation is performed ex-post based on optimization results of ISAaR's scenario $solidEU$, described in *Chapter 2.4.2*. The consumption based emission accounting methodology is based on the concept of flow tracing, explained in *Chapter 2.2*. Energy flows are traced throughout the energy system to determine the energetical composition of consumption processes. Following this methodology the share of a consumption process' EC demand supplied from a specific production process is determined. This information is used to proportionally assign emissions from EC production processes (production emissions) to EC consumption processes. Production emissions are not accounted to the region of production but to the region of consumption, i.e. consumption based emission accounting methodology as described in *Chapter 2.1.3*.

The EMF-calculation is based on a methodology to determine ECs' time resolved EMFs based on ESM results. The methodology is adopted from [69]. The national emission inventory g, see *Chapter 2.1.1*, is calculated according to:

$$\begin{aligned} \underline{g} &= \underline{\underline{B}} \cdot \underline{s} \\ with\ \underline{s} &= \underline{\underline{A}}^{-1} \underline{f} \end{aligned} \tag{4}$$

The final demand vector $\underline{f}$ represents the demand of supplied ECs. The scaling vector $\underline{s}$ is calculated from the technology matrix $\underline{\underline{A}}$, describing energetical exchanges between different processes, and the final EC demand $\underline{f}$. The scaling vector $\underline{s}$ describes each process' total EC demand to deliver the final demand $\underline{f}$. Resulting total emissions $\underline{g}$ are calculated from the environmental intervention matrix $\underline{\underline{B}}$, containing processes' specific emissions, and the scaling vector s. When transferring this approach to ESM the final demand $\underline{f}$ corresponds to FECSs' EC demand. The technology matrix $\underline{\underline{A}}$ describes energy flows within the modelled energy system. The intervention matrix $\underline{\underline{B}}$ is calculated by multiplying fuel inputs per EC with their respective combustion-related EMFs. [69]

3.1.1 Emission Balance

Emission balances are set up to calculate EC specific EMFs while considering interlinkages between ECs. Emission balances are based on the fact that emissions occurring during production of EC demand $E_{in}(ec)$ (production emissions) are accounted to EC demand $E_{out}(ec)$ (outgoing emissions). Outgoing emissions are calculated from the EC specific EMF $emf(ec)$ and the demand of EC. EC demand comprises of EC's final demand from FECSs $P_{demand}(ec)$ and $P_{in}(ec, ec')$. $P_{in}(ec, ec')$ represents the demand of EC ec required for the production of linked ECs ec' due to transformation processes:

$$E_{out}(ec) = emf(ec) * (P_{demand}(ec) + P_{in}(ec, ec')) \tag{5}$$

Production emissions compose of emissions linked to fuel demand and transformation processes required for the production of EC demand. Emissions linked to fuel input are calculated from the amount of fuel required $P_{fuel}(ec)$ and the respective fuel specific EMF emf_{fuel}. Emissions linked to the production of EC ec via the transformation of linked ECs ec' are calculated from the EMFs of linked energy carriers $emf(ec')$ and the demand of linked energy carriers $P_{in}(ec', ec)$:

$$E_{in}(ec) = emf_{fuel} * P_{fuel}(ec) + emf(ec') * P_{in}(ec', ec) \tag{6}$$

The formulated emission balances result in a system of m equations, with m being the number of ECs. Emission balance are set up by equating incoming and outgoing emissions:

$$\begin{aligned} emf(ec) * (P_{demand}(ec) + P_{in}(ec, ec')) \; = \\ emf_{fuel} * P_{fuel}(ec) + emf(ec') * P_{in}(ec', ec) \end{aligned} \tag{7}$$

When applying the approach described in *Equation 7* to ISAaR's optimization results an emission balance is set up for each timestep t, region reg and EC ec modelled within $solidEU$. A timestep t comprises of the year and the hour of the optimization result. An individual emission balance is set up per timestep t, region reg and energy carrier ec according to:

$$\begin{gathered} emf(t, ec, reg) * \\ \left(\sum_{sec} P_{demand}(sec, t, ec, reg) + \sum_{dev} \sum_{ec'} P_{in}(dev, t, ec, ec', reg) + \sum_{reg'} P_{export}(t, ec, reg, reg') \right) \\ = \\ \sum_{dev} (a(dev, t, ec)(emf_{fuel} P_{fuel}(dev, t, ec, reg) + emf(t, ec', reg) P_{in}(dev, t, ec', ec))) + \\ \sum_{reg'} P_{import}(t, ec, reg, reg') emf_{import}(t, ec, reg') \end{gathered} \tag{8}$$

Transformation processes between ECs are considered, with each EC ec being linked to connected ECs ec' via processes dev. Im- and export processes are considered, with regions reg being connected to neighbouring regions reg' via trading capacities. All parameters are obtained from ISAaR's optimization results or external data used within ISAaR, e.g. the fuel specific EMFs emf_{fuel}.

3.1.2 Emission Allocation - Multi-Output Processes

Processes simultaneously generating multiple forms of output energy from the same input energy source are referred to as co-generation units within ISAaR. All co-generation units, modelled within $solidEU$, generate electrical and thermal energy from the combustion of fossil fuel. Co-generation unit's emissions have to be allocated to the generated output ECs to follow the emission flow tracing approach. Co-generation units' production emissions are allocated to the produced ECs by means of an allocation factor a. In the context of this thesis the allocation factor a is determined according to two methodologies.

Energy-Method

The allocation methodology used by the International Energy Agency is referred to as $Energy-Method$ in the context of this thesis. The allocation factor $a_{E,ec}(t, reg, dev)$ is calculated from the ratio of a process $dev's$ energy carrier ec output to the process' total output during timestep t in region reg:

$$\begin{aligned} a_{E,el}(dev, t, reg) &= \frac{P_{Out,el}(dev, t, reg)}{\sum_{ec} P_{Out,ec}(dev, t, reg)};\ a\ \epsilon\ [0; 1] \\ a_{E,th}(dev, t, reg) &= \frac{P_{Out,th}(dev, t, reg)}{\sum_{ec} P_{Out,ec}(dev, t, reg)};\ a\ \epsilon\ [0; 1] \end{aligned} \tag{9}$$

$a_{E,el}$ *Electrical allocation factor: Energy-Method*
$a_{E,th}$ *Thermal allocation factor: Energy-Method*

Carnot-Method

The exergy of generated ECs is reflected by the $Carnot - Method$. The allocation factor is calculated from the electrical and thermal fuel efficiencies η_{el} res. η_{th}, considering the theoretical carnot efficiency η_C. Electric and thermal fuel efficiencies are calculated from the energetic in- and output streams of process dev during timestep t in region reg. The theoretical carnot efficiency is calculated from a process' upper and lower temperature level, $T_u(dev)$ res. $T_l(dev)$:

$$\begin{aligned} a_{C,el}(dev, t, reg) &= \frac{\eta_{el}(dev, t, reg)}{\eta_{el}(t, reg, dev) + \eta_C(dev) * \eta_{th}(dev, t, reg)};\ a\ \epsilon\ [0; 1] \\ a_{C,th}(dev, t, reg) &= \frac{\eta_{th}(dev, t, reg)}{\eta_{el}(t, reg, dev) + \eta_C(dev) * \eta_{th}(dev, t, reg)};\ a\ \epsilon\ [0; 1] \\ \eta_C(dev) &= 1 - \frac{T_u(dev)}{T_l(dev)} \end{aligned} \tag{10}$$

$a_{C,el}$ *Electrical allocation factor: Carnot-Method*
$a_{C,th}$ *Thermal allocation factor: Carnot-Method*

3.1.3 Emission Flow Tracing within EMF-calculation

An EMF-calculation is performed for every emission balance set up, i.e. for every timestep t, ec and region reg modelled within $solidEU$. The EMF-calculation is exemplified for a specific timestep t within this chapter. Hence, the timestep t is not noted within explanatory equations. The explained methodology is executed for every emission balance set up.

The detailed emission balance described in *Equation 8* is transformed into a linear system of equations:

$$\begin{gathered} \underline{\underline{a}} \times \underline{\underline{x}} = \underline{\underline{b}} \\ with\ \underline{\underline{a}} \in \mathbb{R}^{m \times n \times m \times n},\ \underline{\underline{x}} \in \mathbb{R}^{m \times n}\ and\ \underline{\underline{b}} \in \mathbb{R}^{m \times n} \end{gathered} \tag{11}$$

m *Number of energy carriers* ec
n *Number of regions* reg

The target matrix $\underline{\underline{x}}$ describes the EMF of EC ec_i in region reg_j:

$$\underline{\underline{x}}(i,j) = emf(ec_i, reg_j) \tag{12}$$

Emissions occurring during the production of ec_i in region reg_j are described in matrix $\underline{\underline{b}}$ (production emissions):

$$\underline{\underline{b}}(i,j) = \sum_{dev} a(dev, ec_i, reg_j)\,(emf_{dev}(dev, ec_i, reg_j) P_{dev}(dev, ec_i, reg_j)) \tag{13}$$

Production emissions are calculated by assigning a process-, region- and output-energy-carrier-specific emission factor (PSEMF) $emf_{dev}(ec_i, reg_j, dev)$ to the respective production process dev. $Dev's$ production emissions are calculated from its assigned PSEMF and its production profile $P_{dev}(ec_i, reg_j, dev)$. Co-generation processes' production emissions are allocated to the respective output ECs by means of allocation factor $a(dev, ec_i, reg_j)$.

Energy flows throughout the modelled energy system are described in matrix $\underline{\underline{a}}$. Matrix $\underline{\underline{a}}$ is used to allocate production emissions to the respective consumption processes. Matrix $\underline{\underline{a}}$ is calculated by transforming the detailed emission balance described in *Equation 8*:

$$\begin{gathered} \underline{\underline{a}} = \sum_{sec} P_{demand}(sec, ec_i, reg_j) + \sum_{dev}\sum_{ec'} (dev, ec_i, ec', reg_j) + \sum_{reg'} P_{export}(ec_i, reg_j, reg') \\ - \sum_{dev} a(dev, ec_i) P_{in}(dev, ec', ec_i, reg_j) - P_{import}(ec_i, reg', reg_j) \end{gathered} \tag{14}$$

A linear system of equations is set up for each timestep t, ec_i and region reg_j. All data required to set up the equation system is obtained from ISAaR's optimization results. Once the equation system is set up matrix $\underline{\underline{a}}$ is reshaped into a matrix of size $\mathbb{R}^{m*n \times m*n}$ and matrix $\underline{\underline{b}}$ is transformed into a vector of size $\mathbb{R}^{m*n \times 1}$. This step enables the calculation of matrix $\underline{\underline{a}}'s$ generalized inverse, enabling to solve the equation system even when $\underline{\underline{a}}$ is singular. The hourly consumption based EMFs are calculated by multiplying both sides of *Equation 11* with matrix $\underline{\underline{a}}'s$ generalized inverse.

3.2 Application LCA data to ISAaR

3.2.1 Matching: LCA data - ISAaR processes

Production emissions are calculated from a processes' production profile multiplied with its process-, region- and output-energy-carrier-specific emission factor (PSEMF), as described in *Equation 13*. LCA methodologies are integrated into the EMF-calculation with the assignment of LCA based PSEMFs to ISAaR's optimization results. To execute this ex-post assessment, see *Chapter 2.5*, LCA based PSEMFs are evaluated. The entire life cycle up to the point of EC supply is considered within the EMF-calculation. Applying these boundaries to the LCA methodology described in *Chapter 2.3.1* the life cycle model is set to Cradle-to-Gate. Upstream processes from the point of raw material extraction to the point of EC supply are considered.

As one of the world's biggest LCI databases Ecoinvent provides LCA based PSEMFs (Cradle-to-Gate) for a multitude of activities in multiple regions. LCA based PSEMFs are calculated from activity $act's$ lifetime GHG emissions in region reg_j and the lifetime production of an activity's EC ec_i output:

$$PSEMF_{EI}(act, ec_i, reg_j) = \frac{\sum_{LT} GHG(act, ec_i, reg_j)}{\sum_{LT} ec_{i,Out}(act, reg_j)} \tag{15}$$

EI	*Ecoinvent*
LT	*Lifetime*
$PSEMF_{EI}$	*PSEMF calculated within Ecoinvent database*
$\sum_{LT} GHG$	*Lifetime GHG-emissions*
$\sum_{LT} ec_{i,Out}$	*Lifetime production of* ec_i

PSEMFs are calculated per unit of output EC and can therefore be assigned to ISAaR processes' production profile to determine a process' LCA based production emissions. PSEMFs differ between regions due to different assumptions made during the calculation of life cycle emissions.

The matching process of Ecoinvent data to ISAaR processes described within this chapter is implemented within a python-script. The package $brightway2$[1] is used for the interaction between python and the Ecoinvent database. Ecoinvent's database version 3.9.1 with cut-off allocation is used as an LCA database. The impact category defined in IPCC2013 based on GWP100 is used in the context of this thesis [68]. Most ISAaR processes' PSEMFs are adopted from equivalent Ecoinvent activities' LCA based data. In case of few ISAaR processes equivalent activities do not exist within the Ecoinvent database. All data required to perform the matching process between ISAaR processes and Ecoinvent activities is submitted into a matching file. Data is submitted manually into the matching file since there is no possibility to automate this process. Depending on the availability of PSEMFs within the Ecoinvent database and the need for converting PSEMFs to the required format, the matching process is based on data submitted into different sheets of the matching file. The matching of ISAaR processes to Ecoinvent activities is executed individually for each process defined within the matching file.

[1] The package $brightway2$ is described in detail in its *documentation*

In the upcoming chapters the term PSEMF is used without references to output ECs and regions the PSEMF is calculated for. It should be noted that PSEMFs are factors specific to the activity's EC production within a certain region. The assumptions and calculations made in modifying PSEMFs are executed for every EC and region necessary. PSEMFs are constant factors calculated according to the methodology described in *Equation 15*. PSEMFs' adjustments to ISAaR are performed with ISAaR's highly resoluted temporal data. The constant PSEMFs defined within the Ecoinvent database are modified to hourly resoluted PSEMFs based on ISAaR data. In the upcoming chapters the constant PSEMFs are denoted without timestep t, while the highly resoluted adjusted PSEMF are denoted with timestep t. In the upcoming chapters the term $process$ refers to an ISAaR process, while $activity$ refers to an LCA data source's activity.

3.2.1.1 LCA data from Ecoinvent, no conversion required

There is no need for converting PSEMFs if the activity's PSEMF is based on the unit of output EC. ISAaR processes and Ecoinvent activities to be matched are defined within the matching file. A process is defined according to its identification as specified within ISAaR. The activity to be matched is defined by its name as specified within Ecoinvent and the activity's output EC. The output EC has to be set according to ISAaR's energy carrier identification. The database the activity is obtained from is also defined within the matching file. The database's name must contain the activity's database parameters as defined within the matching file. The parameters defined within the matching file describe the database's name and the year the database is valid for. The naming convention has to be considered when first importing the Ecoinvent database into the $brightway2$ project. Otherwise the database along with all its activities is not subjected to the matching process. This methodology enables a simplified integration of prospective LCA into the EMF-calculation, see *Chapter 3.2.3*.

In case of co-generation units there are separate processes modelled within ISAaR. The processes share the same name but differ with regards to their output EC. The same applies to Ecoinvent activities. The individual activities are matched to their respective equivalent ISAaR process.

3.2.1.2 LCA data from Ecoinvent, conversion required

Certain activities' PSEMFs are calculated based on a different functional unit. Storage processes' PSEMFs are calculated per installed capacity rather than per output EC unit, i.e. unit of discharged energy. A conversion is required to make them applicable for use within the EMF-calculation. PSEMFs must be based on output energy unit to determine a process' production emissions. A separate sheet is introduced into the matching file to separate the matching process between whether a conversion is required. ISAaR processes, whose equivalent activities need to be converted, are defined in this sheet. The matching process is set up in the same way as defined in *Chapter 3.2.1.1*. The conversion to PSEMF's required format is described in *Chapter 3.2.5*.

3.2.1.3 LCA data from other sources

ISAaR processes with no equivalent activity existing within the Ecoinvent database are assigned with LCA data from the academic literature. Data required to execute the matching process is submitted into the same sheet as defined in *Chapter 3.2.1.2*. The matching process is set up in the same way as defined in *Chapter 3.2.1.1*. The conversion to PSEMF's required format is described in *Chapter 3.2.5*.

The matching process is described in detail in *Appendix A.1*.

3.2.2 Regional coverage

3.2.2.1 LCA data from Ecoinvent

Each activity is attributed to a specific location within the Ecoinvent database. LCA data of activities describing the same technology differs due to different assumptions made within different regions. Activities are attributed to locations of varying geographical resolution. Activities are either attributed to specific countries or international regions, e.g. Europe. To set up emission balances with upmost accuracy ISAaR processes are matched with Ecoinvent activities assigned to the equivalent location. The matching process described in *Chapter 3.2.1* is expanded with a parameter describing an ISAaR process' res. an activity's location. ENTSO-E's regions as well as the aggregated ENTSO-E region are modelled within $solidEU$, as described in *Chapter 2.4.2*. Certain activities may not exist within all of $solidEU's$ modelled regions.

ISAaR processes are matched to equivalent Ecoinvent activities attributed to the same region. If an activity is not available for the same region as the modelled ISAaR region the ISAaR process is matched to its equivalent activity within the next highest geographical resolution. A list of backup regions has been introduced to automate this step. The backup regions are obtained from the Ecoinvent database. The list of backup regions contains regions in descending geographical resolution. The defined backup regions are Europe without Switzerland, Rest of Europe, Europe, Rest of World and Global. This methodology enables ISAaR processes to be matched with LCA data of the highest regional accuracy. In case an activity of a lower geographical resolution is matched to an ISAaR process the activity's region is changed to fit the region modelled in ISAaR.

3.2.2.2 LCA data from other sources

In case LCA data is derived from sources other than Ecoinvent the activity is solely defined for the region modelled in the LCA data source. The process of researching activities' LCA data for all regions modelled within $solidEU$ would exceed the context of this thesis. In that case the assumption is made that the researched PSEMF is valid for all regions modelled in $solidEU$. ISAaR processes in all modelled regions are matched to the researched LCA data.

3.2.3 Temporal coverage, Integration pLCA

ISAaR processes are matched to activities of the database defined within the matching file. The database is defined by its name and the year it is valid for. This methodology enables the integration of pLCA into the matching process. Prospective databases contain LCA data describing activities in future years based on assumptions made about future technological development. To integrate pLCA into the matching process prospective databases have to be imported into the $brightway2$ project following the naming convention defined in *Chapter 3.2.1.1*. The python-script was developed towards using Ecoinvent as a LCA data source. $premise$ enables the calculation of prospective databases based on Ecoinvent's LCA data. Prospective databases calculated from $premise$ can be imported into the $brightway2$ project to integrate pLCA within the EMF-calculation. Once prospective databases are imported ISAaR processes can be matched to activities within the prospective database.

In the context of this thesis pLCA is not implemented, but the option of implementation is integrated. The database used within the EMF-calculation is Ecoinvent's database version 3.9.1 using cut-off allocation, whose data is assigned to $solidEU's$ base year 2020. ISAaR processes are matched to activities whose database is modelled for the same year as the matched ISAaR process. If an activity's database is not available within the ISAaR process' year the process is matched to the activity in the most recent year available. $solidEU's$ energy system is modelled in 5-year intervals starting with the base year 2020, see *Chapter 2.4.2*. ISAaR processes in 2020 are assigned to LCA data of the imported database assigned to year 2020. ISAaR processes after 2020 are also assigned to activities from 2020 since LCA data is solely assigned to year 2020.

3.2.4 Adjustment Ecoinvent data – ISAaR

LCA based PSEMFs are calculated from GHG-emissions occurring during a process' lifetime and the process' lifetime EC output, as described in *Equation 15*. Assumptions made during the calculation of LCA based PSEMFs impact the resulting PSEMFs. LCA based PSEMFs need to be adjusted to assumptions modelled within ISAaR to be eligible for use within the EMF-calculation.

Almost all ISAaR processes modelled within $solidEU$ can be matched to LCA data from Ecoinvent. In this chapter the process of adjusting PSEMFs from Ecoinvent to assumptions modelled within ISAaR is described. The adjustment to ISAaR based PSEMFs is performed once the matching process is finished.

3.2.4.1 Operational and Constructional Emissions

A process' lifetime emissions are divided into different life cycle phases. In economic theory a process' lifetime costs are divided into capital and operational expenditure (CAPEX / OPEX). When applying this theory to GHG accounting lifetime emissions are divided into emissions occurring during a process' operating phase (operational emissions) and emissions occurring during the construction phase (constructional emissions).

Technosphere flows are assigned to each activity within the Ecoinvent database. Technosphere flows describe a certain activity's exchange either between the activity and the environment or between two activities. Commonly occurring technosphere flows are:

- Facility construction:
  Facility construction processes are modelled as a separate activities
- Sourcing of fuel
- Sourcing of auxiliary materials (e.g. lubricating oil)
- Sourcing of water
- Transport processes
- Waste treatment
- Demand for electrical or thermal energy

An activity's environmental impact comprises of its assigned technosphere flows' impacts, weighted to one unit of the activity's output EC. An activity's PSEMF comprises of its assigned technosphere flows' LCIA results.

PSEMFs are divided into their constructional and operational part during the adjustment to ISAaR. In addition to calculating an activity's total PSEMF, the activity's constructional PSEMF is calculated by executing a separate LCIA calculation on the technosphere flow describing the activity's construction process. An activity's operational based PSEMF is calculated by the subtraction of the activity's total PSEMF and its constructional part:

$$PSEMF_{EI,Op.}(act, ec_i) = PSEMF_{EI,Tot.}(act, ec_i) - PSEMF_{EI,Constr.}(act, ec_i) \tag{16}$$

ec_i	*Activity $act's$ output EC*
$PSEMF_{EI,Op.}$	*Operational PSEMF*
$PSEMF_{EI,Tot.}$	*Total PSEMF*
$PSEMF_{EI,Constr.}$	*Constructional PSEMF*

The segregation is required to adjust a process' constructional emissions to lifetime assumptions modelled within ISAaR, see *Chapter 3.2.4.6*. Adjustments described in *Chapter 3.2.4* are performed on both operational and constructional PSEMFs, if not mentioned otherwise. A process' adjusted total PSEMF is finally calculated from its adjusted constructional and operational PSEMFs.

The segregation of the total PSEMF into an operational and a constructional part also enables the impact evaluation of integrating specific life cycle phases within the EMF-calculation. Different types of PSEMFs used within the EMF-calculation are defined in *Chapter 3.3.1*.

3.2.4.2 Efficiency Adjustment

The PSEMF calculation methodology described in *Equation 15* can be expressed in more detail. An activity's lifetime emissions are allocated to the respective lifetime output energy flows. An activity's lifetime EC production can be described by the activity's lifetime input energy flow and the activity's efficiency in producing the output EC. The integration of this information into *Equation 15* results in a more detailed description of PSEMF-calculation:

$$PSEMF_{EI}(act, ec_i) = \frac{\sum_{LT} GHG(act, ec_i)}{\sum_{LT} ec_{i,out}(act)} = \frac{a_{EI}(act, ec_i) * \sum_{LT} GHG(act)}{\eta_{EI}(act, ec_i) * \sum_{LT} ec_{in}(act)} \tag{17}$$

a_{EI} *Modelled allocation factor Ecoinvent*
η_{EI} *Modelled efficiency Ecoinvent*
$\sum_{LT} ec_{in}$ *Lifetime EC-input*

An activity's lifetime GHG emissions are allocated to the produced ECs ec_i by means of an allocation factor $a_{EI}(act, ec_i)$. The allocation factor of single output activities results to 1. PSEMFs are calculated from an activity's allocated lifetime GHG emissions and the activity's lifetime EC production.

Process efficiencies modelled within ISAaR differ from efficiencies modelled in Ecoinvent. Certain Ecoinvent activities are assigned with a parameter describing the efficiency assumed during their PSEMF calculation. This parameter is imported in conjunction with the activity's LCA data import. The imported parameter describing the activity's modelled efficiency is used to correct the imported PSEMF. An activity's LCA based PSEMF is corrected by erasing the activity's modelled efficiency from the PSEMF calculation described in *Equation 17*:

$$PSEMF_{EI,eta,Cor}(act, ec_i) = PSEMF_{EI}(act, ec_i) * \eta_{EI}(act, ec_i) \tag{18}$$

$PSEMF_{EI,eta,Cor}$ *PSEMF Ecoinvent → Efficiency corrected*

Modelled efficiencies are available for few Ecoinvent activities only. Activities whose efficiencies are not available cannot be adjusted to the respective ISAaR process' efficiency. Modelled efficiencies are available in case of most emission-intensive activities e.g. electricity production from lignite. The activity's corrected PSEMF is adjusted to matched ISAaR process $dev's$ efficiency during the EMF-calculation:

$$PSEMF_{ISAaR,eta}(t, dev, ec_i) = \frac{PSEMF_{EI,Cor}(act, ec_i)}{\eta_{ISAaR}(t, dev, ec_i)} \tag{19}$$

η_{ISAaR} *Modelled efficiency ISAaR, timestep* t
$PSEMF_{ISAaR,eta}$ *PSEMF Ecoinvent → Efficiency adjusted to ISAaR, timestep* t

Efficiencies modelled within ISAaR $\eta_{ISAaR}(dev, ec_i, t)$ are calculated during the EMF-calculation. The efficiency adjustment is performed for each modelled timestep t since ISAaR's modelled efficiencies are varying over time.

3.2.4.3 Allocation Factor Adjustment

Co-generation processes' emissions should be allocated to produced output ECs according to the allocation methodologies described in *Chapter 3.1.2*. Within the Ecoinvent database co-generation activities' PSEMFs are calculated using a modelled allocation factor as described in *Equation 17*. The modelled allocation factor is removed from imported LCA based PSEMFs to allocate emission according to the allocation methodologies defined in *Chapter 3.1.2*.

Allocation factors modelled during Ecoinvent's PSEMF calculation have been researched and defined within the matching file. Certain co-generation activities' thermal allocation factor are not published within the Ecoinvent database. An activity's thermal allocation factor is calculated from the activitiy's EC specific PSEMFs, the published efficiencies and the electrical allocation factor:

$$\begin{aligned} PSEMF_{EI}(act, el) &= \frac{a_{EI,el}(act) * \sum_{LT} GHG(act)}{\sum_{LT} el_{out}(act)} = \frac{a_{EI,el}(act) * \sum_{LT} GHG(act)}{\eta_{EI,el}(act) * \sum_{LT} ec_{in}(act)} \\ PSEMF_{EI}(act, th) &= \frac{a_{EI,th}(act) * \sum_{LT} GHG(act)}{\sum_{LT} th_{out}(act)} = \frac{a_{EI,th}(act) * \sum_{LT} GHG(act)}{\eta_{EI,th}(act) * \sum_{LT} ec_{in}(act)} \\ \rightarrow a_{EI,th}(act) &= a_{EI,el}(act) * \frac{\eta_{EI,el}(act)}{\eta_{EI,th}(act)} * \frac{PSEMF_{EI,el}(act)}{PSEMF_{EI,th}(act)} \end{aligned} \tag{20}$$

$\sum_{LT} el_{out}$ *Lifetime amount of produced electrical energy*
$\sum_{LT} th_{out}$ *Lifetime amount of produced thermal energy*

The calculation of thermal allocation factors is performed within the matching file. It is not possible to import required data, i.e. the allocation factors, and execute the calculation automatically. The modelled allocation factors are used to correct the imported LCA based PSEMFs by erasing the activity's modelled allocation factors from the PSEMF calculation described in *Equation 17*:

$$PSEMF_{EI,AF,Cor}(act, ec_i) = \frac{PSEMF_{EI}(act, ec_i)}{a_{EI}(act, ec_i)} \tag{21}$$

$PSEMF_{EI,AF,Cor}$ *PSEMF Ecoinvent → allocation factor corrected*

The emission allocation is re-implemented during the EMF-calculation by assigning the calculated allocation factor to the corrected PSEMFs:

$$PSEMF_{ISAaR,AF}(t, dev, ec_i) = PSEMF_{EI,AF,cor}(act, ec_i) * a_{ISAaR}(t, dev, ec_i) \tag{22}$$

$PSEMF_{ISAaR,AF}$ *PSEMF Ecoinvent → Allocation factor adjusted to ISAaR, timestep* t

Allocation factors $a(t, dev, ec_i)$ are calculated during the EMF-calculation. The allocation adjustment is performed for each timestep t due to the fact that a process' allocation factor varies over time.

3.2.4.4 Emissions from Electrical Energy and District Heating

Certain activities, e.g. storage processes, incorporate lifetime electrical or thermal energy input in their LCI. The activities are assigned with a technosphere flow describing the activities' lifetime energy carrier input adjusted to one unit of output EC. The environmental impact of input EC demand is considered during these activities' PSEMF calculation. GHG emissions occurring during the production of required input EC demand are implicitly considered within the EMF-calculation. Environmental impacts linked to input EC demand are accounted twice (double counting) when adopting Ecoinvent's LCA based PSEMFs without adjusting them to the methodology used within the EMF-calculation. Environmental impacts linked to required input EC demand, i.e. electrical and thermal energy, are distracted prevent double counting:

$$PSEMF_{EI,el,th,Cor}(act) = PSEMF_{EI}(act) - TF_{EI}(act,el) - TF_{EI}(act,th) \tag{23}$$

$TF(el)$ *res.* $TF(th)$ *Technosphere flows' environmental impacts describing lifetime electrical res. thermal input energy carrier demand*

3.2.4.5 H_2 Ready Processes

Processes using H_2 as a natural gas substitute are referred to as H_2-ready processes within ISAaR. They are modelled separately from their fossil based reference process. H_2-ready processes differ from their reference process, e.g. gas turbine power plants, by the fact that they are fuelled with H_2. The matching and adjustment process is performed separately for each process.

GHG emissions occurring during the production of required H_2 are implicitly considered within the EMF-calculation, similar to electrical energy and district heating, see *Chapter 3.2.4.4.* An H2-ready process' PSEMF is calculated from the fossil based reference process' PSEMF distracted with the environmental impacts of the process' natural gas demand:

$$PSEMF_{EI,h2ready,cor}(act) = PSEMF_{EI}(act) - TF_{EI}(act,gas) \tag{24}$$

$TF(gas)$ *Technosphere flows' environmental impacts describing lifetime natural gas demand*

3.2.4.6 Lifetime Utilization Adjustment

Modelled lifetime utilizations, i.e. lifetime full-load-hours, vary between ISAaR processes and their matched Ecoinvent activities. Different assumptions in lifetime utilization require the LCA based PSEMFs to be adjusted to ISAaR's assumptions. Operational PSEMFs are independent of lifetime utilization since they are not affected by assumed lifetime utilization. The adjustment to ISAaR's lifetime utilization assumptions is exclusively performed on constructional PSEMFs.

The need for adjusting Ecoinvent data to assumptions modelled within ISAaR is based on the fact that an ISAaR process' assigned constructional emissions are equal to constructional emissions of the equivalent Ecoinvent activity:

$$GHG_{ISAaR,Constr.}(dev) = GHG_{EI,Constr.}(act) \tag{25}$$

$GHG_{EI,Constr.}$	*Constructional emissions Ecoinvent*
$GHG_{ISAaR,Constr.}$	*Constructional emissions Ecoinvent $\rightarrow$ assigned to ISAaR*

Lifetime GHG emissions are calculated from $dev's$ res. $act's$ PSEMF and its lifetime EC production:

$$\begin{gathered} PSEMF_{ISAaR,Constr.}(dev) * (FLH_{ISAaR}(dev) * LT_{ISAaR}(dev) * P_{ISAaR}(dev)) = \\ PSEMF_{EI,Constr.}(act) * (FLH_{EI}(act) * LT_{EI}(act) * P_{EI}(act)) \end{gathered} \tag{26}$$

FLH	*Full Load Hours*
LT	*Lifetime*
P	*Nominal Power: Power plant fleet (ISAaR) / Reference unit (Ecoinvent)*
$PSEMF_{EI,Constr.}$	*Constructional PSEMF Ecoinvent*

Ecoinvent's LCA based PSEMFs are adjusted to ISAaR by rearranging *Equation 26*:

$$\begin{gathered} PSEMF_{ISAaR,Constr.}(dev) = \\ PSEMF_{EI,Constr.}(act) * \frac{FLH_{EI}(act) * LT_{EI}(act) * P_{EI}(act)}{FLH_{ISAaR}(dev) * LT_{ISAaR}(dev) * P_{ISAaR}(dev)} \end{gathered} \tag{27}$$

An region's entire plant fleet is described by one ISAaR process. ISAaR processes describe an aggregation of technological units within their geographical boundaries. When setting up the constructional emission balance in *Equation 26* an ISAaR process' modelled power plant fleet is compared to a reference unit assumed within Ecoinvent. Hence, when adjusting PSEMFs according to the energetic ratio, as described in *Equation 27*, ISAaR based PSEMFs are significantly underestimated compared to Ecoinvent's PSEMFs. This problem is solved by the assumption of equivalent nominal power between ISAaR processes and Ecoinvent activities $P_{EI}(act) = P_{ISAaR}(dev)$. The nominal power is cancelled in *Equation 28* and the adjustment to ISAaR based PSEMFs is performed on the ratio of lifetime utilization:

$$PSEMF_{ISAaR,Constr.}(dev) = PSEMF_{EI,Constr.}(act) * \frac{FLH_{EI}(act) * LT_{EI}(act)}{FLH_{ISAaR}(dev) * LT_{ISAaR}(dev)} \tag{28}$$

$PSEMF_{ISAaR,Constr.}$	*Constructional emissions Ecoinvent $\rightarrow$ LT utilization adjusted to ISAaR*

Data regarding lifetime utilization of ISAaR processes and Ecoinvent activities is required to adjust PSEMFs from Ecoinvent to ISAaR . Ecoinvent activities' lifetime utilization is calculated from data defined within the matching file. Ecoinvent activities' lifetime utilizations have been researched from the activities' descriptions within the Ecoinvent database. ISAaR processes' lifetimes, denoted in years of use, are adopted from [70]. To calculate ISAaR processes' lifetime utilizations the assumption is made that a modelled years' optimization results can be adopted for the following years up to the next modelled year. A process' annual utilization is calculated from its production profile and its installed capacity during the respective year. A process' lifetime utilization is aggregated from the annual utilization starting with the base year until the process' end of life. A new life cycle begins in the year following a process' end of life. Life cycles not finished in the final modelled year are extrapolated to the process' lifetime. The factors $factor\_remaining\_lifetime$ and $factor\_exceeding\_lifetime$ have been implemented to consider remaining lifetimes and the possibility of exceeding lifetimes of ISAaR processes:

$$LT_{ISAaR,Adj.}(dev) = LT_{ISAaR}(dev) * \frac{factor\_exceeding\_lifetime}{factor\_remaining\_lifetime} \tag{29}$$

ISAaR process' lifetime and thus lifetime utilization can be adjusted with these factors. In the context of this thesis both factors have are to 1. Life cycles begin in the respective scenario's base year, i.e. in 2020, and they end in the year a process' end of life is reached.

3.2.4.7 Composition - ISAaR process - LCA activities

ISAaR processes can be composed of different Ecoinvent activities. A process' LCA based PSEMF is calculated from matched activities' adjusted LCA based PSEMFs share-weighted with the composition factor defined within the matching file. When implementing pLCA compositions can be defined independently in the modelled years.

The only process whose technological composition is calculated in a different way is onshore wind. ISAaR does not yield any information about a process' plant fleet. Electricity production from onshore wind is described by a multitude of activities depending on the plant's nominal power assumed within Ecoinvent. The assumption is made that in a scenario's base year ISAaR's entire wind onshore fleet is composed of plants in the range of $1-3\ MW$ nominal power. All installation of onshore wind capacity is attributed to plants with nominal power $> 3\ MW$. The composition of the onshore wind process varies between the modelled years depending on the composition of the onshore wind fleet. Wind onshore's composition is calculated for each modelled year according to:

$$\begin{aligned} Cap_{1-3\ MW,2020} &= Cap_{ISAaR,Tot.}(year = 2020) \\ share_{1-3\ MW}(year) &= \frac{Cap_{1-3\ MW,2020}}{Cap_{ISAaR,Tot.}(year)} \\ share_{>3\ MW}(year) &= \frac{Cap_{ISAaR,Tot.}(year) - Cap_{1-3\ MW,2020}}{Cap_{ISAaR,Tot.}(year)} \end{aligned} \tag{30}$$

$Cap_{ISAaR,Tot.}$	*Total installed wind onshore capacity ISAaR*
$share_{1-3\ MW}$	*Process wind onshore's share assigned to Ecoinvent activity wind onshore* $1-3\ MW$
$share_{>3\ MW}$	*Process wind onshore's share assigned to Ecoinvent activity wind onshore* $> 3\ MW$

3.2.5 Adjustment LCA data from other sources

PSEMFs have to be calculated per unit of output EC in order to be eligible for use within the EMF-calculation. In case PSEMFs are based on different parameters adjustments are made to meet these requirements. Adjustments vary depending on how PSEMFs have been calculated within the LCA data sources. The adjustment methodology is defined within a separate sheet of the matching file, see *Chapter 3.2.1.2* and *Chapter 3.2.1.3*.

Ecoinvent Methodology

This methodology is chosen if an ISAaR process is assigned with LCA data from sources other than Ecoinvent. If PSEMFs are calculated per unit of output EC and assumed lifetime utilization is published within the LCA data source the adjustment is performed according to the methodology used for Ecoinvent activities, as described in *Chapter 3.2.4*.

Storage processes

Storage activities' PSEMFs are calculated from activities' lifetime GHG emissions and their installed storage capacities:

$$PSEMF_{EI}(act) = \frac{GHG_{LT}(act)}{Cap_{inst}(act)} \tag{31}$$

Cap_{inst}	*Installed storage capacity*

Processes' installed capacities and energy production differs between modelled years. The adjustment to ISAaR is performed for each modelled year. The researched PSEMF is adjusted with the process' installed capacity and its total EC output in the 5-year period up to the next modelled year:

$$PSEMF_{ISAaR}(year, dev) = PSEMF_{LCA}(act) * \frac{Cap_{inst,ISAaR}(year, dev)}{\sum_{i=year}^{year+4} E_{out,ISAaR}(i, dev)} \tag{32}$$

$PSEMF_{LCA}$	*Researched PSEMF LCA data source*
$\sum_{i=year}^{year+4} E_{out,ISAaR}(i, dev)$	$Dev's$ *discharged energy during 5-year period up to next modelled year*

Heating element

The researched PSEMF of the activity matched to ISAaR process "Heating element" is calculated from the activity's lifetime GHG emissions and the heating element's assumed nominal power:

$$PSEMF_{LCA,HE}(act) = \frac{GHG_{LT}(act)}{P_N(act)} \tag{33}$$

P_N	*Assumed nominal power LCA data source*
$PSEMF_{LCA,HE}$	*Researched PSEMF: Heating element LCA data source*

The PSEMF is adjusted to ISAaR with the process' rated power and its total EC production in the 5-year period up to the next modelled year:

$$PSEMF_{ISAaR,HE}(year, dev) = PSEMF_{LCA,HE}(act) * \frac{P_{N,ISAaR,HE}(year, dev)}{\sum_{i=year}^{year+4} E_{out,ISAaR}(i, dev)} \tag{34}$$

$P_{N,ISAaR,HE}$ *Modelled installed capacity: Heating element ISAaR*

P2Methane

The activity matched to ISAaR process "Power2Methan" is adopted from [71]. The adjustment to ISAaR cannot be performed due to the fact that required data is not published within the data source. The source's PSEMFs are adopted without further adjustment.

PSEMFs are adjusted according to the defined adjustment methodology. Both PSEMFs and adjustment methodology are defined in a separate sheet within the matching file, as described in *Chapter 3.2.1.2* and *Chapter 3.2.1.3*. When looking at the processes listed within the matching file it can be noted that life cycle emissions of all processes matched to other sources exclusively occur during the constructional phase. Researched PSEMFs are entirely allocated to the constructional based PSEMF.

3.2.6 Missing LCA data

Suitable LCA data was not found during the processing period of this thesis in case of certain processes. The following processes were not assigned PSEMFs during the setup of the emission balance:

- Electricity Grid
- H_2 Network
- H_2 Storage

The non-consideration of assigning these processes with PSEMFs does not mean that ECs obtained from these processes are accounted with zero emissions. Emissions related to electrical energy or H_2 obtained via the electricity grid res. H_2 network are implicitly accounted via the linear equation system. Emissions related to the production of obtained EC are traced through the energy system by means of the energy flows described in Matrix $\underline{\underline{a}}$ and allocated to the region of consumption.

The listed processes' upstream emissions are not considered within the EMF-calculation. Emissions linked to the build-up of the electricity grid and the H_2 network are not considered within the EMF-calculation.

3.3 Hourly consumption based EMF-calculation

The calculation of hourly consumption based emission factors (EMF-calculation) is implemented within a jupyter-notebook. The notebook is based on Python, similar to the script used for the matching and adjustment process.

3.3.1 PSEMF-types

Production emissions are calculated according to the methodology described in *Equation 13*. Production processes are assigned with their PSEMFs to determine processes' production emissions. Different types of PSEMFs are assigned to the processes, depending on which kind of emissions and which life cycle phases should be included within the EMF-calculation. The user performing the EMF-calculation chooses the type of PSEMFs to be used:

CO_2 factors (CO2)

ISAaR processes are assigned with their combustion related fuel specific CO_2 EMF. CO_2 emissions are the only environmental impact considered. CO_2 emissions occuring during a processes' operational phase are exclusively considered. Upstream emissions linked to facility construction (UEC) and fuel supply (UEF) are not considered. CO_2-PSEMFs are imported from FfE's database $FREM$. In the context of this thesis this PSEMF type is referred to as CO2-factors.

CO_2 factors + additional GHG factors (CO2GHG)

A fuel specific GHG emission factor is added to the CO2-factors and assigned to each process. With the inclusion of additional GHG factors environmental impacts other than CO_2 emissions are integrated within the EMF-calculation. GHG-emissions occurring during a processes' operational phase are exclusively considered in this approach. The additional GHG factors are adopted from [70] and imported from $FREM$. In the context of this thesis this PSEMF type is referred to as CO2GHG-factors.

LCA factors with RE processes, CO2 + additional GHG factors with other processes (UECEE)

This PSEMF type was introduced to evaluate the impact of integrating RE's upstream emissions within the EMF-calculation. Adjusted LCA based PSEMFs are exclusively assigned to RE processes. In the context of the EMF-calculation RE processes are defined as energy production from photovoltaic units (PV) and wind turbines. Other processes' operational emissions are considered with the assignment of CO2GHG-factors. In the context of this thesis this PSEMF type is referred to as UECEE-factors.

Constructional PSEMFs + CO2 + additional GHG factors with all processes (UECALL)

This PSEMF type was introduced to evaluate the impact of integrating all processes' upstream emission from facility construction into the EMF-calculation. Adjusted LCA based constructional PSEMFs are assigned to all processes. Operational emissions are considered with the assignment of CO2GHG-factors. In the context of this thesis this PSEMF type is referred to as UECALL-factors.

LCA factors, efficiencies adjusted to ISAaR (LCA_adjusted)

This PSEMF type is employed to calculate LCA based hourly consumption based EMFs, as per the first research question of this thesis. This approach enables the impact evaluation of integrating upstream emissions from fuel supply into the EMF-calculation. All processes are assigned with their adjusted total LCA based PSEMFs to determine the energy system's emissions. Emissions along a processes' entire life cycle to the point of EC supply are considered within the EMF-calculation. In the context of this thesis this PSEMF type is referred to as LCA_adjusted-factors.

LCA factors, efficiencies not adjusted to ISAaR (LCA_not_adjusted)

This PSEMF type was introduced to evaluate the impact of adjusting Ecoinvent activities' efficiencies to process efficiencies modelled within ISAaR. All processes are assigned with their adjusted total LCA based PSEMFs, without implementing the efficiency adjustment described in *Chapter 3.2.4.2*. In the context of this thesis this PSEMF type is referred to as LCA_not_adjusted-factors.

DA factors, efficiencies adjusted to ISAaR (DA_adjusted)

This PSEMF type was introduced to calculate hourly consumption based EMFs according to the DA-methodology described in *Chapter 2.6.3*. The DA-methodology in principle follows an LCA based approach. Processes are assigned with their adjusted total LCA based PSEMFs (LCA_adjusted). All processes' constructional emission are set to zero, as well as RE processes' total emissions to follow the DA-methodology. In the context of this thesis this PSEMF type is referred to as DA_adjusted.

3.3.2 Emissions - FECS demand

To this point production processes are the only emissions source considered within the EMF-calculation. Final energy consumption sectors' (FECS) EC demand has to be incorporated to fulfil the EC balance described in *Chapter 2.4.2*. Emissions resulting from FECSs' EC demand are considered to determine the energy system's total emissions. Emissions from FECSs' EC demand are calculated by assigning EC specific operational EMFs (either CO2 or CO2GHG) to the demand processes:

$$GHG_{ISAaR,FECS}(t, ec_i) = Load_{ISAaR,FECS}(t, ec_i) * emf_{Op.}(t, ec_i) \tag{35}$$

$GHG_{ISAaR,FECS}$	*Emissions occurring from FECS' EC demand*
$Load_{ISAaR,FECS}$	*FECS' EC demand*

FECSs' EC demand is modelled separately for each EC within ISAaR. Electrical energy, district heating and H_2 do not cause GHG-emissions during their operational phase when used as an input EC. Their assigned operational EMFs results to 0. Operational EMFs of biomass, methane and SynFuel differ between the modelled years depending on the share of green EC production in EC's yearly mix, see chapter *Chapter 3.3.3*.

3.3.3 Biomass and Green Fuel processes

In the context of this thesis biomass and ECs produced from P2X-processes are defined as green ECs. In the context of this thesis the assumption is made that green EC's lifetime GHG emissions result to zero. The assumption is based on the fact that emission occurring during the operational phase of EC usage are in balance to captured emissions during EC production. Green ECs are assigned with zero-emissions within the EMF-calculation.

An EC's share of green production is calculated from the amount of green EC supply, composing of green import and green production from P2X processes, related to EC's total supply. The green share is calculated with respect to EC's modelled temporal resolution.

$$sg(t, ec_i) = \frac{\sum_t imp_{green}(ec_i) + P2X(ec_i)}{\sum_t imp_{tot}(ec_i) + prod(ec_{out} = ec_i)} \tag{36}$$

sg *EC's share of green production, calculated in EC's temporal resolution*
$prod$ *Production processes producing res. EC*

Biomass' green share results to 1 since it is defined as a green EC. Other EC's green share increases with increasing deployment of green imports and P2X processes.

The EC-mix impacts a process' emissions exclusively during its operational phase. A process' operational PSEMF is adjusted by distracting emissions related to the process' green EC consumption:

$$PSEMF_{Op.,Adj.}(t, dev, ec_{in} = ec_i) = PSEMF_{Op.}(t, dev, ec_{in} = ec_i) * (1 - sg(t, ec_i)) \tag{37}$$

PSEMF$_{Op.,Adj.}$ *Operational PSEMF: Emissions related to green EC consumption distracted*

3.3.4 Temporal Averaging

ECTs are modelled with either hourly, daily or yearly temporal resolution, as described in chapter *Chapter 2.4.2*. ISAaR processes are modelled in the highest temporal resolution of connected ECTs. ISAaR's energy system optimization is performed with hourly resolution. Hence ISAaR processes are assigned with hourly profiles, i.e. timeseries modelled in hourly resolution. ISAaR processes' profiles (hourly resolution) might differ in resolution from the process' modelled temporal resolution. To adjust ISAaR processes' profiles to their respective temporal resolutions each process is averaged over its temporal resolution. This adjustment is performed during the EMF-calculation once ISAaR data has been imported.

Calculated EMFs have to be adjusted to the respective EC's temporal resolution since EC balances are only fulfilled with regards to their modelled temporal resolutions. Calculated EMFs, calculated in hourly resolution, are adjusted to the respective ECs' temporal resolution. This adjustment is performed ex-post within the notebook.

3.3.5 Implementation - EMF-calculation

The EMF-calculation is implemented within a jupyter notebook using Python as a programming language. When going through the notebook the user is first asked to establish a connection to $FREM$. Once the connection is established the user is asked to define input data required to perform the EMF-calculation. Required input data contains the definition of the scenario whose EMFs should be calculated, the allocation methodology and the PSEMF type to be used within the EMF-calculation, see *Chapter 3.1.2* and *Chapter 3.3.1*. Once required input data is defined the scenario's PSEMFs are calculated and adjusted according to the methodologies described in *Chapter 3.2*. The EMF-calculation is performed once the PSEMF-calculation is finished. ISAaR data required to set up emission balances is automatically imported from $FREM$. Calculation results are averaged, see *Chapter 3.3.4*, and exported to $FREM$. A detailed explanation of the notebook and the how the EMF-calculation is executed can be found in *Appendix A.2*. The procedure of performing the EMF-calculation is displayed in *Figure 7*.

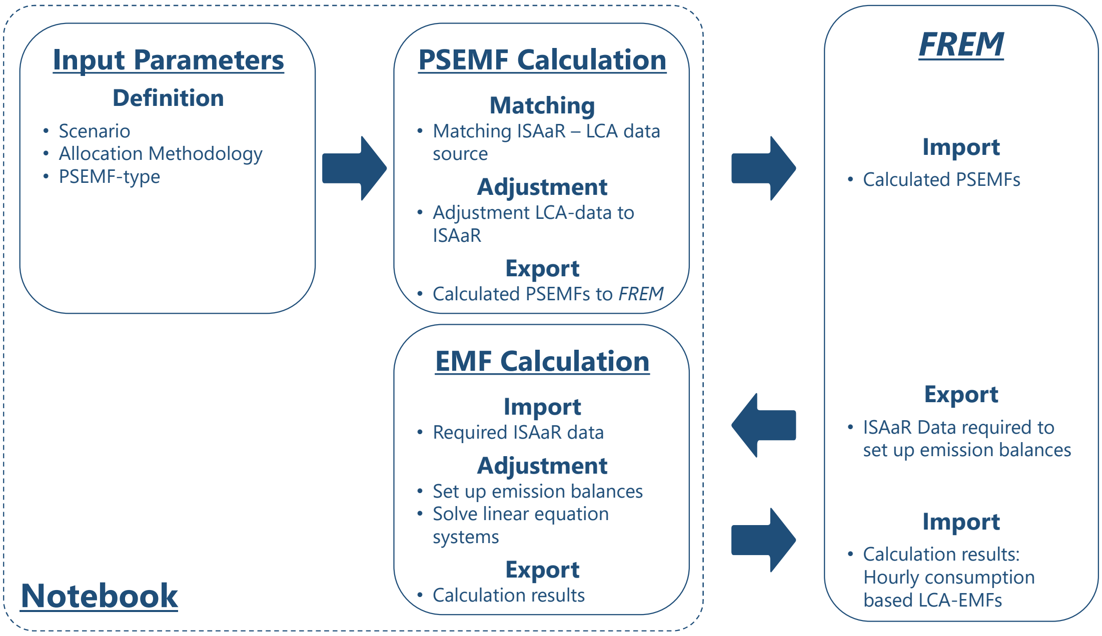

Figure 7: Flow Diagram - EMF-Calculation

The implementation of the methodology is described in detail in *Appendix A.2*.

3.4 Evaluation Green H_2 Production from Electrolysis

The second research question asks for an environmental impact evaluation of H_2 produced from electrolysis. The third research question asks for evaluating differences in the definition of green H_2 according to different regulatory framework. The third research question builds upon the answers obtained from the second research question. As of today the terminology green H_2 is not defined in a standardized way. Regulatory framework for H_2 production used within this thesis is described in *Chapter 2.6.3*. In the context of this thesis green H_2 is solely defined by its carbon footprint.

3.4.1 EMF H_2 Production

H_2 produced from electrolysis is compared to threshold values published in EU-Taxonomy, DA and IRA. Within these frameworks H_2 is defined as green, if produced H_2 causes an environmental impact of max. $3\ \frac{kg\ CO_2e}{kg\ H_2}$, res. $3.4\ \frac{kg\ CO_2e}{kg\ H_2}$, res. $4\ \frac{kg\ CO_2e}{kg\ H_2}$. Differences between the methodologies used to calculate $H_2's$ specific production emissions are explained in *Table 2*.

Electrolysis is a H_2 production process using electrical energy as an input energy source. The environmental impact of H_2 produced from electrolysis is calculated from the environmental impact of the electrical energy used for electrolysis and the electrolyser's efficiency in timestep t:

$$emf_{H_2,electrolysis}(t) = emf_{el}(t) * \eta_{electrolysis}(t)$$
$$\eta_{electrolysis}(t) = \frac{P_{Out,H_2,electrolysis}(t)}{P_{in,el,electrolysis}(t)} \tag{38}$$

$emf_{H_2,electrolysis}$	*EMF H_2 produced from Electrolysis*
$\eta_{electrolysis}$	*Efficiency Electrolysis Process*
$P_{in,el,electrolysis}$	*Electrolysis' energetical input: Electrical energy*
$P_{Out,H_2,electrolysis}$	*Electrolysis' energetical output: H_2*

Electrolysis' upstream emission are considered with the usage of LCA based electrical EMFs. The methodology described in *Equation 38* enables the environmental impact evaluation of the electrolysis process, while considering the process' upstream emissions. Electrical energy's ECT is modelled with hourly resolution within $solidEU$. The EMF-calculation yields electrical energy's EMFs in hourly resolution. As a process connected to electrical energy's ECT electrolysis is modelled with hourly resolution. Hence, the efficiency of the electrolysis process can be calculated with hourly resolution. The efficiency of the electrolysis process is calculated from ISAaR's optimization results describing the process' energetical in- and output flows. The EMF of H_2 produced from electrolysis is also calculated with hourly resolution.

3.4.2 GEA-methodologies - EMF Calculation

The EMF of H_2 produced from electrolysis is directly influenced by the EMF of electrical energy used during the electrolysis process. The EMF-calculation results based on the flow tracing methodology are compared to EMFs calculated according to methodologies from the German Environmental Agency (GEA). GEA's methodologies to calculate EMFs of the German electricity mix are annually published within a report describing the development of German electricity mix' specific GHG emissions. [72]

Electricity Mix

The EMF of the German electricity mix is calculated from direct CO_2 Emissions occurring from electricity production within Germany and the "net amount of electricity available for final energy consumption from the production of electricity in Germany" [72]:

$$emf_{el,Mix} = \frac{CO_{2,el.Prod}}{EL_{Net}} \tag{39}$$

$CO_{2,el.Prod}$	*Direct CO_2 emissions from electricity production*
$EL_{Net,Cons.}$	*Net amount of electricity available for final energy consumption from the production of electricity in Germany*

Production emissions occuring from electricity production are allocated to the produced amount of EC electrical energy. Co-generation units' production emissions are entirely allocated to electrical energy, rather than being allocated to all produced output ECs. Net available electricity for final energy consumption from the electricity production in Germany is calculated from gross electricity production distracted with losses from power plant's on-site consumption, transmission losses and electricity demand from pumping processes. The calculation of net available electricity is mathematically and graphically displayed in *Equation 40* res. *Figure 8*.

$$EL_{Net} = EL_{Gross} - Loss_{PP,onsite} - Loss_{Trans} - Demand_{el.,Pumping} \tag{40}$$

EL_{Gross}	*Gross electricity production*
$Loss_{PP,onsite}$	*Losses from power plant's on-site consumption*
$Loss_{Trans}$	*Transmission losses*
$Demand_{el.,Pumping}$	*Electricity demand from pumping processes*

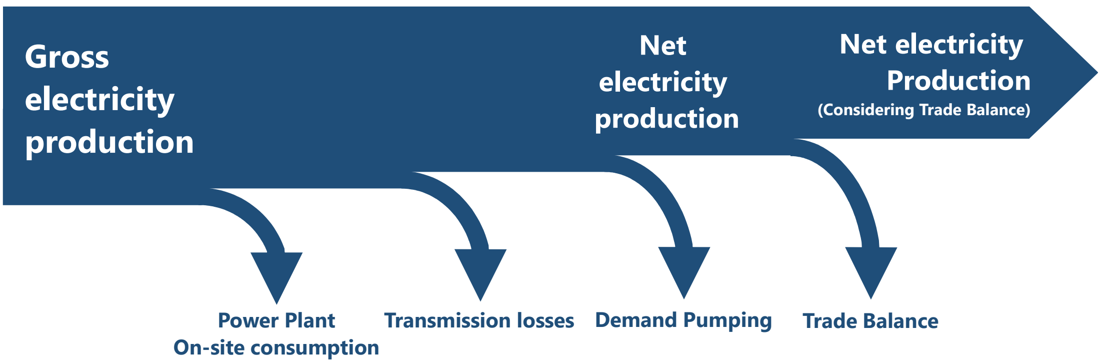

Figure 8: Net Available Electricity for Final Energy Consumption within National Boundaries [72]

In the context of this thesis this methodology is referred to as National Electricity Mix methodology.

Domestic Demand

The EMF of German domestic electricity demand is calculated from direct CO_2 emissions occurring from electricity production within Germany and German domestic electricity demand. German domestic electricity demand is calculated from net available electrical energy within Germany adjusted by the trade balance of electricity in Germany:

$$emf_{el,Domestic} = \frac{CO_2}{EL_{Net} - TB_{el}} \qquad (41)$$
$$TB_{el} = Exp_{el} - Imp_{el}$$

TB_{el} *Trade balance electricity*
Exp_{el} *Electricity exports*
TB_{el} *Electricity imports*

In the context of this thesis this methodology is referred to as Domestic Demand methodology.

Trade Balance

The EMF of Germany's electricity mix considering the German electricity trade balance is calculated from direct CO_2 emissions from electricity production within Germany adjusted with emissions linked to Germany's trade balance and Germany's domestic electricity demand:

$$emf_{el,TradeBalance} = \frac{CO_2 - TB_{el} * emf_{el,Mix}}{EL_{Net} - TB_{el}} \qquad (42)$$

$TB_{el} * emf_{el,Mix}$ *Emissions linked to Trade Balance:*
Interregional trade $\rightarrow$ "exported" res. "imported" emissions

In the context of this thesis this methodology is referred to as Trade Balance methodology.

The GEA applies these methodologies exclusively on German data to annually calculate EMFs of the German electricity mix. CO_2 emissions are the only environmental impact considered by the GEA.

3.4.3 Green H_2 Evaluation Methodology

GEA's methodologies are expanded to an LCA based Cradle-to-Gate approach to follow the requirements of green H_2 production defined in *Chapter 2.6.3*. The expansion to an LCA based approach leads to the inclusion of environmental impacts other than CO_2 emissions within the calculation of electrical energy's EMFs.

The calculation of LCA based EMFs according to GEA's methodologies is performed for every timestep and region modelled within $solidEU$. A region's net amount of electrical energy available for final energy consumption as well as the region's trade balance is calculated from $solidEU's$ optimization results. A region's emissions from electricity production are calculated in the same way as within matrix $\underline{b}$, see *Equation 13*. Co-generation processes' production emissions are entirely allocated to electrical energy. Adjusted LCA factors (LCA_adjusted) are assigned to the production processes to determine LCA based EMFs according to the LCA-methodology, see *Table 2* Classification. Emissions from facility construction and RE demand are adjusted to zero to determine EMFs when applying the DA-methodology. Separate calculations are performed to determine EMFs according to DA- res. LCA-methodology using GEA's methodologies. The methodology used to evaluate green H_2 production from electrolysis according to regulatory framework defined in EU-Taxonomy, DA and IRA is displayed in *Figure 9*.

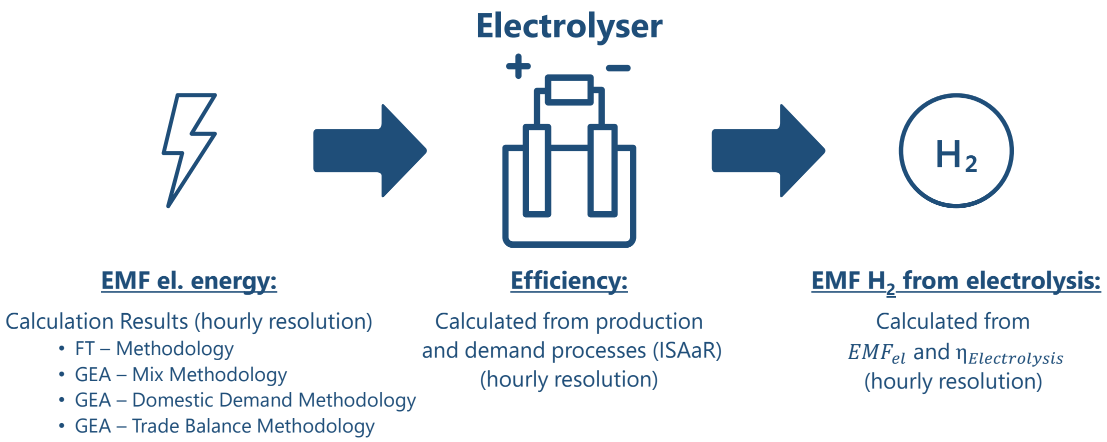

Figure 9: Evaluation: Green H_2 Production from Electrolysis

Chapter 4

Results

Results of the hourly consumption based EMF-calculation are presented, interpreted and evaluated within this chapter. The presented results are based on the $solidEU$ scenario using the carnot allocation methodology.

4.1 Consumption based LCA-EMFs

Hourly and annually resolved consumption based EMFs are presented and interpreted within this chapter. EMFs have been calculated using adjusted LCA based PSEMFs (LCA_adjusted) if not mentioned otherwise. Regions of particular interest are the aggregated ENTSO-E region and Germany.

4.1.1 Annual mean LCA-EMFs

ENTSO-E's annual arithmetic and load weighted mean EMFs are displayed in *Figure 10 a* res. *Figure 10 b*.

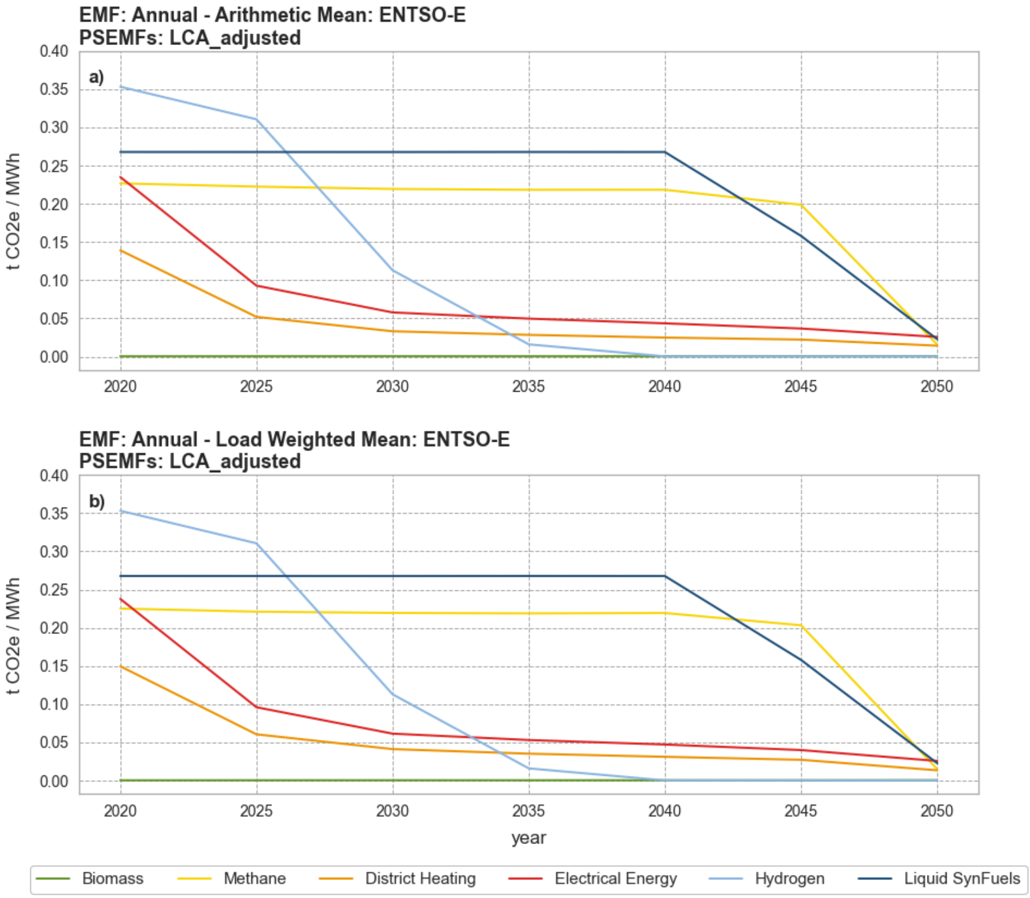

Figure 10: Annual arithmetic (a) and load weighted (b) mean EMFs: ENTSO-E region

The increasing share of RE deployment and sector coupling modelled within later years leads to a decrease of ECs' mean EMFs. Biomass is defined as a green EC and therefore accounted with zero operational emissions, as described in *Chapter 3.3.3*. Biomass' mean EMF is 0 in all modelled years.

Up to the year 2040 ENTSO-E's methane demand is entirely covered by the import of fossil methane. Therefore up to 2040 methane's mean EMF is equal to fossil methane's combustion-related EMF. Methane's mean EMF is decreasing with an increasing share of green methane import starting 2045. In 2050 ENTSO-E's methane demand is entirely covered by the import of green methane. Methane's residual EMF in 2050 is linked to methane production processes' upstream emissions. The conclusions drawn for methane's EMF are also valid for SynFuel's EMF. [50]

Germany's annual arithmetic and load weighted mean EMFs are displayed in *Figure 11 a* res. *Figure 11 b*.

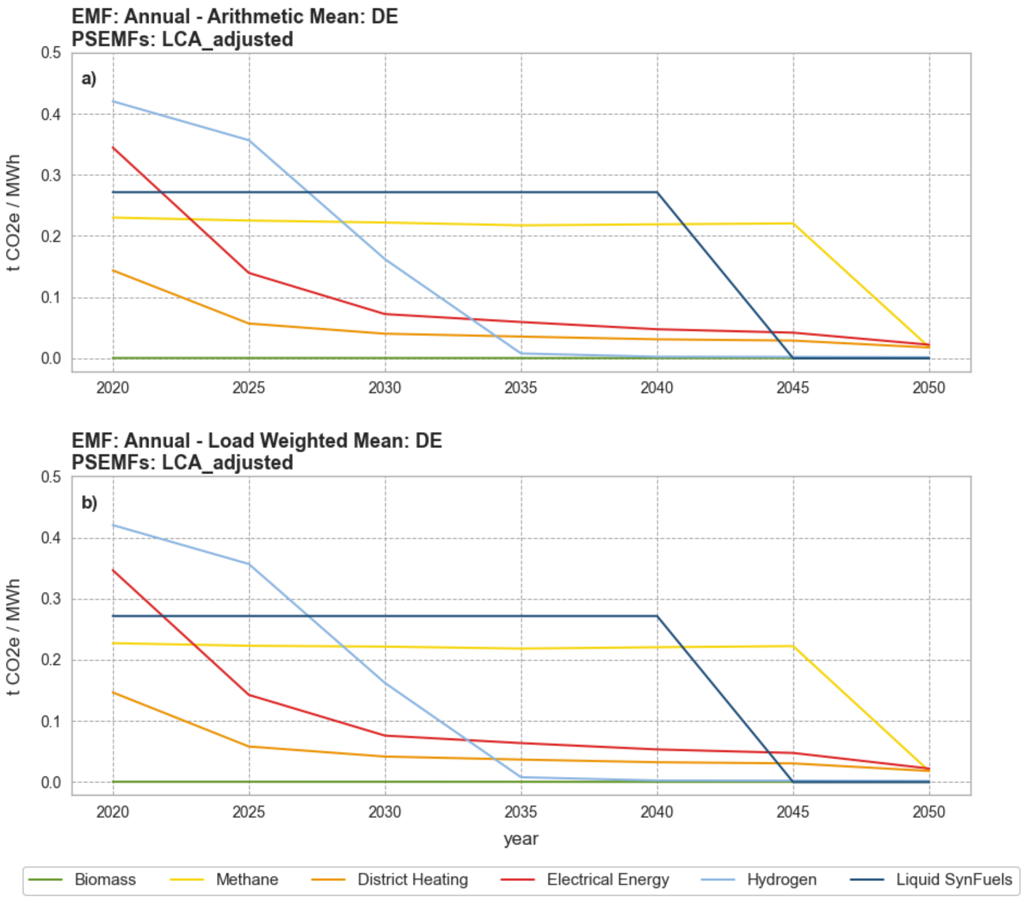

Figure 11: Annual arithmetic (a) and load weighted (b) mean EMFs: Germany

ENTSO-E's EC linkage processes, i.e. sector coupling, and green fuel imports are deployed earlier compared to Germany. The decrease of German methane's mean EMF starts later, i.e. in 2050, compared to ENTSO-E methane's mean EMF, i.e. in 2045. [50]

Up to 2030 German H_2's mean EMF is higher compared to ENTSO-E's mean H_2 EMF. The increased EMFs of H_2 are caused by higher PSEMFs of the steam reforming process, which is the major H_2 production process in both regions until 2030. Higher PSEMFs within Germany result from lower utilization of the process compared to the ENTSO-E region. [50]

From 2045 onwards German SynFuel demand is entirely covered by the import of green SynFuel. Mean EMFs of German Synfuel result to 0 beginning 2045. In 2045 ENTSO-E's SynFuel demand is partly covered by the import of fossil oil and by the import of green SynFuel. In 2050 ENTSO-E's SynFuel demand is covered by green SynFuel import and Power-to-SynFuel processes. ENTSO-E's residual SynFuel EMF in 2050 results from production emissions from Power-to-SynFuel processes, as described in *Chapter 5.3*. [50]

4.1.2 Hourly LCA-EMFs

Hourly consumption based EMFs are presented and interpreted within this chapter. Calculated EMFs are displayed in descending order. EMFs are segregated depending on the EC's modelled temporal resolution. EMFs of ECs modelled with hourly resolution are displayed separately to EMFs of ECs modelled with daily or yearly resolution. Daily and yearly resolution is displayed within the same plot, due to the fact that EMFs of ECs with yearly resolution would yield in a single datapoint otherwise. ECs district heating and electrical energy are modelled with hourly resolution within the looked upon scenario $solidEU$. Methane is modelled with daily resolution, while biomass, H_2 and SynFuels are modelled with yearly resolution.

4.1.2.1 2020

ENTSO-E's res. Germany's hourly consumption based LCA EMFs in 2020 are displayed in *Figure 12* res. *Figure 13*.

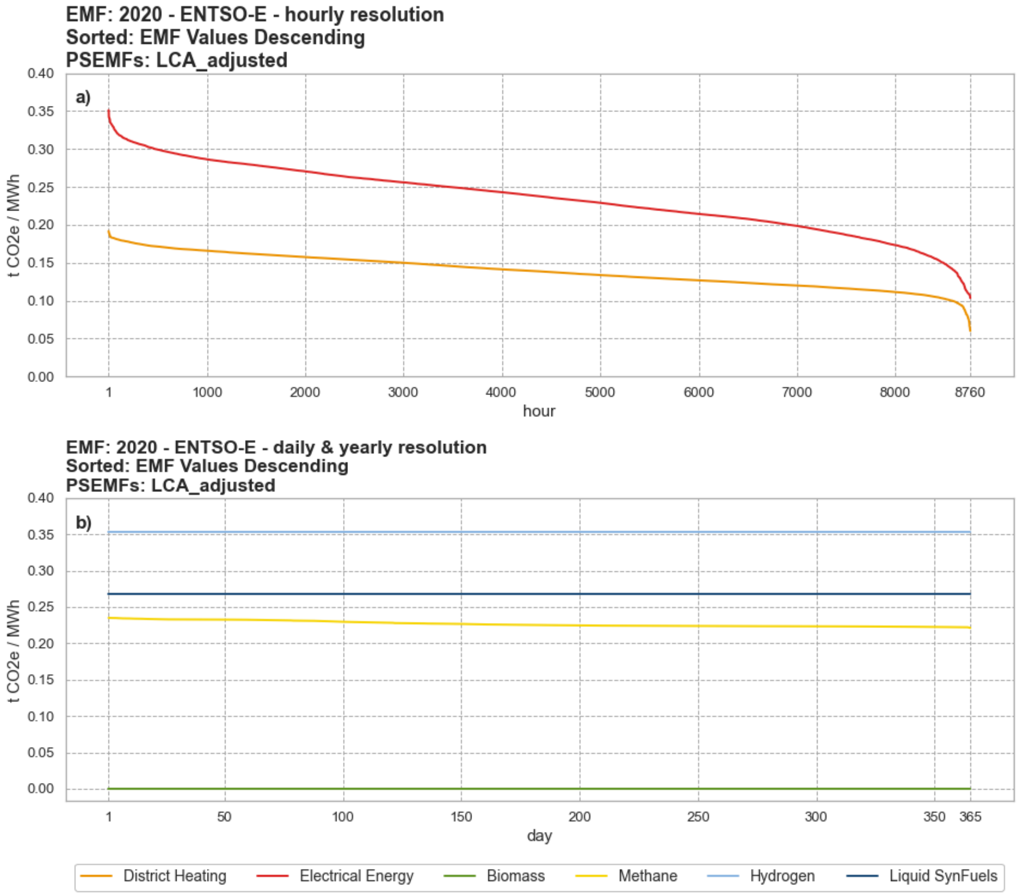

Figure 12: Hourly consumption based LCA-EMFs - ENTSO-E – 2020

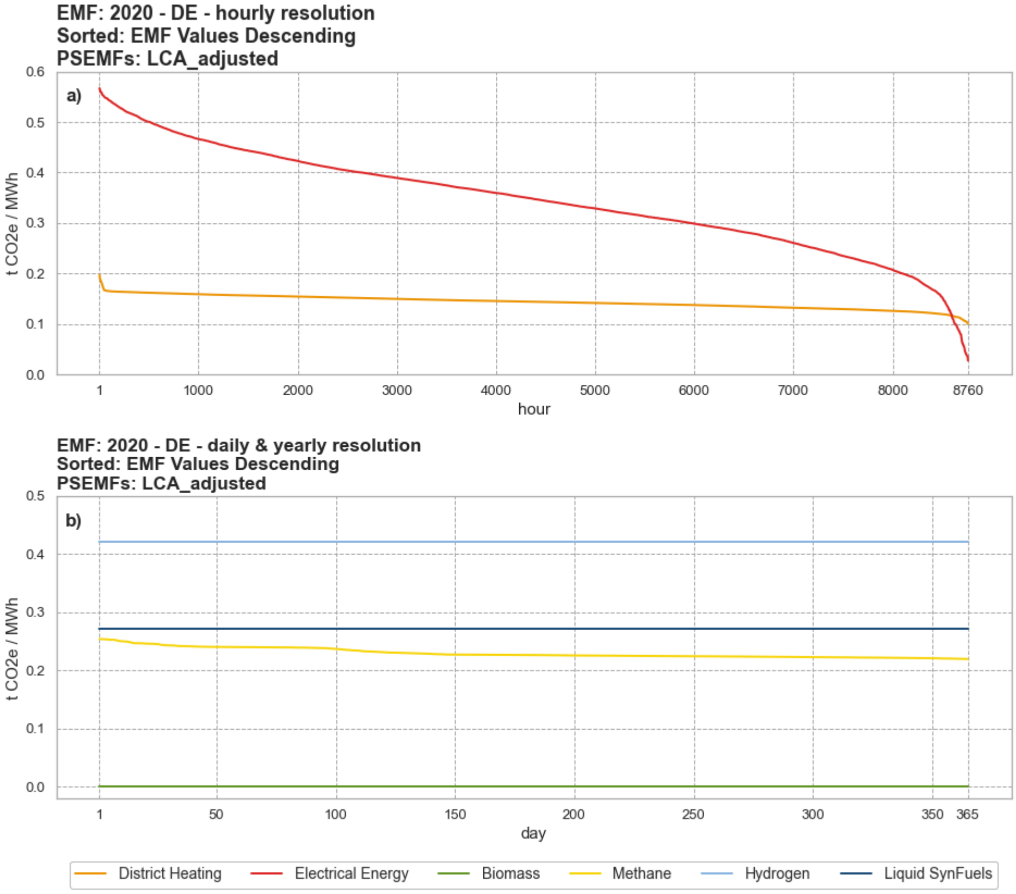

Figure 13: Hourly consumption based LCA-EMFs - Germany – 2020

A balancing effect is identified when comparing EMFs displayed in *Figure 12* and *Figure 13*. The balancing effect emerges from the aggregation of smaller regions to an enlarged region. Electrical energy's EMFs are more extreme within the smaller region Germany compared to the enlarged ENTSO-E region. This is due to higher simultaneity of RE generation occurring within smaller regions. A high simultaneity of RE generation leads to times without any RE generation, as well as times with very high RE generation. Electrical energy demand is entirely covered by fossil generation in times without any RE generation. This results in a drastic increase of electrical energy's EMFs. In times of high RE generation there is little to none fossil generation within the region's energy mix, resulting in a significant decrease of electrical energy's EMFs. When aggregating multiple regions to an enlarged region the aggregated simultaneity of RE generation decreases. Electrical energy demand is neither entirely covered by RE generation nor by fossil generation. Extreme values of electrical energy's EMFs decrease with an enlargement of the assessed region.

4.1.2.2 2050

ENTSO-E's res. Germany's hourly consumption based LCA EMFs in 2050 are displayed in *Figure 14* and *Figure 15*.

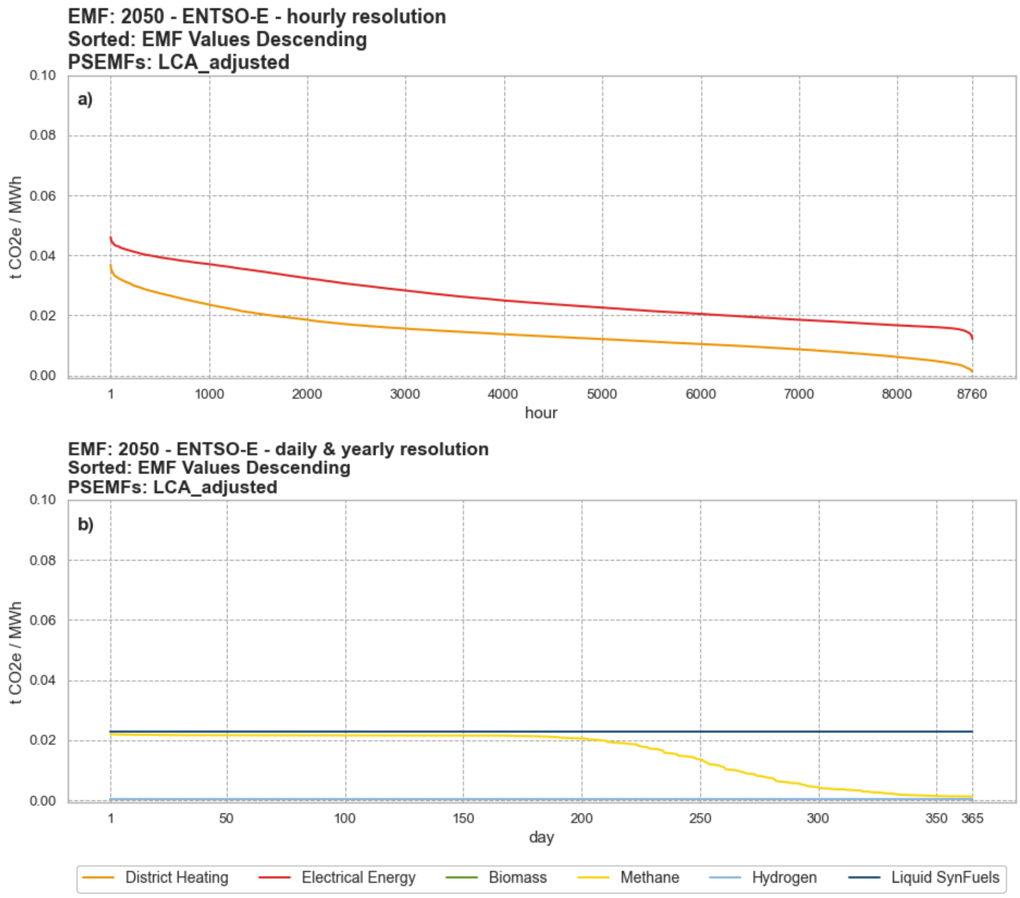

Figure 14: Hourly consumption based LCA-EMFs - ENTSO-E – 2050

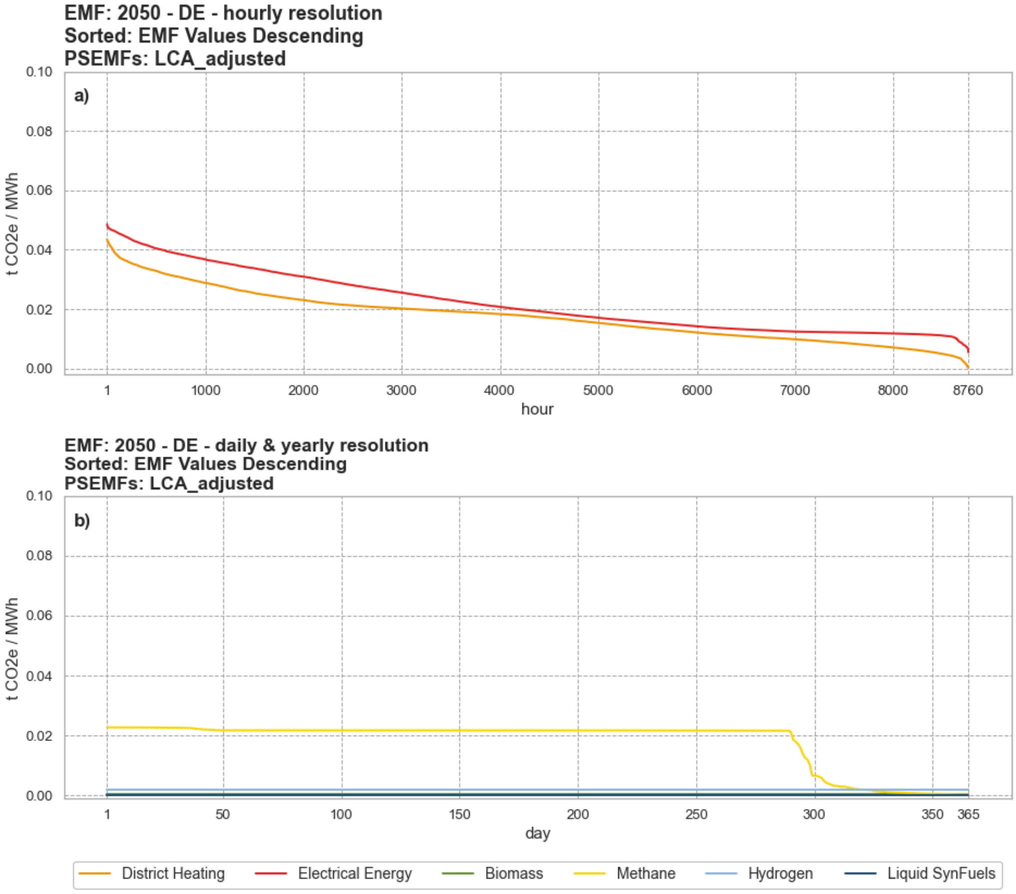

Figure 15: Hourly consumption based LCA-EMFs - Germany – 2050

The decarbonization of the holistic energy system becomes visible when comparing 2020's EMFs displayed in *Figure 12* and *Figure 13* to 2050's EMFs displayed *Figure 14* and *Figure 15*. A strong deployment of RE generation in addition to increasing deployment of sector coupling and interregional trade lead to a significant decarbonization of EC production. In 2050 EC demand is almost entirely covered by RE processes within both assessed regions, both directly and indirectly. Residual EMFs arising in 2050 derive from production processes' upstream emissions UEC and UEF.

4.1.3 Electrical Energy's LCA-EMFs

This chapter focuses on electrical energy's hourly consumption based EMFs. EMFs are presented and interpreted for all regions modelled within $solidEU$. EMFs are displayed both in unsorted and descending order for the years 2020 and 2050.

4.1.3.1 2020

Electrical Energy's EMFs in 2020 are displayed in unsorted res. descending order in *Figure 16* res. *Figure 17*.

Figure 16: EMF Electrical Energy - Unsorted - 2020

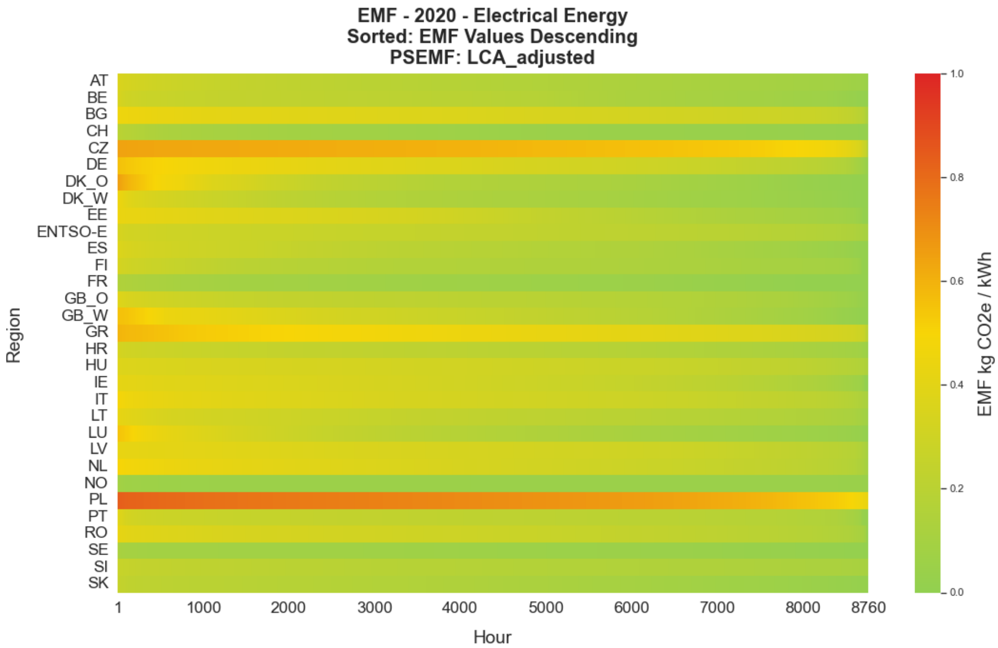

Figure 17: EMF Electrical Energy - Sorted Descending – 2020

Absolute EMFs can be evaluated when analysing sorted results displayed in *Figure 17*. Electrical energy's EMFs are highest in Poland and the Czech Republic. High EMFs result from a major share of electrical energy generation from emission intensive production processes. EMFs are low in times of little fossil based production and high RE generation or in times of high imports from countries with a green energy mix. EMFs are constantly low in countries with a high share of electrical energy production from RE processes, e.g. Norway and Sweden.

Temporal relationships can be evaluated when analysing unsorted results displayed in *Figure 16*. Italy's EMFs are lower during summer season compared to winter. Italy's energy mix in 2020 is significantly influenced from PV generation. PV generation is higher in summer compared to winter season. Hence, Italy's EMFs during summer season are lower than during winter season. The opposing behaviour is asserted when evaluating EMFs of countries, whose energy mix is significantly influenced from wind generation, e.g. Portugal. Wind generation is higher during winter compared to summer season. Hence, EMFs are lower during winter season. Absolute seasonal deviations are comparatively small. This is due to the fact that both wind and PV plants are deployed in all modelled countries. Seasonal effects even out in case both technologies are installed. Seasonal effects can be ascertained in case one technology is deployed to a significant higher extent compared to the other technology. Germany's EMFs do not show significant seasonal effects. In 2020 there is more generation from wind plants compared to PV generation within Germany. Higher generation from wind plants during winter season is compensated with higher absolute demand of electrical energy. Fossil generation is implemented in times of high absolute demand. Hence, the lowering effect on EMFs from wind generation during winter season is counteracted with the integration of fossil generation. [50]

4.1.3.2 2050

Electrical Energy's EMFs in 2050 are displayed in unsorted res. descending order in *Figure 18* res. *Figure 19*.

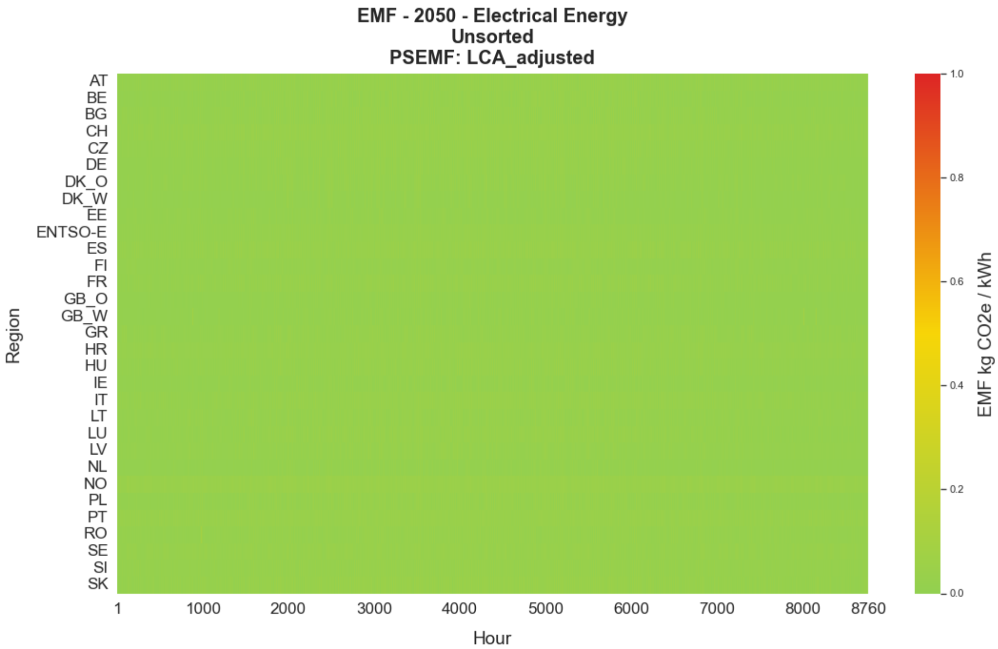

Figure 18: EMF Electrical Energy - Unsorted - 2050

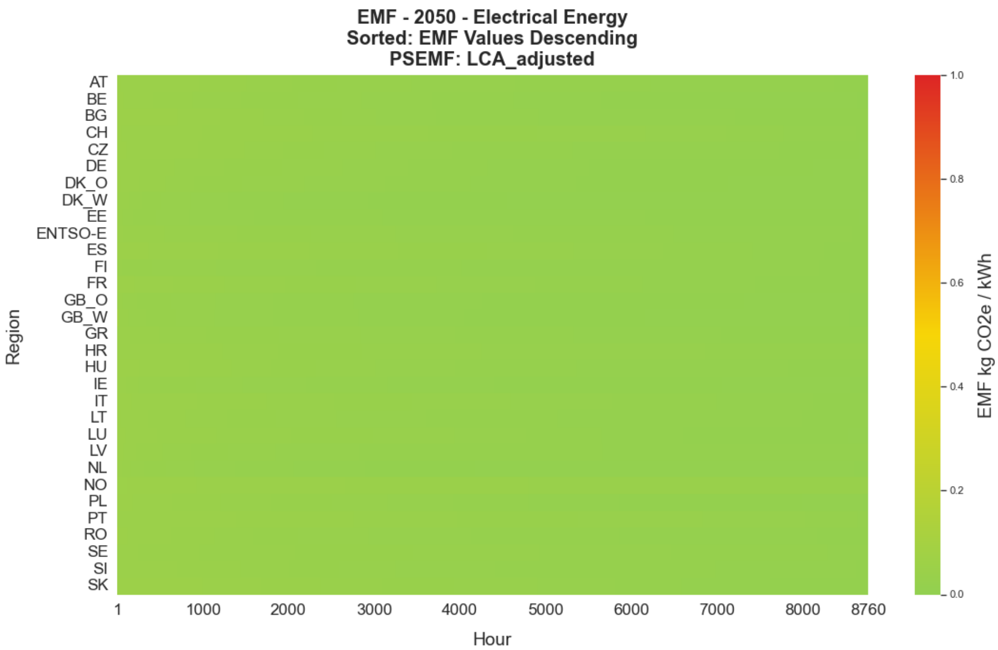

Figure 19: EMF Electrical Energy - Sorted Descending – 2050

In 2050 electrical energy's EMFs are very small in all modelled regions, due to an increasing decarbonization of the holistic energy system, as explained in *Chapter 4.1.2.2*.

4.2 Impact PSEMF-types

From this point onwards German EMF-calculation results are exemplarily presented and interpreted. Most explanations made within the upcoming chapters can also be applied to other country's results.

4.2.1 2020

Consumption based EMFs based on different PSEMF types are compared in *Figure 20*. The comparison displays German electrical energy's calculated EMFs in descending order in 2020.

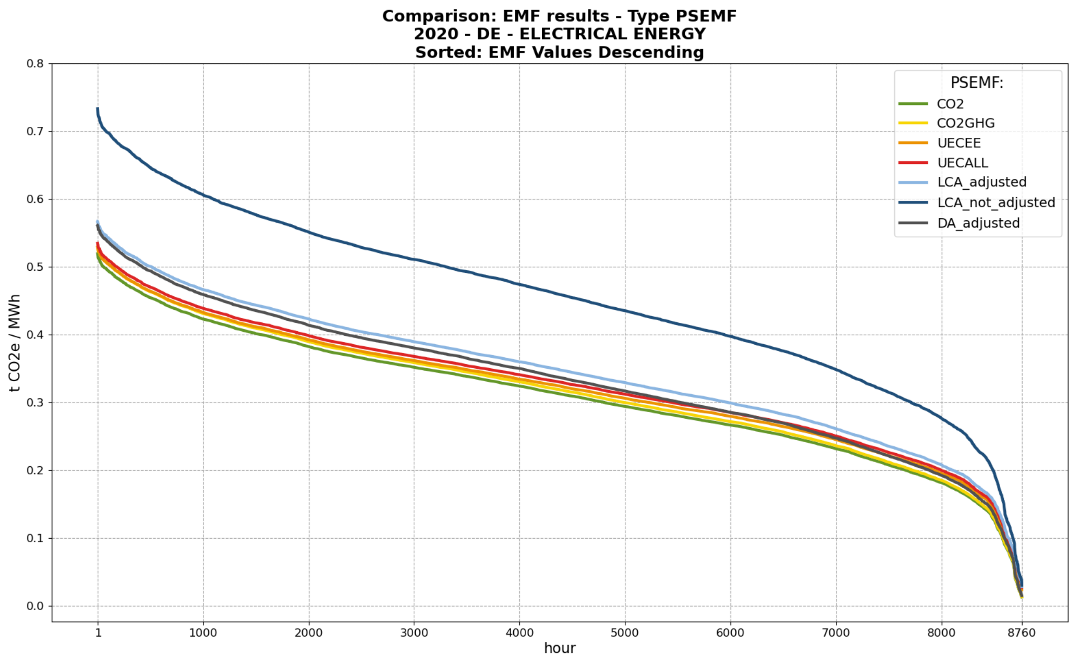

Figure 20: Comparison: EMF Electrical Energy – PSEMF types – Germany- 2020

Calculated EMFs are lowest during times of high RE generation. RE generation is increasing towards the right side of *Figure 20*. Towards the left side of the figure, i.e. in times of little RE generation, an increasing share of electrical energy's demand is covered by fossil generation. Hence, calculated EMFs are increasing towards the left side. The comparison displayed in *Figure 20* enables an impact evaluation of different emission types and different life cycle phases.

The impact of integrating RE's upstream emissions are evaluated when comparing EMFs based on operational GHG-factors, i.e. CO2GHG-factors, to EMFs based on UECEE-factors. The discrepancy between the two graphs displays emissions accounted to RE generation. RE process' emissions solely derive from facility construction. The discrepancy is increasing with increasing RE generation towards the right side of the figure. Emissions accounted to RE generation are directly linked to the amount of RE generation. Thus, emissions accounted to RE generation are increasing towards the right side of *Figure 20*.

The impact of integrating all processes' UEC can be evaluated when comparing EMFs based on LCA_adjusted-factors and EMFs based on DA_adjusted-factors. UEC are not considered by the DA-methodology. The discrepancy between the two graphs describes all processes' UEC. The discrepancy between the two graphs is increasing with increasing RE generation. This is due to the fact that RE processes' lifetime emissions solely derive from UEC. Fossil processes' lifetime emissions mainly occur during the operational phase, i.e. from the combustion of fuel. Therefore the discrepancy is increasing in times of high RE generation, i.e. towards the right side of *Figure 20*.

UEF can be evaluated when comparing calculated EMFs based on UECALL-factors and LCA_adjusted res. LCA_not_adjusted-factors. UECALL-factors consider operational emissions as well as UEC. Fuel supply is not considered by UECALL-factors, but by LCA_adjusted and LCA_not_adjusted-factors. Calculation results based on both LCA-factors i.e. adjusted and not adjusted, are compared to the results based on UECALL-factors to evaluate the impact of adjusting LCA data from Ecoinvent to ISAaR. Calculated EMFs including UEF in average are 39% higher if PSEMFs are not adjusted to ISAaR. If PSEMFs are adjusted to ISAaR the mean increase of calculated EMFs resulting from the inclusion of UEF is 6%. Certain activities' UEF account for up to 40% of the activity's PSEMF [36]. The energy system composes of a multitude of processes, some of whom do not cause any UEF. Hence, the holistic energy system's share related to UEF is significantly lower than the 40% of selected activities. An mean EMF increase of 6% due to the inclusion of UEF is comprehensible. The comparison of calculated EMFs based on PSEMFs adjusted and not adjusted to ISAaR shows the need for adjusting LCA data from Ecoinvent to ISAaR. An average EMF increase of 39% due to the inclusions of UEF is not comprehensible.

4.2.2 2050

Consumption based EMFs based on different PSEMF types are compared in *Figure 21*. The comparison displays German electrical energy's calculated EMFs in descending order in 2050.

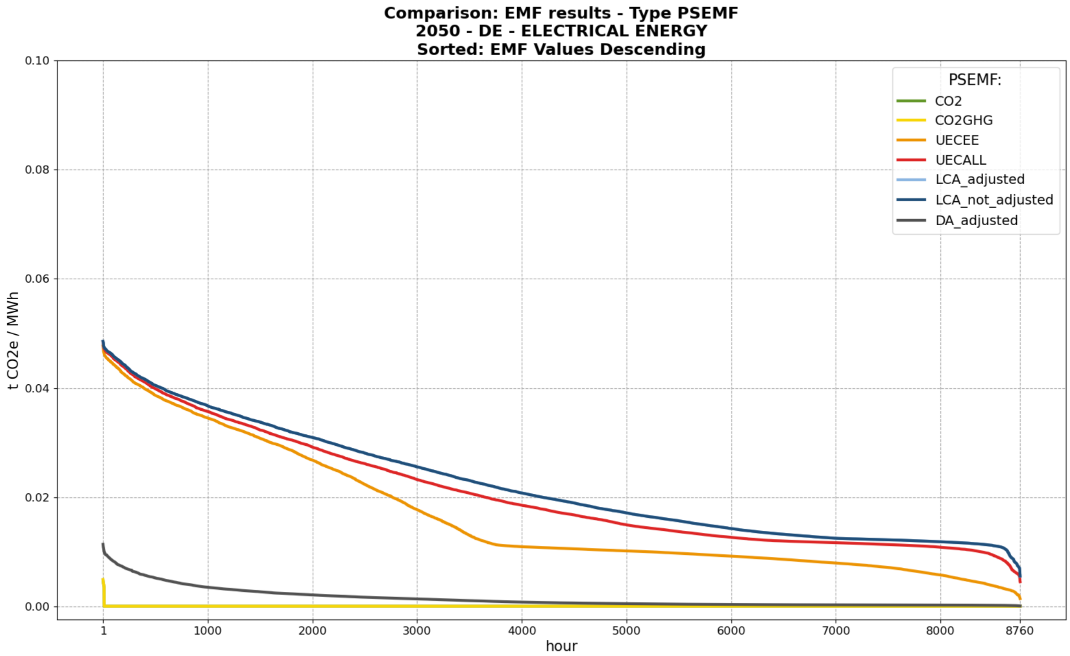

Figure 21: Comparison: EMF Electrical Energy – PSEMF types – Germany- 2050

The calculated EMFs show a significant decarbonization of electrical energy production within Germany in 2050. 81%, res. 14%, res. 2% of German electrical energy demand in 2050 is covered by RE generation, res. imports from European regions, res. thermal power plants. Electrical energy generation from thermal power plants is displayed in *Figure 22*.

Calculated EMFs result to 0 in almost all timesteps if CO2- or CO2GHG-factors are used within the EMF-calculation. Processes' upstream emissions are not considered when using CO2 or CO2GHG-factors. Operational emissions are the only type of emissions considered when applying these PSEMF types. German methane demand in 2050 is entirely covered by the import of green methane [50]. Therefore methane fuelled processes are accounted with zero operational emissions in 2050. Oil fuelled processes are the only electrical energy production process accounted with operational GHG-emissions within the German energy system in 2050. Oil fuelled processes are modelled in few timesteps. EMFs deviating from 0 occur during times with electrical energy production from oil fuelled processes. These EMFs are visualized as spikes occurring in the bottom left corner in *Figure 22*.

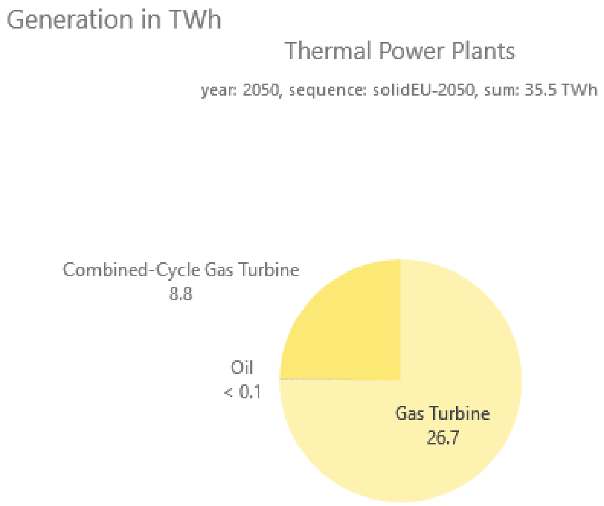

Figure 22: Electricity Production from Thermal Power Plants - Germany - 2050 [50]

Deviations between calculated EMFs based on DA_adjusted and UECEE-factors are attributed to RE processes' UEC. Deviation between EMFs based on UECEE and UECALL-factors are attributed to non-RE processes' UEC.

In 2050 there is no significant difference between calculated EMFs based on LCA_adjusted- and LCA_not_adjusted-factors. This is due to the fact that major emission intensive technologies, e.g. lignite, are not deployed within Germany in 2050, see *Figure 22* [50]. Other electrical energy production processes' PSEMFs are not as strongly influenced by the adjustment to ISAaR. In 2050 the discrepancy between calculated EMFs based on LCA_adjusted res. LCA_not_adjusted-factors decreases to an insignificant amount.

4.3 Green H_2 Production from Electrolysis

The focus of this chapter is on the evaluation of green H_2 production from electrolysis. The evaluation is based on electrical energy's calculated EMFs using adjusted LCA based PSEMFs (LCA_adjusted).

4.3.1 EU-Taxonomy – LCA-Methodology

The amount of green H_2 produced from electrolysis within Germany is displayed in *Figure 23*. Green H_2 is defined according to the regulatory framework published in EU-Taxonomy using LCA-methodology. Flow tracing and GEA's methodologies, see *Chapter 3.4.2*, methodologies have been applied to calculate electricity's EMFs in accordance with LCA-methodology. The percentage above each bar indicates the deviation of that specific bar from the value based on flow tracing within the same year.

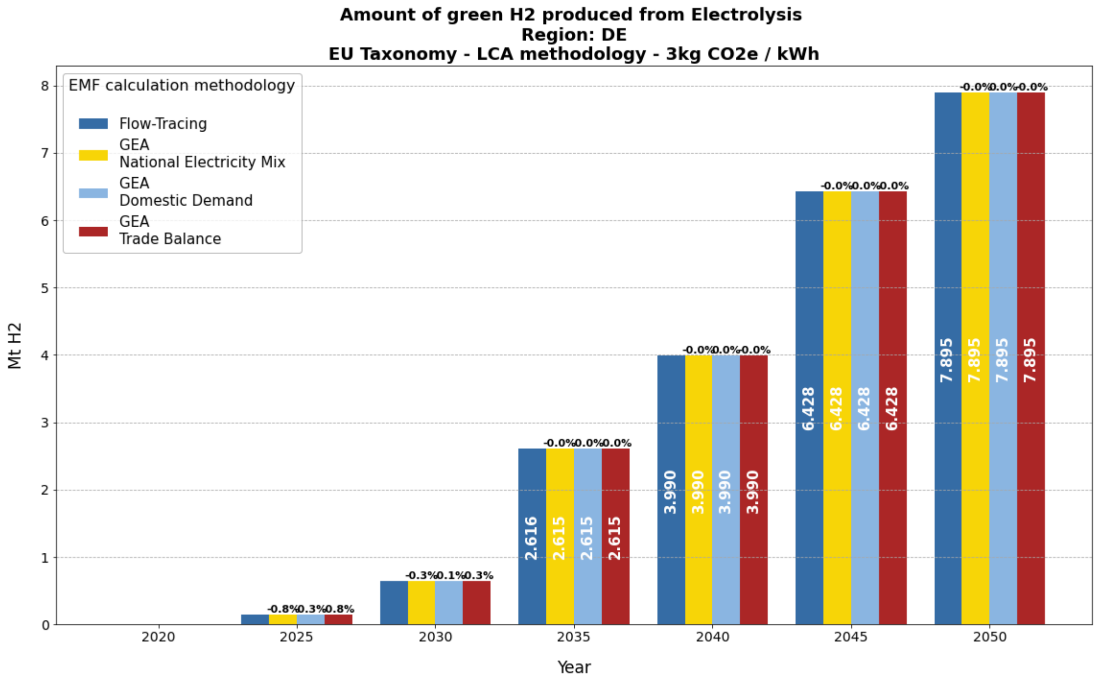

Figure 23: Green H_2 from Electrolysis – Germany – EU-Taxonomy (LCA-Methodology)

ISAaR optimizes the energy system to minimized total system costs. Electrolysis is performed during times of cheap electricity. Electricity prices are low in times of high electricity generation and low electricity demand. This is typically the case during times of peak RE generation. In 2020 RE generation is not deployed to an extent such that electrolysis can be performed economically. An increasing deployment of RE generation leads to an increase in surplus energy, which in turn leads to a higher amount of cheap electricity. Electrolysis becomes more viable during the later modelled years. From 2025 onwards there is enough RE deployment within Germany for electrolysis to be performed economically.

More H_2 is considered green when using flow tracing based EMFs compared to EMFs based on GEA's methodologies. This is due to the fact that within GEA's methodologies emissions from electricity production are entirely allocated to produced electricity. Within the flow tracing methodology emissions from co-generation units are allocated to all produced ECs. Hence, electrical energy's EMFs are higher when using GEA's methodologies compared to flow tracing. This leads to less H_2 considered green when using GEA based EMFs.

Until 2030 Germany is an electricity importing country. This is ascertained by the fact that more H_2 is considered green when evaluating electrical energy's EMFs based on GEA's Domestic Demand methodology compared to GEA's National Mix methodology. This is due to the fact that the German trade balance is negative up to 2030. A negative trade balance occurs in case imports exceed exports. German electricity demand is mostly covered by national RE generation during the later modelled years. The discrepancy between the Domestic Demand and the National Mix Methodology is decreasing towards the later years. From 2035 onwards there is enough RE deployment for the discrepancy to become insignificant.

Absolute deviations between EMF-calculation methodologies are small. Differences between the flow tracing methodology and GEA's methodologies mainly derive from co-generation units' emissions. Within $solidEU$ all co-generation units are fossil based. Electrolysis is mainly performed in times of high RE generation and little fossil generation. During these times there is little generation from co-generation units within the energy mix. Hence, deviations between green H_2 based on flow tracing EMFs and GEA's EMFs are small, i.e. less than 1% in all modelled years. Deviations decrease with increasing RE deployment towards the later years. With increasing RE deployment co-generation units' utilization decreases. Therefore differences between green H_2 based on Flow-Tracing and GEA's methodologies decrease towards the later years. From 2035 onwards there is enough RE deployment for the difference to become insignificant.

4.3.2 Comparison Regulatory Frameworks

The amount for green H_2 produced from electrolysis within Germany is displayed, evaluated and interpreted within this chapter. The evaluation is performed for the years 2025 and 2050. Green H_2 is defined according to all regulatory frameworks presented in *Chapter 2.6.3*. Flow tracing and GEA's methodologies have been used to calculate electrical energy's EMFs according to respective framework's EMF-calculation methodology, i.e. LCA-methodology or DA-methodology. EMFs calculated according to LCA-methodology are referred to as LCA based EMFs, EMFs calculated according to DA-methodology are referred to as DA based EMFs.

4.3.2.1 2025 – Green H_2 Gap

The amount of green H_2 produced from electrolysis within Germany in 2025 is displayed in *Figure 24*. The percentage above each bar represents the deviation of that specific bar from the value based on Flow-Tracing according to the same regulatory framework.

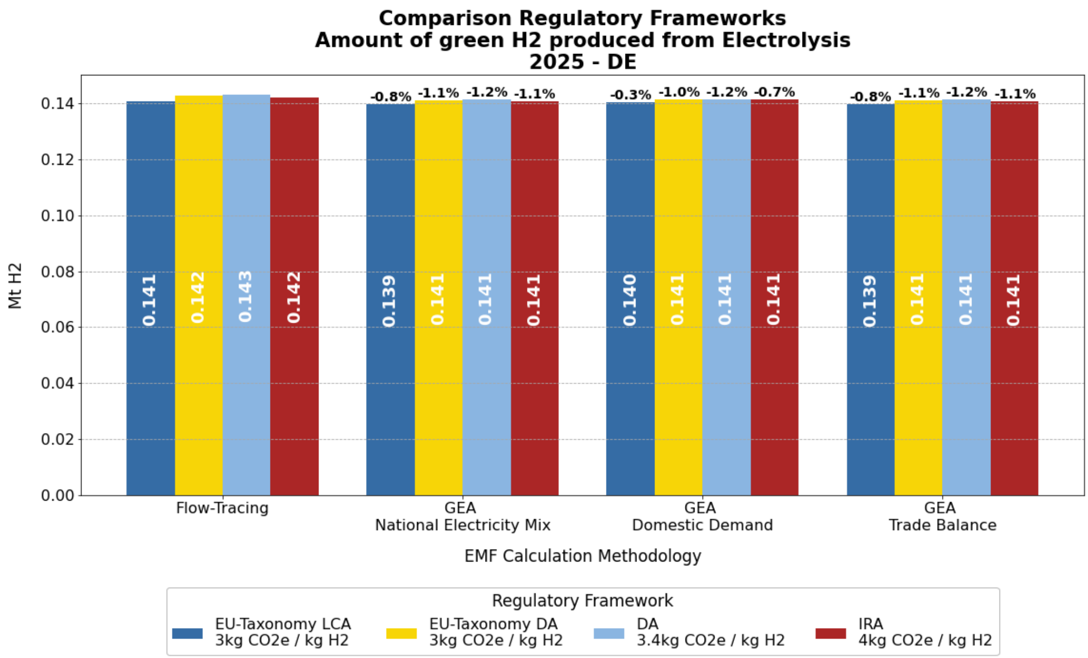

Figure 24: Green H_2 from Electrolysis – Comparison Regulatory Framework – Germany – 2025

Green H_2 production from electrolysis within the ENTSO-E region in 2025 is displayed in *Figure 25* to highlight differences between compared regulatory frameworks.

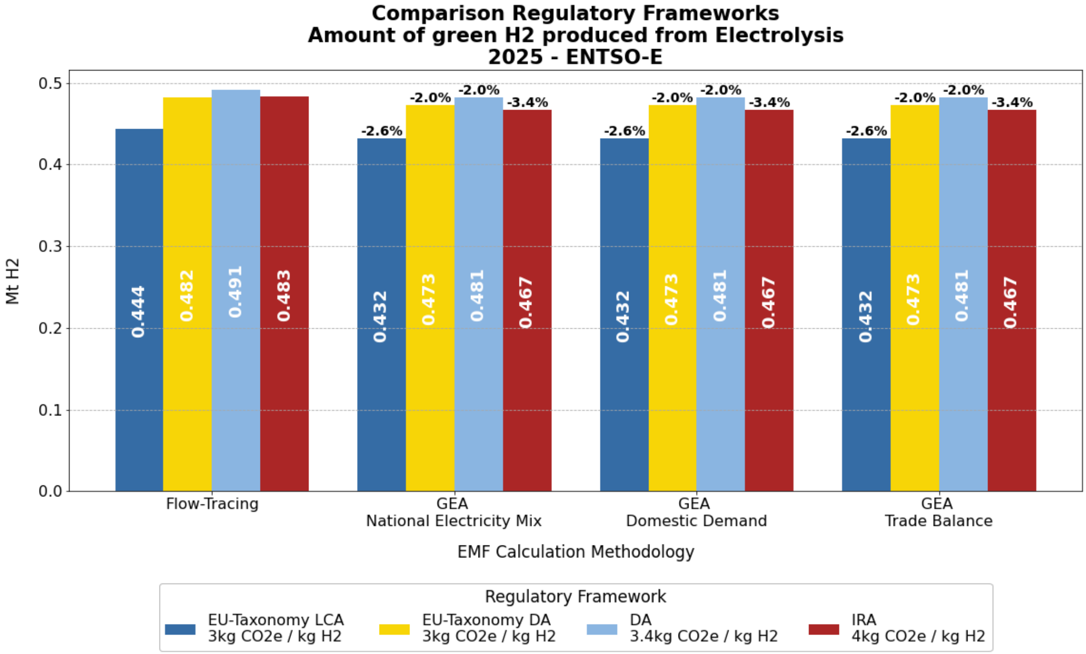

Figure 25: Green H_2 from Electrolysis – Comparison Regulatory Framework – ENTSO-E – 2025

Figure 24 and *Figure 25* allow for a multitude of conclusions to be drawn. The inclusion of emissions from facility construction and renewable electricity (LCA-methodology) has a superior influence compared to higher threshold values of green H_2 production. Less H_2 is considered green according to IRA compared to EU-Taxonomy using DA based EMFs, even though IRA's threshold value of green H_2 production is 33% higher. The inclusion of emissions from facility construction and renewable electricity compensates significantly higher threshold values. The amount of H_2 considered green is highest when applying the regulatory framework presented within the DA and lowest when applying the regulatory framework published in EU-Taxonomy using LCA based EMFs. The high amount of H_2 defined as green according to DA is explained by the fact that UEC are not considered within the methodology, in addition to a high threshold value of green H_2 production. The low amount of H_2 defined as green according to EU-Taxonomy using LCA based EMFs is explained by the fact that UEC are considered, in addition to a low threshold value of green H_2 production.

H_2's average EMFs have been evaluated during times of green H_2 production and during times when H_2 production is not considered green. Additionally, average EMFs have been evaluated during times when H_2 is considered green when using DA based EMFs, but not considered green when using LCA based EMFs. The EMF's share linked to UEC has been calculated. UEC cannot be calculated when using flow tracing methodology. EMFs based on GEA's Trade Balance methodology are displayed in *Table 3*. EMFs of produced H_2 are displayed in the unit $\frac{kg\ CO_2e}{kg\ H_2}$.

	EU-Tax LCA	EU-Tax DA	DA	IRA
H_2 green Avg. EMF H_2	1.19	0.09	0.10	1.21
H_2 green UEC	92.5%	0%	0%	91.9%
H_2 not green Avg. EMF H_2	7.13	6.72	6.92	8.12
H_2 not green UEC	38.3%	0%	0%	35.1%
H_2 green DA H_2 not green LCA Avg. EMF H_2	3.69	0.25	0.25	0.25
H_2 green DA H_2 not green LCA UEC	66.3%	0%	0%	66.3%

Table 3: EMF - H_2 from Electrolysis – Germany – 2025

The following conclusions are drawn exclusively for the results according to EU-Taxonomy's regulatory framework. Average EMFs are lower when using DA based EMFs compared to LCA based EMFs due to the neglect of UEC. When using LCA based EMFs UEC is a characteristic value describing the amount of RE generation within the energy system. This is due to the fact that RE processes' entire lifetime emissions derive from constructional emissions. During times of green H_2 production from electrolysis UEC in average account for 92,5% of electrical energy's EMFs. During times when H_2 production is not considered green the share linked to UEC decreases to 38,3%. This is due to the fact that less RE generation is within the energy system. During times when H_2 production is considered green when using DA based EMFs, but not considered green when using LCA based EMFs UEC account for 66.3% of electricity's EMF. In the context of this thesis this regulatory loophole is referred to as Green H_2 Gap. During times of the Green H_2 Gap there is a mixture of RE and fossil generation within the energy mix. This is assessed by the EMF's mediocre share related to UEC.

In 2025 the Green H_2 Gap occurs in 33 h within Germany. In these 33 hours 1,5 kt of H_2 is produced from electrolysis. This is equivalent to 1% of German H_2 production from electrolysis in 2025. ENTSO-E's Green H_2 Gap occurs in 362 hours in 2025. 40 kt of H_2 is produced in these 362 hours. This is equivalent to 7.6% of ENTSO-E's hydrogen production from electrolysis in 2025.

All modelled region's Green H_2 Gap in the years 2025 and 2050 is displayed in *Appendix A.3*.

4.3.2.2 2050 - Green H_2 Gap

The amount of green H_2 produced from electrolysis within Germany in 2050 is displayed in *Figure 26*. The percentage above each bar represents the deviation of that specific bar from the value based on Flow-Tracing according to the same regulatory framework.

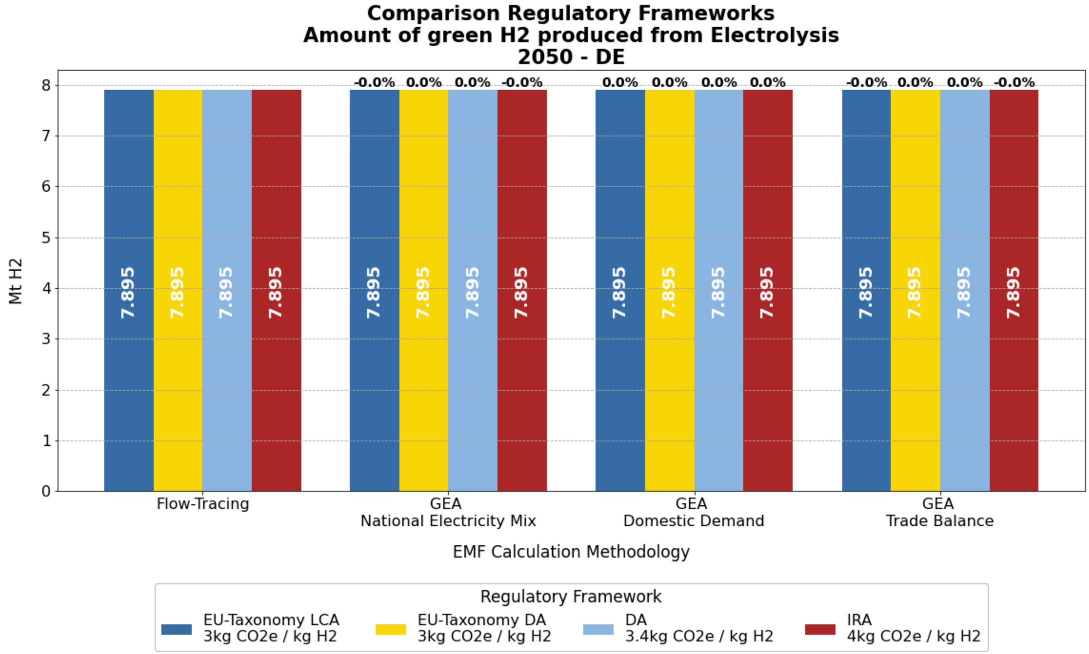

Figure 26: Green H_2 from Electrolysis – Comparison Regulatory Framework – Germany – 2050

In 2050 there is enough RE deployment within Germany for the Green H_2 Gap to disappear. This is ascertained from *Figure 26* due to the fact that green H_2 production does not differ between the applied regulatory frameworks. Deviations between EMF-calculation methodologies disappear in 2050. The disappearance of deviations between EMF-calculation methodologies is explained in *Chapter 4.3.1*.

Chapter 5

Discussion

5.1 Procedure

This thesis asks for three research questions to be answered. The first research question asks for the calculation of hourly consumption based EMFs within a holistic energy system. The EMF-calculation should be based on optimization results from FfE's energy system model ISAaR. LCA methodologies should be applied to integrate upstream emissions from EC production processes. Upstream emissions from facility construction and fuel supply should be considered. This thesis' second research question asks for an environmental impact evaluation of H_2 production from electrolysis based on the calculated hourly consumption based LCA EMFs. The amount of H_2 considered green according to international regulatory framework should be evaluated. This thesis' third research question asks for evaluating differences in the definition of green H_2 between different regulatory frameworks.

The EMF-calculation is based on a methodology adopted from [69]. The adopted methodology has been extended during this thesis' execution:

- Emission balances are set up for each timestep t, region reg and EC ec modelled within the looked upon scenario. An EMF-calculation is performed for each emission balance set up. Therefore the EMF-calculation is automatically performed for each modelled region reg. In [69] the EMF-calculation is exclusively performed for Germany.
- Contrary to the methodology presented in [69] imports are not accounted with a simplified approach. Emissions linked to EC import are accurately calculated from the imported amount of ec with the respective emission factor in region reg' in timestep t: $\sum_{reg'} P_{import}(t, ec, reg, reg') emf_{import}(t, ec, reg')$
- Contrary to the methodology presented in [69] charging processes, both charging and discharging, are considered. Charging processes are considered as additional demand of ec_i in region reg_j within the term: $\sum_{dev} \sum_{ec'} P_{in}(dev, t, ec, ec', reg)$. Discharging processes are implicitly considered in ISAaR's optimization results. Power generation and linked emissions are reduced during storage system's discharges.
- Carnot allocation factors are calculated in hourly resolution according to ISAaR's optimization results. In [69] annual average carnot allocation factors are used.

LCA-data is integrated into the EMF-calculation with the assignment of LCA based PSEMFs. PSEMFs describe a process' specific environmental footprint linked to the production of one unit of output EC. LCA data is adopted from the LCI database Ecoinvent and academic literature. LCA data is based on the life cycle model Cradle-to-Gate. A process' life cycle is defined from the point of raw material extraction to the point of supplying one unit of output EC. Therefore PSEMFs can be assigned to ISAaR processes' production profiles to determine LCA based production emissions. Most ISAaR processes' assigned LCA data is derived from Ecoinvent. ISAaR processes are matched to LCA data of the highest spatial and temporal resolution. LCA data is adjusted to ISAaR to be eligible for use within the EMF-calculation. Adjustments are made with regards to process efficiency, allocation factors, lifetime utilization and emissions linked to sourced input energy carriers, i.e. electrical energy, thermal energy and natural gas. LCA data from other data sources than Ecoinvent is matched and adjusted to ISAaR processes using individual methods.

The calculated hourly consumption based LCA-EMFs are evaluated ex-post. The evaluation enables a multitude of conclusions to be drawn. Calculated EMFs are evaluated within a modelled region to assess correlations between the region's energy mix and its EMFs. Calculated EMFs are evaluated in different years to investigate the impact of energy system transformation on the calculated EMFs. The impact of including different emission types and different life cycle phases is evaluated with a comparison of EMFs based on different PSEMF types.

Green H_2 production from electrolysis is evaluated based on electrical energy's EMFs calculated from flow tracing and GEA's methodologies. In the context of this thesis H_2 is defined as green based on its carbon footprint and threshold values defined in regulatory frameworks. Differences in the amount of H_2 considered green are asserted based on different EMF-calculation methodologies.

5.2 Findings

The first research question has successfully been answered with the calculation of hourly consumption based LCA EMFs. Calculated EMFs are highest in countries with a high share of energy production from fossil fuels. In 2020 highest EMFs arise in Poland and the Czech Republic. EMFs are lowest in countries with a high deployment of RE. Seasonal effects are asserted when evaluating electrical energy's LCA based EMFs. EMFs decrease with increasing RE deployment and sector coupling towards the later modelled years.

The need for adjusting LCA-data from Ecoinvent to assumption modelled within ISAaR has been proven. German electrical energy's EMFs in 2020 increase by 39% due to the inclusion of UEF if LCA data is not adjusted to ISAaR. The mean increase is reduced to 6% if LCA data is adjusted to ISAaR. A mean EMF increase of 6% due to the integration of UEF is comprehensible, while a mean increase of 40% is not reasonable. LCA data's adjustment to ISAaR is especially important in years and regions with a high share of fossil fuel based generation. The difference between adjusting and not adjusting LCA data to ISAaR becomes insignificant if energy demand is entirely met by RE or green fuels, e.g. Germany in 2050.

The second research question has successfully been answered with the evaluation of green H_2 production from electrolysis in Germany in 2025. It has been asserted that the least amount of H_2 is considered green when applying the threshold values from EU-Taxonomy using LCA based EMFs. The low amount of H_2 defined as green according to EU-Taxonomy using LCA based EMFs is explained by the fact that holistic life cycle emissions are considered, in addition to a low threshold value of green H_2 production. Less H_2 is considered green according to IRA compared to EU-Taxonomy using DA based EMFs, even though IRA's threshold value of green H_2 is 33% higher. The inclusion of UEC has a superior influence compared to a significantly higher threshold value of green H_2 production defined in IRA. More H_2 is considered green when using DA based EMFs compared to LCA based EMFs regardless of the threshold values.

The third research question has been answered with the assessment of the Green H_2 Gap. The Green H_2 Gap decreases with increasing RE deployment. In 2025 there is enough RE deployment in Germany for the Green H_2 Gap to occur for 1% of German H_2 production from electrolysis. In 2025 1.5 kt H_2 produced from electrolysis in Germany are defined as green according to DA-methodology, but are not defined as green according to LCA-methodology. The Green H_2 Gap increases to 7,6% of ENTSO-E's H_2 production from electrolysis, res. 40.5 kt H_2, if ENTSO-E's results are evaluated.The unrestricted choice of the accounting methodology according to EU-Taxonomy represents a significant loophole in the declaration of green H_2.

5.3 Outlook

Several problems have arisen during the execution of this thesis. The arosen problems in addition to possible solutions are described within this chapter.

Matching Process

The matching process is implemented for almost all ISAaR processes occurring within the looked upon scenarios $solidEU$ and $BMWStart$. The processes describing electricity grid, H_2 network and H_2 storage could not be matched to equivalent LCA data. These processes' UEC are not yet considered within the EMF-calculation. This thesis can be extended by assigning LCA data to unmatched processes.

Different scenarios might consider ISAaR processes not implemented within the looked upon scenarios $solidEU$ and $BMWStart$. The matching process has to be expanded in case different scenarios should be calculated. Unmatched ISAaR processes implemented within the scenario to be calculated have to be matched to LCA data. This process is described in *Appendix A.1*.

LCA data from sources other than Ecoinvent is assigned to the matched ISAaR process within all modelled regions. LCA data from sources other than Ecoinvent has been researched manually. LCA data has been researched for selected countries due to the restricted amount of time for executing this thesis. The matching process can be further improved if ISAaR processes are matched to LCA data of equivalent regions. LCA data has to be researched for every region an ISAaR process is modelled for. This problem might be solved with future updates of the Ecoinvent database, i.e. added activities. ISAaR processes currently matched to LCA data from other sources could be matched to Ecoinvent data if equivalent activities become available within the Ecoinvent database. In that case the matching file has to be updated to match the ISAaR processes to the newly added Ecoinvent activities.

pLCA can be integrated in future work built upon this thesis. The methodology for integrating pLCA into the matching process has been implemented in the context of this thesis. The methodology for integrating pLCA into the EMF-calculation is described in *Chapter 3.2.3*.

Storage Processes

Storage processes are a key point of improving the EMF-calculation in future work. A methodology could be developed to store EMFs during the charging process and assign them to discharged ECs. This methodology has not been implemented as of today.

Double Counting

The problem of double counting has not entirely been resolved during the execution of this thesis. A methodology was developed to remove activities' environmental impacts from input energy demand is described in *Chapter 3.2.4.4* and *Chapter 3.2.4.5*. Environmental impacts from an activity's electrical energy, thermal energy or natural gas demand are removed from the activity's PSEMF-calculation since they are already accounted within the EMF-calculation. This methodology prevents double counting in case of an activity's top-level technosphere flows. Double counting still occurs within an activity's facility construction process since the construction process, modelled as a separate activity, is a technosphere flow of the activity itself. The construction process' input energy demand is assigned to the construction process, which in return is assigned to the looked upon activity. The input energy demand of an activity's construction process is not removed since it is not directly assigned to the looked upon activity. The energy demand linked to an activity's construction process is accounted twice in case the input energy demand is derived from regions modelled within the looked upon scenarios. In that case an activity's construction process' input energy demand from region reg_j is also accounted as EC demand in region reg_j within the EMF-calculation. A methodology to solve this problem has been developed during the final stage of this thesis. Environmental impacts linked to an activity's construction processes' input energy demand are removed within the methodology. Environmental impacts are exclusively removed in case the input energy demand is derived from regions modelled within the looked upon scenario. As of today the methodology has not been applied yet.

ISAaR's System Boundaries

The demand of Biomass, Methane and SynFuel is partly covered by the import of either fossil or green fuel from outside ISAaR's system boundaries. These ECs are referred to as non-modelled ECs, see *Figure 5*. Non-modelled ECs are accounted with emissions occurring during their operational phase, i.e. they are assigned with either CO2 or CO2GHG-factors.

Fuel imports cause production emissions within the exporting region. Emissions linked to the production of exported EC demand might compound of UEF, UEC, fuel combustion during production processes and linked energy carriers, e.g. P2X processes. Production emissions cannot be determined in case of non-modelled ECs due to the absence of information on how the exported amount of EC has been produced. Therefore production emissions cannot be assigned to the importing region. Non-modelled EC import is accounted with its operational emissions. Operational emissions from non-modelled EC import result to 0 in case the region's EC demand is entirely covered by green import or P2X processes. Production emissions resulting from a region's P2X processes are assigned to the region's EC demand. Production emissions compose of UEC, UEF and operational emissions. This raises the problem that regions with a strong deployment of P2X processes are handicapped compared to regions solely relying on non-modelled green EC imports.

This problem is asserted when comparing SynFuel EMFs displayed in *Figure 10* and *Figure 11*. In 2050 German SynFuel demand is entirely covered by green SynFuel import, while ENTSO-E's SynFuel demand is partly covered by Power-to-SynFuel processes. Both regions' 2050 green share of SynFuels results to 1 and operational emissions of SynFuel-fuelled processes result to 0. ENTSO-E's 2050 SynFuel demand is assigned with emission from Power-to-SynFuel processes within the ENTSO-E region. In 2050 Germany's mean SynFuel EMF results to 0, while ENTSO-E's mean SynFuel EMF deviates from 0. This deviation is entirely linked to ENTSO-E's Power-to-SynFuel process' UEC.

The problem arises due to the fact that certain ECs are not modelled within ISAaR's system boundaries. Non-modelled ECs' production emission cannot be determined due to the absence of information on how the exported EC amount has been produced. Furthermore trade infrastructure is only modelled for ECs electrical energy and H_2 within ISAaR. Even if non-modelled ECs production emissions could be determined they cannot be traced to the consumption region due to the absence of trade infrastructure. These problems are linked to the setup of ISAaR and cannot be solved within the EMF-calculation. The problems are automatically resolved if non-modelled ECs and additional trade infrastructure is integrated into ISAaR.

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Appendix A

Appendix

A.1 Matching Process

ISAaR processes are matched to equivalent Ecoinvent activities if equivalent Ecoinvent activities exist. ISAaR processes are assigned with their matched activities' LCA-data, i.e. PSEMFs stored within the Ecoinvent database. The process of assigning matched LCA data to ISAaR processes is based on data defined within the matching file $matching\_LCA\_to\_ISAaR.xlsx$. ISAaR processes are defined according to their identification specified within ISAaR, i.e. by their id_isaar_typ and $isaar\_typ$. The parameter id_isaar_typ is referred to as dev within the matching file. An Ecoinvent activity is defined by its $name$ as specified within the Ecoinvent database and the activity's output EC. The output EC is set in column id_et according to ISAaR's energy carrier identification:

- id_et = 7: Biomass
- id_et = 21: Methane
- id_et = 71: District Heating
- id_et = 72: Electrical Energy
- id_et = 162: Hydrogen
- id_et = 222: SynFuels (= Liquid Hydrocarbons)

In case LCA-data is obtained from Ecoinvent the activity definition is expanded with the definition of the database the activity is imported from. Prior to executing the matching process, it is necessary to import the relevant Ecoinvent databases into $brightway2$. The name of the database an activity is imported from must contain the values defined in columns $year$ and $scenario$. Processes whose matched activities do not require a PSEMF conversion are defined in sheet $EI\_data\_no\_conversion$. Co-generation processes are matched based on data submitted in sheet EI_data_CHP. The segregation of matching processes within the matching file is due to the fact that co-generation activities' allocation factors cannot be exported automatically. Allocation factors and process efficiencies are required to adjust co-generation activities' LCA-data to assumptions modelled within ISAaR. Allocation factors and process efficiencies have been researched and submitted into sheet EI_data_CHP. The adjustment of co-generation activities' LCA-data is based on data submitted into this sheet. ISAaR processes are matched to their equivalent Ecoinvent activities within the respective sheet.

In case LCA-data is obtained from different sources the activity's $name$ can be set without restrictions. An activity's output EC is defined in column id_et according to ISAaR's energy carrier identification. An activity's LCA data, i.e. the activity's PSEMFs, is defined in columns emf_tot, emf_constr and emf_op. The conversion methodology to convert the activity's PSEMFs to the format required within the EMF-calculation is defined in column $conversion\_methodology$. LCA data from sources other than Ecoinvent is defined in sheet $EI\_data\_conv\_other\_sources$.

The entire process of matching LCA data to ISAaR processes is schematically displayed in *Figure 27*.

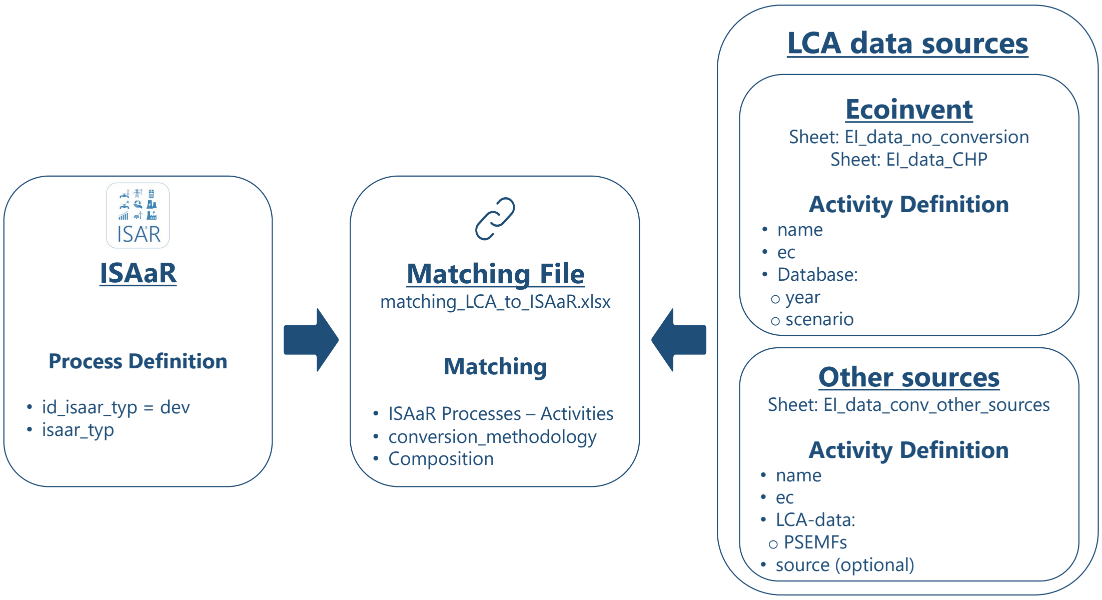

Figure 27: Matching process: Assignment LCA-data to ISAaR Processes

The matching of ISAaR processes to Ecoinvent activities other than co-generation activities is displayed in *Table 4*. *Table 5* displays the matching of ISAaR processes to Ecoinvent's co-generation activities. The matching of ISAaR processes to LCA data from other sources than Ecoinvent is displayed in *Table 6*.

Table 4: Matching: ISAaR Processes - Ecoinvent Activities, without co-generation processes

Matching: ISAaR processes (without co-generation) $\leftrightarrow$ Ecoinvent activities				
ISAaR process		Ecoinvent Activity		Composition
id_isaar_typ	isaar_typ	name	ec	Tech. Comp.
1	AKW	electricity production, nuclear, boiling water reactor	72	0
1	AKW	electricity production, nuclear, pressure water reactor	72	1
3	Beimischung	No matching required: Methane substituted with hydrogen		
9	BK	electricity production, lignite	72	1
11	Dampfreformierung	hydrogen production, steam reforming	162	1
18	fuel_Bio	No matching required: Import implicitly considered (ECT-balance)		
19	fuel_Gas	No matching required: Import implicitly considered (ECT-balance)		
22	Gasturbine	electricity production, natural gas, conventional power plant	72	1
26	Geothermie	electricity production, deep geothermal	72	1
27	GuD	electricity production, natural gas, combined cycle power plant	72	1
28	Heizwerke	heat production, natural gas, at industrial furnace $> 100kW$	71	1
28	Heizwerke	heat production, natural gas, at boiler modulating $> 100kW$	71	0
28	Heizwerke	heat production, natural gas, at boiler modulating $< 100kW$	71	0
28	Heizwerke	heat production, natural gas, at boiler condensing modulating $> 100kW$	71	0
28	Heizwerke	heat production, natural gas, at boiler condensing modulating $< 100kW$	71	0
35	Laufwasser	electricity production, hydro, run-of-river	72	1
36	Muell_ind_Abwaerme	electricity, from municipal waste incineration to generic market for electricity, medium voltage	72	1

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36	Muell_ind_Abwaerme	heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	71	1
38	Netz	No matching performed yet		
41	Oel	electricity production, oil	72	1
45	PSW_mit_nat_Zufluss	electricity production, hydro, pumped storage	72	1
46	PSW_ohne_nat_Zufluss	electricity production, hydro, pumped storage	72	1
50	SK	electricity production, hard coal	72	1
52	Sonstige Fossile	No matching required: Not considered within EMF-calculation		
53	Speicherwasser	electricity production, hydro, reservoir, non-alpine region	72	1
64	Wind_Onshore	electricity production, wind, $< 1MW$ turbine, onshore	72	see *Chapter 3.2.4.7*
64	Wind_Onshore	electricity production, wind, $1 - 3MW$ turbine, onshore	72	see *Chapter 3.2.4.7*
64	Wind_Onshore	electricity production, wind, $> 3MW$ turbine, onshore	72	see *Chapter 3.2.4.7*
65	Wind_Offshore	electricity production, wind, $1 - 3MW$ turbine, offshore	72	1
66	import_green_synfuel	No matching required: Import implicitly considered (ECT-balance)		
67	import_green_methane	No matching required: Import implicitly considered (ECT-balance)		
68	import_fossil_oil	No matching required: Import implicitly considered (ECT-balance)		
70	Waermepumpe	heat production, air-water heat pump 10kW	71	1
70	Waermepumpe	heat production, borehole heat exchanger, brine-water heat pump 10kW	71	0
76	H2_Speicher	No matching performed yet		
77	H2_Netz	No matching performed yet		
96	Gasturbine_H2Ready	electricity production, natural gas, conventional power plant	72	1

Table 5: Matching: ISAaR Processes - Ecoinvent Activities, co-generation processes

Matching: ISAaR co-generation processes ↔ Ecoinvent activities				
ISAaR process		Ecoinvent Activity		Composition
id_isaar_typ	isaar_typ	name	ec	Tech. Comp.
6	BioBHKW	heat and power co-generation, biogas, gas engine	72	0.73
6	BioBHKW	heat and power co-generation, biogas, gas engine	71	0.73
6	BioBHKW	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	72	0.27
6	BioBHKW	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	71	0.27
80	SK_KWK	heat and power co-generation, hard coal	72	1
80	SK_KWK	heat and power co-generation, hard coal	71	1
81	BK_KWK	heat and power co-generation, lignite	72	1
81	BK_KWK	heat and power co-generation, lignite	71	1
82	GuD_KWK	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	72	1
82	GuD_KWK	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	71	1
83	Gasturbine_KWK	heat and power co-generation, natural gas, conventional power plant, 100MW electrical	72	1
83	Gasturbine_KWK	heat and power co-generation, natural gas, conventional power plant, 100MW electrical	71	1
97	Gasturbine_H2Ready_KWK	heat and power co-generation, natural gas, conventional power plant, 100MW electrical	72	1
97	Gasturbine_H2Ready_KWK	heat and power co-generation, natural gas, conventional power plant, 100MW electrical	71	1

Table 6: Matching: ISAaR Processes - LCA data from other sources, Ecoinvent data with conversion required

Matching: ISAaR processes ↔ LCA data from other sources and Ecoinvent data with conversion							
ISAaR process		Ecoinvent Activity					
id_isaar_typ	isaar_typ	name	reg_name	ec	Tech. Comp.	Source	Conversion Methodology
2	Batterie	battery production, Li-ion, LFP, rechargeable, prismatic	RoW	72	1	Ecoinvent	Storage processes
2	Batterie	battery production, Li-ion, NCA, rechargeable, prismatic	RoW	72	0	Ecoinvent	Storage processes
2	Batterie	battery production, Li-ion, NMC111, rechargeable, prismatic	RoW	72	0	Ecoinvent	Storage processes
2	Batterie	battery production, Li-ion, NMC811, rechargeable, prismatic	RoW	72	0	Ecoinvent	Storage processes
15	Elektrolyse	hydrogen production, PEM electrolysis	DE	162	1	[73]	Ecoinvent methodology
42	P2SG	synfuel production, P2SF	GLO	222	1	[74]	Ecoinvent methodology
43	Heizelement	heat production, flow heater	DE	71	1	[75]	Heating element
44	Power2Methan	gas production, P2G	AT	21	1	[71]	P2Methane
73	PV_Freiflaeche	electricity production, photovoltaic, open ground installation	DE	72	1	[76]	Ecoinvent methodology
74	PV_Gebaeude	electricity production, photovoltaic, slanted-roof installation	DE	72	1	[76]	Ecoinvent methodology
93	Emob_bidirektionales_Laden	Emob_bidirektionales_Laden	RoW	72	1	Ecoinvent	Storage processes
93	Emob_bidirektionales_Laden	Emob_bidirektionales_Laden	RoW	72	0	Ecoinvent	Storage processes
93	Emob_bidirektionales_Laden	Emob_bidirektionales_Laden	RoW	72	0	Ecoinvent	Storage processes
93	Emob_bidirektionales_Laden	Emob_bidirektionales_Laden	RoW	72	0	Ecoinvent	Storage processes

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94	Emob_gesteuertes_Laden	Emob_gesteuertes_Laden	RoW	72	1	Ecoinvent	Storage processes
94	Emob_gesteuertes_Laden	Emob_gesteuertes_Laden	RoW	72	0	Ecoinvent	Storage processes
94	Emob_gesteuertes_Laden	Emob_gesteuertes_Laden	RoW	72	0	Ecoinvent	Storage processes
94	Emob_gesteuertes_Laden	Emob_gesteuertes_Laden	RoW	72	0	Ecoinvent	Storage processes
99	Batterie_2nd_Life	No matching required: Batteries already exist					

A.2 EMF-Calculation Code Set-Up

Setting Input parameters

The EMF-calculation is implemented within the notebook $emf\_ISAaR.ipynb$. The calculation starts by establishing a connection to $FREM$ to access data from ISAaR's optimization runs. Username and password are required to access $FREM$. Once, the connection is established input parameters have to be defined. The user is asked to define the scenario whose EMFs should be calculated. The scenario is defined by its identification number $id\_sequence$ as specified within ISAaR. EMFs are calculated for all modelled years within the defined scenario unless specific years to be calculated are explicitly defined in list sz_log_list. Then, the emission allocation methodology and the PSEMF type to be used within the EMF-calculation are defined, see *Chapter 3.1.2* and *Chapter 3.3.1*. As a next step PSEMFs can be calculated, as defined in defined in *Chapter 3.2*. The PSEMF calculation and adjustment to ISAaR is performed within the notebook by importing the python-script $calc\_LCA\_emf\_ISAaR.py$. The PSEMF-calculation is an optional step since it is a long-lasting process. This step should be skipped if the scenario's PSEMFs have already been calculated before and are stored within $FREM$. If the PSEMF calculation is executed, the calculated PSEMFs are exported to $FREM$. The PSEMFs used within the EMF-calculation are imported from $FREM$. As a last step prior to the EMF-calculation the user can choose whether query results should be stored. The naming of the stored query files and calculation results is automated.

The EMF-calculation is set up in a way such that all ISAaR scenarios can be calculated. The spatiotemporal resolution of the EMF-calculation is defined by imported ISAaR data. It may occur that certain processes modelled within the scenario to be calculated are not implemented within the matching process. As of today the matching process is implemented for all processes occurring within the scenarios $solidEU$ $(id\_sequence = 778)$ and $BMW-start$ $(id\_sequence = 1047)$. Before calculating other scenario's EMFs the user has to ensure that the matching process is implemented for all processes within the scenario to be calculated. The matching file has to be updated if the matching process is not implemented for all processes occurring within the scenario to be calculated. Non matched processes are assigned with PSEMFs of zero. The sequence's PSEMFs have to be re-calculated to integrate the updated matching process into the EMF-calculation.

Calculation process

The EMF calculation process begins once required input parameters are defined. Required data to set up the linear equation system defined in *Chapter 3.1.3* is imported into the notebook by a multitude of SQL commands. The SQL commands are stored within the file $query\_file.py$ and imported into the notebook. Allocation factors are calculated according to the defined allocation methodology. The final adjustment of LCA based PSEMFs to ISAaR is implemented during the setup of matrix $\underline{\underline{b}}$. Calculated LCA based PSEMFs are assigned with ISAaR based allocation factors and process efficiencies to finish the adjustment process to ISAaR, see *Chapter 3.2.4.2* and *Chapter 3.2.4.3*. The adjusted ISAaR based PSEMFs are assigned to the processes to determine the energy system's emissions.

Once all required data is imported the linear equation system is set up and modified according to the methodology defined in *Chapter 3.1.3*. The linear equation system is solved and calculated EMFs are stored. If queries are defined to be stored the query results are stored.

Adjusting calculation Results

The calculated hourly consumption based EMFs are adjusted to ECs' temporal resolutions, see *Chapter 3.3.4*, and exported to $FREM$.

Plotting

The notebook concludes with some code to create different plots for displaying the calculated EMFs. In the first cell yearly mean EMFs and yearly load-weighted EMFs are calculated and plotted. Additionally, annual descending EMF curves are calculated and plotted within this cell. The comparison of calculated EMFs based on different PSEMF types, see *Chapter 3.3.1*, is implemented within the second cell. Calculation results are imported and plotted in a single figure to evaluate impacts of the integration of certain emission types or certain life cycle stages. Storage locations are defined automatically for each plot.

The EMF-calculation methodology is holistically displayed in *Figure 28*.

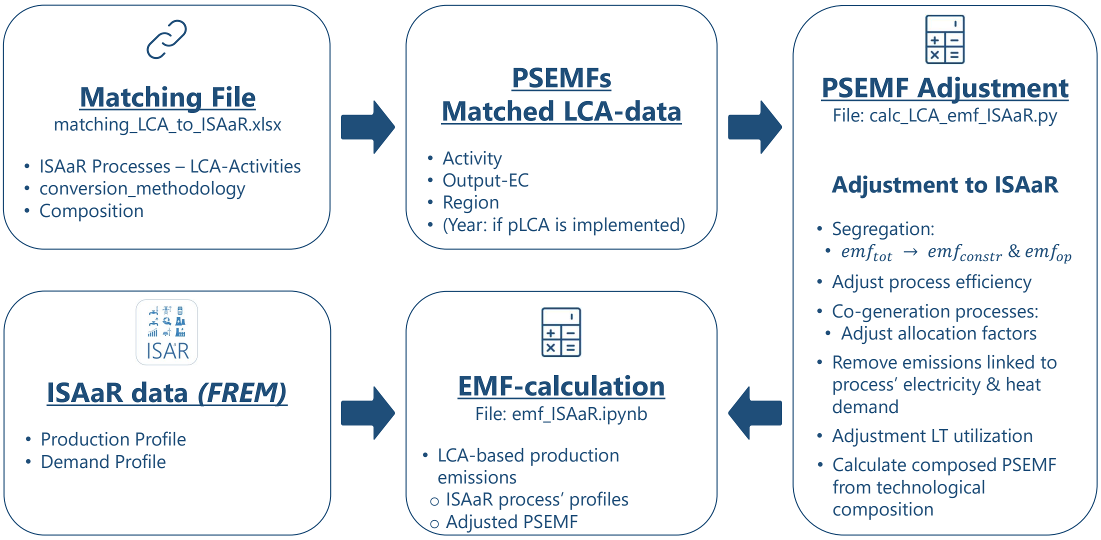

Figure 28: Flow Diagram: EMF calculation

A.3 Green H_2 Gap

The Green H_2 Gap in 2025 and 2050 is displayed in *Table 8*. The annual Green H_2 Gap is evaluated for each region modelled within $solidEU$. The amount of H_2 defined as green according to EU-Taxonomy based on DA-methodology, but not as green based on LCA-methodology is displayed. It is compared to the total amount of H_2 produced from electrolysis. H_2 amounts are displayed in the unit $kt\ H_2$.

Table 8: Green H_2 Gap in 2025 & 2050

Green H_2 Gap								
	2025				2050			
Region	No. Hours	H_2 green DA not green LCA	Total H_2	Share Green H_2 Gap	No. Hours	Green H_2 not green LCA	Total H_2	Share Green H_2 Gap
ENTSO-E	362	40.6	536.1	7.6 %	0	0	32581.2	0 %
AT	0	0	0	No Electrolysis	506	13.2	140.4	9.4 %
BE	0	0	0	No Electrolysis	539	0.2	3.5	5.6 %
BG	0	0	0	No Electrolysis	912	11.8	68	17.3 %
CH	0	0	0	No Electrolysis	0	0	0	No Electrolysis
CZ	0	0	0	No Electrolysis	1	0	304.2	0 %
DE	33	1.5	144.4	1 %	11	0	7895	0 %
DK_O	0	0	0	No Electrolysis	0	0	0	No Electrolysis
DK_W	0	0	0	No Electrolysis	19	0.2	887.6	0 %
EE	0	0	0	No Electrolysis	270	1.9	74.9	2.5 %
ES	221	6.4	75.3	8.5 %	33	0	2186.1	0 %
FI	0	0	0	No Electrolysis	0	0	345.5	0 %
FR	5	0.3	175.9	0.2 %	15	0	5757.6	0 %
GB_O	0	0	0	No Electrolysis	1	0	2641.3	0 %
GB_W	0	0	0	No Electrolysis	159	4.3	433.1	1 %
GR	0	0	0	No Electrolysis	0	0	525.9	0 %
HR	0	0	0	No Electrolysis	2	0	231.4	0 %
HU	0	0	0	No Electrolysis	14	0.5	434.3	0.1 %
IE	0	0	0	No Electrolysis	2	0	132.3	0 %

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IT	0	0	0	No Electrolysis	0	0	3223.6	0 %
LT	0	0	0	No Electrolysis	482	8.2	117.1	7 %
LU	0	0	0	No Electrolysis	0	0	0	No Electrolysis
LV	0	0	0	No Electrolysis	250	2.9	197.9	1.5 %
NL	0	0	72.7	0 %	4	0	2424.8	0 %
NO	0	0	0	No Electrolysis	1125	59.7	376.6	15.9 %
PL	0	0	0	No Electrolysis	22	0	2075.5	0 %
PT	1567	44.2	67.8	65.2 %	760	44	263	16.7 %
RO	0	0	0	No Electrolysis	107	5.9	881.6	0.7 %
SE	0	0	0	No Electrolysis	10	0	321.1	0 %
SI	0	0	0	No Electrolysis	0	0	0	No Electrolysis
SK	0	0	0	No Electrolysis	5	0.1	637.8	0 %