FH MÜNSTER
University of Applied Sciences

Faculty of
Energy · Building Services ·
Environmental Engineering

Coupling Energy System Modeling with Life Cycle Assessment

Bachelor Thesis

April 15, 2024
Franziska Koert
franziska.koert@fh-muenster.de

First supervisor: Prof. Dr. Peter Vennemann
Second supervisor: Prof. Dr.-Ing. Elmar Brügging

This publication emerged as part of a bachelor's thesis and is available in a slightly modified form under the DOI: https://doi.org/10.25974/fhms-17880.

Contents

List of Figures

List of Tables

List of Algorithms

Abbreviations

AoP area of protection

ASHP air source heat pump

CF characterization factor

DALYs disability adjusted life years

DAL Database Analyser and Launcher

DB dichlorobenzene

EAFESA Environmental Framework for Energy System Assessment

EF Environmental Footprint

ELCD European Life Cycle Database

ESM energy system modeling

EU European Union

GCHP ground-coupled heat pump

GEMIS Global Emission Model for Integrated Systems Analysis

GHG greenhouse gas

GUI graphical user interface

ILCD International Reference Life Cycle Data System

IPCC Intergovernmental Panel on Climate Change

IO input-output

LAEND Life Cycle Assessment based Energy Decision

LCIA life cycle impact assessment

LCA life cycle assessment

LCT life cycle thinking

LAEND Life Cycle Assessment based Energy Decision

MCDA multi-criteria decision analysis

MES multi-energy systems

NEEDS New Energy Externalities Developments for Sustainability

OEFSR organization environmental footprint sector rules

oemof Open Energy Modelling Framework

PEFCR product environmental footprint category rules

ProBas Prozessorientierte Basisdaten für Umweltmanagement-Instrumente

PV photovoltaic

SESMG Spreadsheet Energy System Model Generator

SESMG-Data Spreadsheet Energy System Model Generator - Database

SWHP surface water heat pump

TMY typical meteorological year
US-Tool Urban District Upscaling Tool
UUID universally unique identifier

Abstract

When simulating and optimizing urban energy systems, the focus is usually on minimizing financial costs or greenhouse gas (GHG) emissions. As energy systems transition towards a growing share of renewable energy sources and technological complexity, environmental impacts that affect more than just GHG emissions, such as resource extractions, water and land use impacts or impacts on human health, are becoming increasingly relevant.

To address this gap, this thesis introduces an automated coupling procedure for energy system modeling (ESM) and life cycle assessment (LCA). The implementation includes general recommendations and a practical coupling of the Open Energy Modelling Framework (oemof) based Spreadsheet Energy System Model Generator (SESMG) with a suitable LCA software.

The LCA procedure involves goal and scope definition, inventory analysis, impact assessment, and interpretation. To adapt these steps to different energy system models, the LCA should be attributional, process-based and territorial. Further, the openLCA software by GreenDelta serves as a suitable soft-linking tool. The main challenge of the coupling procedure is the inventory analysis. Data collection faces limitations, reasoned by the commercialization and high maintenance efforts in open-source databases. After evaluating free databases, the Prozessorientierte Basisdaten für Umweltmanagement-Instrumente (ProBas) database of the Umweltbundesamt emerged as the most suitable choice for the coupling. However, also this database lacks traceability of datasets or compatibility with a comprehensive impact assessment.

A generalized framework for the LCA application of energy systems was developed. The framework is based on an ex-post LCA assessment that considers the combination of the two approaches within every step of the procedure. Main considerations of this framework include automatic calculations of the inventory analysis and the impact assessment for different energy technologies, as well as calculations summed up for all technologies of energy system scenarios. Further, technology mapping and data harmonization are essential considerations for the automatic coupling and double counting of impacts needs to be avoided.

Subsequently, the framework is realized with the adaption of the SESMG. Its database-independent realization allows compatibility with different databases in openLCA. For the selected ProBas database, the tool can be used with different available energy technologies. The use of unit processes is encouraged for data harmonization. Result interpretation of the LCA (in general or with the SESMG) should not solely focus on the absolute values of the impact categories, but rather on the comparative strengths among scenarios and technologies.

The successful application to a reference single-family building using the ProBas database revealed varied environmental impacts, in relation with a higher reduction in GHG emissions, with an increase of 11 % in terrestrial acidification impacts in the emission-optimized scenario. These findings emphasize a more comprehensive perspective on environmental impacts and provide a valuable validation of the developed methodology.

Future research should include the improvement of data harmonization, the inclusion of more datasets for a more customized analysis of energy systems and more applications. The coupled approach offers a promising avenue for gaining deeper insights into optimizing urban energy systems.

Graphical Abstract

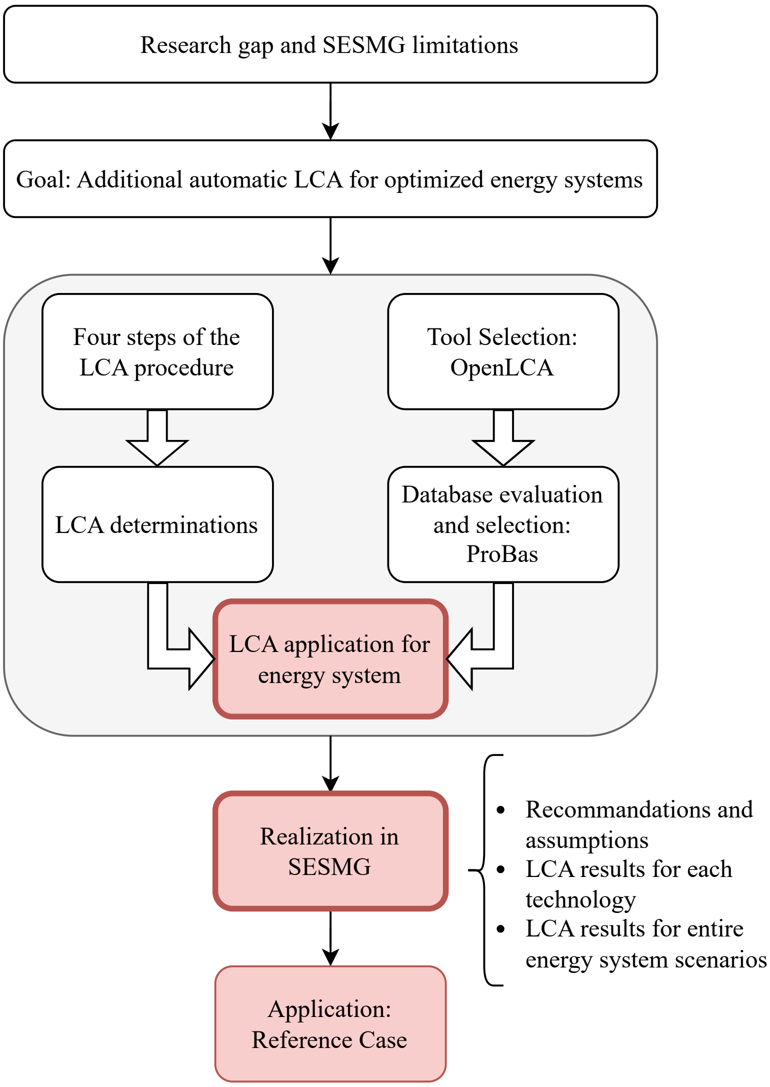


Figure 1.: Graphical abstract for the content of this thesis. Red parts of the illustration represent main results of this thesis, that were used to draw conclusions. Abbreviations: SESMG = Spreadsheet Energy System Model Generator, LCA = life cycle assessment, ProBas = Prozessorientierte Basisdaten für Umweltmanagement-Instrumente. Own illustration.

Key Words *Energy system modeling, Urban energy system, Life cycle assessment, Spreadsheet Energy System Model Generator, OpenLCA, Databases, ProBas*

1. Introduction

With over 70 % of global greenhouse gas (GHG) emissions attributed to cities [1] and the expected increase in the urban population reaching 68 % by 2050 [2], cities act not only as a source of environmental challenges but also pose a key opportunity in contributing towards ambitious climate goals [1]. To address future challenges, cities must undergo comprehensive restructuring, particularly in their urban energy systems, involving a transition towards renewable energy technologies [1]. The transformation towards a sustainable energy consumption is highlighted by the urgency of the European Union (EU) to nearly double the share of renewable sources in gross final energy consumption, from the current 23 % to over 42 % by 2030 [3]. This shift aims not only to reduce GHG emissions but also contributes to other environmental impacts. Particularly, the impacts of renewable energy technologies extend to water, ground, wildlife, and landscapes, with intricate connections existing among these categories [4, 5]. These environmental trade-offs are increasingly recognized in political measures, evident in initiatives like the European Green Deal [6]. While public discourse often focuses on the role of energy supply systems in contributing to climate change through GHG emissions, these systems exert significant influence on various other environmental impacts [7].

To analyze the different combinations of technologies that can be implemented in energy systems, energy system modeling (ESM) is a suitable method [8, 9]. Energy system models are already integral to policy-making processes, aiding decision-makers in shaping effective energy policies [10]. The increasing complexity of future systems and the rising demands that extend beyond the direct consequences of climate change necessitate an expansion to include environmental aspects [11, 12]. Addressing this gap, a solution lies in the integration of a life cycle assessment (LCA), which quantifies all environmental impacts throughout the entire life cycle of a product or system [13]. The potential of coupling the two approaches was also mentioned by the Intergovernmental Panel on Climate Change (IPCC) as an option to assess a variety of environmental impacts of energy systems [14].

Currently, a prevailing limitation in research is the predominant focus on minimizing costs within the simulation and optimization of energy system models, often neglecting additional environmental impacts [15, 16]. While certain models have begun incorporating production based GHG emissions and life cycle based emissions in the last years, other environmental impacts remain underrepresented [17–19]. The number of scientific articles covering the topic of coupling ESM and LCA, especially focusing on larger spatial systems and the power sector [11, 16, 20], has experienced exponential growth since the 1990s [5]. However, Lotteau et al. analyzed that there where no direct applications of LCAs of energy systems in the scale of a neighborhood until 2015 [21].

The Spreadsheet Energy System Model Generator (SESMG) [22], developed by the work group of ESM at the FH Münster - University of Applied Sciences is a modeling tool utilized for optimizing urban energy systems. In a case study in Herne, Germany, a LCA methodology was applied after defining various possible energy system scenarios for a neighborhood [23] using the mentioned tool. This contributed to a better understanding of the environmental impacts associated with energy technology choices. Building upon this foundation, laid by Quest et al. [23], this study aims to advance the coupling of ESM and LCA further. The previous study employed the two approaches independently, which resulted in the need for detailed knowledge about both approaches. In contrast, the objective here is to enhance the methodology by implementing an automated integration for systematically evaluating additional impacts within energy system models.

The primary audience of this study remains the field of ESM, with the overarching goal of redefining the area of LCA from scratch. The objective is to comprehend this field anew and explore its potential integration as an expansion within ESM tools. Therefore this thesis deals with the question: "How can additional environmental impacts of different energy system scenarios be assessed and analyzed?".

Finally, this work clearly differs from previous studies, given that the majority of ESM tools do not take additional environmental parameters, aside from GHG emissions into account [15, 17, 24]. This lack of research was also discovered in the review of different assessment indicators of the SESMG, which came to the conclusion that "other sustainability aspects than GHG emissions (e.g., space, water, different raw materials) are not directly considered in this analysis" [24].

After presenting the needed background information about ESM (see section 2.1), LCA (see section 2.2) and the coupling of the approaches (see section 2.3), the thesis proceeds with essential steps in tool and database selection (see section 3.1) to develop a comprehensive LCA application (see section 3.3). This general application is subsequently realized in the ESM tool SESMG (see section 3.4) and the methodology is validated through a practical study of a reference case (see section 4.1). The discussion critically examines challenges and limitations (see chapter 5), and the conclusion elaborates key findings for the general coupling of ESM and LCA as well as for the realization in the SESMG (see chapter 6) before a final outlook for future research is presented (see chapter 7).

2. Background

2.1. Energy System Modeling (ESM)

2.1.1. Urban Energy Systems

Urban energy systems can be defined as "the combined process of acquiring and using energy in a given spatial entity with a high density and differentiation of residents, buildings, commercial sectors, infrastructure, and energy sectors (e.g., heat, electricity, fuels)" [24]. They are also referred to as mixed-use multi-energy systems (MES) because they integrate diverse energy sources and technologies to ensure efficient and sustainable energy supply for urban environments [25, 26].

As urban energy systems shift towards sustainability by incorporating of renewable sources with volatile production, utilization of energy storage, sector coupling, and the growing importance of new sectors, their composition becomes more complex [15]. The growing number of possible combinations of energy technologies makes the task of identifying optimal configurations increasingly challenging [15, 26]. Traditionally, these systems are designed by considering sectors separately and by comparing few different scenarios with selected combinations of technologies. However, this conventional approach fails in ensuring the optimization of targeted values or in identifying the optimal solution to design an energy system [9]. Therefore a holistic planning strategy is essential, one that takes into account all energy sectors and their interaction with each other, various planning objectives, and the spatial context [8, 26].

2.1.2. Energy System Models

Definition Energy system models serve as a simplified representation of the actual energy system [27, 28]. The objective of ESM is to depict the interactions among different sectors in order to improve the understanding of an energy system integration [26]. Model generators are instrumental tools in constructing these models [8]. The tools possess predefined analytical and mathematical properties, contributing to the accurate representation of urban energy systems [8, 29]. To map the mentioned complexity of these systems, employing the MES approach is recommended. The approach involves the simultaneous consideration and integration of various energy sources within a single framework [26, 28].

Characteristics Various properties and categorizations can be used to classify tools for energy system models [28, 30, 31]. In terms of the methodology, most models in the field of planing urban energy systems use an optimization approach whereas different scenarios are created and rated according to an objective function [29]. An important characteristic influencing how the sustainability of different model scenarios is measured, lies in the assessment criteria. Diverse indicators are available for designing and analyzing the targeted system [24]. While numerous energy system models primarily optimize for a single objective, often focusing on minimizing energy costs [15], this approach falls short in delivering a holistic evaluation of urban energy systems, as it tends to neglect other critical factors. Multi-objective models are needed to broaden the perspective of sustainability [24]. To define suitable boundaries for the considered system, it is recommended to cover all conversion processes up to the final energy within the energetic boundaries. Furthermore, when optimizing emissions, the boundaries of the target values should integrate life cycle accounting [32]. Another dimension of classification includes structural and technological details which focus for example on the geographical coverage, the time horizon of the model, or the spatial and temporal resolution [28]. The application of a holistic planing approach results in a need for rapid computing resources. Consequently, there are usually constraints on the temporal and spatial resolution required for the system [33]. Other additional characteristics are not further addressed here.

Multi-Objective Optimization To create multi-objective models, it is possible to either use combined indicators, where different metrics are unified into a single value for optimization, or to conduct a constraint optimization where one or more additional indicators limit the optimization process [24]. The second option is reached by applying the epsilon-constraint method [34]. Typical indicators for the multi-objective optimization encompass the reduction of energy use, GHG emissions, and financial costs [15]. As an example, the model minimizes financial costs first. In subsequent runs, it minimizes GHG emissions, treating them as a constraint [24]. The first run creates the cost-optimized scenario, followed by the reduction of the permitted GHG emissions in multiple steps (e.g., 20 % steps) until the value is so low that no target scenario can be determined, resulting in the emission-optimized scenario. The gradual reduction of emissions leads to the creation of multiple "best-known-Pareto-points" that can be connected into one Pareto front shown in Figure 2.1. Typically, the traditional scenario has recognizably higher costs and emissions [24, 35, 36].

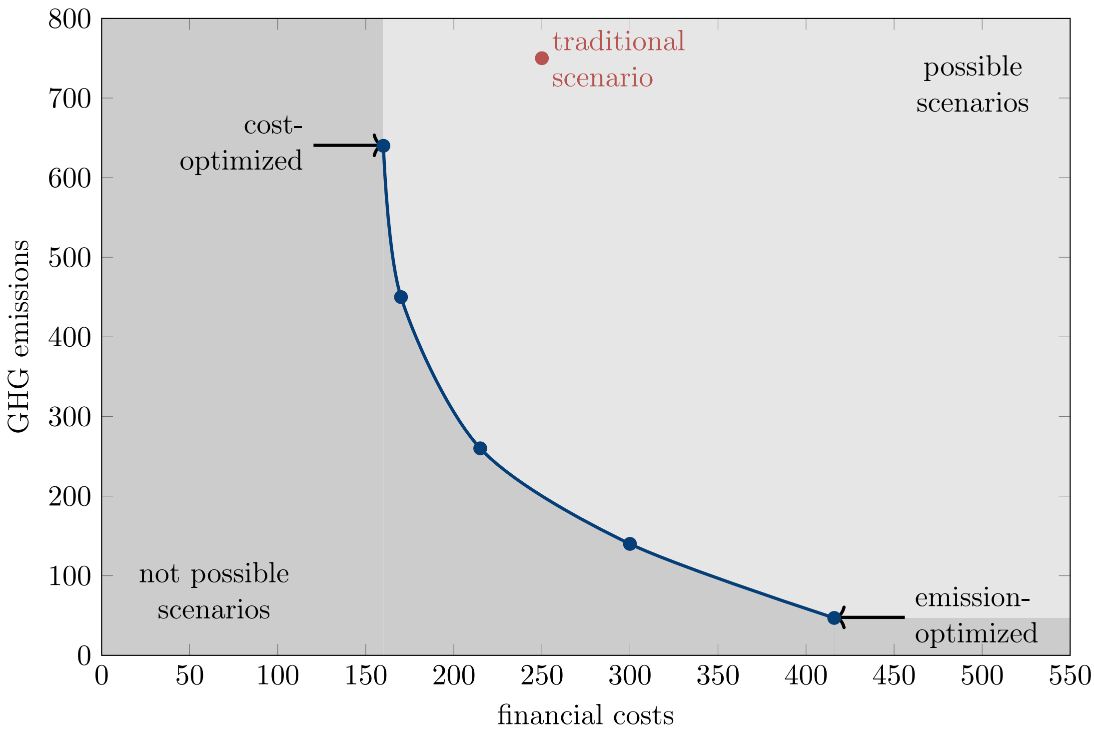


Figure 2.1.: Pareto front. All scenarios above the front are technical possible. Different points between the cost-optimized and emission-optimized scenario represent the "best-known-Pareto-points". The exact shape of the Pareto front, the costs and the emissions depend on the specific energy system. Abbreviation: GHG = greenhouse gas. Taken from [32].

Possible targets in line with the explained Pareto front, include:

- Costs of energy supply
- GHG emissions from energy supply
- Costs at a given GHG limit

2.1.3. Spreadsheet Energy System Model Generator (SESMG)

Tool Description In a review of existing methods and approaches, Klemm et al. concluded that there is a lack of tools to rightfully model MES in mixed-used urban districts [28]. This research gap resulted in the development of the SESMG [22], a model generator enabling the implementation of Open Energy Modelling Framework (oemof)[1] energy system models. The open-source framework oemof provides a versatile framework for designing, modeling and optimizing a variety of energy system models. Oemof is structured based on graph theory, a mathematical framework for representing and analyzing relationships between interconnected entities using graphs (see SESMG documentation[2] for explanation of different graph components). The SESMG additionally uses a bottom-up approach, involves building a model from individual components and uses multi-objective optimization with the epsilon-constraint method [37]. As an ESM tool, it encompasses all available technologies of modern energy systems and uses numerical solution methods to adjust the ranges for each of these technologies until the system reaches an optimum of a specific target. Typically financial costs and GHG emissions are used for the multi-objective optimization, but the SESMG can utilize any quantity as a target criterion [28].

The program flow can be divided into three sub-steps, as shown in Figure 2.2 (see SESMG documentation[3] for more information about the sourcecode):

- Pre-processing: All elements of the energy system are defined in the model definition (xlsx-file), which can be manually created by defining all needed components along with their technical, economical and ecological values. Alternatively, the model definition can be simplified using the Urban District Upscaling Tool (US-Tool)[4], that contains all building-specific parameters. This tool automatically creates the model definition in combination with a set of case-independent standard parameters (standard parameter sheet). The model definition can be passed on to "processing" with the graphical user interface (GUI). Afterwards, all the individual elements are combined into a mathematical optimization problem.
- Processing: An external solver solves the linear problem (or integer problem for district heating options) before forwarding the results to the result processing. Based on the model definition different temporal and spatial simplification can be applied. The user also has the option to employ pre-modeling to reduce the computing resources by applying a highly simplified model for the first optimization. Alternatively, the epsilon-constraint method conducts a model run with different weights of the optimization criteria.

[1] Website - oemof: `https://oemof.org/`.
[2] Documentation - SESMG - Structure of Energy Systems: `https://spreadsheet-energy-system-model-generator.readthedocs.io/en/latest/01.01.00_structure_of_energy_systems.html`.
[3] Documentation - SESMG - Sourcecode Documentation: `https://spreadsheet-energy-system-model-generator.readthedocs.io/en/latest/04.00.00_sourcecode_documentation.html`.
[4] Documentation - SESMG - Urban District Upscaling: `https://spreadsheet-energy-system-model-generator.readthedocs.io/en/latest/01.04.00_urban_district_upscaling.html`.

- Post-processing: The obtained results undergo preparation and automatic analysis. This phase returns several result files, as well as a graphical analysis of the final energy amounts or the Pareto front points which can get accessed again via the GUI.

Further information about the application of the tool as well as about the different steps of the workflow, including details about the results or the GUI can be found in the documentation[5].

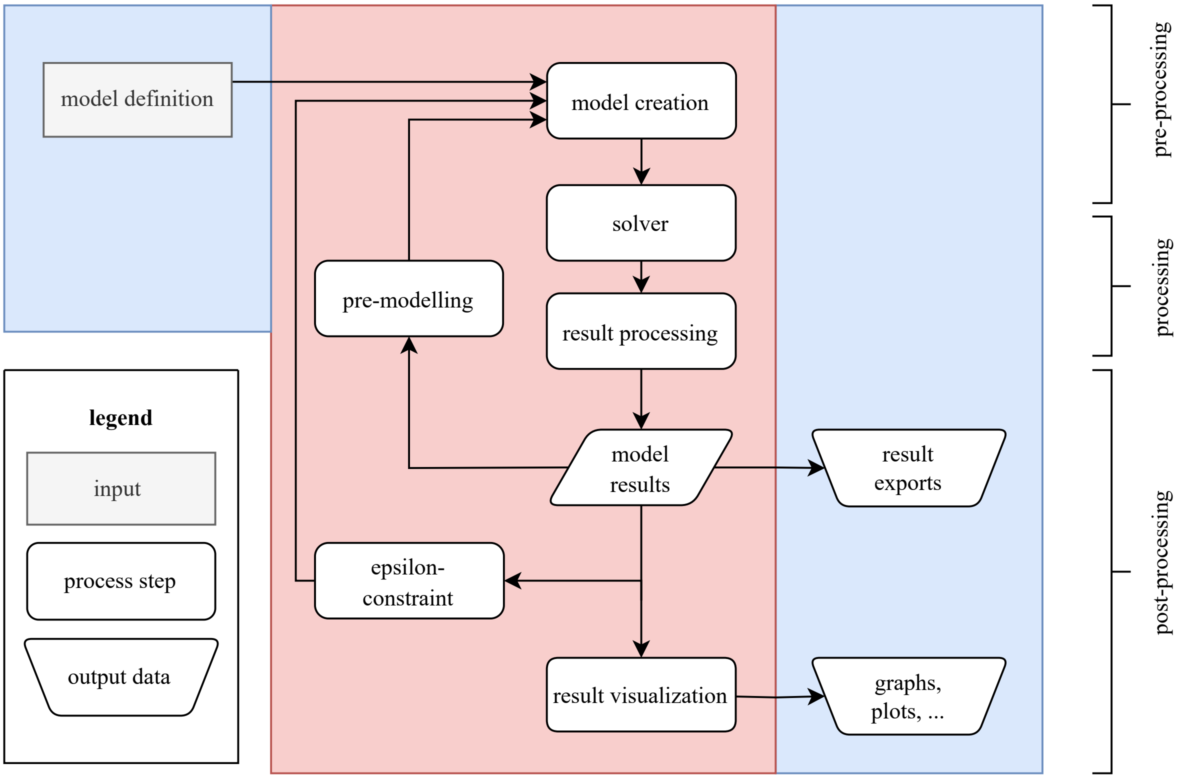


Figure 2.2.: Modeling workflow SESMG. Data represented as trapezoids (model results) can be accessed. Own illustration adapted from [32].

Strengths and Limitations The SESMG presents several strengths that contribute to its significance in the domain of ESM:

- Progress: The SESMG maps the links and interactions of sustainable urban energy systems at model level and minimizes different target variables using optimization algorithms in order to close the aforementioned research gap in ESM [28].
- Data collection: Users are automatically provided with required technical and economic parameters, which can be assumed by default and do not depend on the energy system under consideration with the help of the US-Tool. This will be facilitated even more in the future due to the ongoing development of the Spreadsheet Energy System Model Generator - Database (SESMG-Data)[6]. This comprehensive database provides a plugin for the SESMG including an automated generation of the standard parameter sheet and a creation of a parameter overview for practical studies.

[5] Documentation - SESMG: https://spreadsheet-energy-system-model-generator.readthedocs.io/en/latest/index.html.
[6] GitHub - SESMG-Data: https://github.com/SESMG/SESMG-Data.

- User friendliness: The tool is published under an open-source license. In contrast to oemof, it requires no programming knowledge, because the input is table-based [37]. The GUI not only lowers the entry barrier but also enhances result visualization, ensuring accessibility and ease of use.
- Application and development: Over recent years, the SESMG has been successfully applied in various case studies, demonstrating its adaptability and effectiveness across diverse scenarios and neighborhoods [38]. The tool further exhibits a commitment to ongoing development such as the integration of district heating networks with an additional Python module [39] or the development of the pre-modeling [33], showcasing its adaptability and versatility in addressing evolving needs.

However it is crucial to acknowledge certain limitations:

- Assessment criteria [24]: The focus on costs and GHG emissions as optimization targets, illustrated in Figure 2.1, constraints a more comprehensive assessment. Different studies already discovered this limitation and call for further research in terms of different criteria [24, 28]. This involves the need of the implementation of environmental factors [23]. Additionally, the optimization aims to reduce system wide economic costs, which excludes the possibility of considering different stakeholders separately [32, 40].
- Data Validation: The complexity of required information, as well as diverse data sources makes data processing challenging. Despite the existence of SESMG-Data, datasets inside the database remain not standardized or outdated due to limitations of open-source datasets.
- Further limitations [32]: The mobility sector is excluded in this tool, which can lead to incomplete insights into the interactions and potential synergies between energy systems [41]. Additionally, legal adjustments cannot be automatically considered for the implementation of different technologies and require additional coordination with policy experts [32]. Another previously discussed limitation includes the high computing times for a optimization process [33].

The improvement approach addressed in this thesis focuses on the selection of the mentioned assessment criteria, particularly emphasizing the consideration of GHG and life cycle emissions in ESM.

2.2. Life Cycle Assessment (LCA)

2.2.1. Definitions

Life Cycle Thinking The concept of life cycle thinking (LCT) considers the entire life cycle of a product or system, including raw material extraction, manufacturing, utilization, maintenance, end-of-life, and disposal stages [13]. LCT aims to identify sources of environmental burdens and to reduce them at the source of the burden itself [13]. This can be achieved by implementing perspectives of a circular economy. A circular system minimizes the use of resources, reduces waste and emissions, and conserves energy by systematically closing loops for materials and energy [42, 43].

Life Cycle Assessment The application of LCT to a specific project results in the idea of a LCA [12, 44]. In reality, environmental assessments are often limited to the utilization phase, particularly, when evaluating energy generation processes [12, 30]. However, a LCA overcomes this limitation by measuring environmental impacts of a product or service over its whole life cycle [13]. The comprehensive consideration of all stages is referred to as "cradle to grave" [45, 46]. Another concept , developed as "cradle to cradle" also includes the stage of the reuse potential of a product or service [13, 47]. The main purpose of LCAs is to prevent burden shifting, where environmental impacts are transferred to other stages rather than reduced [47]. Other names for a LCA are "life cycle approach", "cradle to grave analysis", or "eco-balance" [13]. The idea of a LCA was first introduced in the late 1960s and early 1970s [13, 48] due to the energy price crises and the social aim to decrease pressure on the environment [49]. Since its inception, the methodology has undergone improvement and expansion. During the 1990s it started to be incorporated in decision and policy making and particularly in the last century numerous advances in LCA methodology have been accomplished [13].

Product System The illustration in Figure 2.3 shows a typical product system within the context of a life cycle perspective. A product system in LCA consists of all processes, activities, and resources associated with a specific product or service. This system serves as the subject of analysis to evaluate environmental impacts throughout its entire life cycle [13, 47].

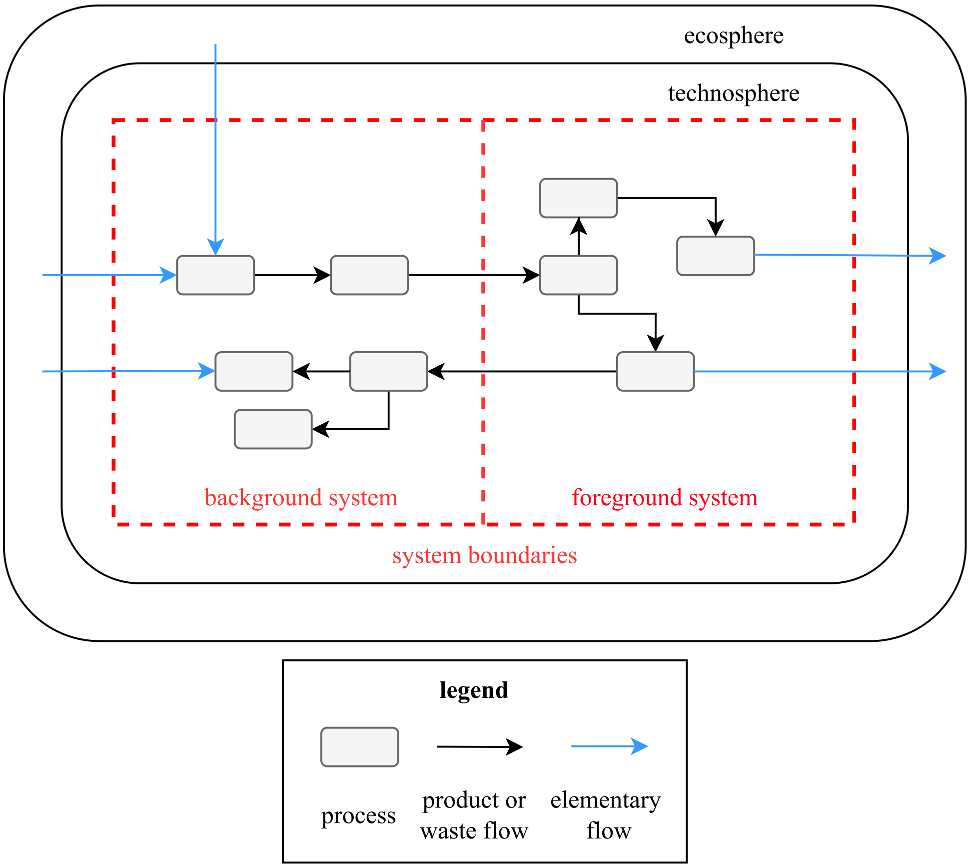


Figure 2.3.: Generic product system. Life cycle model illustrating the division between ecosphere and technosphere as well as the boundaries of the product system (in red) with the division between background and foreground system. Own illustration adapted from [47].

A product system consists of the following parts:

- Technosphere and ecosphere: The technosphere of the system encompasses all human-created components, while the ecosphere includes everything not originating from human activities. The ecosphere contains qualities meant to be protected by the LCA. This quality is therefore often called area of protection (AoP) [47].
- Foreground and background system: The foreground system refers to the specific processes of a product system that are unique to that particular product. The background system includes processes that are commonly included in the life cycles of many different products [47].
- Unit process: A unit process in LCA refers to a clearly defined operational unit within the product system. It represents a step or an activity in the life cycle of a product or service [45].
- Flows: As illustrated in Figure 2.3, a singular process receives input and generates output data. This data is classified into various flows. Flows interconnect multiple unit processes [45, 47]. The different types of flows are shown in Table 2.1. Elementary flows can be defined as flows that are drawn from the ecosphere or released to the ecosphere [44], while products or waste flows can act as material and energy input flows for other processes [47].

Table 2.1.: Different flows of the inventory analysis.

Input flows	**Output flows**
Materials	Products
Energy	Waste
Resources[a]	Emissions[a]

[a] Elementary flow.

2.2.2. Procedure

The conduct of LCA is governed by the environmental management standards ISO 14040 [45] and ISO 14044 [50]. These standards provide a comprehensive framework and offer guidelines and principles. The International Reference Life Cycle Data System (ILCD), an European initiative, provides a handbook that serves as a valuable companion to these standards, enriching the LCA process with best practices and additional insights [44]. According to the environmental standards a LCA consists of four phases, as shown in Figure 2.4. The goal and scope definition is followed by the inventory analysis and the impact assessment. All steps are assessed, and conclusions are drawn in the interpretation step, as depicted by the different arrows in the figure. The following explanation provides an excerpt of the mentioned key steps and necessary considerations of a LCA.

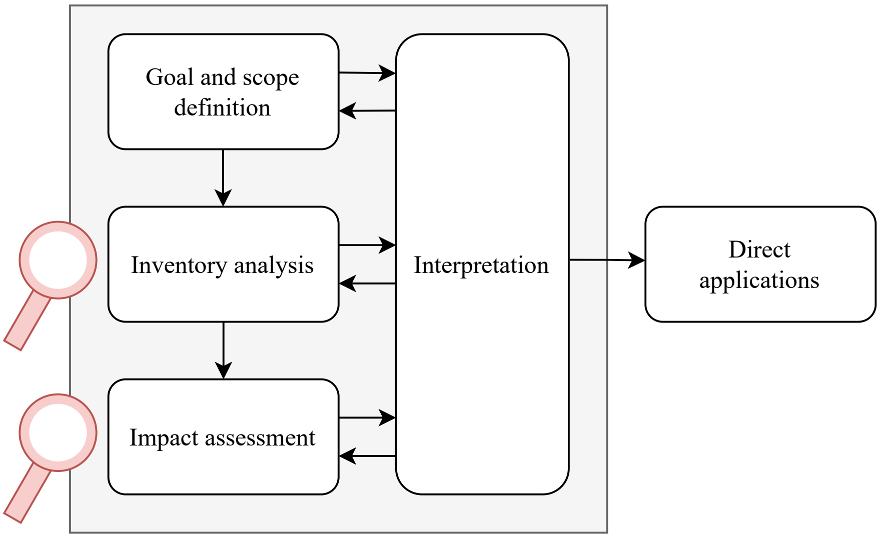


Figure 2.4.: LCA procedure. Framework with the four mandatory steps of a LCA. Arrows indicate the order of the steps. Magnifier represents the steps that are later broken down into further intermediate steps. Own illustration adapted from ISO 14040 standard [45].

Step 1: Goal and Scope Definition

The initial phase provides the conceptual framework for later conducting the inventory phase of a LCA. This happens in two individual sub-steps.

Goal In the goal definition the intended application and the target audience are addressed [45]. It is important to define the decision context as well as the reason for carrying out the study [47]. The definition of the goal is crucial as it shapes and influences all subsequent phases of the LCA [44].

Scope Within the scope of the examination, various steps are taken into account [45, 47, 50]:

- Definition of the product system: The system involves assembling modules composed of unit processes with elementary and product flows, effectively modeling the life cycle of a product. The typical approach is to construct the foreground system process by process.
- Function and functional unit: The function refers to the primary purpose or task of the product system, specifying what it is designed for. The functional unit is a quantitative representation of the function. For example, in the case of a single photovoltaic panel, the functional unit could be the production of 1 kWh electricity [51]. The quantified output associated with a functional unit is called reference flow.
- System boundaries: Inside the boundaries are all activities and processes that belong to the life cycle of the product or system under investigation.
- Allocation method, impact assessment and data quality: These principles are determined in the following phases.
- Assumptions and limitations of the study: Addressing uncertainties and a transparent communication of results is needed to cover explicit choices and constraints from the beginning.
- Aspects of a critical review: The review involves an examination of the study's methodology, assumptions, and data quality to ensure its credibility and reliability.

Step 2: Inventory Analysis

The main purpose of the inventory analysis is to collect all information to describe the product system [43]. As shown in Figure 2.5, after identifying the main processes for the LCA model in the goal and scope definition, data collection is crucial to depict environmental impacts [47]. Afterwards, the data can be used to calculate the inventory analysis. Depending on the predefined principles, allocation of some flows might become necessary. The result of the inventory analysis is a summary of the resources used as inputs and the emissions generated as outputs throughout the life cycle of the product, relative to the functional unit [46].

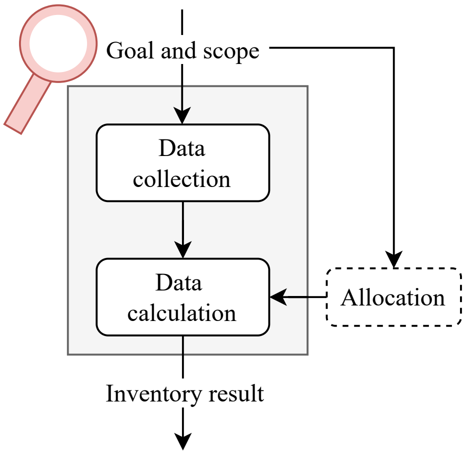


Figure 2.5.: Sub-steps of the inventory analysis. Dashed line represents an optional step. Magnifier represents affiliation to Figure 2.4. Own illustration based on ISO 14040 [45] and ISO 14044 [50].

Data Collection In general, data for the inventory analysis can be categorized into primary data, obtained from measurements of the main activities within the system boundaries, and secondary data, derived from external sources [13]. Usually, when defining the system boundaries of a LCA model, secondary data is predominantly used to describe the background system, while primary data is preferred to provide the foreground system with appropriate information [52]. However, the existence of primary data is often limited due to the complexity and cost intensity of measuring all inputs and outputs for individual data points [47]. Therefore a lot of data that is used for both background and foreground processes is gathered through online research and accessing public sources. The easiest and most reliable possibility to access (secondary) data is by finding a suitable database [13] as they often have already addressed the barriers of data collection and the handling of multiprocessing [47].

The selection of the database is one of the most labor-intensive stages of a LCA [46] and it significantly influences the reliability and accuracy of the environmental environmental data used in the assessment [52]. Since the release of the environmental management standards [45, 50], a considerable number of databases have been developed [46, 53] and databases can be adequate to fulfill many project requirements. However, it might be necessary to adapt the data to align with the different studies [13]. Additionally, the availability of databases remains restricted, and especially assessments containing technologies at an early stage of development encounter the problem of data gaps [54]. The lack of an internationally accepted structure, format, and documentation is another problem while identifying suitable databases for certain purposes [55]. For example, Martinez-Rocamora et al. discovered that for the building industry most databases have several further problems, including a difference between the locations of the data and the location of the study, a lack of transparency and the unsuitability for their project

[53]. The most widely used databases in literature are ecoinvent [56] and GaBi [57], renowned for their completeness and comprehensiveness [23, 47, 53, 58]. However, both databases are not publicly accessible and require paid licenses due to the high costs associated with maintaining data quality, highlighting the limitations in database selection [54].

Another important consideration is the difference between unit process datasets and aggregated process datasets (often called system processes) [13]. Aggregated process datasets combine multiple unit process datasets into a single process with a unified reference flow output. Many databases include such average data to streamline memory usage and reduce complexity [46, 47]. Nevertheless, using these averages can pose challenges in tailoring data to specific projects and product systems, resulting in a loss of transparency [47].

Data Calculation The collected data needs to be validated with respect to geographical, time-related and technological viability [13]. Then the data is assigned to the chosen process modules as well as to the chosen functional unit. If gaps appear, it is possible to adapt the system boundaries afterwards to change the selection of chosen processes [45].

Allocation As illustrated in Figure 2.5, the allocation represents an optional step in the inventory analysis. Allocation is necessary, if a process in a product system has multiple outputs, and not all of them are used by the reference flow of the study [47]. To handle this so called multiprocessing, different allocation principles can be used [45]:

- System expansion: The system boundaries are expanded to consider the outputs of a process as co-products. The environmental burdens are then assessed for each co-product separately.
- Subdivision: This method involves dividing the environmental impacts of a process among its different products based on a predetermined allocation factor. Each product is then individually assessed for its environmental performance.

Step 3: Impact Assessment

The purpose of the impact assessment is to analyze the outcomes derived from the inventory analysis to understand the environmental impacts of the study [45, 46]. Figure 2.6 illustrates the sub-steps of the impact assessment, including three mandatory and three optional steps. The result of the impact assessment is the category indicator result, a numerical score for the examined environmental impacts. In addition to the environmental standards the technical report ISO/TR 14047 provides examples and additional guidance for this phase of a LCA [59].

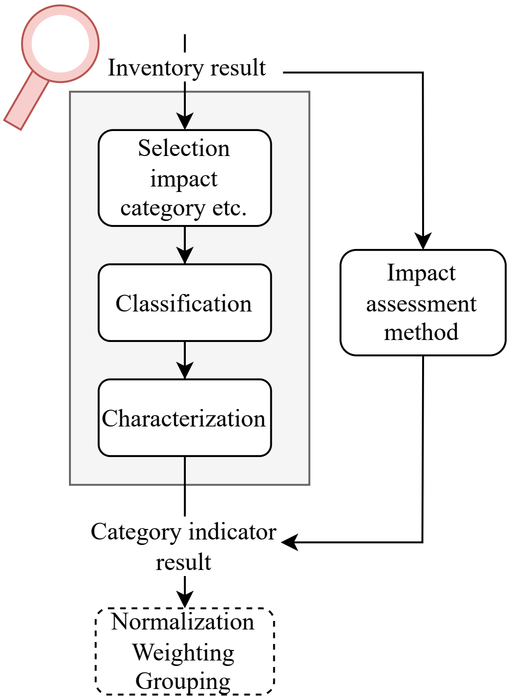


Figure 2.6.: Sub-steps of the impact assessment. The impact assessment method works as a shortcut for the impact assessment. Dashed line represents optional steps. Magnifier represents affiliation to Figure 2.4. Own illustration based on ISO 14040 [45] and ISO 14044 [50].

Selection of Impact Categories, Category Indicators, and Characterization Model The selection of these three terms, which are defined in Table 2.2, needs to be in common sense with the selected goal and scope of the study [50]. Initially, impact categories can be associated with either input flows (e.g., fossil fuel consumption) or output flows (e.g., climate change, human toxicity) [45]. The category indicators should represent impacts of the chosen impact category as good as possible and can be chosen somewhere between the inventory results and the endpoints along the environmental mechanism, as shown in Figure 2.7. Midpoint indicators represent intermediate environmental impacts, while endpoint indicators link different midpoint indicators and capture broader and final environmental effects [59]. Endpoint indicators are defined at the level of AoPs, as also shown in Figure 2.7. These areas encompass a group of category endpoints with widely accepted societal values and typically cover aspects of the natural environment, human health, or resources [60]. In general, it is recommended to conduct the impact assessment on midpoint and endpoint indicators. However, it is common practice to focus on midpoint indicators due to the large uncertainties associated with endpoint indicators, stemming from the necessary additional modeling efforts [46, 59]. Some possible impact categories for indicators are shown in Figure 2.7. The specific selection depends on the goals and scope of the study. The third term, the characterization model, also takes temporal and spatial relationships between the inventory results and the impact indicators into account [50].

After defining the impact categories, the category indicators, and the characterization model, environmental standards recommend evaluating the environmental relevance by examining the qualitative impact of the category indicator on the category endpoint. This involves providing insights into the extent to which the indicator influences the endpoint in a qualitative manner [47, 59].

The different definitions are further explained in Table 2.2, illustrated by the application of the impact category climate change.

Table 2.2.: Definitions of important terms of the impact assessment. The example covers one possible impact category (climate change). In relation to [45] and [47].

Term	Definition	Example
inventory result	result of the inventory analysis representing the environmental inputs and outputs related to the functional unit	amount of GHG emissions from a manufacturing process
impact category	class representing a specific environmental issue of concern	climate change
characterization model	mechanism to describe the relation between the inventory results and the category indicators, used to derive the CFs	baseline scenario by the IPCC for the global warming potential of different greenhouse gases
category indicator	quantifiable representation of an impact category	increase of infrared radiative forcing (W/m^2)
characterization factor (CF)	factor that transfers the inventory result to the standardized unit of the category indicator	global warming potential for each GHG emission (kg CO_2 eq/kg emission)
indicator result	numerical score obtained through the quantification of the category indicator with the CF	sum of the global warming potential (kg CO_2 eq)
category endpoint	aspect of one AoP describing an environmental problem	years of life lost, loss of coral reefs, etc.
environmental relevance	degree of correlation between the impact category indicator value and the corresponding category endpoint	Infrared radiative forcing elevates the atmospheric concentration of greenhouse gases

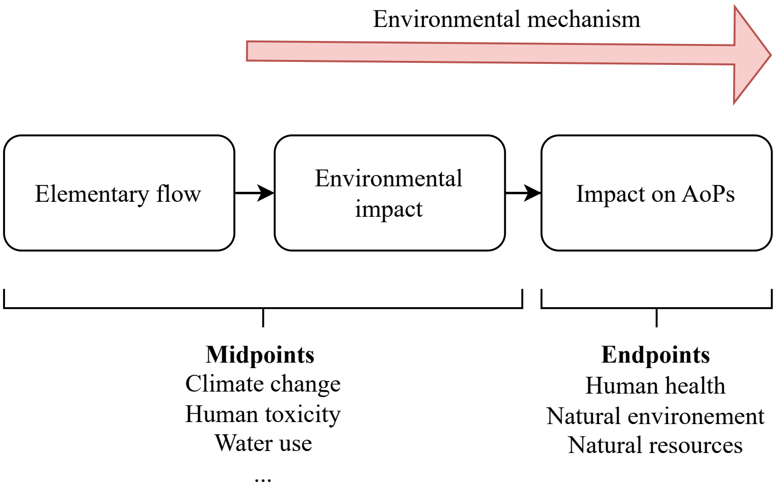


Figure 2.7.: Selection of midpoint and endpoint indicators. The midpoint indicators represent examples of possible midpoints. Endpoint indicators represent the impact of the AoP. Abbreviation: AoPs = areas of protection. Own illustration based on [44, 47]

Classification The classification of elementary flows is done by assigning inventory results to the impact categories on which they have an impact on [45]. This step requires professional knowledge about the different substances and their consequences and is therefore typically done by a LCA software [47].

Characterization The results of category indicators are calculated [59]. Therefore elementary flows of the product system are assigned to a degree to which they contribute to an impact, by multiplying the amount of elementary flows in an impact category with a CF. These results are summed to a total impact score for the respective impact category (also called indicator result) [60, 61].

$$IR = \sum_i (CF_i \cdot E_i)$$

with:

IR Indicator result

CF Characterization factor

E Environmental impacts (category indicator)

This process assists in presenting various environmental impacts in a consistent manner, facilitating the comparative analysis of different impact categories [47].

Optional There are three optional steps of the impact assessment [59, 62]:

- Normalization: Comparing impacts to those of a reference country or industry to provide a better perspective.
- Weighting: Assigning different or equal weights to each category indicator, based on subjective choices.
- Grouping: Categorizing impact categories into clusters or groups, allowing for sorting or ranking based on predefined goals.

One form of weighting is the monetization of LCA results analogous to the use of single values in the multi-objective optimization in ESM (see subsection 2.1.2). This method aims to enable trade-offs between different impact categories by creating a single score that expresses environmental impacts in monetary items [63]. In other words, it seeks to quantify the loss of economic welfare attributable to the impacts [23]. However, there are a lot of different monetization methods resulting in scores with a wide range of results. Studies show monetary values per capita and year for an average EU citizen range between 224 € up to almost 8 000 € [63]. Consequently, it is recommended by the guidelines of the environmental standards to use these scores only for internal communication within an organization. This caution arises from the acknowledgment that monetization may not accurately and comprehensively represent the entirety of the environmental impact of a product or service [45, 50].

Impact Assessment Method ISO 14040 [45] and ISO 14044 [50] contain several further recommendations for the selection of impact categories, category indicators, and characterization models, as well as for the classification and characterization. Given the complexity and multitude of factors to consider, practitioners frequently prefer established impact assessment methods [13]. As shown in Figure 2.6 these methods simplify subsequent stages of the impact assessment process as they have already incorporated considerations into their frameworks [47]. Since the inception of the first impact assessment method, a number of these methods has been developed, like IMPACT World+ [64], ReCiPe [65], or the Environmental Footprint (EF) method [66]. Those methods differ in their emphasis on environmental categories, their application of LCA forms (see subsection 2.2.3), or their inclusion of different life cycle stages [47]. Therefore, the selection involves careful consideration of diverse elements to ensure the relevance and accuracy of the chosen method for a given study [62].

An example that is often used in scientific literature is the ReCiPe method [17, 23, 63, 67]. It refers to the "method for the characterization of environmental impacts - midpoint and endpoint method" [61]. This method considers impact categories for indicators at midpoint or endpoint level, as shown in Figure 2.8. More information about the midpoint indicators can be found in Appendix B. The endpoint categories are expressed in disability adjusted life years (DALYs) for human health, relative species loss over space and time for the ecosystem and additional financial costs for future extraction of metal and fossil resources in units of dollars for resources [65]. Midpoints or endpoints can be represented at different archetypes of human behavior, where perspective H is normally chosen for default values as it considers the most common policy principles with regard to time frame and other issues. ReCiPe was initially defined in 2008, but got adapted in 2016 [61].

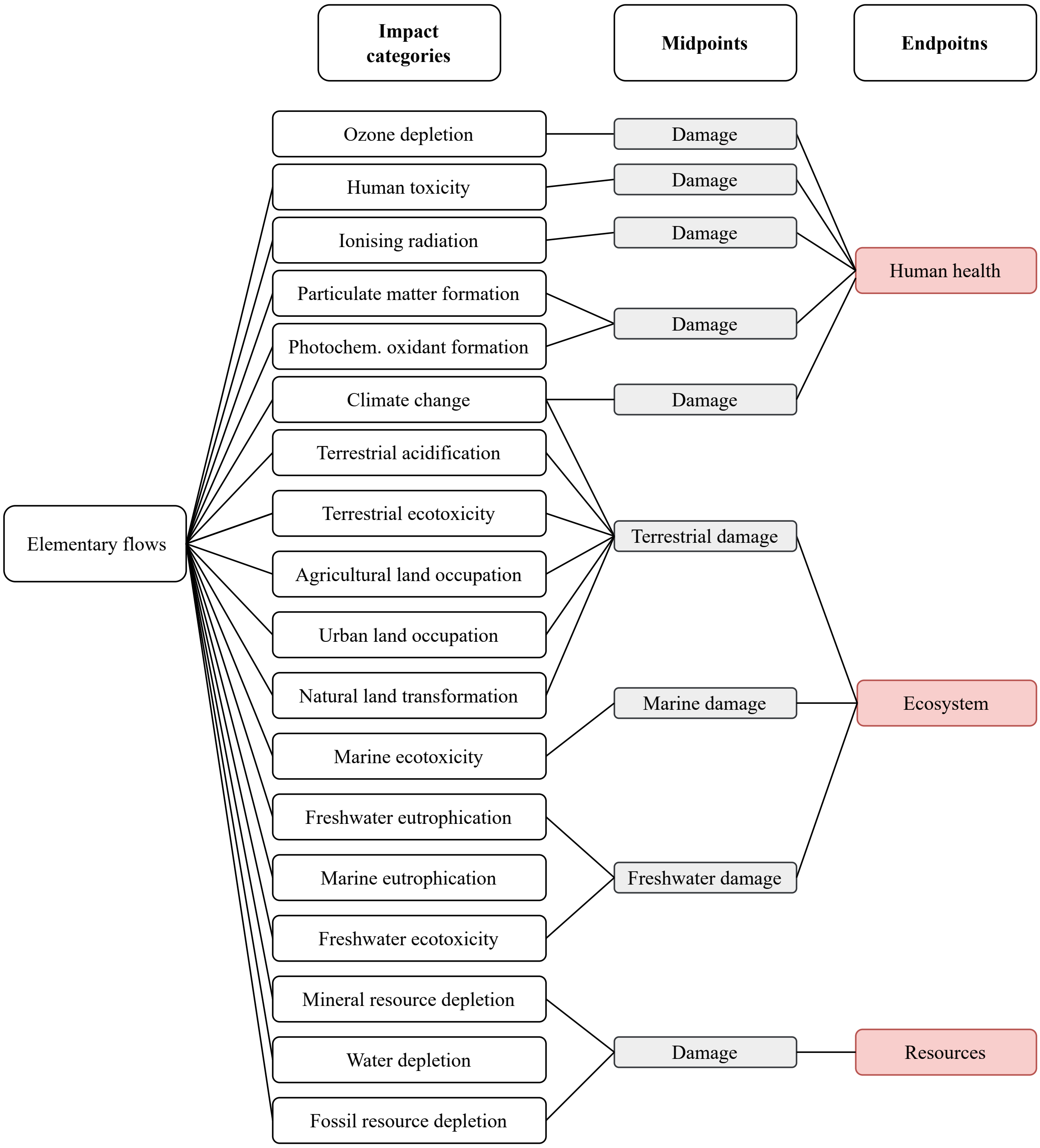


Figure 2.8.: ReCiPe2008 impact categories. Overview of the impact categories at midpoint and endpoint level. For some impact categories there is no mid-to-endpoint connection (e.g., marine eutrophication, water consumption). Abbreviation: Photochem. = Photochemical. Own illustration adapted from [65].

Step 4: Interpretation

The interpretation draws conclusion from results of the inventory analysis as well as of results from the impact assessment [47]. It is not the last step of a LCA, but links the results of the other three phases [52]. During interpretation, it is necessary to revisit the goal and scope definition to assure the accordance with the objective of the study. Further it includes [45]:

- Examination of inventory analysis and impact assessment results.
- Completeness check, consistency check, sensitivity analysis.
- Limitations and recommendations.

The interpretation excludes weighting and normalization which are often used to interpret LCA results. Instead, it focuses on the independent summary of the results in relation to the defined phases [52].

2.2.3. Forms of LCA

Attributional and Consequential LCA There are two different types of LCA considering the aim of the study - attributional or consequential LCA.

Attributional LCA aims to provide information on what environmental burdens can be attributed to a specific product life cycle [68]. This method typically utilizes average data to quantify environmental burdens [52]. In contrast, consequential LCA seeks to provide information on the environmental burdens that occur, directly or indirectly, as a consequence of a decision [68]. Consequential LCA usually employs marginal data that is specific to the intended consequences of the decisions [52].

In the past, attributional LCA has been more commonly applied in practice. This is based on the fact that for a consequential study, information is needed about how the market reacts to fluctuations in demand and supply. Obtaining such information is often difficult [47].

Integrated LCA The term refers to the concept that LCA is connected with other model approaches [68], such as ESM or material flow analysis [16]. The integrated LCA framework normally considers not only environmental impacts but also incorporates social and economic dimensions throughout the entire life cycle of a product or service [68].

Territorial LCA Building upon the product-oriented approach that traditionally focuses on smaller scales, there is a natural progression to extend this methodology to larger meso- and macro-scale objects [69]. This evolution lead to the development of a territorial LCA approach [70]. Loiseau et al. defines two types of territorial LCA. Type A includes environmental impacts of an activity that occur within a specified territory, while type B encompasses impacts of all production and consumption activities within the territory, including also cross-sectoral impacts [70].

Hybrid LCA Process-based LCA is the standard form of a LCA [71]. The data is generated in a bottom-up approach, starting with the different flows of each component of the product system [72]. The disadvantages are common data gabs, missing knowledge, and a possible underestimation of environmental burdens due to those uncertainties [55].

The aim of an input-output (IO) LCA is to consider the inputs and outputs of a chosen system in terms of economical values [71]. Therefore data collection is done in the way of a top-down approach, resulting in highly aggregated datasets [72].

Hybrid LCA combines process-based LCA and IO LCA. In hybrid LCA, macroeconomic data is commonly employed in the background system to provide a more detailed representation of the process-based foreground system [47]. This approach is used to overcome limitations of process-based data. Due to the availability of national input and output tables for different sectors, it is possible to expand the system boundaries of the background system [13, 72].

2.2.4. OpenLCA

There are multiple software tools and techniques to design the framework for a LCA [13]. An example of a software used to conduct a LCA is the tool openLCA by GreenDelta[7]. The current version of this software is openLCA 2.0.3. One of its major advantages is its accessibility as it is open-source and freely accessible to the public [47]. It can be used for a broad range of functionalities. Users can model life cycles, adjust inventories, and assess environmental impact categories of different processes and products[8].

Another advantage is the ability to interact with the software via a programming interface using packages of the olca client[9]. It can be used by any application in any programming language. The olca-ipc package is used for the inter-process communication with openLCA and further includes the olca-schema package[10], which can be used for reading and writing datasets.

An additional feature by the GreenDelta company is openLCA Nexus, an online repository for LCA data. It contains free and commercial datasets[11].

2.3. Model Coupling of LCA and ESM

2.3.1. Advantages and Growing Importance

As pointed out in the introduction, current research on simulating energy systems tends to prioritize cost optimization, often overlooking broader environmental impacts. However, there are a variety of advantages from integrating LCA into typical ESM. The transition towards a renewable energy system, moving away from fossil fuel production, significantly impacts various environmental factors [11, 16]. This transition can lead to higher material requirements, affecting the impact category metal depletion [5, 11, 23]. Zang et al. focused on different power generation schemes based on biomass, resulting in varying impacts, especially in terms of ozone depletion and human toxicity [73]. These examples underline the increasing significance of non-climate environmental impacts in shaping the course of the transition [72]. The consideration of these impacts leads to additional trade offs due to the interaction between the impact categories [17]. An energy system that reduces all possible environmental impacts does currently not exist. Therefore, different combinations of technologies can ultimately lead to the lowest possible impacts [30, 74]. Another important advantage of considering perspectives of a LCA in ESM is the prevention of burden shifting [5]. This is particularly important when examining renewable energies, where a significant portion of environmental impacts occurs outside the usage or generation phase. This is exemplified by technologies like wind power or photovoltaic (PV) systems [5].

[7] Website - openLCA: `https://www.openlca.org/`.
[8] User manual - openLCA: `https://greendelta.github.io/openLCA2-manual/`.
[9] Documentation - olca-ipc: `https://greendelta.github.io/openLCA-ApiDoc/ipc/`.
[10] Documentation - olca-schema: `https://greendelta.github.io/olca-schema/intro.html/`.
[11] Website - openLCA Nexus: `https://nexus.openlca.org/`.

2.3.2. Challenges

From the combination of the two approaches arise the following challenges [12, 28]:

- System boundaries: LCA takes all flows into consideration, while ESM only considers energy input flows.
- Data collection: The two approaches differ in their data requirements, as LCA considers energy and material flows of technologies in a much more detailed way. Particularly for analyzing the environmental impacts in the energy sector, databases lack disclosure for different electrical technologies [72].
- Double counting: When two or more components attribute the same impact to a shared process, this might lead to an overestimation of the environmental burden inside the system or within different systems [75, 76].
- Spatial and temporal scale: ESM classifies usecase specific spatial and temporal scale, while LCA normally does not take regional and temporal differences into account, because local values dependent on weather, population or other information, are often not available [75]. Moreover, ESM also has to take the spatial and temporal resolution of the modeling process into account [33], while this can be neglected in LCA [75].
- Model logic: LCA typically does not model the connection of technologies and does not consider potential impacts resulting from linking components of the energy system.

These challenges limit the possibilities to rightfully combine these two scientific approaches and result in further simplifications needed for this study. Due to the mentioned growing interest, several guidelines on the coupling have emerged in recent years, guiding users and developers in potentially overcoming these challenges [12, 58, 77]. As an example Xu avised the Environmental Framework for Energy System Assessment (EAFESA) to use the advantages of both LCA and ESM, addressing previously elucidated challenges [12].

2.3.3. Possibilities of the Implementation

There is a general difference between the ways of linking these two approaches with each other. Soft linking involves the transfer of information from one model to another, whereas hard linking implies merging of different models into a new integrated model [20].

Another classification can be made considering the actual coupling of ESM and LCA [12, 16, 17].

- Ex-post analysis: The outputs obtained from energy optimization are utilized as inputs for a comprehensive environmental analysis (energy system thinking).
  - Stand-alone analysis: The LCA is conducted afterwards and independently. An example for this option is the case study published by Quest et al. [23].
  - Multi-criteria decision analysis (MCDA): A decision is based on additional environmental impacts as well as on the outcomes derived from ESM optimization. An example for this option is the study by Volkart et al. [78].

- Endogenous analysis: The ESM is fed with information from LCA datasets that are considered within the optimization. This option assumes a consequential LCA, as the influencing factors are directly incorporated into the decisions arising from the ESM (life cycle and energy system thinking) [30].
  - Monetization of environmental impacts: Energy systems are conventionally optimized based on costs, but these costs incorporate environmental impacts by converting them into monetary units. This has mostly been done in the power sector. An example for this option are the studies by Brown et al. [79] or García-Gusano et al. [74] who integrate monetization of the impact categories climate change and human health.
  - Multi-objective optimization: Aiming to address uncertainties associated with the monetization approach, this optimization considers environmental impacts as a separate goal. An example for this is Rauner and Budzinski [36]. So far this approach has mostly focused on GHG emissions, overlooking other LCA indicators.
  - Blanco et al. also proposes the idea of a third approach where the ESM incorporates targets for various impact categories in the optimization [17], a concept that had not been explored until the release of their paper.

The advantages of an endogenous analysis is the feedback between environmental impacts and the optimization problem [17]. However, monetization is highly uncertain [63]. Even though multi-objective optimization can address this issue, it encounters significant complexity challenges. Therefore, until now, most studies have been realized in the field of ex-post studies [17]. In principle, it is recommended to initially examine ESM outputs with LCA and subsequently integrate environmental indicators back into the ESM [12, 58].

2.3.4. Life Cycle Assessment based Energy Decision (LAEND)

Tool Description The landscape of tools incorporating a life cycle approach into energy system models is limited [12, 17]. An example illustrating the concept of an endogenous analysis is the LAEND tool[12] , developed by Pforzheim University. LAEND couples sustainability assessment and optimization with a focus on environmental considerations [31]. This tool is built upon the open-source toolbox oemof [82] and utilizes the LCA software openLCA [83].

The modeling and optimization of energy systems with incorporation of environmental impacts, shown in the Figure 2.9, consists of several steps and sub-process steps (see LAEND documentation[13] for more information about the tool). Based on several user decisions, the modeling workflow may follow different pathways. These choices are manifested through distinct input files and the selection of different options within the main configuration folder. During the modeling process, results are saved in a result folder with mostly xlsx-files.

The two most important functions of the LAEND tool are *main()* and *optimizeForObjective()*.

The *main()* function executes all preparations that are independent of the optimization objectives. First, the local specifications of the energy system are imported. This enables the user to make different decisions based on the characteristics of the energy system. The temporal settings include the start and end year of the modeling process. The location settings include the time zone, longitude, and latitude of the energy system. Further, LAEND uses a typical meteorological year (TMY) comprising meteorological data for a single year, with hourly values

[12] GitHub - LAEND_v031: https://github.com/inecmod/LAEND/commits/main/.
Version until commit "Update utils.p" (b0c43e4), new commits were released at 01.03.2024 and are not part of this thesis.

[13] Documentation - LAEND_v031:
https://github.com/inecmod/LAEND/commit/51eac2ec14315711eb29eedfc8fc77e2b3bdfe6b.

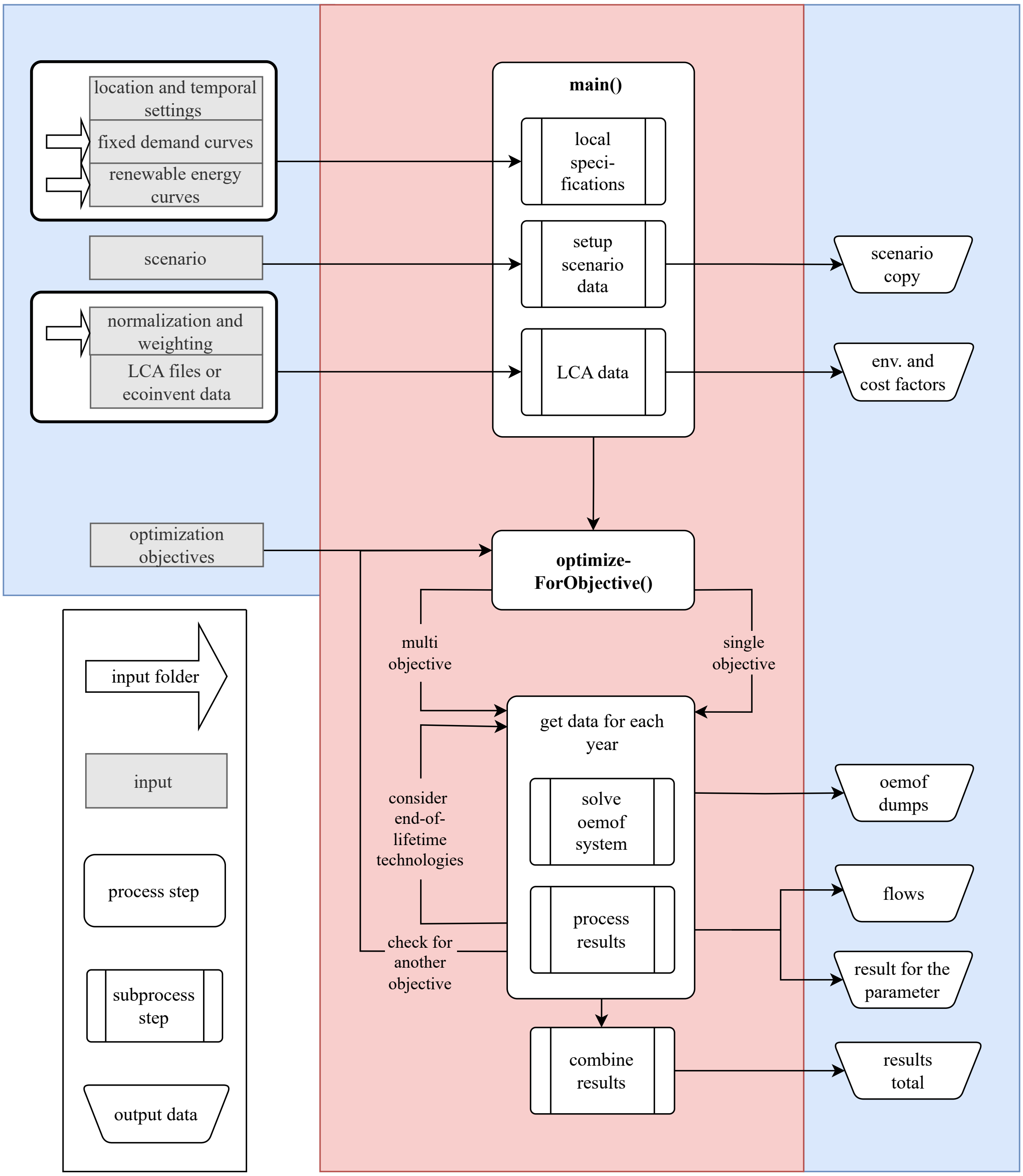


Figure 2.9.: Modeling workflow Life Cycle Assessment based Energy Decision (LAEND) Tool. The two main functions of the tool are printed in bold. Abbreviations: LCA = life cycle assessment, env. = environmental, oemof = Open Energy Modelling Framework. Own illustration based on [80, 81].

for the specified location of the energy system. These values are generated from a database with a much longer period in order to depict reality as closely as possible [84]. The TMY serves a dual role, acting as a filter for PV data by defining the weather settings and as the source for selecting fixed demand curves and renewable energy curves. Consequently, the user can import new fixed load curves by changing the TMY, as well as the load curves in the input folder.

Once local specifications are adjusted, the scenario data is set up accordingly. The scenario.xlsx serves as the main input table for LAEND, including all components of the current energy system organized in different sheets. It also incorporates additional sheets for buses (nodes of the energy system) and references to demand curves and time series. A copy of the scenario input file is saved in the results folder for further documentation. The last step of the main function is to import all required LCA datasets. One input file contains normalization and weighting factors for conducting optional steps of the impact assessment (see "Step 3: Impact Assessment" in subsection 2.2.2). These factors derive from two published papers of the Publications Office of the EU and are used to combine multiple impact categories into a single impact score [85, 86]. The LCA data, which includes the inventory results with resource and emission flows for all components of the energy system, is imported in two ways. It can be linked to the openLCA software [83] and the ecoinvent database [56], or used directly from several saved xlsx-files. The first option can be realized with the olca package (see subsection 2.2.4). The program already includes files for selected technologies of an energy system, allowing its use without requiring an ecoinvent license, as a second option. The outputs of the LCA data import include environmental factors (category indicator results) and cost factors for every technology and every possible optimization objective.

The second important function *optimizeForObjective()* runs the optimization for each objective. The user can select between different objectives for the optimization. The optimization objectives encompass system costs and environmental impacts. The environmental impacts can be represented either through a single impact category of the EF 2.0 impact assessment method [87], or through three single scores that account for multiple impact categories (see "Step 3: Impact Assessment" in subsection 2.2.2). These multi-objective goals involve the different normalization and weighting factors. For each objective an objective-specific energy system model is created and optimized for one single year. Therefore, all fundamental components within the energy system are created from a set of investment options. The oemof system is solved and the oemof dumps, data outputs generated during the simulation, are also saved in the result folder. These dumps can be restored for individualized results. Subsequently, the optimization from the first year is carried forward as the status quo for the second year, and the entire process is repeated. At this point, the end-of-lifetime of different technologies is also taken into account. If the lifetime is not exceeded, the graph is constructed based on prior investments, and new investment options are incorporated. The results are processed by the program and two different result files are created. The flows result file contains dispatch results for each optimized hour, while the general results xlsx-file comprises two sheets the environmental and financial impacts of the energy system. Additionally, it provides information on the capacity and energy flows for each technology, with a focus on minimizing the chosen objective parameters. After processing results for one objective, the program checks for additional objectives and repeats the process. In the end, the result files are copied into one xlsx-file for easier analysis.

Strengths and Limitations

Strengths of the LAEND tool:

- Multi-objective optimization: The consideration of multiple objectives with a single indicator, allowing for the derivation of an optimal energy system. This addresses a research gap outlined in literature and integrates environmental aspects into the optimization process (see subsection 2.3.1).

- Utilization of oemof: Similar to the SESMG, the LAEND tool adopts the oemof approach, a literature-defined method for energy system modeling [28].
- Open-Source Intention: The tool aims to employ open-source datasets. However, its implementation is currently limited by the requirement of an ecoinvent license for conducting further updates.
- Programming Interface: The LAEND tool provides the flexibility of using a programming interface via the olca package (see subsection 2.2.4) with the openLCA software.

Limitations of the LAEND tool:

- Unfinished programming: The tool is currently in an unfinished state, impacting its usability and reliability.
- Limited openness: The openness of the LAEND tool is restricted due to a mandatory ecoinvent license for updating LCA data.
- Single Score for multi-objective optimization: The optimization is limited through the single score that considers a weighting between environmental impacts and costs.
- Limited documentation and testing: The tool lacks comprehensive documentation and testing, and there are no available case studies for users to reference.

3. Implementation of LCA in SESMG

3.1. Concept Creation

3.1.1. Determinations

In order to integrate a LCA analysis in the SESMG, LCA concepts (see subsection 2.2.3) need to be selected to address challenges of coupling the two approaches.

- Ex-post LCA: For the research question, using LCA as an additional factor suffices for analyzing and designing energy systems. Given the current lack of consideration for environmental aspects beyond GHG emissions within the SESMG, a gradual integration is necessary. During the optimization process, the number of indicators should be limited to a tolerable level [24]. It is also recommended by frameworks like EAFESA [12] to start from an energy-system perspective, where ESM results serve as an input for the followed LCA (see subsection 2.3.3). Additionally, including LCA indicators in the optimization process with an endogenous analysis requires a validated data basis. These information cannot be provided with current data limitations [30].
- Integrated LCA: The developed approach is an integrated LCA [68], as the output of ESM is used as an input for the LCA.
- Attributional LCA: This approach allows reliance on databases that provide average data [46, 52]. On the contrary, consequential LCA would need information about how the market reacts to different compositions of the electricity mix (see subsection 2.2.3) [47, 68]. Such information, crucial for consequential LCA, cannot be adequately provided by average data [52].
- Process-based LCA: This approach facilitates the consideration of environmental impacts attributed to different processes [88]. IO LCA or hybrid LCA is not applicable, primarily because highly disaggregated datasets for the energy sector are lacking, and there is an increased complexity in implementation [12, 55].
- Territorial LCA: In many studies, a sector-specific examination is typically conducted within the framework of territorial LCA [89]. Given the focus on energy provision and consumption within a specific territory, type A is chosen [70].

3.1.2. Tool Selection

There were two possibilities to integrate LCA in the SESMG.

Firstly, the possibility of utilizing an existing tool capable of processing SESMG results for an independent ex-post LCA was explored. The LAEND tool [80] was evaluated as a potential standalone solution for this purpose. However, several limitations, such as restricted access to the ecoinvent database, and the inclusion of LCA parameters in the optimization process, rendered the tool unsuitable for this objective (see subsection 2.3.4). Despite these drawbacks, certain aspects of LAEND could serve as a guide for developing an own automated ex-post LCA methodology for energy systems.

Secondly, the option of integrating a LCA software tool into the SESMG through soft-linking was pursued. This led to the decision to employ the open-source software openLCA [83] which was also utilized in the LAEND tool. OpenLCA is currently the only known open-source software available to model life cycles [13, 47] (for more advantages see subsection 2.2.4).

3.2. Database

Data selection is a significant burden for obtaining meaningful results (see "Step 2: Inventory Analysis" in subsection 2.2.2). Consequently, the methodology begins with a prioritized consideration of the database selection. The choice of the openLCA software narrowed down database options to those compatible with the software.

3.2.1. Evaluation

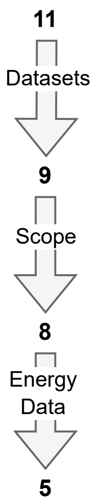


Figure 3.1.: Databases filtering. Own illustration.

For this study, only free databases were examined. OpenLCA Nexus provides free licenses for 11 databases[14]. This comprises ten options categorized as 'free databases' (not explicitly categorized as open-source) and the Prozessorientierte Basisdaten für Umweltmanagement-Instrumente (ProBas) database, listed under 'for purchase databases' which can also be used through a free license. In order to identify a suitable database, a preliminary filtering of these databases was conducted based on the criteria shown in Figure 3.1.

- Datasets: Inclusion of data and not just methods (excluding the impact assessment methods IMPACT World+ and openLCA life cycle impact assessment (LCIA)).
- Scope: Coverage data for Germany, the European Union, or global cases (excluding OzLCI2019 which focuses on Australasians regional supply).
- Energy Data: Presence of data related to multiple processes in an energy system (excluding ARVI, Agribalyse and bioenergiedat).

[14] All listed databases in this section can be accessed at openLCA Nexus.
Website - openLCA Nexus: https://nexus.openlca.org/

The filtering process resulted in five potential databases for the goal of combining the database with ESM:

- European Life Cycle Database (ELCD)[15]: European database of the Joint Research Center which is the European Commission's scientific and technical research center, with 190 datasets. This database complements other data sources in the ILCD Data Network [44].
- New Energy Externalities Developments for Sustainability (NEEDS)[16]: Life cycle inventories of future electricity supply in Europe, with 794 system and 139 unit processes [90, 91].
- Exiobase[17]: Global, detailed multi-regional environmentally extended IO database, developed by the Exiobase consortium [92], including datasets for 200 products and 163 industry processes [92].
- EF[18]: Secondary inventory datasets adhering to EF standards from various providers (also developed by the European Commission), with more than 3000 datasets [93].
- ProBas[19]: German database provided by the German Federal Environment Agency (Umweltbundesamt), contains 17 000 datasets (in the year 2013) which derive from multiple different projects [94].

All considered databases are summarized and evaluated in Table 3.1. In order to compare these databases a set of decisive features is proposed. The chosen features in accordance with Martinez-Rocamora et al. [53] are:

- Type: The database can be either process-based or IO-based.
- Scope: The scope describes the territory where the processes are located (for further information see "Step 1: Goal and Scope Definition" in subsection 2.2.2).
- Completeness: The completeness describes to which extent datasets cover the energy system. The subcategories are as follows:
  - Excellent: Data covers heat and electricity, renewable and fossil energy technologies, data for materials and transportation; allows selection between different technologies.
  - Acceptable: Data covers some parts of the energy system, but a noticeable data gap is identified after the initial examination.
  - Insufficient: Data only covers a few components of the energy system.
- Transparency: The transparency combines traceability with the description of a methodological process that is created with help of the database [53].
- Impact assessment method: The method indicates whether a database is compatible with a specific impact assessment offered by openLCA Nexus. If there is no fitting impact assessment method, the impacts would need to be evaluated separately under development of an costume impact assessment.
- Update: The update includes the latest data update of a database to ensure the currency of datasets.
- License: The license describes the form of license required to access the database.

[15] Website - openLCA Nexus - ELCD: https://nexus.openlca.org/database/ELCD.
[16] Website - openLCA Nexus - NEEDS: https://nexus.openlca.org/database/NEEDS.
[17] Website - openLCA Nexus - Exiobase: https://nexus.openlca.org/database/exiobase.
[18] Website - openLCA Nexus - EF: https://nexus.openlca.org/database/Environmental%20Footprints.
[19] Website - openLCA Nexus - ProBas: https://nexus.openlca.org/database/ProBas.

Database	Type	Scope	Completeness	Transparency	Impact Assessment Method	Updates	License	Further Anformation
ELCD	process-based	Europe	insufficient	undefined[a]	no own method	ELCD 3.2 (2015-2018) [95]	freely accessible to public	none
NEEDS	process-based	Europe, country specific data	acceptable[b]	undefined[a]	no own method	project 2004-2009 with prospective data	freely accessible to public	hard to combine with other databases
Exiobase	IO-based	global, country specific data	acceptable[c]	detailed documentation [92], several case studies [58]	own methods [96]	Exiobase 3.8.2 (2022)	paid licenses, but free older version (Exiobase 3.4)	hard to combine with other databases
EF	process-based	Europe	acceptable or excellent[d]	comprehensive documentation, some case studies [97]	own methods [93]	EF 3.1 (2023); EF 2.0 (2019) [93]	requires the paid feature of the Database Analyser and Launcher (DAL)	datasets are not final yet [97]
ProBas	process-based	Germany	acceptable[e]	comprehensive documentation, mistakes in the openLCA methodology [94]	own adapted methods [94]	corrections with ProBas+ (2016) [98]	free academic license	based on Global Emission Model for Integrated Systems Analysis (GEMIS) database [99]

[a] Not further examined.
[b] Covers data for the future electricity supply, material supply and transport services, but no data for small-scale technologies like PV systems or heating transformers [90].
[c] Super-categories like electricity by coal, gas, solar or biomass and values for distribution and trade services of energy.
[d] Super-categories like end-of-life treatment, energy carriers and technologies [97], no assignment to 'excellent' or 'acceptable', because the data is not freely available.
[e] Covers data for heat, electricity and mechanical energy, waste and transportation for different years and technologies.

Table 3.1.: Evaluation of free databases available in openLCA. Information without citation derive from the openLCA Nexus website [100] and the analysis of the different databases.

3.2.2. Selection

The ELCD database is unsuitable due to its limited dataset which lacks data for renewable energy technologies (see Table 3.1). The NEEDS database was designed between 2004 and 2009 for the analysis of a national or global energy system and does not contain data for single houses or neighborhoods [91]. Further, it can not be combined with any given impact assessment method (see Table 3.1).

⇒ Both databases are therefore not suitable for the coupling of ESM with an open-source database.

The Exiobase database is the only database that documents flows on a global scale and follows an IO inventory approach (see Table 3.1). Most models use the process-based approach [12], because the inclusion of macroeconomic IO data increases the complexity of the LCA [88] (see subsection 2.2.3). Therefore, Exiobase is often used as a supplementary database and is only partially suitable as a standalone database [7, 58].

⇒ Due to the decision of conducting a process-based LCA, the database is not suitable for the coupling.

The EF database presents some essential advantages, listed in Table 3.1. With highly detailed flows, encompassing over 10 000 inputs and outputs for a single process [101], it theoretically enables integration of other international datasets that share similar or identical flow nomenclature. Additionally, it employs a fully functional impact assessment method, which was also used by the earlier presented LAEND tool (see subsection 2.3.4). To evaluate the completeness (see subsection 3.2.1) a comprehensive comparison between the technologies in ProBas and EF, the two remaining databases, was conducted (see Appendix C). It revealed that 88 % of the categories of technologies commonly used in small-scale energy systems, like the ones examined in the case study by Quest et al. [23], can be represented using the EF database (EF 2.0 and EF 3.1) available in openLCA. In contrast, ProBas only covers records for 75 % of these categories, notably lacking data on battery storage systems and thermal storage systems (see Appendix C). This poses a significant disadvantage since battery storage systems were identified as a main contributor to the ecosystem damage in the study by Quest et al. [23]. Also other literature already defined battery storage systems as a source of many environmental impacts [102]. Despite its advantages, the EF database could not be used, due to the following reasons[20]:

- Paid license for the DAL[21]: The DAL is an additional tool for openLCA that is needed to access certain databases and costs 250 €/year plus an additional maintenance fee.
- Time limitation: Even if access to the database is granted, use of the datasets is only assured till the 31st of December 2025. After this period, an additional license agreement might be necessary, or the ongoing agreement has to be redefined with the software provider [103].
- Permitted use: The license only allows use in line with the current product environmental footprint category rules (PEFCR) as well as organization environmental footprint sector rules (OEFSR). These methods enable companies to measure and communicate their environmental performance. However, these studies demand a thorough comprehension of regulations and standards [104]. The use of the database can also be requested for other purposes [103]. However, after detailed consultation with experts of the openLCA software, this excludes any scientific use or use in the context of research. As openLCA only

[20] Despite several consultations with openLCA software experts.
[21] Website - openLCA Nexus - DAL: https://nexus.openlca.org/utility/Database%20Analyser%20and%20Launcher.

manages the integration of data and is not the provider of datasets [101, 103, 105], data use is restricted. The DAL makes datasets freely available, but the publication of datasets or results derived from them must adhere to the guidelines of the European Commission and cannot be legally guaranteed.

⇒ Mainly due to the license requirements the database is not suitable for the coupling.

Due to the limitations of the EF database, the ProBas database remained as the final database. The main advantages include free accessibility, an acceptable technology coverage compared to alternative databases, and potential of an own impact assessment method (see Table 3.1). Another important feature of this database is the ongoing commitment for database improvement by the Umweltbundesamt. They regularly improve datasets and corrected several flows of the datasets in their online data repository[22] in 2021. They publish additional information about their work and already recognized a lack of technologies in the field of battery storage systems [106], making future updates possible. While efforts have been made to enhance the database, certain limitations persist. Some were already mentioned in the database documentation [94], others became increasingly visible through the implementation of individual data records. The update of the database with ProBas+ managed to solve some of these mistakes and added 1 800 additional data sets [98][23].

⇒ Despite these challenges, this option appears to be the most viable for achieving the integration of LCAs with the SESMG.

3.2.3. Limitations of Prozessorientierte Basisdaten für Umweltmanagement-Instrumente (ProBas)

The following limitations and flaws within the ProBas database were discovered while working with the database. For some limitations there are possible solutions of dealing with these sources of error. The exact handling of mistakes is considered in more detail in subsection 3.4.2.

Unit and System Processes According to openLCA and to the definition in subsection 2.2.1, unit processes represent an individual activity or operation within a life cycle and are therefore meant to be connected to each other within a product system. In openLCA, a system process is a collection of multiple unit processes (see openLCA documentation[24] for examples of different processes). While implementing ProBas datasets from the online repository of the Umweltbundesamt in the software, most processes were divided in unit and system processes [98]. Theoretically, this means that calculations of a system process should lead to the same results as calculations of a unit process that is connected to the right additional processes. This is done as an example for the gas heating transformer in subsection 3.4.2. However, relying solely on unit processes leads to inaccurate impact assessment results and negative outcomes for various impact categories, regardless of the chosen impact assessment method. For example, calculated impacts of the dataset "El-Wärmepumpe-mono-Erdreich-DE-2010-mix" are more than five times lower in some impact categories in the unit process compared to the system process.

⇒ Handling: OpenLCA recognizes these mistakes and recommends utilizing only system processes when manually constructing the foreground system. Additionally, unit processes can be updated or modified by the user in the database [107].

[22] Website - Umweltbundesamt ProBas: `https://probas.umweltbundesamt.de/datenbank/#/`.
The following sections, if not specified differently, always refer to the ProBas version in the openLCA software.
[23] In the following thesis, the name of the database is simplified to ProBas, representing the ProBas+ version of 2016.
[24] Documentation - openLCA 2.0 - Processes:
`https://greendelta.github.io/openLCA2-manual/processes/index.html`.

Linking Properties OpenLCA offers the option to construct a product system (which is defined by the software as "a set of processes connected by flows, performing one or more defined functions and modeling the life cycle of a product" [108]) by automatically connecting processes using linking properties. This is an optional feature for unit processes. However, this feature does not effectively function with the ProBas database due to inadequate linking property information for most datasets [94]. This limitation leads to errors when attempting to use this option.

⇒ Handling: To address this issue, it is advisable to refrain from using the linking properties option and instead manually link processes. For example, this could involve manually connecting the gas input and the gas heating transformer as it is done in subsection 3.4.2.

Outdated Datasets The datasets of ProBas in openLCA differ from those available in the online database with the same name. This discrepancy arises from the data transfer in 2016 and the adaptions that were made by the software producers [98]. The datasets are regularly updated on the website of the Umweltbundesamt [99], as already mentioned above. However, these updates are not considered in openLCA leading to huge significant differences between these two sources. An example for this is shown in Table 3.2.

Table 3.2.: Comparison between ProBas in openLCA and the online data repository by the Umweltbundesamt[25]. Example of the dataset "Solar-PV-multi-Rahmen-mit-Rack-DE-2030_LCI". Values taken for the reference flow of 1 TJ electricity. Just a few flows selected as examples.

Flow example	Value openLCA	Value Umweltbundesamt
"Erze" (ores)	4 017 kg	725 kg
"Wasser" (water)	149 413 kg	85 964 kg
"Kohlendioxid" (carbon dioxide)	20 058 kg	45 082 kg
"Methan" (methane)	63.8 kg	11 kg
"Stickoxide" (nitrogen oxide)	33.4 kg	11.4 kg

⇒ Handling: There is no possibility to check whether the datasets were correctly imported in openLCA, as the original structure of the database does not exist anymore. This hinders the traceability of datasets. Consequently, it implies that datasets are outdated and potentially flawed, given that some technologies may have undergone significant changes, leading to discrepancies in values.

Aggregated Flows Flows in the ProBas database lack detailed information compared to other databases. This is mainly due to the reason that the flows are highly aggregated. Certain flows such as "Staub" (dust) or "Mineralien" (minerals) pose challenges for analysis due to unclear compositions.

⇒ Handling: While generally not problematic, the lack of detailed information is inherent in the database's methodology. Highly aggregated datasets from the Umweltbundesamt make it impossible to deeply analyze environmental impacts of different flows, as for example "Staub" (dust) could be composed by many different elementary flows.

[25] Website - Umweltbundesamt ProBas - Solar-PV-multi-Rahmen-mit-Rack-DE-2030: https://data.probas.umweltbundesamt.de/datasetdetail/process.xhtml?uuid=a976e93d-afce-4e7a-b32b-3477b87be658&version=02.44.152&stock=PUBLIC&lang=de.

Impact Assessment Despite adapting the impact assessment methods to the nomenclature of the ProBas database, there is no impact assessment that comprehensively covers all input and output flows of the required processes. Significant flows like "Erze" (ores) or "Fe-Schrott" (iron scrap) in energy technologies are not assigned to any environmental impact with a corresponding CF, rendering the impact assessment results incomplete.

⇒ Handling: Manually addressing the currently disregarded material flows is feasible to a limited extent, even after consulting openLCA customer service. This process involves applying distinct CFs to the aggregated material flows, making it both time-consuming and error-prone. Yet, without undertaking this manual intervention, the outcomes of the input-based impact categories lack significance.

3.3. LCA Application

3.3.1. Framework

The methodology for this thesis was adapted from the EAFESA framework (see subsection 2.3.2) that consists of the four main steps which are also described in the environmental standards and illustrated in Figure 3.2. The uniqueness of the framework lies in the exchange of information at each of these individual steps. Despite the fact that the ESM precedes the LCA in the process, it is important to consider the connection of the approaches when applying the LCA.

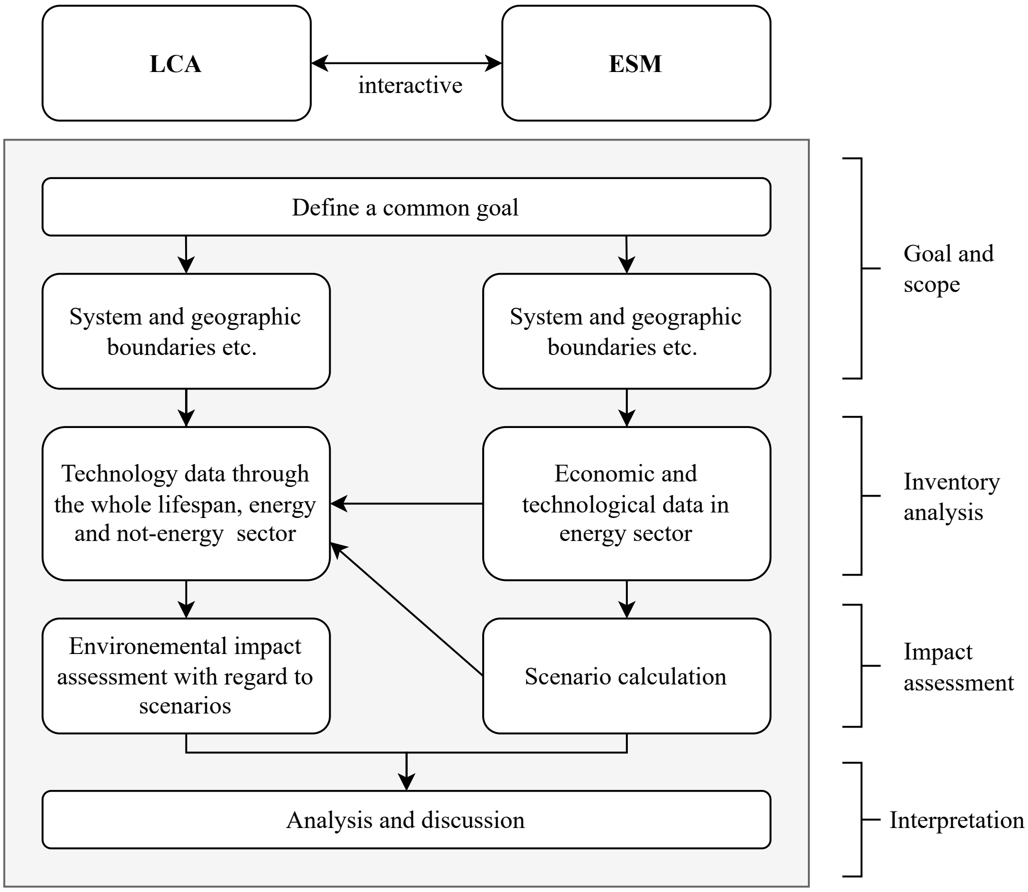


Figure 3.2.: EAFESA framework. Guidance how to integrate ESM outputs to LCA. Arrows represent the typical direction of the coupling. Abbreviations: LCA = life cycle assessment, ESM = energy system modeling. Own illustration adapted from [12].

To overcome the challenges outlined in subsection 2.3.2 two particular steps are essential when following the framework:

- Technology mapping: If technologies are modeled at a higher level of aggregation in one of the models and are considered in both approaches, they need to be disaggregated. For instance, if a LCA represents a technology as a single unit while the energy system model provides a more detailed breakdown, technology mapping involves breaking down the aggregated technology to match the granularity of the energy system model. This is also possible the other way around, depending on the selected databases.
- Data harmonization: Data that is considered in both approaches needs to be harmonized to establish a consistent and unified dataset (ideally after the technology mapping). This involves aligning the data formats, units, and temporal or spatial resolutions.

The application of the guideline outlined in Figure 3.2 encompasses the procedural steps for assessing the environmental impacts, of a generic energy system optimized with an ESM tool. Due to the interactions between the approaches, specifically the inventory analysis and the impact assessment are suitable for an automation.

Typically, these steps remain unaffected by the choice of the database. Nonetheless, in subsection 3.2.3 the ProBas database was identified as the only suitable option for this study. Any specific details or limitations arising from this selection and the use of this database within the openLCA software are outlined in boxes.

3.3.2. Step 1: Goal and Scope

In accordance with the framework illustrated in Figure 3.2, the goal and scope of the study are collectively defined for both LCA and ESM.

Goal

- Intention: Environmental impacts that derive from an additional LCA of energy system scenarios, can be used for analyzing the differences between them as whole systems as well as the composition of different energy technologies separately.
- Target audience: The field of ESM acts as the main target audience for the coupling of these two approaches. This is the reason why the additional calculation attempts to limit the level of user knowledge required for a LCA.

Scope

- Product system: All components that are defined in the energy system model should be considered by the conducted LCA, following the territorial LCA approach type A. Therefore, every technology that needs to be considered with environmental impacts has its own product system. The exact allocation which parts of the energy system need to be considered for the LCA depends on the ESM tool. Therefore, an option for this is shown in Figure 3.3 and further explained in section 3.4.

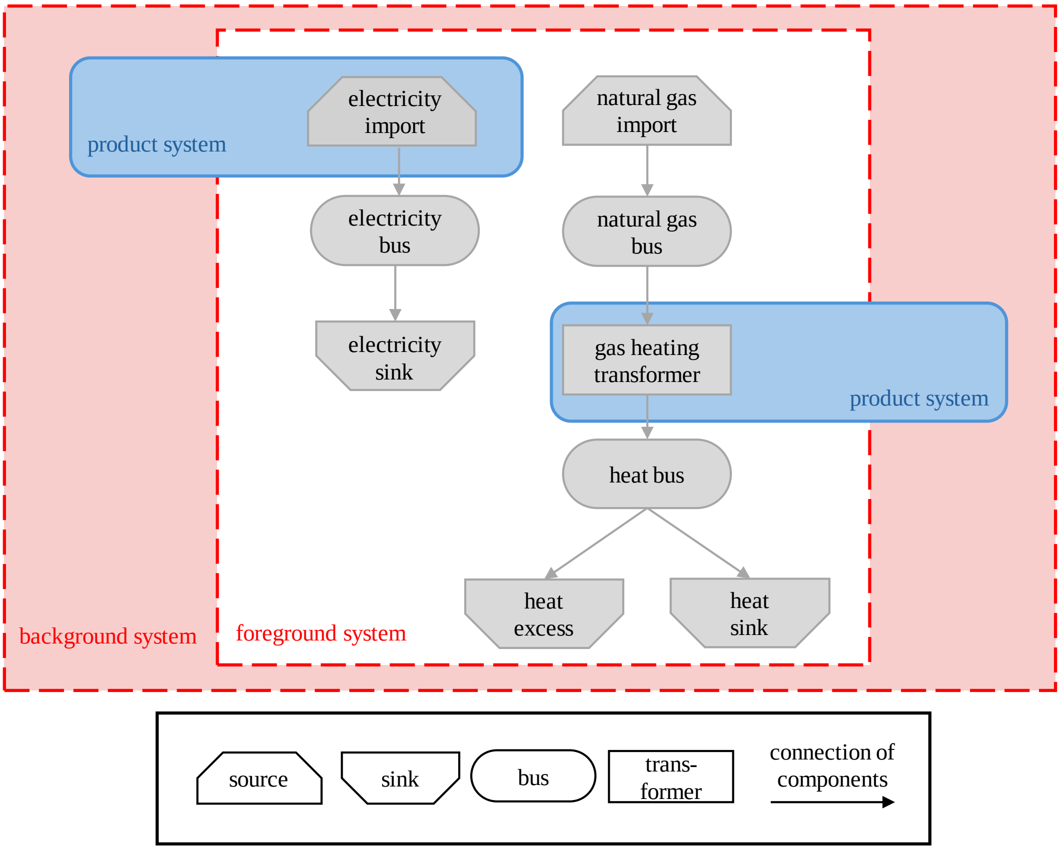


Figure 3.3.: Product systems in an exemplary energy system (including electricity mix and gas heating transformer components). Division into foreground and background system and definition of several product systems. The illustration follows the graph theory from oemof to model energy system components and their interactions as directed graphs. Own illustration.

- Function and functional unit: The general function of the different product systems is the supply of electricity and heat for the current system. In relation to Quest et al., the functional unit is defined as the "energy supply of electricity and heat to cover the energy demand of the system for one year" [23].
- System boundaries: The foreground system consists of all components that derive from the results of the ESM tool. Boundaries of an exemplary energy system are shown in Figure 3.3. The background system is derived from data of a database. Ideally, this database considers the whole process chain of the components [58].

ProBas

ProBas mainly uses GEMIS datasets. These datasets include processes that encompass the entire process chain from the extraction of resources that are converted into primary energy or raw materials up to the disposal process [109]. However, due to the mistakes in the linking of unit processes with other processes (see subsection 3.2.3), mainly system processes can be used. Because the datasets are highly aggregated, these processes already include all considerations of the background system. This leads to a less detailed system and makes the processes of the background system not displayable or adaptable.

- Allocation: Allocation is applied according to the norm only when processes with multiple outputs occur.

ProBas

Allocation is handled automatically by the openLCA software by using system expansion for multi-output processes (see "Step 3: Impact Assessment" in subsection 2.2.2). Processes with multiple outputs are considered as "Gross" processes. ProBas calculates environmental impacts by subtracting conventional "Bonus" processes for each output, creating a "Net" process where the substituted byproduct is treated as a credit (see website Umweltbundesamt[26] for an allocation example). This principle does not need to be considered manually by the user of the database [98].

- Impact assessment: The impact assessment is conducted using an impact assessment method that aims to assign as many considered flows as possible to the relevant impact assessment categories.

ProBas

The impact assessment is limited by the available methods compatible with the database. In openLCA, 17 different methods were adapted to the nomenclature in ProBas[27]. However, there is no method that rightfully represents the resource and emission flows used in the system (see subsection 3.2.3). Consequently, in the impact assessment, specific adjustments are necessary to better capture the unique characteristics of highly aggregated flows.

- Data quality: The data quality is recognized as a significant issue hindering the validity of the results, which should be taken into account when analyzing the outcomes of the LCA. This was already mentioned as a challenge for coupling the approaches in subsection 2.3.2.

ProBas

Due to the database's compilation from various sources, only brief descriptions are available for individual data points. This inherent limitation, coupled with documented errors in the database's methodology, compromises the overall data quality. These factors underscore the need for careful interpretation and acknowledgment of potential inaccuracies when utilizing ProBas data with openLCA in any analysis.

[26] Website - Umweltbundesamt ProBas - Solar-PV-multi-Rahmen-mit-Rack-DE-2030: https://data.probas.umweltbundesamt.de/datasetdetail/process.xhtml?uuid=a976e93d-afce-4e7a-b32b-3477b87be658&version=02.44.152&stock=PUBLIC&lang=de.

[27] Website - open LCANexus - Impact Assessment Methods: https://www.openlca.org/lcia-methods-databases/.

- Assumptions and limitations:
  - System boundaries: Currently all environmental impacts inside the boundaries are assigned to the chosen system, following the territorial approach A. Additionally, the environmental impacts follow the consumption-based accounting, which has the advantage that it considers the export of electricity produced inside the boundaries [24, 110].
  - Linear scaling: A linear scaling is used to scale the inventory flows and environmental impacts. This adjustment is achieved by multiplying the original flows with the quantities of energy that result from the optimization process of the energy system.
  - Material flows such as waste, water, wastewater, and building material are not considered.

3.3.3. Step 2: Inventory Analysis

The inventory analysis for the ESM tool results in economic and technological data of the energy sector, containing different energy supplies to fulfill the earlier mentioned function of the product systems. The inventory analysis of the LCA is done afterwards by adding additional input and output flows to the different components of the energy system, with consideration of the following steps:

- Data collection: In general, all components that can be used to supply heat and electricity are aimed to be connected to LCA datasets. Ideally, these datasets enable technology mapping and data harmonization. This means having a variety of unit processes available to represent different technologies with varying levels of detail. These processes can then be used to match the composition of the energy scenario and to adapt data values. To gain a detailed understanding of how this can be integrated into a tool, see section 3.4 for more information.

  ProBas

  Not all component types can be mapped with ProBas, as analyzed in Appendix C. This limits the process of technology mapping. Moreover, the desired data harmonization is hindered by aggregated datasets and mistakes in the unit processes of the database. This is because adaptations of flows can only be realized through unit processes.

- Data calculation: The flows are assigned to different technologies of the scenario calculation. The inventory results for the components of the energy system are further summed up across technologies to compare the energy system as a whole.

  ProBas

  The calculation is limited to system processes in the database. Due to the mistakes of the linking properties within the openLCA application, automatic connections of processes need to be avoided.

3.3.4. Step 3: Impact Assessment

In principle, the impact assessment combines different flows from the inventory results with the energy scenario calculations, as illustrated by the arrows in Figure 3.2 by the arrows. A comprehensive analysis across various impact categories is needed to understand overall environmental consequences [12, 45]. The impact assessment is conducted with an impact assessment method which leads to the neglection of the other steps. This is preferred to reduce the complexity and time effort. The three optional (normalization, weighting, grouping) steps are currently not conducted, but remain optional for further discussion.

ProBas

Multiple impact assessment methods are available in openLCA that can be utilized within the ProBas database. The most suitable method for this database is one that can assess the impacts of most of the flows, partly addressing the mistake of the impact assessment methods adapted for ProBas. Therefore, the assignment of different flows to the impact categories was analyzed using a simple energy system example consisting of electricity import, gas import, gas heating transformer, PV system and ground-coupled heat pump (GCHP). This analysis led to the selection of the ReCiPe2008 midpoint H method (see "Step 3: Impact Assessment" in subsection 2.2.2) since it covers the most flows, with 31 out of 64 flows used in the exemplary energy system (see Appendix D). Additionally, midpoint indicators were chosen because ReCiPe2008 lacks endpoint-to-midpoint factors, which could hinder the validity in considering endpoint indicators [61]. The further analysis in Appendix E highlights the insufficient representation of some flows. Even in ReCiPe midpoint H, half of the flows are not utilized in the impact assessment. Consequently, manual assignments were made for certain flows to their respective impact categories. For instance, the flow "Eisenschrott" (iron scrap) underwent the following manual changes:

- Classification: In reference to [65] iron is assigned to the impact category metal depletion.
- Characterization: The CF was taken from [65] as well. The methodology lists CF = 1 for iron in the category. This assignment was also added in the impact assessment method in the openLCA software manually.

This manual assignment was not possible for all flows. Appendix E shows which flows could be added to the impact assessment. Even after the manual assignment, 26 % of the flows remained too aggregated or vague to determine an accurate CF. These flows are not addressed further in the impact assessment. Additionally, note that the manual assignment was only done for flows of a simple example system chosen for the development of the impact assessment in Appendix D. The integration of more technologies would even increase the amount of flows that are lacking a CF for the assessment methods.

3.3.5. Step 4: Interpretation

In this thesis the interpretation of the LCA is done in the discussion (see chapter 5). As shown in Figure 3.2, the results of both methodological approaches must be combined in the interpretation. This makes statements about the environmental impact of the different technologies as well as of the system possible.

3.4. Realization in SESMG

The application of an ex-post automatic LCA is done with soft-linking (see subsection 2.3.3) of the SESMG and openLCA. The following implementation steps can be distinguished:

- Incorporation into SESMG structure.
- Programming individual LCA steps with the olca packages.
- Selection of datasets for the mapping of different technologies.

3.4.1. SESMG Structure

In general, the realization of the LCA is done independently from the database. This means that the LCA calculation can theoretically be conducted for individual projects using commercial databases, with a few necessary user-initiated changes. Therefore, boxes are utilized again to define steps affected by the choice of the ProBas database.

As shown in Figure 3.4, the two main interfaces between the tools include the model definition and the obtained results for the components of the optimized energy system, expressed in terms of energy amounts. The results from the openLCA software act as results for step 2 and step 3 of the earlier explained application of the LCA in Figure 3.2.

Due to the requirements of the olca client, the SESMG was updated to run with Python 3.11. Currently, the extension runs in an specific branch of the SESMG (see Appendix A).

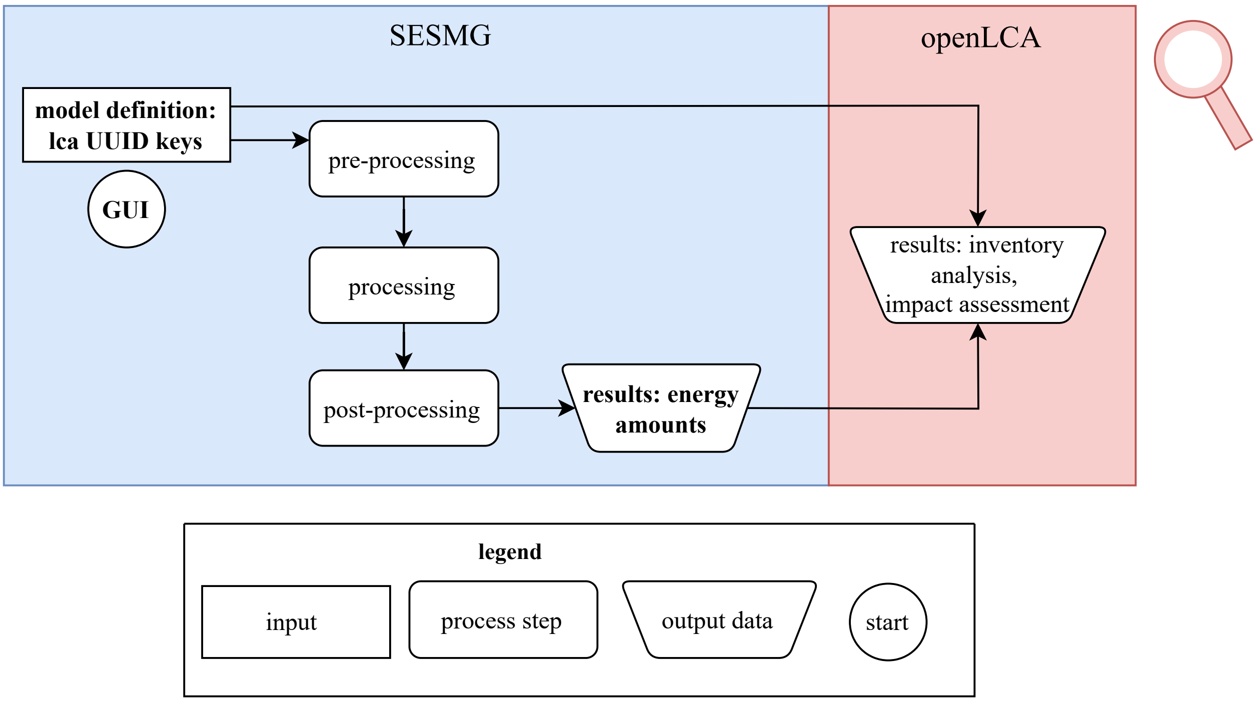


Figure 3.4.: Methodology for coupling the SESMG with openLCA. Blue represents the ESM part, red the LCA part. Model definition and energy amounts act as interfaces between the approaches. Magnifier represents that the steps by the openLCA software are later broken down into several sub-steps (see subsection 3.4.2). Abbreviations: SESMG = Spreadheet Energy System Model Generator, ESM = energy system modeling, LCA = life cycle assessment, UUID = uniiversally unique identifier, GUI = graphical user interface. Own illustration based on Figure 2.2.

Model Definition The model definition, which contains all parameters needed for the creation of the energy system (see subsection 2.1.3), is used to link the components of the energy systems to the appropriate dataset in the openLCA software via universally unique identifier (UUID) keys. These are sequences of characters and letters that identify a process in the software.

This has several advantages:

- Comprehensive overview: The model definition contains parameters for all components of the energy system [38], making it an ideal location to systematically include UUID keys for the components that can be calculated with an additional LCA.This advantage was also acknowledged by the EAFESA framework and the LAEND tool, both of which use an input file for model creation to link components to life cycle data.
- Optimization integration: The allocation of components occurs at the initial stage of a simulation or optimization process. This ensures the potential for generating future results based on LCA datasets, enabling integration into the optimization process as part of multi-objective optimization.
- Integration with SESMG-Data: The model definition simultaneously acts as an outcome from the US-Tool in conjunction with the SESMG-Data database. This setup opens the possibility of directly incorporating UUID keys into the model definition through SESMG-Data in the future.
- Database independence: The amount of UUID keys is limited to a minimal amount, making a change of datasets or the entire database theoretically possible by only changing the keys. This further limits the susceptibility to errors.

GUI The application is implemented in the GUI with a select box, enabling the user to specify whether LCA results should be added. If the box is selected, the calculation is conducted in the post-processing of the SESMG either for a simulation or for a Pareto optimization. If a Pareto optimization is selected, the outcomes across various impact categories are presented within the "Result Processing" of the GUI. This feature allows users to observe not only the quantities of heat and electricity generated by each component at different points along the Pareto front but also to understand how each component contributes to the specific impact category. An example of how this is visualized is shown in Appendix F.

ESM Results The process of linear scaling involves adjusting the inventory flows and environmental impacts based on the energy output of specific technologies (see subsection 3.4.2). These results are already generated by the SESMG (components csv-file)[28]. Scaling is possible when the process in openLCA has a heat or electricity output selected as the quantitative reference. The quantitative reference serves as the benchmark for proportionally aligning all related inputs and outputs[29].

The linear scaling is explained in the following:

$$\text{flows per process} \xrightarrow{\text{* output [1/kWh]}} \text{flows per component}$$

[28] Documentation - SESMG - Application: https://spreadsheet-energy-system-model-generator.readthedocs.io/en/latest/02.02.00_application.html#results.
[29] Documentation - openLCA 2.0 - Processes: hhttps://greendelta.github.io/openLCA2-manual/processes/index.html.

The consideration of environmental impacts depends on consumption-based accounting (see subsection 3.4.2). This is in combination with the different components of the energy system, which are handled differently for the assessment of their environmental impacts:

- Sources: Sources represent the provision of energy, as material imports (e.g., oil import), the electricity import, and other sources of energy (e.g., PV). Their environmental impacts need to be considered.
- Transformers, storages: Those components are integral parts of the energy system, and their environmental impacts must be considered.
- Sink: Sinks of heat and electricity need to be considered in situations, where a bus has surplus energy. The release of this energy, often in the form of electricity fed into the grid, is represented with an excess sink. As the electricity is consumed at another place, the environmental impacts need to be subtracted for the system.
- Links: Links are not treated separately in the LCA, since their impacts are already accounted for, by the outputs of sources and transformers. They are not physical components of the system but rather represent the connections within the energy flow.
- Buses: Buses function as equilibrium points in the energy system, ensuring a balance between energy production and consumption. They do not need to be considered.

Double counting poses a possible challenge when coupling ESM and LCA (see subsection 2.3.2). To avoid double counting within a system, sources that are considered in multiple technologies with an UUID key are automatically subtracted from the original source component (see Appendix A for more information on how this is done exactly).

ProBas

Due to the use of system processes, material imports (e.g., oil import) are already considered in the product systems of other energy technologies (e.g., oil heating transformer). Therefore, double counting is simply avoided by not matching an UUID key to these material imports. However, for the consumption of electricity from the grid, the avoidance of double counting is useful. Consumption is taken into account by subtracting the electricity that is already considered in other system processes from the electricity import, in order to calculate the results of the used electricity inside the system.

$$\text{electricity import} \xrightarrow{\text{- electricity used for components}} \text{electricity demand}$$

LCA Results In accordance with the existing SESMG structure [38], results of the inventory analysis and the impact assessment are saved in the folder of the current run. The results are always scaled up to the time span considered in the model definition, which is typically a period of one year. A xlsx-file is generated, including the results of the individual material flows sorted into input and output flows with the respective values and units, the results of the impact categories for the entire system as well as the breakdown of the technologies within the system. Additionally, if a Pareto optimization is selected, the results for the different runs are summarized per impact category and saved in a separate xlsx-file in the result folder. This file is also used in order to display the results in the GUI (see Appendix F).

3.4.2. LCA Steps

General Steps

According to Figure 3.5, the program distinguishes between a unit or system process, based on the UUID key. This distinction influences the way to create product systems. For a unit process, the creation of a product system involves additional sub-steps. However, the key advantage lies in the ability to perform technology mapping and data harmonization. In contrast, with system processes, adjusting individual input flow values to align with those used in the energy scenario is not feasible.

Due to the mistakes of unit processes (see subsection 3.2.3), it is necessary to check components for the consistency of results from unit and system processes. If the results differ by several orders of magnitude, unit processes are considered not feasible (as also recommended by the openLCA costumer service).

For ten analyzed processes, "Gas-Heizung-DE-2030" emerged as the only unit process where the magnitudes of impact categories are acceptable. For all other product systems, selecting unit processes lead to much lower results. This is partly due to the higher number of material input flows, leading to a higher potential for errors. The gas heating performer is used as an example to fully understand the difference between unit and system processes.

As illustrated in Figure 3.5, the product systems are designed based on the processes and the result calculation includes the results of the inventory analysis and the impact assessment.

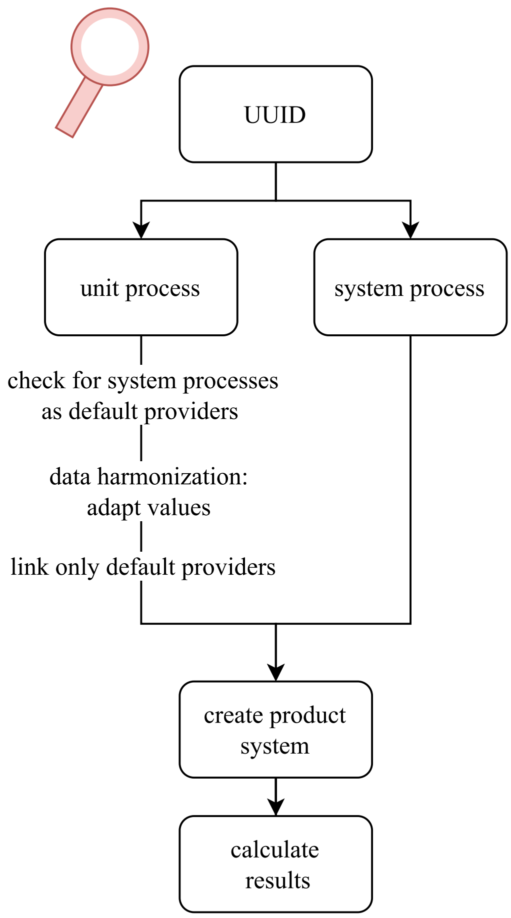


Figure 3.5.: LCA steps for the interface with openLCA. Dependent on whether comprehensible unit processes for technologies exist. Magnifier represents affiliation to Figure 2.2. Abbreviation: UUID = universally unique identifier. Own illustration.

Example: Gas Heating Transformer

In the SESMG, a gas heating transformer is a "GenericTransformer", defined by oemof, that is used for linear transformers with constant efficiencies [82].

The energy amounts for the transformer typically include a value for the gas input in kWh as well as a value for the output of heat in kWh. As mentioned above, this requires technology mapping, implying that datasets for the LCA should cover the same level of detail as the results of the SESMG. Data harmonization includes adapting given values from the energy scenario also in the openLCA software.

System Process The system process of the gas heating transformer does not include information about the value for the gas input, making adaptions impossible. By selecting a system process, undocumented assumptions of ProBas about the gas input are automatically adopted.

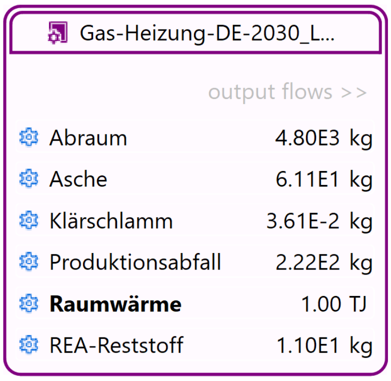


Figure 3.6.: Model graph of the product system created from a unit process of "Gas-Heizung-DE-2030_UP". Created in the openLCA application.

Unit Process The unit process includes the environmental impacts for the transformation of gas to heat, as well as the connection to the material input flows that are needed. In the example, four materials are needed to produce heat with the transformer ("Elektritzität" (electricity), "Erdgas" (gas), "Polyvinchlorid" (polyvinchloride) and "Stahl" (steel)), as illustrated in Figure 3.7.

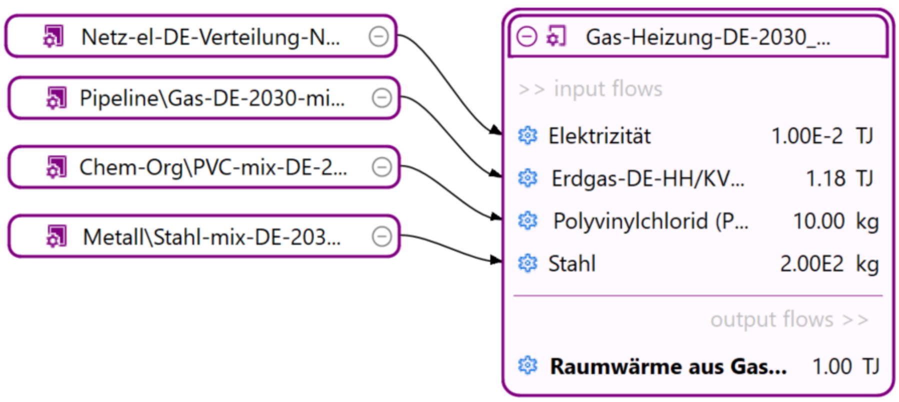
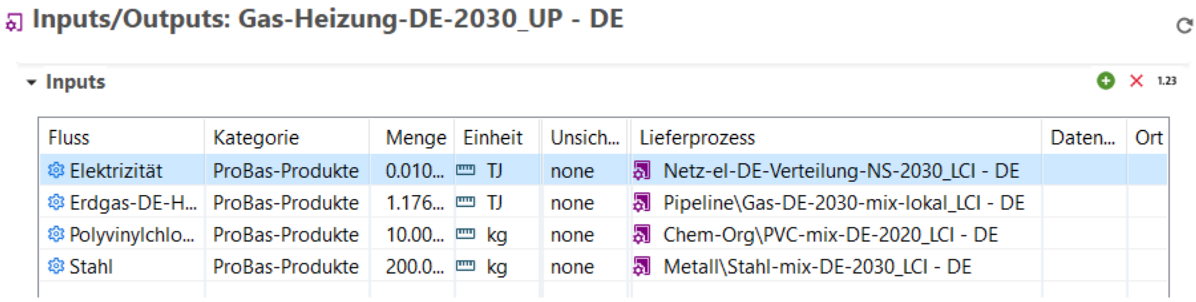


Figure 3.7.: Model graph of the product system created from a unit process of "Gas-Heizung-DE-2030_LCI". Created in the openLCA application.

System Processes as Default Providers Default providers are the pre-selected providers for material input flows of a process, (see Table 2.1 for definitions of different flows). The different default providers are shown in the column “Lieferprozess” (provider) in Figure 3.8. They can again be divided into unit or system processes. Due to the mistakes in the database (see subsection 3.2.3) provider linking, which means automatically connecting processes for the whole supply chain, is not recommended. Therefore, it is necessary to check manually whether all providers are system processes. This prevents the software from automatically connecting all processes and considers only one additional step along the supply chain.



Inputs/Outputs: Gas-Heizung-DE-2030_UP - DE

Inputs

Fluss	Kategorie	Menge	Einheit	Unsich...	Lieferprozess	Daten...	Ort
Elektrizität	ProBas-Produkte	0.010...	TJ	none	Netz-el-DE-Verteilung-NS-2030_LCI - DE		
Erdgas-DE-H...	ProBas-Produkte	1.176...	TJ	none	Pipeline\Gas-DE-2030-mix-lokal_LCI - DE		
Polyvinylchlo...	ProBas-Produkte	10.00...	kg	none	Chem-Org\PVC-mix-DE-2020_LCI - DE		
Stahl	ProBas-Produkte	200.0...	kg	none	Metall\Stahl-mix-DE-2030_LCI - DE		

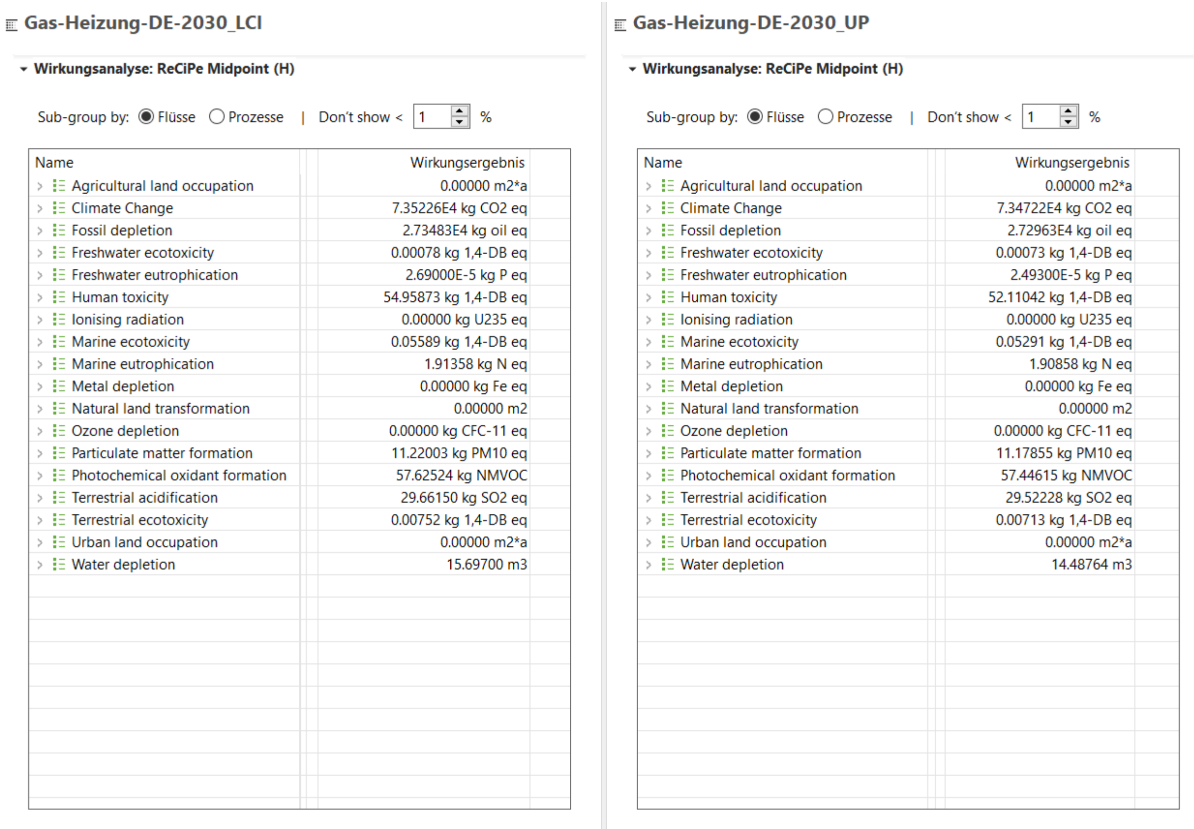
Figure 3.8.: Input flows of the gas heating transformer. Dataset: “Gas-Heizung-DE-2030_UP”. Created in the openLCA application.

Data Harmonization Values for the material input flows can now be adapted to values from the energy scenario. For the transformer this involves the automatic adaptation of the value for the gas input flow (see Algorithm 3).

Link only Default Providers When calculating the product system, it is necessary to only link default providers to avoid mistakes in the linking of processes. This can be selected within the openLCA application (see openLCA documentation[30] for more information about provider linking). The calculated product system contains four processes with the adapted value for the gas flow.

Result Comparison The results differ between the two possibilities of processes, as shown in Figure 3.9. Both methods of creating a product system, result in values for impact categories approximately within the same order of magnitude. The results for the unit process are slightly lower reaching between 92 % (water depletion) to almost 100 % of the values from the system process (e.g., climate change, marine eutrophication). The fact that the results are similar confirms the correctness of the data sets, as the manual linking of another step of the supply chain worked.

[30] Documentation - openLCA 2.0 - Creating a new product system: https://greendelta.github.io/openLCA2-manual/prod_sys/Creating.html.



Gas-Heizung-DE-2030_LCI

Wirkungsanalyse: ReCiPe Midpoint (H)

Sub-group by: Flüsse Prozesse | Don't show < 1 %

Name	Wirkungsergebnis
Agricultural land occupation	0.00000 m2*a
Climate Change	7.35226E4 kg CO2 eq
Fossil depletion	2.73483E4 kg oil eq
Freshwater ecotoxicity	0.00078 kg 1,4-DB eq
Freshwater eutrophication	2.69000E-5 kg P eq
Human toxicity	54.95873 kg 1,4-DB eq
Ionising radiation	0.00000 kg U235 eq
Marine ecotoxicity	0.05589 kg 1,4-DB eq
Marine eutrophication	1.91358 kg N eq
Metal depletion	0.00000 kg Fe eq
Natural land transformation	0.00000 m2
Ozone depletion	0.00000 kg CFC-11 eq
Particulate matter formation	11.22003 kg PM10 eq
Photochemical oxidant formation	57.62524 kg NMVOC
Terrestrial acidification	29.66150 kg SO2 eq
Terrestrial ecotoxicity	0.00752 kg 1,4-DB eq
Urban land occupation	0.00000 m2*a
Water depletion	15.69700 m3

Gas-Heizung-DE-2030_UP

Wirkungsanalyse: ReCiPe Midpoint (H)

Sub-group by: Flüsse Prozesse | Don't show < 1 %

Name	Wirkungsergebnis
Agricultural land occupation	0.00000 m2*a
Climate Change	7.34722E4 kg CO2 eq
Fossil depletion	2.72963E4 kg oil eq
Freshwater ecotoxicity	0.00073 kg 1,4-DB eq
Freshwater eutrophication	2.49300E-5 kg P eq
Human toxicity	52.11042 kg 1,4-DB eq
Ionising radiation	0.00000 kg U235 eq
Marine ecotoxicity	0.05291 kg 1,4-DB eq
Marine eutrophication	1.90858 kg N eq
Metal depletion	0.00000 kg Fe eq
Natural land transformation	0.00000 m2
Ozone depletion	0.00000 kg CFC-11 eq
Particulate matter formation	11.17855 kg PM10 eq
Photochemical oxidant formation	57.44615 kg NMVOC
Terrestrial acidification	29.52228 kg SO2 eq
Terrestrial ecotoxicity	0.00713 kg 1,4-DB eq
Urban land occupation	0.00000 m2*a
Water depletion	14.48764 m3

Figure 3.9.: Result comparison for the dataset "Gas-Heizung-DE-2030". Results include all categories from the impact assessment method ReCiPe2008 midpoint H. Left side shows results from the system process, right side from the unit process with default provider linking. Result visualization is taken from the openLCA application.

3.4.3. Code Excerpt

As the difference between unit and system processes poses a major challenge, the following code extraction underlines the handling of this, making an implementation of better unit processes possible for future applications. The algorithms only show an excerpt of the code (see Appendix A for the entire sourcecode). The *nodes_ data* dictionary includes the sheets of the model definition and the *components_ list* includes the results from the optimization process as the two main interfaces, defined in section 3.4.

Firstly, Algorithm 1 adds the UUID keys of the *nodes_ data* dictionary to the right technologies in the *components_ list* DataFrame. Additionally, information about the input and the output for the technology are mapped, as they are later needed to avoid double counting (not included in the code excerpt). The code in Algorithm 2 creates a dictionary out of the components_list that contains all information needed for subsequent LCA calculations. The data harmonization is done in Algorithm 3. This includes checking if the UUID key refers to a unit process and if this unit process has an input, represented by another dataset. Then the value (called exchange amount) of this input is directly updated in the dataset in the openLCA application.

Algorithm 1: Adding UUIDs to components

```
Data: nodes_data, components_list
Result: components_list with added UUIDs
Create an empty dictionary: uuid_mapping;
for each sheet in nodes_data do
    // Skip sheets not needed for LCA calculation
    if sheet is relevant then
        for each row in the current sheet do
            Extract values for row_first_value, row_uuid_value, input_value, and
             output_value;
            Check for "input" or "output" columns and assign values to input_value and
             output_value;
            Add {'uuid': row_uuid_value, 'input': input_value, 'output': output_value}
             to uuid_mapping;
Remove '_shortage' from components_list['ID'];
// Add uuids and input values to components_list
Map components_list['ID'] to uuid_mapping, filling missing values with {'uuid': None,
 'input': None, 'output': None};
Apply the mapping to create new columns 'uuid', 'input', and 'output' in
 components_list;
return components_list
```

Algorithm 2: Creating LCA dictionary

```
Data: filtered_components
Result: lca_dict
Create empty lca_dict;
for each row in filtered_components do
    Extract uuid, component_id, output_value_old, and change_input_flow;
    Convert output_value_old to TJ;
    Get process_ref based on uuid;
    Extract component_type from process_ref;
    Fill lca_dict with relevant information;
return lca_dict
```

Algorithm 3: Changing values of input processes

Data: lca_dict

Result: Updated lca_dict without components already considered in another product system

```
Create a copy of the dictionary (lca_dict_copy);
for each component in lca_dict_copy do
    Extract values for change_input_flow, output_value, uuid, and component_type;
    Check if the component is a unit process with an input that needs harmonization;
    if true then
        Get the corresponding uuid and output of the input flow from lca_dict;
        Get the right input flow;
        for each exchange in the input flow do
            Check if there are inputs and outputs with a default provider;
            if true then
                Get the default provider's reference and its ID;
                Check if the default provider can be harmonized with the selected uuid;
                if true then
                    Update the exchange amount based on the ratio of selected_output to
                      output_value;
                    Print a message indicating the update of values in the process flows;
                    Change the value(s) in the database;
        Remove the input flows that are already considered from lca_dict to avoid double
          counting;
return Updated lca_dict
```

3.4.4. Technologies

The primary focus of this thesis is on technologies suitable for small-scale energy systems. This strategic choice serves as an initial testing ground for the implementation. The decision to prioritize small-scale systems is motivated by both the uncertainties in the available data (see subsection 3.2.3), and the considerable effort required in selecting appropriate datasets.

The selection of datasets for different technologies followed the listed rules, that are also recommended for further technology selections:

1. Selecting the newest dataset (most of the technologies have datasets with validity dates from 2000 up to 2030).
2. Comparing the dataset of the CO_2 emissions in ProBas with the CO_2 emissions provided in the current dataset (2030) on the website of the Umweltbundesamt [99]. Due to no updates of ProBas in openLCA since 2016, many datasets were already improved and corrected on the website. If the difference between emissions from the two sources was more than 100 %, other datasets within openLCA with a lower difference were preferred. In case this lead to another selected dataset, it is noted in Table 3.3. These reasons may also account for possible inaccuracies in the results.

The Table 3.3 lists all currently implemented technologies, along with further information about the dataset selection.

Table 3.3.: Technologies with working LCA datasets from ProBas. Note that the gas heating transformer is the only example of a unit process (see "Example: Gas Heating Transformer" in subsection 3.4.2). Abbreviations: LCI = life cycle inventory, UP = unit process.

Technology	Dataset name in ProBas	Reason for selection
Sources		
electricity import	Netz-el-DE-Verteilung-NS-2020	The 2020 dataset was prefered over the newest dataset (2030) due to more realistic CO_2 emissions compared to [111].
gas import	Pipeline-DE-2030-mix-lokal_LCI	The gas import is considered for the applied example of the gas heating transformer.
solar thermal system decentral roof-mounted	SolarKollektor-Flach-DE-2030_LCI	Apparently, a storage is already included in the dataset without providing further information, but no alternative technology was available.
PV system decentral roof-mounted	Solar-PV-multi-Rahmen-mit-Rack-DE-2010_LCI	The 2010 dataset was preferred over the newest datasets (2020 and 2030) due to more realistic CO_2 emissions when compared to the Umweltbundesamt [99].
Transformers		
gas heating system	Gas-Heizung-DE-2030_UP	The dataset was preferred over the datasets considering the calorific value, due to technical reasons.
oil heating system	Ö-Heizung-DE-2030_LCI	The dataset was preferred over the datasets considering the calorific value, due to technical reasons.
electric heating system	El-Heizung-DE-2030-mix_LCI	Selection due to the predefined rules.
pellet heating system	Holz-Pellet-EU-Heizung-2030_LCI	No dataset available for Germany. Wood is the most common type of biomass used for pellets [112].
GCHP	El-Wärmepumpe-mono-Erdreich-DE-2010-mix_LCI	There was no dataset available for 2020 or 2030.
air source heat pump (ASHP)	El-Wärmepumpe-mono-Luft-DE-2010-neu_LCI	To enable a comparison with the other heat pump, a dataset for 2010 was selected. Additionally, CO_2 emissions were found to be extremely low in the 2030 dataset.

It is crucial to acknowledge that the current focus on small-scale energy systems is not a permanent constraint, but rather a deliberate step taken to ensure the reliability and accuracy of the initial model [113]. As the development progresses, there is a desire for future work to expand its scope, shifting attention towards neighborhoods and larger energy systems [21]. Table 3.4 deals with currently not considered technologies and efforts to later integrate them in the LCA application as well.

The categorization of technologies according to the hurdle of future implementation in the last column can be helpful for future work with the SESMG. Especially, technologies that are categorized as **possible** implementation technologies are theoretically available in the ProBas database in openLCA and call for further work.

Table 3.4.: Technologies currently not considered in the LCA application.

Technology	**Reason**	**Future implementation**
oil import, biogas import, biomass import, hydrogen import, wood import	already considered within the system processes	difficult[a]
PV system central ground-mounted, solar thermal system central ground-mounted, screw turbine	no priority for a single house	**possible**
central gas heating plant, district heat house station, electric radiator, combined heat and power plant, biomass plant, electrolysis, fuel cell, methanization, woodstove	no priority for a single house	**possible**
surface water heat pump (SWHP)	no dataset available	not possible
hydrogen storage, natural gas storage, battery storage (central, decentral), thermal storage (central, decentral)	no datasets available	difficult[b]
district heating network	no priority for a single house	**possible**
insulation	cannot be scaled by an energy amount	difficult[c]

[a] These imports are available as own system processes in the database, but the unit processes need to be validated manually in order to use them.
[b] Implementing own datasets by combining several processes, for example, for the battery storage, is possible but labor-intensive due to the high number of material flows [23, 114].
[c] More research into the behavior of insulating materials in relation to the energy system is needed to find a solution to this problem.

3.4.5. Utilization

In order to use the LCA calculation option in the SESMG the user needs an openLCA software and an academic license of the ProBas database.

Then, the server of the software needs to be started within the application[31]. The model definition needs to contain the needed UUID keys.

If technologies are considered inside the energy system that are currently not implemented in the model, the user should aim to follow the earlier described steps for implementing new technologies (see subsection 3.4.4).

If the user wants to implement more unit processes to consider technology mapping and data harmonization, it is recommended to follow the comparison between the processes as done in the example of the gas heating transformer (see "Example: Gas Heating Transformer" in subsection 3.4.2).

All subsequent steps are done by the SESMG automatically. This process is also described in the documentation of the SESMG[32].

In summary, the tool facilitates LCA calculations of energy systems. However, to analyze results or to include more technologies and functions, expert knowledge is needed.

3.5. Assumptions and Limitations

To conduct LCA calculations for optimized energy system scenarios, certain assumptions were necessary to adapt the calculations to any energy system. These additions complement the predefined assumptions in subsection 3.4.2:

- Data harmonization: Data harmonization is employed with the utilization of unit processes, but its applicability is limited. The current methodology allows data harmonization only for energy amounts of the ESM results. All other parameters in the LCA remain unaffected by the parameters of the SESMG.
- Standardized data: Only standard data sets are currently used for each technology, which are assigned to the technology by a single UUID key. The program cannot select these automatically but is dependent on manual assignment.

[31] Documentation - olca-ipc - Introduction: https://greendelta.github.io/openLCA-ApiDoc/ipc/.

[32] Documentation - SESMG - Additional features: https://spreadsheet-energy-system-model-generator.readthedocs.io/en/latest/02.04.00_additional_features.html.

ProBas

- Impact assessment: Mistakes of the impact assessment were only solved partially. Flows of the inventory analysis that are not assigned to an impact category cannot be analyzed under consideration of their contribution to the impact categories.
- Technology mapping: The exclusion of unit processes for many technologies (see subsection 3.4.2) makes it impossible to consider electricity that is produced inside the system (e.g., PV) for different components that have an electricity input. This is solved by subtracting this input from the electricity import (see subsection 3.4.1). Therefore, if more electricity is produced by a PV system than imported from the grid, environmental impacts are subtracted from the impacts of the whole system. Technically, this leads to a correct consideration of environmental impacts, as shown in Figure 3.10. However, this can only be mapped to a limited extant in the results. The impacts for the electricity import might turn into negative impacts, also leading to negative results in the impact amounts graph.
- LCA stages: The validation of included LCA stages is limited, as the code can currently not assure to which extend LCA stages are considered. The assumptions for the consideration of life cycle stages are automatically adopted from the database. In openLCA, the functionality of ProBas is further limited by the exclusion of traceability for different data sets (see subsection 3.2.3).

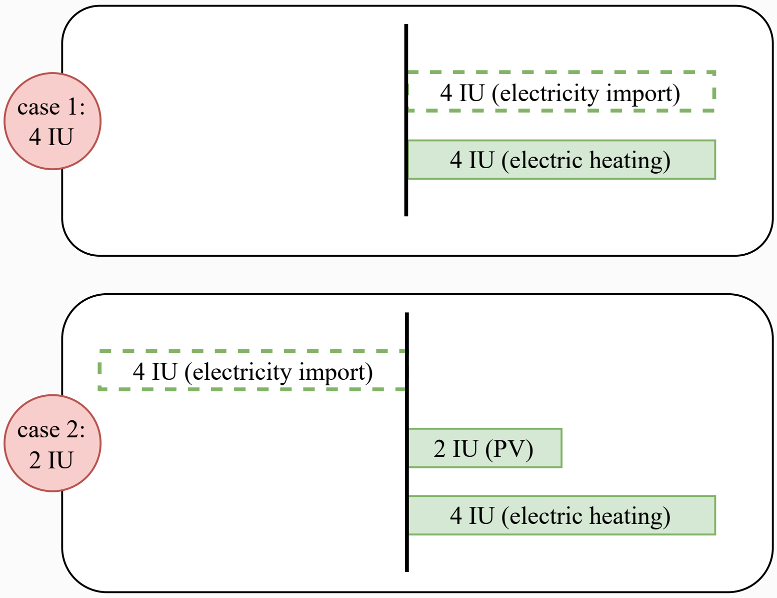


Figure 3.10.: Example for a negative electricity impact. Dashed line represents subtracted impacts. In case 1, all electricity for the electric heating transformer is subtracted from the electricity import (4 IU for the system). In case 2, the electricity for the electric heating transformer is provided by the PV system with a lower impact. The impact from the electricity import is still subtracted, as the impacts of the electric heating transformer cannot be changed (2 IU for the system). This calculation is correct, but leads to negative impacts for the electricity import. Abbreviations: IU = impact unit, PV = photovoltaic. Own illustration.

4. Application

4.1. Reference Case

In the reference case, the developed methodology for coupling ESM and LCA (see section 3.3) is systematically applied to a single building. Rather than an extensive discussion of results, this chapter emphasizes the functionality and implementation of the developed approach.

For this reason, the goal and scope include a general demonstration of how the methodology operates in assessing the environmental impacts of various technologies and scenarios. The inventory analysis and the impact assessment are done automatically with the developed integration in the SESMG. The last step represents the interpretation of the results, which is done in the discussion (see section 5.4).

The reference case includes a fictional single family building. The assumed energy demands for a four-person household in a single family building without electric water heating are estimated as follows [115, 116]:

- Heat demand: 30 000 kWh
- Electricity demand: 4 000 kWh

In the base case the building is supplied only by electricity from the grid and heat by a gas heating transformer. This represents the German heating standard [117]. The initial simulation captures this case with a fixed gas heating transformer capacity of 12 kW.

Afterwards, the optimization process is carried out without timeseries simplifications (see "Tool Description" in subsection 2.1.3). Scenarios are calculated for the cost-optimized scenario, three additional Pareto points with emission reductions at 25 % (S1), 50 % (S2) and 75 % (S2) compared to the cost-optimized scenario and the emission-optimized scenario (S4).

The model definition includes all technologies outlined in the energy graph, illustrated in Figure 4.1. This ensures that the developed methodology is tested under known assumptions and limitations. Due to the mistake of the ProBas database (see subsection 3.2.3), the gas heating transformer is the only process were the use of a unit process enables technology mapping and data harmonization up to a limited extend (see subsection 3.4.2). Additionally, the consideration of a thermal storage system is limited to the heat generated by the solar thermal collector (see Table 3.3). To address this, the model definition is adapted by dividing the heat bus into two separate buses. The first bus is solely connected to the solar thermal collector, enabling the connection to a thermal storage system designed specifically for solar thermal heat, shown in Figure 4.1. The second bus is connected to the remaining heat providing technologies.

For parameters of the technologies, standard parameters were chosen based on the practical study conducted with the SESMG in the city Horstmar [22]. This study presents the current state of research concerning default parameters.

The model definition of the reference case as well as the results for the different Pareto runs can be accessed via the released GitHub repository (see Appendix A).

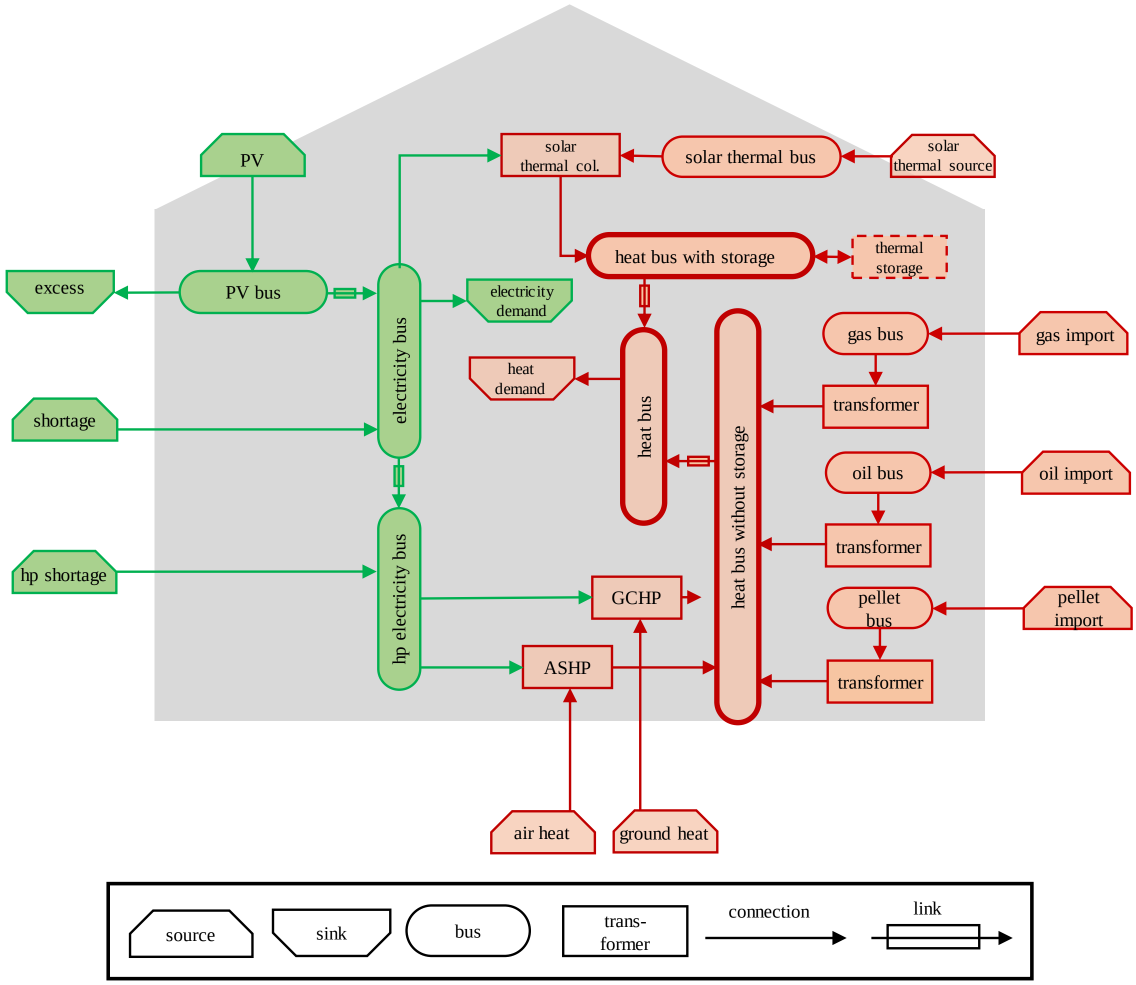


Figure 4.1.: Energy graph of the reference case. Containing all technologies from Table 3.3. Green represents electricity related components, red represents heat related components. Bold lines highlight the division of the heat bus into two buses. Abbreviation: PV = photovoltaic, solar thermal col. = solar thermal collector, hp = heat pump, ASHP = air source heat pump, GCHP = ground-coupled heat pump. Own illustration.

4.2. Results

4.2.1. ESM Results

The results from the ESM, illustrated in Figure 4.2, demonstrate that significant reductions in GHG emissions are achievable with minimal additional costs. The scenario optimized for emission minimization leads to a disproportionately high cost increase, with expenses more than seven times higher than those associated with achieving a 75 % reduction in emissions. This typically leads to a favorability of one of the other Pareto points with more balanced results of costs and emissions, like S4, highlighted in Figure 4.2.

In the optimized scenarios, the composition of technologies consists of the following technologies: electricity import, PV system, GCHP, ASHP, electric heating transformer, pellet heating transformer, and solar thermal collector with the associated thermal storage. The gas heating and oil heating transformer were not designed for any of the scenarios. For more information on which technologies are exactly designed in the different scenarios see energy and heat amounts in the results of the reference case in Appendix A.

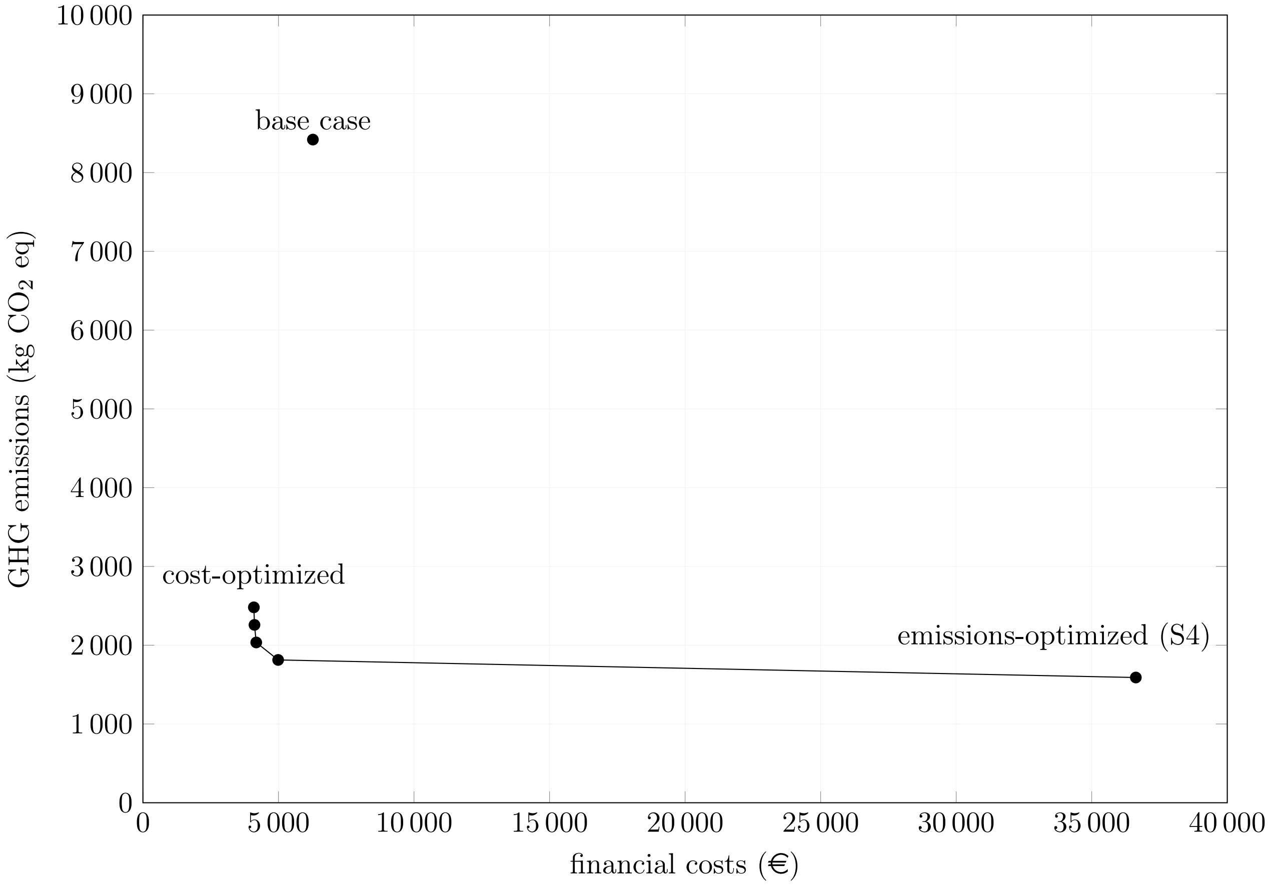


Figure 4.2.: Pareto front reference case. Results of the base case and the different optimized scenarios (S1, S2, S3, S4) of the reference energy system for costs and GHG emissions.

4.2.2. Comparison of Pareto Points

Inventory Analysis Given that ProBas does not consider certain material flows within the impact categories, and manual assignment of these flows was only possible for a limited number (see Appendix D), it might be beneficial to analyze these flows separately for a more comprehensive understanding. As an illustrative example, the flows "Mineralien" (minerals) and "Erze" (ores) were selected because they contribute to the production of various metals typically associated with the metal depletion impact category [65]. Table 4.1 illustrates the variability in quantities of these two flows across different scenarios. Notably, the amount of minerals decreases as the share of GHG emission reduction increases. Conversely, the quantity of ores initially rises, reaching peak values of 101 kg and 99 kg in S2 and S3. This values might be reasoned by the energy amounts of the GCHP that requries high copper values for its production [118].

Table 4.1.: Results of the flows “Mineralien” (minerals) and “Erze” (ores). They present exemplary flows that are not included in the impact assessment.

Scenario	Cost-optimized	S1	S2	S3	S4
“Mineralien” (minerals) (kg)	414	334	249	155	178
“Erze” (ores) (kg)	98	101	99	95	90

Impact Assessment The impact categories not validated in Appendix B were removed from the analysis of the results because they cannot currently be mapped correctly with the use of ProBas datasets. This resulted in 13 remaining impact categories for analyzing the energy scenarios.

In Figure 4.3, the impacts of the five optimized scenarios are compared to the base case scenario (simulation). It becomes visible, that not all impact category results decrease with a lower value of GHG emissions. In most scenarios, impacts related to climate change and metal depletion are notably reduced when compared to the base case. The highest reduction is reached in the emission-optimized scenario with a reduction of 20.64 % of climate change impacts and 83.51 % of metal depletion (CC and MD in Figure 4.3) impacts. However, it can be observed that all other impact categories demonstrate increased values in the optimized scenarios. The highest increase occurs for the cost-optimized scenario in the categories water depletion, freshwater ecotoxicity, and human toxicity.

An increased emphasis on emission reduction generally leads to decreased environmental impacts across most categories, as demonstrated in the illustration. For example, the emission-optimized scenario (dark green) has the lowest value in the majority of impact categories. The assignment of these influences to the different technologies is done in further course of this thesis (see subsection 4.2.3).

The increase in most of the impact categories is mainly attributed to the limited variety of technologies considered in the base case scenario, where only the electricity import and the gas heating transformer contribute to environmental impacts. However, the base case encompasses significantly higher costs and emissions compared to all other scenarios (see Figure 4.2). In the application of energy-system thinking (see subsection 3.1.1), the primary objective is not to rely solely on environmental impacts for energy system design decisions. Instead, the aim is to utilize them as a tool to identify advantages and disadvantages among various scenarios and technologies, all of which represent improvements over the base case.

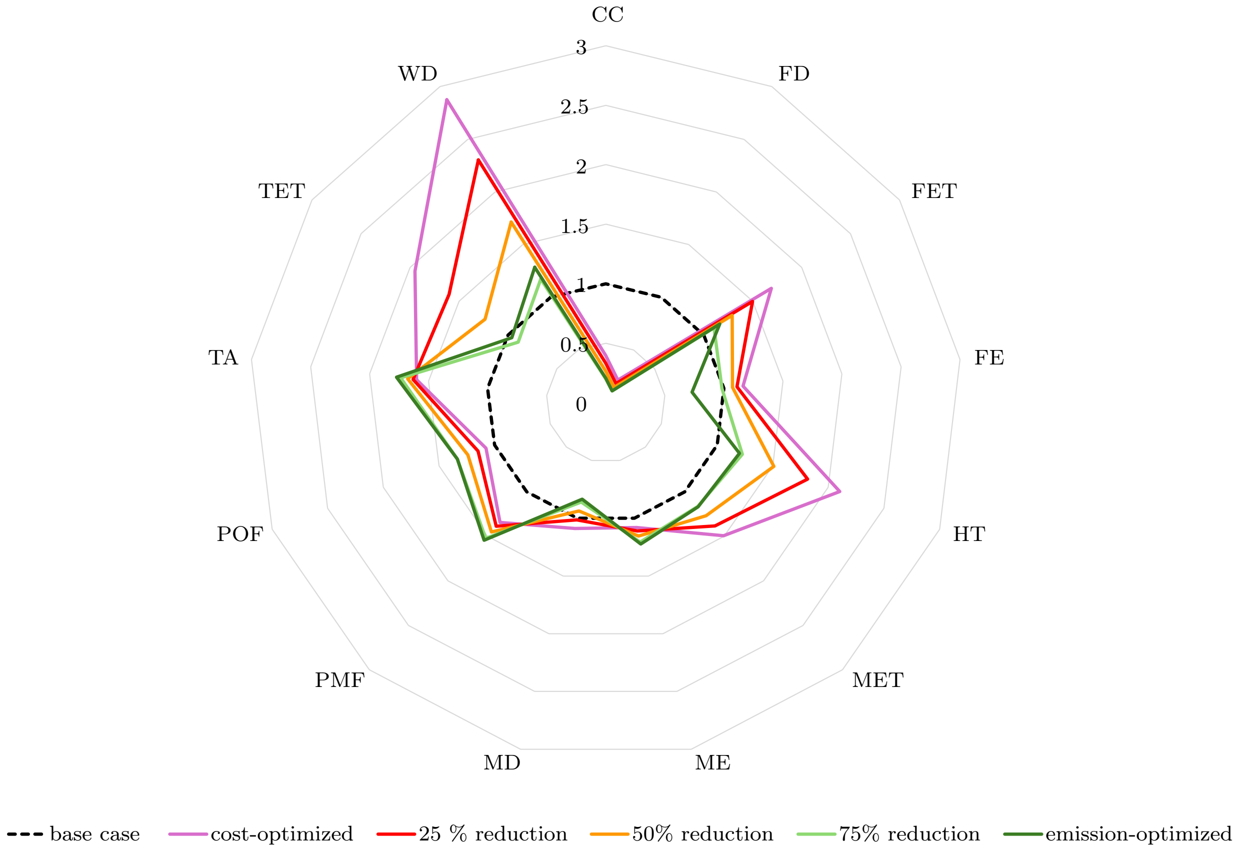


Figure 4.3.: Comparison of scenarios with the base case. Most environmental impacts do not decrease with a lower value of GHG emissions. Dotted line represents 100 %. Abbreviations: CC = climate change, FD=fossil depletion, FET = freshwater ecotoxicity, FE = freshwater eutrophication, HT = human toxicity, MET = metal depletion, ME = marine eutrophication, MD = metal depletion, PMF = particulate matter formation, POF = photochemical oxidant formation, TA = terrestrial acidification, TET = terrestrial ecotoxicity, WD = water depletion. Own illustration.

Therefore, a second comparison was conducted, shown in Figure 4.4. In this illustration the base case is excluded and the cost-optimized scenario represents the 100 % line, to show the variations in environmental impacts that result from the implementation of these scenarios. The main result that can be taken from this comparison is that values of impact categories are either rising with higher emission reduction or declining. Four impact categories that exhibit increased values can be identified, signaling areas where the shift towards lower GHG emissions in optimized energy systems might lead to unintended environmental consequences. These categories include:

- Terrestrial acidification (11 % more impacts in the emission-optimized scenario)
- Petrochemical oxidant formation (24 % more impacts in the emission-optimized scenario)
- Particulate matter formation (15 % more impacts in the emission-optimized scenario)
- Marine eutrophication (13 % more impacts in the emission-optimized scenario)

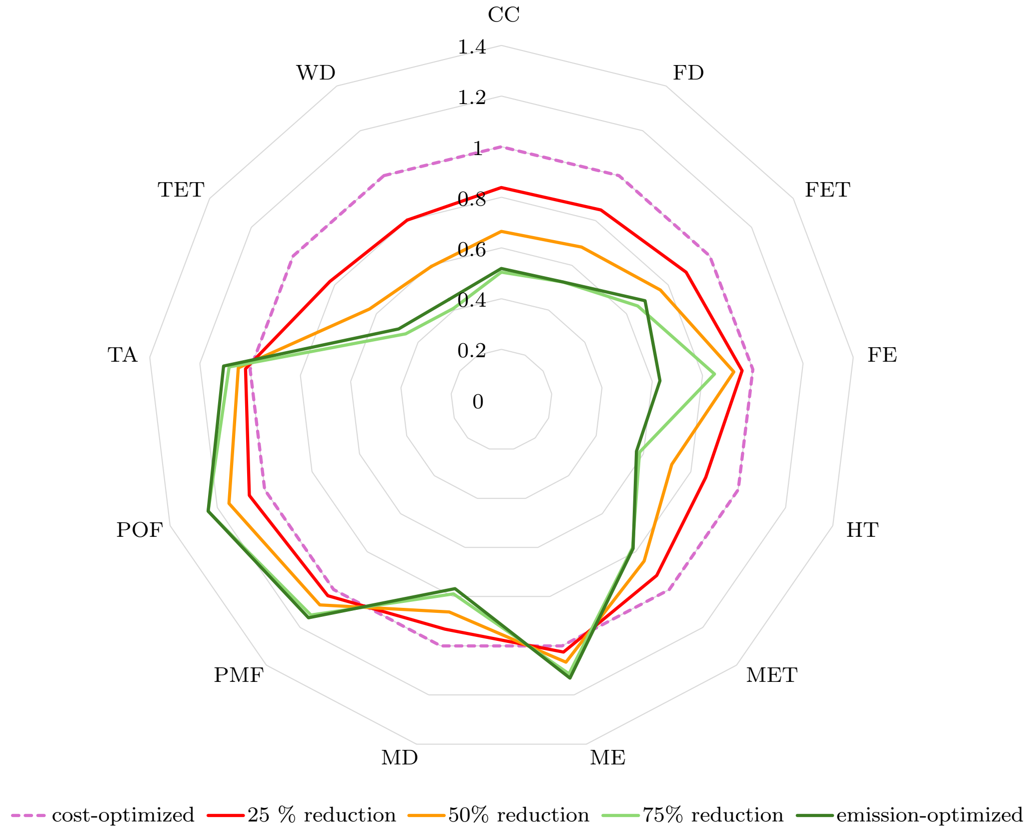


Figure 4.4.: Comparison of scenarios with the cost-optimized scenario. Impacts either rise or decrease with a higher emission reduction. Dotted line represents 100 %. Abbreviations: CC = climate change, FD = fossil depletion, FET = freshwater ecotoxicity, FE = freshwater eutrophication, HT = human toxicity, MET = metal depletion, ME = marine eutrophication, MD = metal depletion, PMF = particulate matter formation, POF = photochemical oxidant formation, TA = terrestrial acidification, TET = terrestrial ecotoxicity, WD = water depletion. Own illustration.

4.2.3. Comparison of Technologies

In the result section of the GUI (see section 3.4), the course of all 13 impact categories is visualized for the optimized scenarios separately per impact category, including the share of contribution per technology. Exemplary impact categories are chosen to showcase their functionality in evaluating the environmental implications of various scenarios and technologies.

Climate Change The impact category climate change evaluates effects of GHG emissions on climate change, measured in kg CO_2 eq [65] (see Appendix B).

In alignment with the life cycle emissions considered in the SESMG (see Figure 4.2), the results indicate a decrease in climate change impacts. Figure 4.5 illustrates that the impacts of the category decrease from 9 623 kg CO_2 eq in the base case, to 3 825 kg CO_2 eq in the cost-optimized scenario, and 1 986 kg CO_2 eq in the emission optimized scenario. These values are higher (between 9.5 and 54 %) than the results of the SESMG for the different scenarios, but remain in the same order of magnitude.

The observed higher values in GHG emissions can be attributed to the reliance on one single database as a constant data source for the LCA, while the optimization process of the SESMG employs diverse data sources for the different technologies. Although these data entries may offer enhanced traceability and currency, they could vary in terms of LCA stages and considered flows.

While the GCHP contributes the highest share, it may not necessarily be the primary contributor to the category indicator result. This can be explained by the limitation in data technology mapping (see section 3.5), that results in the inclusion of the electricity input within the environmental impacts of the given technologies. This partly explains the high CO_2 eq emissions from the heat pump because a substantial amount of electricity is required for its heat conversion.

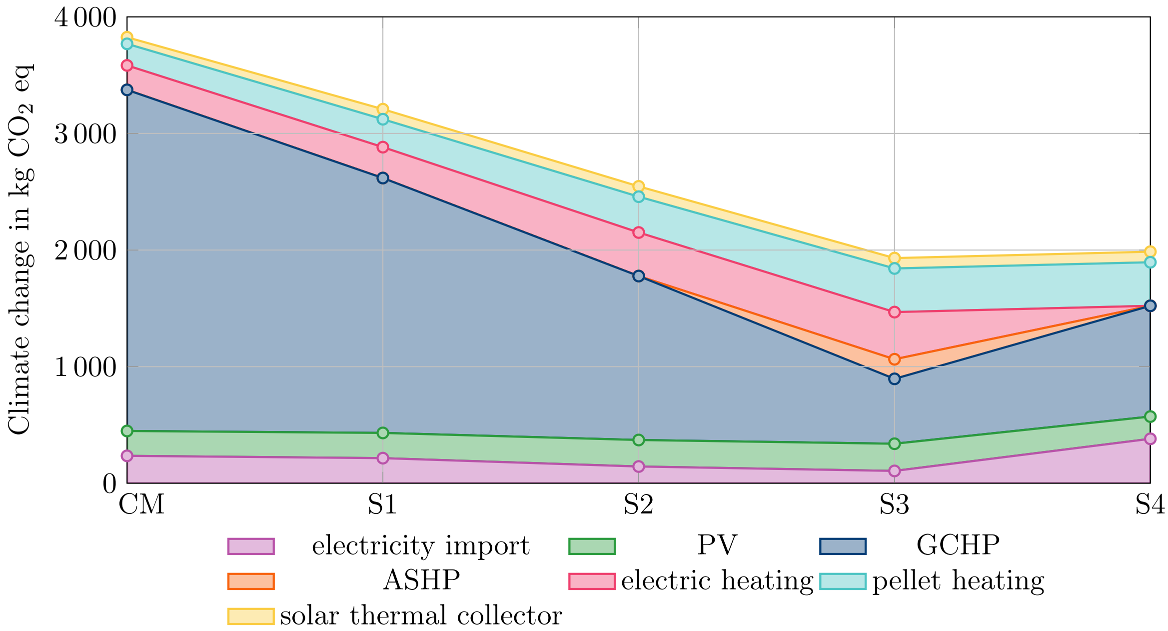


Figure 4.5.: Impacts in the category climate change. Abbreviations: CM = cost-minimized scenario, ASHP = air source heat pump, PV = photovoltaic, GCHP = ground-coupled heat pump. Own illustration.

Human Toxicity Human toxicity assesses the potential adverse effects of substances on human health. The impact category is measured in kg 1.4-dichlorobenzene (DB) eq and is used to compare and quantify the impacts of various substances on the impact category [65] (see Appendix B).

Similar to the category of climate change, the sum of contributions to human toxicity decreases along the Pareto curve from 45.7 to 26.1 1.4-DB eq, as shown in Figure 4.6. In all scenarios, the two major contributors to this category are the PV system and the GCHP. This can be partially explained by the overrepresentation of the GCHP system due to its electricity import.

However, this limitation does not apply to the PV system, which predominantly shapes the category. The PV system contribution remains relatively stable across scenarios, attributed to the consistent sizing of the PV system in all scenarios. In the scenario with a 75 % reduction in emissions, often regarded as a more realistic case (see Figure 4.2), the PV system emerges as the primary contributor. It accounts for 31.5 % of the amount of kg 1.4-DB eq. This may be explained with the alignment of scientific findings. Scenarios with an increased PV electricity amount exhibit higher or fluctuating values for human toxicity, mainly due to large toxicity-related impacts stemming from material production [5, 11, 16, 23].

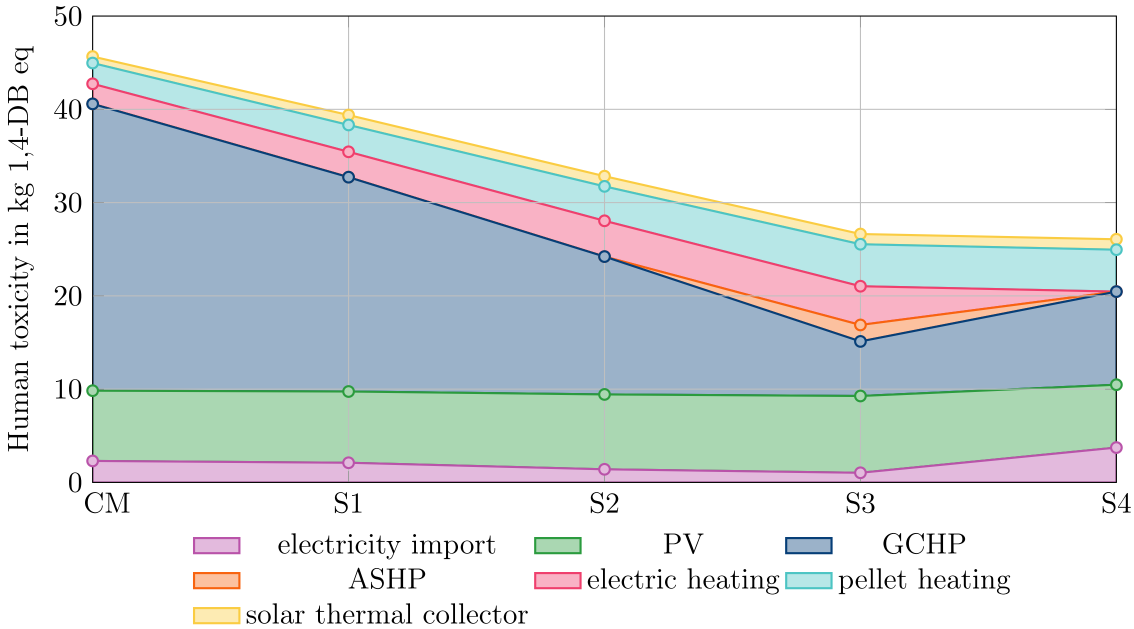


Figure 4.6.: Impacts in the category human toxicity. Abbreviations: CM = cost-minimized scenario, ASHP = air source heat pump, PV = photovoltaic, GCHP = ground-coupled heat pump. Own illustration.

Terrestrial Acidification Acidficiation is the atmospheric deposition of inorganic materials which leads to an increase of acidity in soil. It is measured in kg SO_2 eq [65] (see Appendix B).

The impact category terrestrial acidification poses one example of a category where the cateogry indicator result rise with a higher share of emission reduction in the optimization.

Illustrated in Figure 4.7, the category indicator result rises from 9.0 kg SO_2 eq in the cost-optimized scenario to almost 10.0 kg SO_2 eq in the emission optimized scenario. As emissions decrease in this scenario, the usage of pellet heating increases, emerging as the primary contributor to the environmental impacts within this midpoint category. This may be explained in correlation with research in literature because mainly the pre-treatment of pellets and the combustion heating stage are linked to large emissions of SO_2 [112, 119].

The second highest contributor in all scenarios, is the GCHP (overestimation). All other categories remain constant according to their designed output value in the scenario.

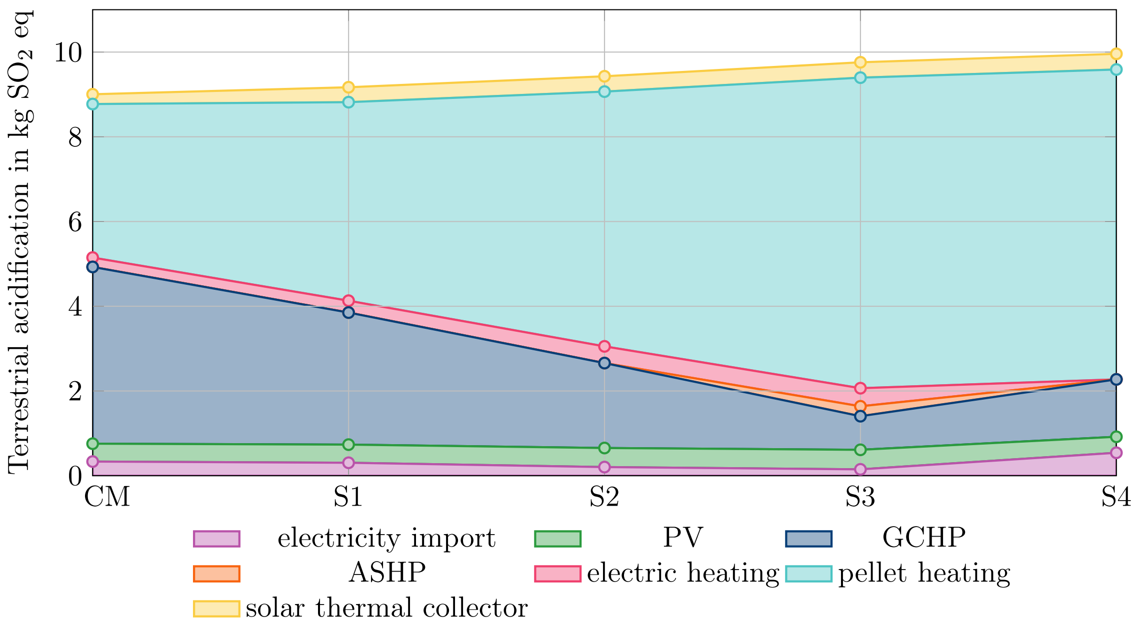


Figure 4.7.: Impacts in the category terrestrial acidification. Abbreviations: CM = cost-minimized scenario, ASHP = air source heat pump, PV = photovoltaic, GCHP = ground-coupled heat pump. Own illustration.

Other Impact Categories The three additional categories, that increase with a higher reduction of GHG emissions (marine eutrophication, photochemical oxidant formation, and particulate matter formation) exhibit behavior similar to the terrestrial acidification category. In all these impact categories (see Appendix B), the impacts rise with a higher share of reduction, primarily attributed to the increased output of the pellet heating system.

Given that this reference case primarily serves as a representation of the application, further research is required to contextualize the results of all impact categories.

5. Discussion

5.1. Uncertainties of LCA Data

Data Collection The acquisition of data has proven to be the biggest obstacle in linking the two approaches of ESM and LCA (see section 3.2) [46, 47, 52].

This is primarily reasoned by the required structure of datasets, as they include a much higher number of data entries compared to data typically required by ESM tools. As a result, research of single values is connected to high effort. Another barrier for the data collection, is the limited availability of databases which were defined as the easiest option to overcome structural challenges of data handling (see subsection 3.3.3) [13]. Availability of open-source data is limited and most databases are commercialized, making this part extremely challenging, especially for researchers who have no options to acquire primary data sources [52, 104]. Furthermore, dealing with different databases requires expert knowledge to understand, adapt, and analyze them effectively (see subsection 3.2.1). These challenges in selecting data are made even harder by the existing difficulties in acquiring inventory datasets, given the limited availability of open-source software for LCA calculations (see subsection 2.2.4).

In summary, even though the data collection was already examined as a major challenge for coupling ESM and LCA (see subsection 2.3.2), overcoming this barrier is quite more challenging. If a study requires secondary data, the use of a database is mandatory. Therefore, results from coupling the two approaches should always be analyzed taking into account the data basis.

ProBas Database Due to errors in the database, the utilization of ProBas introduced numerous uncertainties in the LCA data (see subsection 3.2.3). The fundamental limitation arises from the lack of traceability of the database within the openLCA software. The absence of individual data source tracking and the inability to verify data alignment with the current state of the ProBas database from the Umweltbundesamt [99], hinder thorough validation of datasets. The lack of clarity in documenting and rectifying errors limits the use of unit processes, which is crucial for technology mapping and, consequently, obtaining meaningful results in the LCA (see section 3.5). A possible solution might involve manually importing the current ProBas database into openLCA. However, the intricate structure with interconnections between various processes makes the manual creation only adaptable for software experts. The same principle applies for the manual import of additional GEMIS data. Both approaches require further work by the software providers.

Despite claims that the datasets encompass environmental impacts from the beginning of an extraction process to the disposal of a product [109], it remains challenging to ascertain the accuracy of the entire process chain from "cradle to grave" in the database. An example for this is the consideration of waste flows (see Table 2.1). In openLCA, many datasets from the Umweltbundesamt refer to the GEMIS 4.2 version, where waste flows are listed [109]. Consequently, these are also listed in the inventory result as end-of-life treatment flows, such as "Klärschlamm" (sewage sludge) or "Abraum" (spoil). However, there is a lack of uniform consideration for further treatment or emissions resulting from the disposal processes of these flows.

The second important limitation is the impact assessment. Despite efforts to enhance the evaluation of environmental impacts (see Appendix B and Appendix D), the assessment is heavily constrained by the exclusion of numerous highly aggregated flows. For the unimplemented flows, further steps are required to analyze their environmental impacts. However, to do so, obtaining information about these flows from the Umweltbundesamt is essential. Currently, such information is lacking.

Despite these challenges, efforts were made in section 3.4 to circumvent errors as much as possible to generate additional results using the ProBas database. The ongoing limitations and uncertainties associated with ProBas hinder the significance of results and may require additional research, for example if statements are needed on impact categories that are not currently mapped. This underscores the need for improvements in data transparency, traceability, and completeness for robust LCA applications.

5.2. LCA Application for Energy Systems

Ex-post LCA The implementation of a LCA was limited to an ex-post assessment (see subsection 3.1.1). However, multi-objective optimization might not only be helpful in assessing environmental impacts but also in using budgets for each life cycle impact during the optimization process. The main advantages of this is the feedback between the environmental impacts and the optimization problem (see subsection 2.3.3). Nevertheless, uncertainties in data collection for the LCA complicate this implementation, as quantitative results lack consistency and might lead to over- or underestimations of environmental impacts in the optimization process. The primary objective should be to use environmental impacts to identify advantages and disadvantages among different scenarios and technologies.

OpenLCA Software OpenLCA provides several interesting features for conducting LCAs that have not been completely explored within the scope of this thesis. These include the option of an own classification of data quality[33], which might help to overcome the mentioned data collection challenges. Another feature is the generation of customized results, that might act as additional visualizations in the GUI[34].

However, the labeling of 'free databases' in openLCA Nexus is misleading. The EF database should not be categorized as a free database, as it initially requires the paid DAL license and is not suitable for research purposes (see subsection 3.2.2). Additionally, even though the software was crucial for the automatic implementation in the SESMG and provided many advantages (see subsection 2.2.4), a renunciation of the software could open further data sources for investigation.

Given the limited availability of open-source software options, openLCA emerges as a recommended tool for conducting a LCA in the domain of energy systems, particularly when a programming interface is necessary. However, future endeavors should delve into unlocking the full potential of the software and assessing the labor intensity associated with integrating data from literature sources.

[33] Documentation - openLCA 2.0 - Data Quality:
`https://greendelta.github.io/openLCA2-manual/advanced_top/data_quality.html`.

[34] Documentation - openLCA 2.0 - Calculation and Result Analysis:
`https://greendelta.github.io/openLCA2-manual/res_analysis/index.html`.

5.3. Assessment of Limitations and Assumptions

There were two types of assumptions and limitations that occurred during this thesis, the ones related to the general application of a LCA to energy systems (see section 3.3), and the other limitations and assumptions of the methodological realization in the SESMG (see section 3.5).

Linear Scaling The process of scaling environmental impacts through multiplication with the reference flow of the dataset, rests on the assumption of a linear relationship between inventory flows or environmental impacts and equipment size (see section 3.3, subsection 3.4.1). This approach is commonly employed in literature [120]. In reality, environmental impacts do not strictly follow linear relationships. While it may be convenient to assume linearity, acknowledging the deviation from such simplifications is crucial for a more accurate understanding of environmental complexities [120, 121]. To assess more appropriate scaling factors, scaling procedures exist [121].

In addition, environmental impacts are often assumed to exhibit linearity through the application of CFs to the different material input flows (see subsection 3.4.2). In reality, certain substances do not contribute to an effect in a linear fashion, as exemplified by the ReCiPe impact category terrestrial acidification. When acidic emissions lower the pH of the soil, this can affect the availability of nutrients and lead to changes in the plant community. This effect is not linear as it depends on various factors, including the specific plant species present in a given area [65].

Scaling procedures and the abandonment of CFs are currently no practicable solution at the present time, as a LCA is still a modeled representation of reality. In addition, the data basis has a far greater influence on the results.

Data Harmonization Most variables in the LCA are not harmonized with parameters in the SESMG (section 3.5). This lack of synchronization becomes evident when changes occur in input values, such as the gas import, failing to trigger corresponding adjustments in other material input flows like the steel or electricity demand for the transformer production (see “Example: Gas Heating Transformer” in subsection 3.4.2). Addressing this discrepancy requires the establishment of functional relationships between different material flows. This task is often not practical because separate research for each technology is needed. Taking the example of a gas heating transformer, a high efficiency might result from additional components like pumps or control systems, that would require a higher steel demand for production [122].

Taking functional relationships between individual material flows into account might pose a possibility to improve the data harmonization and should, therefore, be taken into account for future research (see chapter 7).

Standardization Currently, each technology that needs to be considered for the LCA is manually matched to a standardized dataset with the UUID key in the model definition (see subsection 3.4.1). This practice of linking a manually selected dataset introduces discrepancies in parameters like capacity or lifespan, which may not align with the specific characteristics of parameters in the SESMG. A potential solution to address this, and the challenges posed by limited data harmonization, described above, involves the automated selection of the most suitable dataset. In an ideal scenario, a database contains, for example, multiple PV datasets. Based on the values specified in the model definition, the dataset with the least deviation could be automatically chosen.

Furthermore, standardization constrains the specific consideration of local conditions. Regional inventory datasets have a substantial influence on the results. Gibon et al., for example, found that GHG emissions for a single solar power plant could vary widely, ranging from 33 to 95 g CO_2 eq/kWh between different countries [77]. When different locations are available for the selection of energy technologies, an automated approach, incorporating Geographic Information System data, could account for these variations. Spatial information can be attached to processes and their associated elementary flow [123]. This selection would enable a more nuanced representation of the environmental impacts associated with diverse geographical contexts.

Implementing such solutions is challenging due to the limited availability of datasets (see subsection 3.2.2). Even widely used databases, such as ecoinvent, often have low coverage of energy technologies, offering only a single available inventory dataset per technology class [58]. This underscores the need for a broader and more comprehensive availability of datasets, especially for emerging and diverse energy technologies.

However, some automatic selections of datasets might be possible and should, therefore, be taken into account for future research (see chapter 7).

System Boundaries The assignment of environmental impacts to the point of consumption (see section 3.5), heavily influences the results of the LCA. The separation of production and consumption of energy technologies allows for the potential assignment of environmental burdens at both levels [110]. Consumption-based accounting offers the advantage of considering all impacts associated with energy consumption, while production-based accounting may lead to emission reductions achieved through outsourced activities [76].

This approach neglects the environmental impacts of the PV system's electricity generation, which is fed into the grid. This assumption relies on the neighboring system, accounting for the share of renewables within the electricity import. To avoid double counting between systems, widespread adoption of the same accounting (here consumption-based accounting) is necessary [76, 124].

Furthermore, this approach assumes that the neighbored system considered the current electricity mix. Given the challenges in implementing this in LCA databases (see section 3.2), as discussed in various instances throughout this thesis, datasets are rarely up-to-date.

An alternative approach could involve dividing environmental impacts into periodic and variable impacts, similar to the division of emissions in the SESMG. For specific environmental impacts, such as those related to the PV system, periodic emissions could still be assigned to the system (e.g., accordance with end-of-life considerations), while variable emissions are addressed within the consumption-based approach. This distinction may offer a more nuanced understanding of environmental impacts. In contrast, if this approach is considered differently in various systems, this might lead to double counting between systems as well.

In summary, this assumption can be neglected as it is in alignment with the consumption-based approach that is already used in the SESMG.

5.4. Reference Case

Due to mistakes of the ProBas database and the assumptions that needed to be made in order to accomplish the LCA integration in the SESMG, the meaningfulness of the application (see section 4.1) is reduced to a small relevance.

5.4.1. Interpretation

The interpretation of the reference case aligns with the predefined steps in the LCA procedure (see subsection 3.3.5).

Examination of Inventory Analysis and Impact Assessment Results In general, the application case allows for concrete insights by comparing scenarios and individual Pareto points. From the inventory analysis, the material input flows "Mineralien" (minerals) and "Erze" (ores) were analyzed, showing fluctuating values in the ores flow. The two flows can be considered additionally to the impact assessment results, as they might indicate a high metal depletion impact in some scenarios (see subsection 4.2.2). Further, the graphical representation of impact amounts enhanced the understanding of the contributions of each technology to different categories. In case of the category climate change, this graphical breakdown, previously absent, enhances our understanding of the specific technologies influencing the amount of GHG emissions. While such insights could be derived from the SESMG results as well, the graphical presentation offers a more intuitive and explicit depiction now. The comparison of technologies in exemplary categories, such as climate change, human toxicity, and terrestrial acidification, reveals key contributors to environmental impacts. For instance, the PV system is a major contributor to human toxicity, while the pellet heating transformer plays a significant role in terrestrial acidification (see subsection 4.2.3). In summary, the impact assessment results in the return of logical outcomes, providing valuable insights into the influence of specific technologies on environmental impacts.

Completeness and Consistency Check The LCA was done completely for the already implemented technologies in Table 3.3. The consistency of data cannot be guaranteed with ProBas datasets (see subsection 3.2.3). However, the calculation of the inventory analysis and impact assessment results was consistently performed according to the developed methodology.

Sensitivity Analysis Given the predefined goal of functionality and implementation of the developed approach (see section 4.1), the sensitivity analysis includes the comparison between different Pareto points for the given energy system scenarios (see subsection 4.2.3). Future sensitivity analyses could explore the impact of excluding specific technologies (e.g., GCHP or pellet heating) on various impact categories. Additionally, technologies with multiple datasets in ProBas could be evaluated with different datasets (standardization).

Limitations and Recommendations The lack of a battery storage and a thermal storage that can only be used for the energy of the solar thermal system (see Table 3.4) hinder the SESMG from designing a realistic energy system scenarios. As a result, the scenarios show only minor differences in their technology composition. In reality, the economic and emission benefits of a heat pump, especially when combined with thermal storage, are significant [32, 125]. Unfortunately, this specific transition cannot be accurately reflected in the current modeling framework.

Further, the results are limited by negative electricity impacts (see section 3.5). In the reference case, this lead to a small amount of environmental impacts attributed to the electricity import and an overrepresentation of the GCHP in most of the impact categories. The heat pump has a high electricity input that is automatically considered with environmental impacts of the average electricity mix.

The application of the reference case did not lead to specific recommendations for technologies; a deeper analysis of the results would be required for such recommendations

5.4.2. Comparison with Literature

General Laurent et al. [5] conducted a comprehensive review of LCA results from energy system technologies, concluding that certain impact categories are associated with higher values when there is a higher share of renewables in the energy system:

- Categories that typically record lower impacts due to a higher share of renewables include climate change and eutrophication. In the reference case, the share of renewables remains relatively stable across the different Pareto points. The categories climate change and freshwater eutrophication are still decreasing with a higher reduction of GHG emissions. The rise in marine eutrophication is attributed to the pellet heating transformer.
- In literature, varied results are observed in toxicity-related, land use, and water use categories. Due to the use of system processes, land use and water use categories could not be analyzed (see Appendix B). The impact category human toxicity was reduced overall in the reference case, with renewables identified as the main contributor to this category.
- The category metal depletion often exhibits an increase in impact [11, 16, 23]. An explicit verification was challenging in the applied reference case due to the presence of renewable energy components (PV system, heat pumps) in all scenarios. Additionally, many material flows that typically contribute to this impact category are excluded in ProBas. Therefore, the material input flows "Mineralien" (minerals) and "Erze" (ores) were additionally analyzed (see subsection 4.2.2) and identified the GCHP as a possible source for fluctuating values. However, the aggregated flows make specific quantitative statements about this impact difficult.

Herne In Herne, Germany, a significant portion of environmental impacts is attributed to the battery storage system [23]. Because of its absence in the reference case, direct result comparison with this study lacks robustness. Moreover, the analysis of the reference case is limited to a single building. To enhance the comparability with findings of the Herne study, the steps outlined in the conclusion (see chapter 6) are essential. These steps facilitate the representation of larger systems and contribute to a more comprehensive assessment.

6. Conclusion

LCA Application Life cycle assessment (LCA), encompassing goal and scope definition, inventory analysis, impact assessment, and interpretation, proves to be a suitable method for capturing and categorizing the environmental impacts of energy system models (see section 5.2). For example, the increases in categories like terrestrial acidification or marine eutrophication (see subsection 4.2.3) can be recognized and avoided in practical implementation by varying the composition of energy technologies. To establish the linkage between the two approaches, the following steps should consistently be considered:

1. **Collect data**: If primary data acquisition is not possible, use databases as a source for data collection. However, this acts as the main hurdle for the LCA. Accordingly, analyze databases transparently, considering their weaknesses. Interpret results with a full awareness of these limitations (see section 5.1).
2. **Perform an ex-post assessment**: In the LCA procedure all steps need to consider the combination of both approaches. Particularly, the inventory analysis and the impact assessment are suitable for an automatic combination with an energy system modeling (ESM) tool. The ex-post assessment should include the calculation of multiple product systems for the different technologies, as well as a summary of these calculations for the entire system (see section 3.3). The impact assessment should always cover as many flows of the inventory analysis as possible. For the automated coupling, it is recommended to use the openLCA software (see section 5.2).
3. **Overcome challenges**: Ensure optimal consideration of technology mapping and data harmonization by aligning LCA data with the current state of ESM. When coupling, avoid double-counting by establishing a logical and consistent allocation of environmental impacts, dependent on the system boundaries (e.g., consumption based accounting) (see section 3.3).
4. **Do research about environmental impacts**: To derive concrete recommendations for the design of energy systems, more research about the environmental impacts is needed. Even though a LCA is conducted to capture a broad range of impacts, some categories might be more important than others (see section 5.4).
5. **Interpret results**: The results should be used as an additional decision-making criterion. Sensitivity analysis with varying technology compositions or parameters might enhance the insight into the results (see section 5.4). To avoid potential misinterpretation, the emphasis is not on the absolute values of the impact categories but rather on the strength of the comparisons among the scenarios.

Realization in SESMG In the specific case of using the LCA application within the Spreadsheet Energy System Model Generator (SESMG) (see section 3.4) along with the Prozessorientierte Basisdaten für Umweltmanagement-Instrumente (ProBas) database in openLCA, the following steps must be taken into account. Also, these steps aid users of other ESM tools in overcoming challenges for coupling the approaches:

1. **Choose database**: The user has to chose the most fitting database. If a commercial database is not available, it is recommended to use the ProBas database within openLCA, given its free availability and broader technology coverage compared to other free databases (see section 5.1). However, due to errors identified in the database, the implementation was strategically designed to also allow compatibility with alternative databases.
2. **Include technologies**: Technologies listed in Table 3.4 can be added one by one to the model definition with a corresponding universally unique identifier (UUID) key. If more technologies are needed to analyze the energy system, central energy technologies and district heating networks can possibly be implemented for the analysis of larger systems (see Table 3.4). However, a plausibility check should be carried out after each additionally implemented technology. The user needs to assure that environmental impacts are neither neglected nor double counted.
3. **Check for unit processes**: Unit processes pose the opportunity of technology mapping between the LCA and the ESM. To avoid mistakes in the use of unit processes, they should be checked for validity. In the context of ProBas, this involves manually creating the unit process and then comparing it with the system process, based on the results of the impact assessment (see subsection 3.4.2).
4. **Adapt the impact assessment**: The adaption of the ReCiPe2008 method in ProBas (see Appendix D) should be used. For alternative energy systems, it is essential to consistently check flows for their assignment to impact categories or to analyze them separately, as demonstrated in the reference case (see subsection 4.2.2).
5. **Consider result limitations**: After the LCA was conducted, results should always take into account the used data basis. In the context of ProBas in openLCA, it is important to note that relying solely on the graphical representation in the graphical user interface (GUI) when analyzing results may be misleading. Misinterpretation might occur if there is an increase in electricity production within the system boundaries (see section 5.4).

7. Outlook

Two out of the four limitations and assumptions should be addressed in the future:

- Data harmonization (see section 5.3): To account for functional relationships between individual material flows, additional information on the datasets of the technologies is required. These information might be integrated in a comprehensive database. Once Spreadsheet Energy System Model Generator - Database (SESMG-Data) is available as an open-source database, a long-term goal could be its integration with a database in the openLCA software. This would enable a common interface to check different parameters prior to conducting the technology mapping and data harmonization.
- Standardization (see section 5.3): An automated selection of the most suitable dataset requires a deeper analysis of different datasets within the ProBas database, and a comparison between the datasets.

The following enumeration opens possible research topics that could be implemented in the field of coupling ESM and LCA in the future:

- Implementation in optimization (see section 5.2): To accomplish this, the Environmental Framework for Energy System Assessment (EAFESA) frameworks provides additional guidance [12].
- Endpoint indicators or single indicators (see section 5.3 and section 5.4): Subsequent research could explore the impact of diverse energy system compositions on ReCiPe endpoint indicators, encompassing effects on human health, ecosystems, and resources [65]. Additionally, other individual indicators or the monetization of impacts may be examined for their potential benefits in the impact assessment.
- OpenLCA features (see section 5.2): OpenLCA allows the categorization of data quality using color codes independently from the database. This feature could be implemented in future studies if the database provides information about the initial source of the dataset.
- Specific SESMG improvements[35]: Improvements of the code could include GUI enhancements such as automatic database and impact assessment category selection. Future adaptations could also encompass alternative visualization forms and setting up a dedicated server for the openLCA application. Furthermore, impacts in the category of climate change can be utilized to verify currently implemented emission values. This thesis uncovered higher emissions for an energy system compared to the values obtained from the SESMG. This outcome prompts a reexamination of the presently employed data sources for emission calculations, once SESMG-Data is available.

[35] GitHub - SESMG - Wishlist: https://github.com/SESMG/SESMG/issues/216.

Acknowledgment

I would like to take this opportunity to express my gratitude to everyone who supported me in writing my bachelor thesis. Special thanks go to Prof. Dr. Peter Vennemann, Prof. Dr.-Ing. Elmar Brügging and Dr. Christian Klemm, who gave me the opportunity to write this thesis. I would also like to thank Jan Niklas Tockloth, Gregor Becker and Benjamin Blankenstein for numerous discussions about the content and and support for this thesis. A special acknowledgement goes to Dr. Christian Klemm for supporting me consistently till the end of my thesis. I extend my gratitude to Fabio Lange, my sister Pauline Koert, Benjamin Blankenstein, Jan Niklas Tockloth and Gregor Becker for proofreading my bachelor thesis. I would also like to thank the developers of the AI tools ChatGPT and DeepL Write, which I used for text editing. I would like to extend my sincere gratitude to my family, friends and roommates. Their positive energy significantly contributed to my perseverance, and I deeply appreciate their friendship and support. I would like to thank the sdw (Stiftung der Deutschen Wirtschaft),the HHV-Stiftung (Hans Herman Voss-Stiftung), and the University of Applied Sciences Münster (Faculty of Energy, Building Services, Environmental Engineering) for their financial and moral support during my studies.

This thesis would not have been possible without the collective support, guidance, and encouragement from each of you.

Bibliography

[1] International Energy Agency. *Empowering Cities for a Net Zero Future: Unlocking Resilient, Smart, Sustainable Urban Energy Systems*. Tech. rep. 2021. URL: https://www.iea.org/reports/empowering-cities-for-a-net-zero-future.

[2] UN DESA. *Anteil der Bevölkerung in Städten weltweit von 1985 bis 2015 und Prognose bis 2050 [Graph]*. May 2018. URL: https://de-statista-com.ezproxy.fh-muenster.de/statistik/daten/studie/37084/umfrage/anteil-der-bevoelkerung-in-staedten-weltweit-seit-1985/ (visited on 02/05/2024).

[3] European Commission. *Renewable Energy Directive - Key Facts*. URL: https://energy.ec.europa.eu/topics/renewable-energy/renewable-energy-directive-targets-and-rules/renewable-energy-directive_en (visited on 01/24/2024).

[4] F. Asdrubali, G. Baldinelli, F. D'Alessandro, and F. Scrucca. "Life Cycle Assessment of Electricity Production from Renewable Energies: Review and Results Harmonization". In: *Renewable and Sustainable Energy Reviews* 42 (Feb. 2015), pp. 1113–1122. ISSN: 1364-0321. DOI: 10.1016/j.rser.2014.10.082.

[5] A. Laurent, N. Espinosa, and M. Z. Hauschild. "LCA of Energy Systems". In: *Life Cycle Assessment*. Ed. by M. Z. Hauschild, R. K. Rosenbaum, and S. I. Olsen. Cham: Springer International Publishing, 2018, pp. 633–668. ISBN: 978-3-319-56475-3. DOI: 10.1007/978-3-319-56475-3_26.

[6] European Commission. *The European Green Deal*. 2019. URL: https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_en (visited on 01/23/2024).

[7] G. Luderer, M. Pehl, A. Arvesen, T. Gibon, B. L. Bodirsky, H. S. De Boer, O. Fricko, M. Hejazi, F. Humpenöder, G. Iyer, S. Mima, I. Mouratiadou, R. C. Pietzcker, A. Popp, M. Van Den Berg, D. Van Vuuren, and E. G. Hertwich. "Environmental Co-Benefits and Adverse Side-Effects of Alternative Power Sector Decarbonization Strategies". In: *Nature Communications* 10.1 (Nov. 2019). ISSN: 2041-1723. DOI: 10.1038/s41467-019-13067-8.

[8] J. Keirstead, M. Jennings, and A. Sivakumar. "A Review of Urban Energy System Models: Approaches, Challenges and Opportunities". In: *Renewable and Sustainable Energy Reviews* 16.6 (Aug. 2012), pp. 3847–3866. ISSN: 1364-0321. DOI: 10.1016/j.rser.2012.02.047.

[9] Z. Lukszo, E. Bompard, P. Hines, and L. Varga. "Energy and Complexity". In: *Complexity* 2018 (June 2018), pp. 1–2. ISSN: 1076-2787, 1099-0526. DOI: 10.1155/2018/6937505.

[10] S. C. Bhattacharyya and G. R. Timilsina. "A Review of Energy System Models". In: *International Journal of Energy Sector Management* 4.4 (Nov. 2010), pp. 494–518. ISSN: 1750-6220. DOI: 10.1108/17506221011092742.

[11] P. Berrill, A. Arvesen, Y. Scholz, H. C. Gils, and E. G. Hertwich. "Environmental Impacts of High Penetration Renewable Energy Scenarios for Europe". In: *Environmental Research Letters* 11.1 (Jan. 2016). ISSN: 1748-9326. DOI: 10.1088/1748-9326/11/1/014012.

[12] L. Xu. "Coupling Life Cycle Assessment with Energy System Analysis". In: *Dissertation* (2023). DOI: 10.5445/IR/1000157936.

[13] S. N. Pati. *Life Cycle Assessment: Future Challenges*. 1st ed. Boca Raton: CRC Press, June 2022. ISBN: 978-1-00-320675-0. DOI: 10.1201/9781003206750.

[14] J. Sathaye et al. "Renewable Energy in the Context of Sustainable Development". In: *Renewable Energy Sources and Climate Change Mitigation: Special Report of the Intergovernmental Panel on Climate Change*. Ed. by C. von Stechow, G. Hansen, K. Seyboth, O. Edenhofer, P. Eickemeier, P. Matschoss, R. Pichs-Madruga, S. Schlömer, S. Kadner, T. Zwickel, and Y. Sokona. Cambridge: Cambridge University Press, 2011, pp. 707–790. ISBN: 978-1-107-02340-6. DOI: 10.1017/CBO9781139151153.013.

[15] X. Zhang, M. Lovati, I. Vigna, J. Widén, M. Han, C. Gal, and T. Feng. "A Review of Urban Energy Systems at Building Cluster Level Incorporating Renewable-Energy-Source (RES) Envelope Solutions". In: *Applied Energy* 230 (Nov. 2018), pp. 1034–1056. ISSN: 03062619. DOI: 10.1016/j.apenergy.2018.09.041.

[16] E. Hertwich. "Understanding the Climate Mitigation Benefits of Product Systems: Comment on "Using Attributional Life Cycle Assessment to Estimate Climate-Change Mitigation..."" In: *Journal of Industrial Ecology* 18.3 (May 2014), pp. 464–465. ISSN: 1088-1980, 1530-9290. DOI: 10.1111/jiec.12150.

[17] H. Blanco, V. Codina, A. Laurent, W. Nijs, F. Maréchal, and A. Faaij. "Life Cycle Assessment Integration into Energy System Models: An Application for Power-to-Methane in the EU". In: *Applied Energy* 259 (Feb. 2020). ISSN: 0306-2619. DOI: 10.1016/j.apenergy.2019.114160.

[18] M. Pehl, A. Arvesen, F. Humpenöder, A. Popp, E. G. Hertwich, and G. Luderer. "Understanding Future Emissions from Low-Carbon Power Systems by Integration of Life-Cycle Assessment and Integrated Energy Modelling". In: *Nature Energy* 2.12 (Dec. 2017), pp. 939–945. ISSN: 2058-7546. DOI: 10.1038/s41560-017-0032-9.

[19] C. Unsihuay-Vila, J. Marangon-Lima, A. Zambroni De Souza, and I. Perez-Arriaga. "Multistage Expansion Planning of Generation and Interconnections with Sustainable Energy Development Criteria: A Multiobjective Model". In: *International Journal of Electrical Power & Energy Systems* 33.2 (Feb. 2011), pp. 258–270. ISSN: 0142-0615. DOI: 10.1016/j.ijepes.2010.08.021.

[20] D. García-Gusano, D. Iribarren, M. Martín-Gamboa, J. Dufour, K. Espegren, and A. Lind. "Integration of Life-Cycle Indicators into Energy Optimisation Models: The Case Study of Power Generation in Norway". In: *Journal of Cleaner Production* 112 (Jan. 2016), pp. 2693–2696. ISSN: 0959-6526. DOI: 10.1016/j.jclepro.2015.10.075.

[21] M. Lotteau, P. Loubet, M. Pousse, E. Dufrasnes, and G. Sonnemann. "Critical Review of Life Cycle Assessment (LCA) for the Built Environment at the Neighborhood Scale". In: *Building and Environment* 93 (Nov. 2015), pp. 165–178. ISSN: 0360-1323. DOI: 10.1016/j.buildenv.2015.06.029.

[22] C. Klemm, G. Becker, J. Tockloth, J. Budde, and P. Vennemann. *The Spreadsheet Energy System Model Generator (SESMG): A Tool for the Optimization of Urban Energy Systems*. Zenodo. Sept. 2023. DOI: 10.5281/ZENODO.8344791.

[23] G. Quest, R. Arendt, C. Klemm, V. Bach, J. Budde, P. Vennemann, and M. Finkbeiner. "Integrated Life Cycle Assessment (LCA) of Power and Heat Supply for a Neighborhood: A Case Study of Herne, Germany". In: *Energies* 15.16 (Aug. 2022). ISSN: 1996-1073. DOI: 10.3390/en15165900.

[24] C. Klemm and F. Wiese. "Indicators for the Optimization of Sustainable Urban Energy Systems Based on Energy System Modeling". In: *Energy, Sustainability and Society* 12.1 (Dec. 2022), p. 3. ISSN: 2192-0567. DOI: 10.1186/s13705-021-00323-3.

[25] D. Kumar, ed. *Urban Energy Systems: Modeling and Simulation for Smart Cities*. 1st ed. Wiley, Aug. 2023. ISBN: 978-1-119-84759-5. DOI: 10.1002/9781119847595.

[26] P. Mancarella, G. Andersson, J. Pecas-Lopes, and K. Bell. "Modelling of Integrated Multi-Energy Systems: Drivers, Requirements, and Opportunities". In: *2016 Power Systems Computation Conference (PSCC)*. Genoa, Italy: IEEE, June 2016, pp. 1–22. ISBN: 978-88-941051-2-4. DOI: 10.1109/PSCC.2016.7541031.

[27] M. Günther and K. Velten. *Mathematische Modellbildung und Simulation: eine Einführung für Wissenschaftler, Ingenieure und Ökonomen*. Lehrbuch Physik. Weinheim: Wiley-VCH Verlag GmbH & Co. KGaA, 2014. ISBN: 978-3-527-41217-4.

[28] C. Klemm and P. Vennemann. "Modeling and Optimization of Multi-Energy Systems in Mixed-Use Districts: A Review of Existing Methods and Approaches". In: *Renewable and Sustainable Energy Reviews* 135 (Jan. 2021). ISSN: 1364-0321. DOI: 10.1016/j.rser.2020.110206.

[29] S. Pfenninger, A. Hawkes, and J. Keirstead. "Energy Systems Modeling for Twenty-First Century Energy Challenges". In: *Renewable and Sustainable Energy Reviews* 33 (May 2014), pp. 74–86. ISSN: 13640321. DOI: 10.1016/j.rser.2014.02.003.

[30] I. M. Algunaibet and G. Guillén-Gosálbez. "Life Cycle Burden-Shifting in Energy Systems Designed to Minimize Greenhouse Gas Emissions: Novel Analytical Method and Application to the United States". In: *Journal of Cleaner Production* 229 (Aug. 2019), pp. 886–901. ISSN: 0959-6526. DOI: 10.1016/j.jclepro.2019.04.276.

[31] D. Birnkammer. *Extending the Multi-Objective Model LAEND to Account for Sector Coupled Heat and Electricity Supply of Residential Quarters under Consideration of Decarbonization Strategies*. Oct. 2021.

[32] C. Klemm. "Optimization of Sustainable Urban Energy Systems: Model Development and Application". In: *Dissertation* (Sept. 2023). DOI: 10.5281/ZENODO.8255615.

[33] C. Klemm, F. Wiese, and P. Vennemann. "Model-Based Run-Time and Memory Reduction for a Mixed-Use Multi-Energy System Model with High Spatial Resolution". In: *Applied Energy* 334 (Mar. 2023). ISSN: 0306-2619. DOI: 10.1016/j.apenergy.2022.120574.

[34] G. Mavrotas. "Effective Implementation of the ϵ-Constraint Method in Multi-Objective Mathematical Programming Problems". In: *Applied Mathematics and Computation* 213.2 (July 2009), pp. 455–465. ISSN: 0096-3003. DOI: 10.1016/j.amc.2009.03.037.

[35] M. Fadaee and M. Radzi. "Multi-Objective Optimization of a Stand-Alone Hybrid Renewable Energy System by Using Evolutionary Algorithms: A Review". In: *Renewable and Sustainable Energy Reviews* 16.5 (June 2012), pp. 3364–3369. ISSN: 1364-0321. DOI: 10.1016/j.rser.2012.02.071.

[36] S. Rauner and M. Budzinski. "Holistic Energy System Modeling Combining Multi-Objective Optimization and Life Cycle Assessment". In: *Environmental Research Letters* 12.12 (Dec. 2017). ISSN: 1748-9326. DOI: 10.1088/1748-9326/aa914d.

[37] C. Klemm, G. Becker, J. N. Tockloth, J. Budde, and P. Vennemann. "The Spreadsheet Energy System Model Generator (SESMG): A Tool for the Optimization of Urban Energy Systems". In: *Journal of Open Source Software* 8.89 (Sept. 2023). ISSN: 2475-9066. DOI: 10.21105/joss.05519.

[38] C. Klemm and G. Becker. *Sourcecode Documentation of the SESMG Algorithm*. 2022. URL: https://spreadsheet-energy-system-model-generator.readthedocs.io/en/latest/index.html (visited on 01/14/2024).

[39] G. Becker, C. Klemm, and P. Vennemann. "Open Source District Heating Modeling Tools—A Comparative Study". In: *Energies* 15.21 (Nov. 2022). ISSN: 1996-1073. DOI: 10.3390/en15218277.

[40] J. N. Tockloth. *Gestaltungsmöglichkeiten zukünftiger lokaler Energiemärkte*. Steinfurt, Germany: Springer Gabler Wiesbaden, 2024. ISBN: 978-3-658-43760-2.

[41] M. Muratori, P. Jadun, B. Bush, D. Bielen, L. Vimmerstedt, J. Gonder, C. Gearhart, and D. Arent. "Future Integrated Mobility-Energy Systems: A Modeling Perspective". In: *Renewable and Sustainable Energy Reviews* 119 (Mar. 2020). ISSN: 1364-0321. DOI: 10.1016/j.rser.2019.109541.

[42] M. Geissdoerfer, P. Savaget, N. M. Bocken, and E. J. Hultink. "The Circular Economy – A New Sustainability Paradigm?" In: *Journal of Cleaner Production* 143 (Feb. 2017), pp. 757–768. ISSN: 0959-6526. DOI: 10.1016/j.jclepro.2016.12.048.

[43] S. S. Muthu, ed. *Life Cycle Assessment & Circular Economy*. Environmental Footprints and Eco-design of Products and Processes. Cham: Springer Nature Switzerland, 2023. ISBN: 978-3-031-33982-0. DOI: 10.1007/978-3-031-33982-0.

[44] European Commission. Joint Research Centre. Institute for Environment and Sustainability. *International Reference Life Cycle Data System (ILCD) Handbook: General Guide for Life Cycle Assessment - Detailed Guidance*. LU: Publications Office, 2010. URL: https://data.europa.eu/doi/10.2788/38479 (visited on 12/21/2023).

[45] DIN EN ISO 14040:2021-02. *Environmental Management - Life Cycle Assessment - Principles And Framework*. Feb. 2021.

[46] G. Finnveden, M. Z. Hauschild, T. Ekvall, J. Guinée, R. Heijungs, S. Hellweg, A. Koehler, D. Pennington, and S. Suh. "Recent Developments in Life Cycle Assessment". In: *Journal of Environmental Management* 91.1 (Oct. 2009), pp. 1–21. ISSN: 0301-4797. DOI: 10.1016/j.jenvman.2009.06.018.

[47] M. Z. Hauschild, R. K. Rosenbaum, and S. I. Olsen, eds. *Life Cycle Assessment: Theory and Practice*. Cham: Springer International Publishing, 2018. ISBN: 978-3-319-56475-3. DOI: 10.1007/978-3-319-56475-3.

[48] R. G. Hunt. *Resource and Environmental Profile Analysis of Nine Beverage Container Alternatives, Final Report*. Washington: Environmental Protection Agency; for sale by the Supt. of Docs., U.S. Govt. Print. Off., 1974. URL: https://catalog.hathitrust.org/Record/011409108 (visited on 12/27/2023).

[49] R. Frischknecht, F. Wyss, S. Büsser Knöpfel, T. Lützkendorf, and M. Balouktsi. "Cumulative Energy Demand in LCA: The Energy Harvested Approach". In: *The International Journal of Life Cycle Assessment* 20.7 (July 2015), pp. 957–969. ISSN: 0948-3349, 1614-7502. DOI: 10.1007/s11367-015-0897-4.

[50] DIN EN ISO 14044:2006 + Amd 1:2017 + Amd 2:2020. *Environmental Management Life Cycle Assessment – Requirements and Guidelines*. Feb. 2021.

[51] S. Gerbinet, S. Belboom, and A. Léonard. "Life Cycle Analysis (LCA) of Photovoltaic Panels: A Review". In: *Renewable and Sustainable Energy Reviews* 38 (Oct. 2014), pp. 747–753. ISSN: 1364-0321. DOI: 10.1016/j.rser.2014.07.043.

[52] M. A. Curran, ed. *Interpretation, Critical Review and Reporting in Life Cycle Assessment*. LCA Compendium – The Complete World of Life Cycle Assessment. Cham: Springer International Publishing, 2023. ISBN: 978-3-031-35727-5. DOI: 10.1007/978-3-031-35727-5.

[53] A. Martínez-Rocamora, J. Solís-Guzmán, and M. Marrero. "LCA Databases Focused on Construction Materials: A Review". In: *Renewable and Sustainable Energy Reviews* 58 (May 2016), pp. 565–573. ISSN: 1364-0321. DOI: 10.1016/j.rser.2015.12.243.

[54] S. Hellweg and L. Milà I Canals. "Emerging Approaches, Challenges and Opportunities in Life Cycle Assessment". In: *Science* 344.6188 (June 2014), pp. 1109–1113. ISSN: 1095-9203. DOI: 10.1126/science.1248361.

[55] G. F. Menzies, S. Turan, and P. F. G. Banfill. "Life-Cycle Assessment and Embodied Energy: A Review". In: *Proceedings of the Institution of Civil Engineers - Construction Materials* 160.4 (Nov. 2007), pp. 135–143. ISSN: 1747-6518. DOI: 10.1680/coma.2007.160.4.135.

[56] G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz, and B. Weidema. "The Ecoinvent Database Version 3 (Part I): Overview and Methodology". In: *The International Journal of Life Cycle Assessment* 21.9 (Sept. 2016), pp. 1218–1230. ISSN: 1614-7502. DOI: 10.1007/s11367-016-1087-8.

[57] Sphera. *GaBi Databases.* URL: http://www.gabi-software.de/databases/gabi-databases/ (visited on 01/03/2024).

[58] T. Junne, S. Simon, J. Buchgeister, M. Saiger, M. Baumann, M. Haase, C. Wulf, and T. Naegler. "Environmental Sustainability Assessment of Multi-Sectoral Energy Transformation Pathways: Methodological Approach and Case Study for Germany". In: *Sustainability* 12.19 (Oct. 2020). ISSN: 2071-1050. DOI: 10.3390/su12198225.

[59] PD ISO/TR 14047:2012. *Environmental Management. Life Cycle Assessment. Illustrative Examples on How to Apply ISO 14044 to Impact Assessment Situations.* Tech. rep. BSI British Standards, June 2021. DOI: 10.3403/30232967.

[60] M. Z. Hauschild and M. A. J. Huijbregts. "Introducing Life Cycle Impact Assessment". In: *Life Cycle Impact Assessment.* Ed. by M. Z. Hauschild and M. A. Huijbregts. Dordrecht: Springer Netherlands, 2015, pp. 1–16. ISBN: 978-94-017-9744-3. DOI: 10.1007/978-94-017-9744-3_1.

[61] M. A. J. Huijbregts, Z. J. N. Steinmann, P. M. F. Elshout, G. Stam, F. Verones, M. Vieira, M. Zijp, A. Hollander, and R. Van Zelm. "ReCiPe2016: A Harmonised Life Cycle Impact Assessment Method at Midpoint and Endpoint Level". In: *The International Journal of Life Cycle Assessment* 22.2 (Feb. 2017), pp. 138–147. ISSN: 1614-7502. DOI: 10.1007/s11367-016-1246-y.

[62] R. K. Rosenbaum. "Selection of Impact Categories, Category Indicators and Characterization Models in Goal and Scope Definition". In: *Goal and Scope Definition in Life Cycle Assessment.* Ed. by M. A. Curran. Dordrecht: Springer Netherlands, 2017, pp. 63–122. ISBN: 978-94-024-0855-3. DOI: 10.1007/978-94-024-0855-3_2.

[63] R. Arendt, T. M. Bachmann, M. Motoshita, V. Bach, and M. Finkbeiner. "Comparison of Different Monetization Methods in LCA: A Review". In: *Sustainability* 12.24 (Dec. 2020). ISSN: 2071-1050. DOI: 10.3390/su122410493.

[64] C. Bulle, M. Margni, L. Patouillard, A.-M. Boulay, G. Bourgault, V. De Bruille, V. Cao, M. Hauschild, A. Henderson, S. Humbert, S. Kashef-Haghighi, A. Kounina, A. Laurent, A. Levasseur, G. Liard, R. K. Rosenbaum, P.-O. Roy, S. Shaked, P. Fantke, and O. Jolliet. "IMPACT World+: A Globally Regionalized Life Cycle Impact Assessment Method". In: *The International Journal of Life Cycle Assessment* 24.9 (Sept. 2019), pp. 1653–1674. ISSN: 1614-7502. DOI: 10.1007/s11367-019-01583-0.

[65] M. Goedkoop, R. Heijungs, M. Huijbregts, A. Schryver, J. Struijs, and R. Zelm. *ReCiPe 2008: A Life Cycle Impact Assessment Method Which Comprises Harmonised Category Indicators at the Midpoint and the Endpoint Level.* Jan. 2008. URL: https://www.researchgate.net/publication/302559709_ReCiPE_2008_A_life_cycle_impact_assessment_method_which_comprises_harmonised_category_indicators_at_the_midpoint_and_the_endpoint_level.

[66] European Commission. Joint Research Centre. *Updated Characterisation and Normalisation Factors for the Environmental Footprint 3.1 Method.* LU: Publications Office, 2023. URL: https://data.europa.eu/doi/10.2760/798894 (visited on 11/22/2023).

[67] J. Fischer. *Comparing Wind and Solar Energy Impacts on the Environment: A LCA Approach Using openLCA Platform*. Apr. 2021.

[68] J. B. Guinée, S. Cucurachi, P. J. Henriksson, and R. Heijungs. "Digesting the Alphabet Soup of LCA". In: *The International Journal of Life Cycle Assessment* 23.7 (July 2018), pp. 1507–1511. ISSN: 1614-7502. DOI: 10.1007/s11367-018-1478-0.

[69] J. B. Guinée and R. Heijungs. "Life Cycle Sustainability Analysis: Framing Questions for Approaches". In: *Journal of Industrial Ecology* 15.5 (Oct. 2011), pp. 656–658. ISSN: 1088-1980. DOI: 10.1111/j.1530-9290.2011.00398.x.

[70] E. Loiseau, L. Aissani, S. Le Féon, F. Laurent, J. Cerceau, S. Sala, and P. Roux. "Territorial Life Cycle Assessment (LCA): What Exactly Is It about? A Proposal towards Using a Common Terminology and a Research Agenda". In: *Journal of Cleaner Production* 176 (Mar. 2018), pp. 474–485. ISSN: 0959-6526. DOI: 10.1016/j.jclepro.2017.12.169.

[71] S. Nakamura and K. Nansai. "Input–Output and Hybrid LCA". In: *Special Types of Life Cycle Assessment*. Ed. by M. Finkbeiner. Dordrecht: Springer Netherlands, 2016, pp. 219–291. ISBN: 978-94-017-7610-3. DOI: 10.1007/978-94-017-7610-3_6.

[72] E. Masanet, Y. Chang, A. R. Gopal, P. Larsen, W. R. Morrow, R. Sathre, A. Shehabi, and P. Zhai. "Life-Cycle Assessment of Electric Power Systems". In: *Annual Review of Environment and Resources* 38.1 (Oct. 2013), pp. 107–136. ISSN: 1545-2050. DOI: 10.1146/annurev-environ-010710-100408.

[73] G. Zang, J. Zhang, J. Jia, E. S. Lora, and A. Ratner. "Life Cycle Assessment of Power-Generation Systems Based on Biomass Integrated Gasification Combined Cycles". In: *Renewable Energy* 149 (Apr. 2020), pp. 336–346. ISSN: 09601481. DOI: 10.1016/j.renene.2019.12.013.

[74] D. García-Gusano, I. R. Istrate, and D. Iribarren. "Life-Cycle Consequences of Internalising Socio-Environmental Externalities of Power Generation". In: *Science of The Total Environment* 612 (Jan. 2018), pp. 386–391. ISSN: 0048-9697. DOI: 10.1016/j.scitotenv.2017.08.231.

[75] M. F. Astudillo, K. Vaillancourt, P.-O. Pineau, and B. Amor. "Integrating Energy System Models in Life Cycle Management". In: *Designing Sustainable Technologies, Products and Policies*. Ed. by E. Benetto, K. Gericke, and M. Guiton. Cham: Springer International Publishing, 2018, pp. 249–259. ISBN: 978-3-319-66981-6. DOI: 10.1007/978-3-319-66981-6_28.

[76] S. Harris, J. Weinzettel, A. Bigano, and A. Källmén. "Low Carbon Cities in 2050? GHG Emissions of European Cities Using Production-Based and Consumption-Based Emission Accounting Methods". In: *Journal of Cleaner Production* 248 (Mar. 2020). ISSN: 0959-6526. DOI: 10.1016/j.jclepro.2019.119206.

[77] T. Gibon, R. Wood, A. Arvesen, J. D. Bergesen, S. Suh, and E. G. Hertwich. "A Methodology for Integrated, Multiregional Life Cycle Assessment Scenarios under Large-Scale Technological Change". In: *Environmental Science & Technology* 49.18 (Sept. 2015), pp. 11218–11226. ISSN: 1520-5851. DOI: 10.1021/acs.est.5b01558.

[78] K. Volkart, N. Weidmann, C. Bauer, and S. Hirschberg. "Multi-Criteria Decision Analysis of Energy System Transformation Pathways: A Case Study for Switzerland". In: *Energy Policy* 106 (July 2017), pp. 155–168. ISSN: 0301-4215. DOI: 10.1016/j.enpol.2017.03.026.

[79] K. E. Brown, D. K. Henze, and J. B. Milford. "How Accounting for Climate and Health Impacts of Emissions Could Change the US Energy System". In: *Energy Policy* 102 (Mar. 2017), pp. 396–405. ISSN: 0301-4215. DOI: 10.1016/j.enpol.2016.12.052.

[80] H. Hottenroth, I. Tietze, L. Lazar, and S. Lewerenz. *LAEND_v031*. URL: https://github.com/inecmod/LAEND/commits/main/ (visited on 11/21/2023).

[81] H. Hottenroth and D. Birnkammer. *LAEND Documentation v.0.3.1*. May 2022. URL: https://github.com/inecmod/LAEND/commit/51eac2ec14315711eb29eedfc8fc77e2b3bdfe6b (visited on 11/21/2023).

[82] oemof developer group. *A Modular Open Source Framework to Model Energy Supply Systems*. Oct. 2023. URL: https://oemof.org/ (visited on 11/21/2023).

[83] *openLCA.Org | openLCA Is a Free, Professional Life Cycle Assessment (LCA) and Footprint Software with a Broad Range of Features and Many Available Databases, Created by GreenDelta since 2006*. URL: https://www.openlca.org/ (visited on 01/07/2024).

[84] T. Huld, E. Paietta, P. Zangheri, and I. Pinedo Pascua. "Assembling Typical Meteorological Year Data Sets for Building Energy Performance Using Reanalysis and Satellite-Based Data". In: *Atmosphere* 9.2 (Feb. 2018), p. 53. ISSN: 2073-4433. DOI: 10.3390/atmos9020053.

[85] E. Crenna, R. Pant, S. Sala, and M. Secchi. *Global Normalisation Factors for the Environmental Footprint and Life Cycle Assessment*. Luxembourg: Publications Office of the European Union, 2017. ISBN: 978-92-79-77213-9.

[86] European Commission. Joint Research Centre. Institute for Environment and Sustainability. *Development of a Weighting Approach for the Environmental Footprint.* Publications Office, 2018. URL: https://data.europa.eu/doi/10.2760/945290 (visited on 11/21/2023).

[87] S. Biganzioli, F. D. Laurentiis, S. Diaconu, and L. Zampori. *Supporting Information to the Characterisation Factors of Recommended EF Life Cycle Impact Assessment Methods: Version 2, from ILCD to EF 3.0*. LU: European Comission, 2018. ISBN: 978-92-79-98584-3. URL: https://data.europa.eu/doi/10.2760/002447 (visited on 03/06/2024).

[88] T. J. Mattila. "Use of Input–Output Analysis in LCA". In: *Life Cycle Assessment*. Ed. by M. Z. Hauschild, R. K. Rosenbaum, and S. I. Olsen. Cham: Springer International Publishing, 2018, pp. 349–372. ISBN: 978-3-319-56475-3. DOI: 10.1007/978-3-319-56475-3_14.

[89] B. Zhang, S. Su, Y. Zhu, and X. Li. "An LCA-based Environmental Impact Assessment Model for Regulatory Planning". In: *Environmental Impact Assessment Review* 83 (July 2020). ISSN: 0195-9255. DOI: 10.1016/j.eiar.2020.106406.

[90] C. Rodríguez. *NEEDS in openLCA*. 2017. URL: https://nexus.openlca.org/documents.

[91] *New Energy Externalities Development for Sustainability | NEEDS Project | Fact Sheet | FP6*. URL: https://cordis.europa.eu/project/id/502687 (visited on 01/28/2024).

[92] R. Wood, K. Stadler, T. Bulavskaya, S. Lutter, S. Giljum, A. De Koning, J. Kuenen, H. Schütz, J. Acosta-Fernández, A. Usubiaga, M. Simas, O. Ivanova, J. Weinzettel, J. Schmidt, S. Merciai, and A. Tukker. "Global Sustainability Accounting—Developing EXIOBASE for Multi-Regional Footprint Analysis". In: *Sustainability* 7.1 (Dec. 2014), pp. 138–163. ISSN: 2071-1050. DOI: 10.3390/su7010138.

[93] GreenDelta. *Database Notes – Environmental Footprint (EF) Database*. 2019. URL: https://nexus.openlca.org/documents.

[94] S. Weyand and A. Ciroth. *Die 'ProBas' Datenbank in openLCA.Pdf*. July 2014. URL: https://nexus.openlca.org/documents.

[95] European Commission. *European Platform on LCA: EPLCA*. URL: https://eplca.jrc.ec.europa.eu/ELCD3/ (visited on 11/22/2023).

[96] A. Ciroth and J. Bunsen. *A Multi-Regional Input-Output Database in openLCA*. 2019. URL: https://nexus.openlca.org/documents.

[97] F. Recanati and A. Ciroth. *Secondary Data in openLCA*. Aug. 2019. URL: https://nexus.openlca.org/documents.

[98] A. Ciroth. *ProBas+ in openLCA*. Jan. 2016. URL: https://nexus.openlca.org/documents.

[99] Umweltbundesamt. *ProBas - Prozessorientierte Basisdaten Für Umweltmanagementsysteme*. URL: https://www.probas.umweltbundesamt.de/php/index.php (visited on 12/06/2023).

[100] *openLCA Nexus: The Source for LCA Data Sets*. URL: https://nexus.openlca.org/databases (visited on 11/22/2023).

[101] openLCA. *Webinar: Release of the Environmental Footprint (EF) 3.1 Database*. Dec. 2023. URL: https://www.youtube.com/watch?v=btVoTrJZ1dk (visited on 02/19/2024).

[102] M. Raugei, E. Leccisi, and V. M. Fthenakis. "What Are the Energy and Environmental Impacts of Adding Battery Storage to Photovoltaics? A Generalized Life Cycle Assessment". In: *Energy Technology* 8.11 (Nov. 2020). ISSN: 2194-4296. DOI: 10.1002/ente.201901146.

[103] CEPE aisbl. *End User License Agreement (EULA) for the Databases Included in the Environmental Foodprint 3.1 Database*. URL: https://nexus.openlca.org/database/Environmental%20Footprints#!.

[104] European Commission. *Commission Recommendation (EU) 2021/2279*. Dec. 2021. URL: https://eur-lex.europa.eu/eli/reco/2021/2279/oj (visited on 02/09/2024).

[105] European Commission. *European Platform on LCA: Superseded Environmental Footprint Reference Packages*. Nov. 2019. URL: https://eplca.jrc.ec.europa.eu/LCDN/EF_archive.html (visited on 02/09/2024).

[106] L. Rausch and U. R. Fritsche. *Aktualisierung von Ökobilanzdaten für Erneuerbare Energien im Bereich Treibhausgase und Luftschadstoffe*. Tech. rep. Öko-Institut e.V., June 2012. URL: https://iinas.org/app/downloads_from_old_page/bio/oeko/2012_LCA-EE-BMU.pdf.

[107] *Recent Questions - Ask.openLCA - Question and Answer (Q&A) on Life Cycle Assessment (LCA) - A Life Cycle Assessment (LCA) Community*. URL: https://ask.openlca.org/questions (visited on 02/13/2024).

[108] *Introduction - openLCA 2 Manual*. URL: https://manuals.openlca.org/openlca/introduction/index.html (visited on 01/07/2024).

[109] U. R. Fritsche and K. Schmidt. *Handbuch Zu GEMIS*. Darmstadt: Öko-Institut e.V., May 2007. URL: http://www.gemis.de/g44handbuch.07.pdf (visited on 02/20/2024).

[110] S. J. Davis and K. Caldeira. "Consumption-Based Accounting of CO_2 Emissions". In: *Proceedings of the National Academy of Sciences* 107.12 (Mar. 2010), pp. 5687–5692. ISSN: 1091-6490. DOI: 10.1073/pnas.0906974107.

[111] E. Örtl. *CO_2-Emissionen pro Kilowattstunde Strom stiegen in 2022*. May 2023. URL: https://www.umweltbundesamt.de/themen/co2-emissionen-pro-kilowattstunde-strom-stiegen-in (visited on 02/28/2024).

[112] P. Quinteiro, L. Tarelho, P. Marques, M. Martín-Gamboa, F. Freire, L. Arroja, and A. C. Dias. "Life Cycle Assessment of Wood Pellets and Wood Split Logs for Residential Heating". In: *Science of The Total Environment* 689 (Nov. 2019), pp. 580–589. ISSN: 0048-9697. DOI: 10.1016/j.scitotenv.2019.06.420.

[113] J. DeCarolis, S. Babaee, B. Li, and S. Kanungo. “Modelling to Generate Alternatives with an Energy System Optimization Model”. In: *Environmental Modelling & Software* 79 (May 2016), pp. 300–310. ISSN: 1364-8152. DOI: 10.1016/j.envsoft.2015.11.019.

[114] M. Gutsch and J. Leker. “Global Warming Potential of Lithium-Ion Battery Energy Storage Systems: A Review”. In: *Journal of Energy Storage* 52 (Aug. 2022). ISSN: 2352-152X. DOI: 10.1016/j.est.2022.105030.

[115] co2online. *Heizspiegel*. 2022. URL: https://www.heizspiegel.de/fileadmin/hs/heizspiegel-2023/heizspiegel-2023-flyer.pdf (visited on 02/21/2024).

[116] co2online. *Stromverbrauch eines 4-Personen-Haushalts in Deutschland nach Gebäudetyp 2022*. May 2023. URL: https://de-statista-com.ezproxy.fh-muenster.de/statistik/daten/studie/558288/umfrage/stromverbrauch-einen-4-personen-haushalts-in-deutschland/ (visited on 02/21/2024).

[117] Statistische Ämter des Bundes und der Länder. *Verteilung der primär verwendeten Energieträger zur Beheizung der Wohnräume von Eigentümer- und Mieterhaushalten[1] in Deutschland im Jahr 2022 [Graph]*. Aug. 2023. URL: https://de-statista-com.ezproxy.fh-muenster.de/statistik/daten/studie/1419933/umfrage/verwendete-energietraeger-zum-heizen-der-wohnraeume-nach-miete-und-eigentum/ (visited on 02/25/2024).

[118] J. A. Lozano Miralles, R. López García, J. M. Palomar Carnicero, and F. J. R. Martínez. “Comparative Study of Heat Pump System and Biomass Boiler System to a Tertiary Building Using the Life Cycle Assessment (LCA)”. In: *Renewable Energy* 152 (June 2020), pp. 1439–1450. ISSN: 09601481. DOI: 10.1016/j.renene.2019.12.148.

[119] K. Cen, F. Chen, D. Chen, Z. Gan, X. Zhuang, and H. Zhang. “Life Cycle Assessment of Torrefied Cornstalk Pellets Combustion Heating System”. In: *Fuel* 320 (July 2022). ISSN: 0016-2361. DOI: 10.1016/j.fuel.2022.123968.

[120] L. Gerber, M. Gassner, and F. Maréchal. “Systematic Integration of LCA in Process Systems Design: Application to Combined Fuel and Electricity Production from Lignocellulosic Biomass”. In: *Computers & Chemical Engineering* 35.7 (July 2011), pp. 1265–1280. ISSN: 0098-1354. DOI: 10.1016/j.compchemeng.2010.11.012.

[121] H. Bahlawan, W.-R. Poganietz, P. R. Spina, and M. Venturini. “Cradle-to-Gate Life Cycle Assessment of Energy Systems for Residential Applications by Accounting for Scaling Effects”. In: *Applied Thermal Engineering* 171 (May 2020). ISSN: 1359-4311. DOI: 10.1016/j.applthermaleng.2020.115062.

[122] N. Aste, M. Buzzetti, P. Caputo, and M. Manfren. “Local Energy Efficiency Programs: A Monitoring Methodology for Heating Systems”. In: *Sustainable Cities and Society* 13 (Oct. 2014), pp. 69–77. ISSN: 2210-6707. DOI: 10.1016/j.scs.2014.04.006.

[123] C. François, N. Gondran, and J.-P. Nicolas. “Spatial and Territorial Developments for Life Cycle Assessment Applied to Urban Mobility—Case Study on Lyon Area in France”. In: *The International Journal of Life Cycle Assessment* 26.3 (Mar. 2021), pp. 543–560. ISSN: 1614-7502. DOI: 10.1007/s11367-020-01861-2.

[124] P. Holzapfel, V. Bach, and M. Finkbeiner. “Electricity Accounting in Life Cycle Assessment: The Challenge of Double Counting”. In: *The International Journal of Life Cycle Assessment* 28.7 (July 2023), pp. 771–787. ISSN: 0948-3349, 1614-7502. DOI: 10.1007/s11367-023-02158-w.

[125] N. Zhu, P. Hu, L. Xu, Z. Jiang, and F. Lei. “Recent Research and Applications of Ground Source Heat Pump Integrated with Thermal Energy Storage Systems: A Review”. In: *Applied Thermal Engineering* 71.1 (Oct. 2014), pp. 142–151. ISSN: 1359-4311. DOI: 10.1016/j.applthermaleng.2014.06.040.

[126] United Nations. "United Nations: Montreal Protocol on Substances That Deplete the Ozone Layer - Adjustments and Amendment". In: *International Legal Materials* 32.3 (May 1993), pp. 874–887. ISSN: 1930-6571. DOI: 10.1017/S0020782900016338.

[127] L. F. Cabeza and M. Chàfer. "Technological Options and Strategies towards Zero Energy Buildings Contributing to Climate Change Mitigation: A Systematic Review". In: *Energy and Buildings* 219 (July 2020). ISSN: 0378-7788. DOI: 10.1016/j.enbuild.2020.110009.

[128] H. De Bruijn, R. Van Duin, M. A. J. Huijbregts, J. B. Guinee, M. Gorree, R. Heijungs, G. Huppes, R. Kleijn, A. De Koning, L. Van Oers, A. Wegener Sleeswijk, S. Suh, and H. A. Udo De Haes, eds. *Handbook on Life Cycle Assessment: Operational Guide to the ISO Standards*. Vol. 7. Eco-Efficiency in Industry and Science. Dordrecht: Springer Netherlands, 2002. ISBN: 978-0-306-48055-3. DOI: 10.1007/0-306-48055-7.

A. Digital Appendix

A.1. GitHub - Release

The developed program can be accessed via the permanent release link:

https://github.com/SESMG/SESMG/releases/tag/v1.0.1rc2

A.2. GitHub - SESMG - Branch

Additionally, the program currently runs in a separate branch of the SESMG. This link might not be permanently accessible, but includes the folder structure of the program as well as the different commits that might help in understanding code improvements:

https://github.com/SESMG/SESMG/tree/python311_integrateLCA

The following files for the reference case are also included in the GitHub repository:

- model_definition_reference_case.xlsx
- results_reference_case-folder (Figure A.1 shows which results might be interesting for a deeper understanding of the reference case)

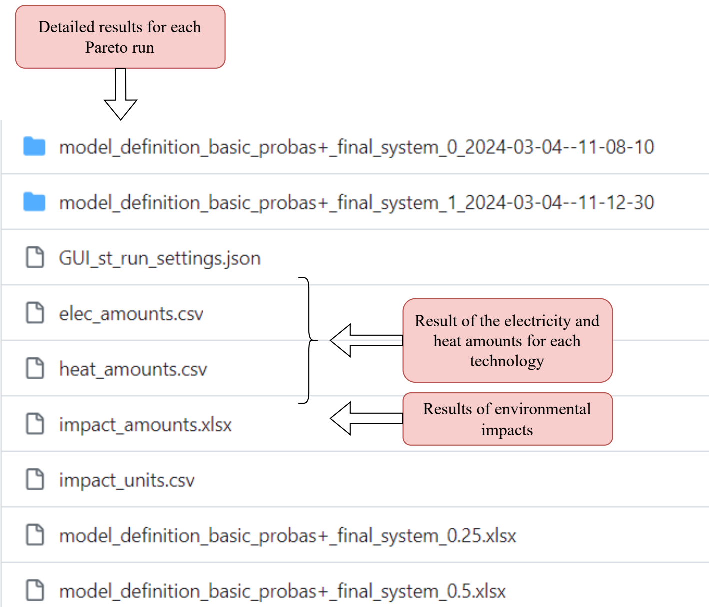


Figure A.1.: Files for a deeper analysis of results from the reference case.

In the future, the branch will be merged with the main branch of the SESMG for a permanent access:

https://github.com/SESMG/SESMG

B. Impact Categories of ReCiPe2008

Table B.1.: Impact categories of ReCiPe2008. For definitions of the terms in the columns see Table 2.2. Adapted from [65].

Impact category[a]	Description	Reference unit[b]	Category indicator	Validation ProBas
OD	anthropogenic substances, persisting in the atmosphere, escalate the rate of ozone destruction	kg CFC-11 eq	stratospheric ozone concentration	no[c]
HT	toxicity considers accumulation in the human food chain and toxicity of chemical substances	kg 1,4-DB eq	hazard-weighted dose	unsure
IR	releases of radioactive material to the environment	kg U235 eq	absorbed dose	no[d]
PMF	fine Particulate Matter with a diameter of less than 10 m causes health problems	kg PM10 eq	PM10 intake	yes
POF	ozone, formed as a result of photo-chemical reactions is a health hazard to humans	kg NMVOC	photo-chemical ozone concentration	yes
CC	alterations in temperature, and atmospheric conditions, primarily driven by human activities such as GHG emissions affect health and ecosystem	kg CO_2 eq	infra-red radiative forcing	yes
TA	deposition of inorganic substances, such as sulfates, nitrates, and phosphates, cause a change in acidity in the soil	kg SO_2 eq	base saturation	yes
TET	ecotoxicity considers the environmental persistence and the toxicity of chemical substances.	kg 1,4-DB eq	hazard-weighted concentration	unsure
ALO	occupation of a certain area of land during a certain time	m^2*a	occupation	no[e]
ULO	occupation of a certain area of land during a certain time	m^2*a	occupation	no[e]
NLT	transformation of a certain area of land	m^2	transformation	no[e]
MET	ecotoxicity considers the environmental persistence and the toxicity of chemical substances.	kg 1,4-DB eq	hazard-weighted concentration	unsure
FE	nutrient enrichment of the aquatic environment	kg P eq	phosphorus concentration	unsure
ME	nutrient enrichment of the aquatic environment	kg N eq	nitrogen concentration	unsure
FET	ecotoxicity considers the environmental persistence and the toxicity of chemical substances.	kg 1,4-DB eq	hazard-weighted concentration	unsure
MD	depletion of minerals or metals	kg Fe eq	grade decrease	unsure
WD	water shortage	m^3	amount of water	yes
FD	depletion of group of resources that contain hydrocarbons	kg oil eq	lower heating value	yes

[a] Abbreviations: OD = ozone depletion, HT = human toxicity, IR = ionizing radiation, PMF = particulate matter formation, POF = photochemical oxidant formation, CC = climate change, TA = terrestrial acidification, TET = terrestrial ecotoxicity, ALO = agricultural land occupation, ULO = urban land occupation, NLT = natural land transformation, FE = freshwater eutrophication, ME=marine eutrophication, FET = freshwater ecotoxicity, MD = metal depletion, , WD = water depletion, FD = fossil depletion.
[b] Abbreviations: CFC-11 = trichlorofluoromethane, DB = dichlorobenzene, U = uranium, PM = particulate matter, NMVOC = non-methane volatile organic compounds, P = phosphorus, Fe = iron.
[c] Only consideration of one flow in ProBas, substances to decrease ozone are phased out by the Montreal Protocol [126].
[d] No consideration of ion flows in ProBas.
[e] Only consideration in unit processes.

C. Comparison of Technologies in ProBas and Environmental Footprint (EF)

Table C.1.: Comparison of available energy technologies in the ProBas database and the EF database, based on technologies analyzed by Quest et al. [23] ("combined heat and power", "heat pipes" and "heat network" were excluded). The components "thermal storage system" and "solar thermal collector" were included because they represent important energy technologies for buildings contributing to climate change mitigation [127]. "Heat pumps" and "gas heating system" are used as examples for different kind of transformers. The ProBas examples not necessarily represent the selected datasets for this thesis (see Table 3.3).

Component	**Quest et al.**	**ProBas Example**	**EF Example**
electricity mix	electricity from Grid	"Netz-el-DE-Verteilung-NS-2030"	"Electricity grid mix 1kV-60kV technology mix consumption mix, to consumer 1kV - 60kV" (EF.3.1)
gas mix	natural gas mix	"Pipeline-Gas-DE-2030-mix"	"Natural gas mix technology mix consumption mix, to consumer medium pressure level ($<$ 1 bar)" (EF 3.1)
gas heating system	heat gas boiler	"Gas-Heizung-DE-2030" and many heating system datasets	multiple datasets for the boiler production (EF 3.1)
PV system	PV system with multiple datasets	"Solar-PV-multi-Rahmen-mit-Rack-DE-2030"	multiple datasets (EF 3.1 and EF 2.0)
battery storage system	battery storage system with more than 40 datasets	not existing	"Li-ion (1kWh), consumption mix, battery production, usage and end- of- life" (EF 2.0)
heat pumps	SWHP and GCHP with multiple datasets	"El-Wärmepumpe-mono-Erdreich-DE-2010-mix" and many heat pump datasets	"electric ground source heat pump (gshp) operation combined vertical and horizontal exchange loop production mix 1 MJ of thermal energy, 4 % losses" (EF 3.1)
thermal storage system	not considered in the case study	only in combination with solar thermal collector	different datasets depending on the type of the storage system
solar thermal collector	not considered in the case study	"SolarKollektor-Flach-DE-2030"	no information found
Categories covered		**6** (75 %)	**7** (88 %)

D. Comparison of Impact Assessment Methods for ProBas

Table D.1.: Assignment of flows of an energy system to the impact assessment methods. The energy system consists of: electricity mix, gas mix, gas heating transformer, PV system, GCHP. The calculations were performed using the older ProBas version, as ProBas+ academic license became available later. Flows according to the nomenclature of ProBas. Abbreviations: BL = baseline, EP = endpoint, MP = midpoint, CEM = Cumulative Energy Demand, EcSM = Ecological Scarcity Method.

Flows	CML (BL)	CML (non BL)	eco-indicator E	eco-indicator H	eco-indicator I	ReCiPe EP E	ReCiPe EP H	ReCiPe EP I	ReCiPe MP E	ReCiPe MP H	ReCiPe MP I	TRACI 2.1	ILCD EP	ILCD MP	CEM	EcSM
As (Abwasser)						1	1	1	1	1	1		1	1		
Biomasse-Anbau mit Heizwert															1	
Pb (Luft)						1	1	1	1	1	1		1	1		1
N2O	1	1	1	1	1	1	1	1	1	1	1		1	1		1
Wasser									1	1	1					
Atomkraft															1	
PAH (Luft)		1	1	1	1	1	1	1	1	1	1					1
PCDD/F (Luft)	1	1														
SO_2	1	1	1	1	1	1	1	1	1	1	1	1	1	1		1
Perfluoraethan	1	1	1	1	1	1	1	1	1	1	1		1	1		1
Ni (Luft)						1	1	1	1	1	1		1	1		
Erdgas mit Heizwert						1	1	1	1	1	1	1			1	
Wasserkraft															1	
Geothermie															1	1
Hg (Luft)						1	1	1	1	1	1		1	1		1
Cr (Luft)						1	1	1	1	1	1		1	1		
CO_2	1	1	1	1	1	1	1	1	1	1	1					
NMVOC	1	1	1	1	1	1	1	1	1	1	1		1	1		1
Steinkohle						1	1	1	1	1	1	1		1		
Hg (Abwasser)						1	1	1	1	1	1		1	1		1
Cd (Abwasser)						1	1	1	1	1	1		1	1		
CH4	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
Staub																
As (Luft)						1	1	1	1	1	1		1	1		
Erdöl mit Heizwert						1	1	1	1	1	1	1			1	
Braunkohle						1	1	1	1	1	1				1	
Erdgas (ProBas)						1	1	1	1	1	1	1			1	
Biomasse-Reststoffe mit Heizwert															1	
NOx	1	1	1	1	1	1	1	1	1	1	1	1	1	1		1
Cd (Luft)						1	1	1	1	1	1		1	1		1
H2S	1	1														1
HCl	1	1										1				1
Pb (Abwasser)						1	1	1	1	1	1		1	1		1
Cr (Abwasser)						1	1	1	1	1	1		1	1		
Perfluormethan	1	1	1	1	1	1	1	1	1	1	1		1	1		1
HF	1	1				1	1	1	1	1	1	1				1
NH3	1	1	1	1	1	1	1	1	1	1	1	1	1	1		1
CO	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
BSB5												1				
CSB												1				1
AOX																1
P	1					1	1	1	1	1	1	1				1
N	1								1	1	1	1				1
Assigned flows	16	15	11	11	11	29	29	29	31	31	31	15	20	20	11	21

E. ReCiPe2008 Adaptions

Table E.1.: Flows that could manually be assigned to the impact categories in ReCiPe2008 [65]. CML refers to the Center of Environmental Science, Leiden University, Netherlands. The CFs of this impact assessment method are documented in [128].

Manually assigned flows	Impact category	CF	Source
Schwefelwasserstoff Elementary flows/air/unspecified	terrestrial acidification	1.88	taken from CML
	human toxity	0.22	taken from CML
Dioxine und Furane unspezifisch Elementary flows/air/unspecified	freshwater ecotoxity	2.13E+06	taken from CML
	human toxity	1.93E+09	taken from CML
	marine ecotoxity	2.96E+08	taken from CML
	terrestrial ecotoxicity	1.20E+04	taken from CML
Chlorwasserstoff Elementary flows/air/unspecified	terrestrial acidification	8.80E-01	taken from CML
	human toxicity	5.00E-01	taken from CML
Fe-Schrott Elementary flows/ProBas elementary flows/resource	metal depletion	1	taken from ReCiPe, assumption: 100% iron
Eisen-Schrott Elementary flows/ProBas elementary flows/resource	metal depletion	1	taken from ReCiPe, assumption: 100% iron

F. Graphical User Interface (GUI)

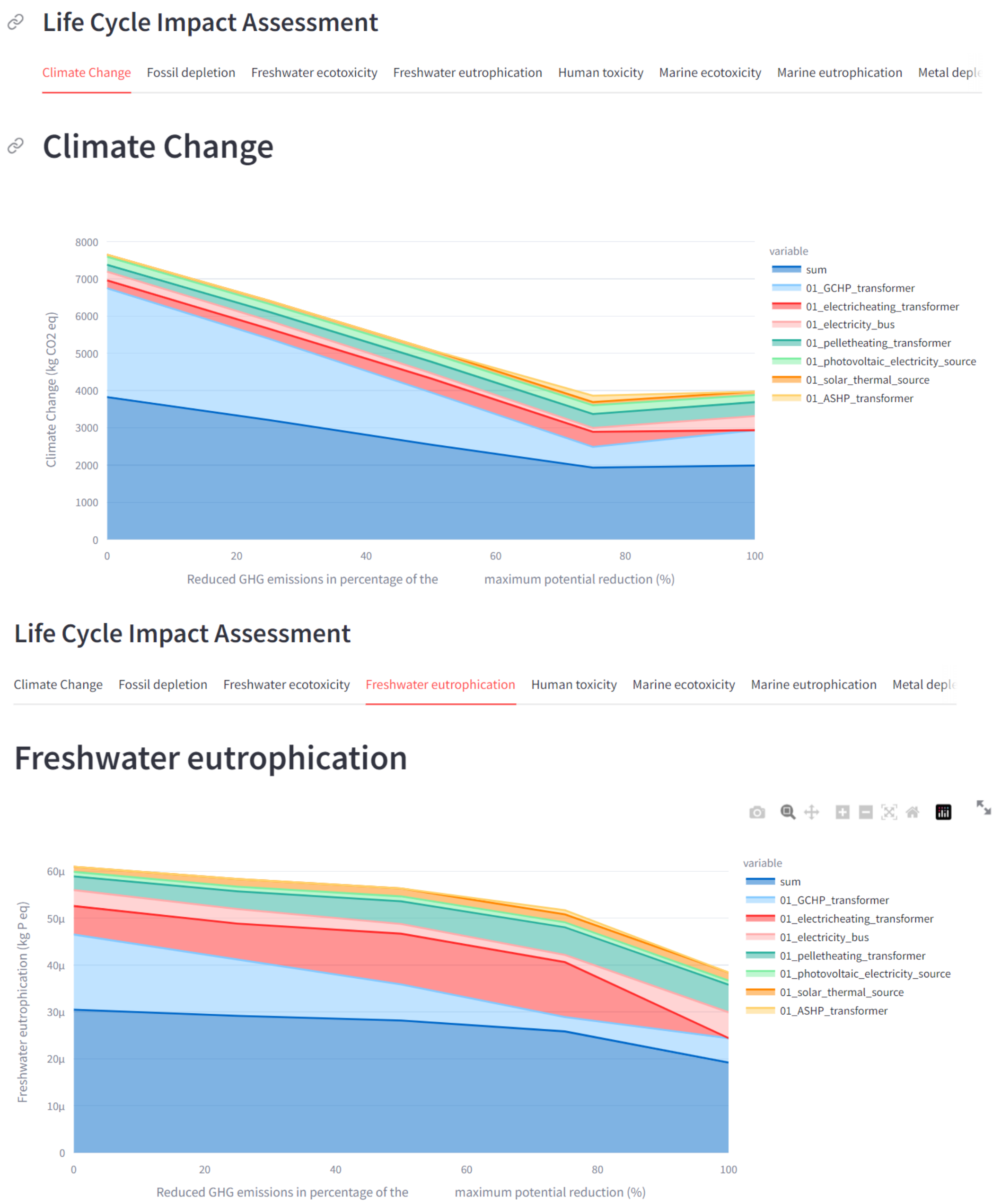
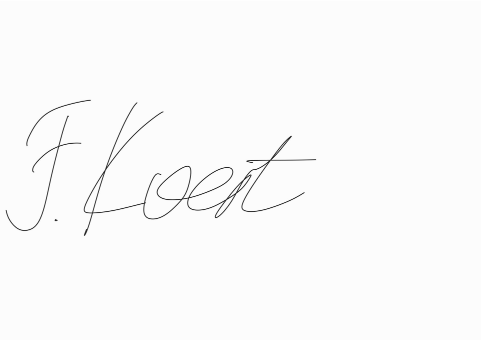


Figure F.1.: GUI implementation. Screenshots for the results of the reference case. Examples show the impact categories climate change and freshwater eutrophication.

Declaration on oath

I herewith declare that I have composed the present thesis myself and without use of any other than the cited sources and aids. Sentences or parts of sentences quoted literally are marked as such; other references with regard to the statement and scope are indicated by full details of the publications concerned.

The thesis in the same or similar form has not been submitted to any examination body and has not been published. This thesis was not yet, even in part, used in another examination or as a course performance.



Franziska Koert
Münster, March 7, 2024