



Master Thesis

**ERP-Control Domain:
Activity-Based Life Cycle-Accounting
Methodology applied to Injection Molding
Technology**

carried out for the purpose of obtaining the degree of

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English Abstract

Plastic production and disposal are responsible for around 3.3% of global greenhouse gas (GHG) emissions, making it a significant emitter in the production industry. For enterprises that must report their GHG emissions, the GHG Protocol requires them to measure emissions related to their produced products and based on the energy consumption. An important MIT study provides benchmarks for the energy consumption of the injection molding (IM) process, and other studies further refine these calculations with additional information. All of these studies use mathematical formulas to express the energy consumption calculations. The existing Enterprise Resource Planning (ERP) systems lack the functionalities to measure and report these emissions effectively, and the problem of integrating these calculations into an Enterprise Information System (EIS) remains unsolved, which is necessary to align the calculation metrics with the broader business system. The Activity-Based Life Cycle-Accounting (AB-LC-ACC) Methodology addresses this integration problem by specifying and implementing a calculation model that fits into the EIS. From the AB-LC-ACC methodology, the Activity-Based Costing provides the accounting fundamentals for the cost and GHG accounting, the Life-Cycle Assessment provides the impact measurement of the GHG emissions, and the Domain Engineering (DE) principles provide the framework for this specification and implementation. To conceptualize the model, the domain analysis step from DE is applied by specifying the domain and defining the terminology, including the language spoken in it. The 'ERP-Control' domain, which integrates the Enterprise Resource Planning (ERP) and the Production Planning and Control (Control) domains and is specified in the ECSI standardization, is used for this analysis. To enable the implementation of the conceptual model, the infrastructure specification step from DE is applied to operationalize this knowledge by adding the calculation metrics and parameter system to the conceptual ERP-Control model, which is extended with the necessary attributes and functionalities. Finally, to implement this operationalized ERP-Control model in the infrastructure implementation step, a data science-capable programming language is used to code it into the information system. The GHG accounting model that is developed with the AB-LC-ACC Methodology is demonstrated with a prototypical implementation of a plastic bowl production with the injection molding technology.

Keywords: AB-GHG Accounting, AB-LC-ACC Methodology, Carbon Footprint, ECSI Standardization, ERP-Control Domain, GHG Emission, GHG Protocol, Injection Molding

Deutsche Kurzfassung

Die Herstellung und Entsorgung von Kunststoff verursacht etwa 3,3 % der globalen GHG (Greenhouse Gas)-Emissionen und ist somit ein bedeutender Verursacher innerhalb der Produktionsbranche. Unternehmen müssen die GHG-Emission ihrer Produkte basierend auf ihrem Energieverbrauch (EV) messen und berichten. Eine wichtige MIT-Studie liefert Referenzwerte zum Energieverbrauch des Spritzgussverfahrens, und weitere Studien verfeinern diese Berechnungen mithilfe zusätzlicher Informationen. Alle diese Untersuchungen verwenden mathematische Formeln, um die Berechnungen zum EV zu beschreiben. Die bestehenden ERP (Enterprise Resource Planning) Systeme bieten bislang nicht die notwendigen Funktionen, um diese Emissionen effektiv zu messen und zu berichten. Hinzu kommt die ungelöste Frage, wie sich diese Berechnungen in ein Enterprise Information System (EIS) integrieren lassen, um die Berechnungskennzahlen in das übergeordnete Geschäftssystem einzubetten. Die Activity-Based Life Cycle-Accounting (AB-LC-ACC) Methodologie adressiert dieses Integrationsproblem, indem sie ein Berechnungsmodell spezifiziert und implementiert, das in das EIS passt. Dabei liefern die Prinzipien des Activity-Based Costing (ABC) die Grundlagen für Kosten- und GHG-Accounting, während die Life-Cycle Assessment (LCA) Methodik die Messung der GHG-Auswirkungen ermöglicht und die Domain Engineering (DE) Prinzipien den Rahmen für Spezifikation und Implementation bereitstellen. Um das Modell zu konzeptualisieren, wird der Domain Analysis-Schritt aus dem DE angewendet, indem die Domäne spezifiziert und die Terminologie – einschließlich der in ihr verwendeten Sprache – definiert wird. Für diese Analyse dient die „ERP-Control“-Domäne, welche das Enterprise Resource Planning (ERP) und die Production Planning and Control (Control)-Domänen integriert und in der ECSI Standardization spezifiziert ist. Um die Implementation des konzeptuellen Modells zu ermöglichen, wird der Infrastructure Specification-Schritt aus dem DE angewendet, um dieses Wissen zu operationalisieren – indem die Berechnungsmetriken und das Parametersystem zum konzeptuellen ERP-Control Modell hinzugefügt werden, das um die notwendigen Attribute und Funktionalitäten erweitert wurde. Schließlich wird, um dieses operationalisierte ERP-Control Modell im Infrastructure Implementation-Schritt umzusetzen, eine data science-fähige Programmiersprache verwendet, um es in das Informationssystem zu codieren. Das mit der AB-LC-ACC Methodology entwickelte GHG Accounting-Modell wird anhand einer prototypischen Implementation einer Kunststoffschlüsselproduktion mittels Spritzgusstechnologie demonstriert.

Schlagwörter: AB-GHG Accounting, AB-LC-ACC Methodology, Carbon Footprint, ECSI Standardization, ERP-Control Domain, GHG Emission, GHG Protocol, Spritzgussverfahren

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Abbreviations

3-LoEC	<i>3-Levers of Emission Control</i>
AB-LC-ACC	<i>Activity-Based Life Cycle-Accounting</i>
ABC	<i>Activity-Based Costing</i>
CFP	<i>Carbon Footprint</i>
DDD	<i>Domain-Driven Design</i>
DE	<i>Domain Engineering</i>
EC	<i>Energy Consumption</i>
EIS	<i>Enterprise Information System</i>
ELiab	<i>Emission Liability</i>
ERP	<i>Enterprise Resource Planning</i>
ESRS	<i>European Sustainability Reporting Standards</i>
EmCo	<i>Emission Coefficient</i>
FG	<i>Finished Good</i>
FG-uCFP	<i>Product's Unit-Carbon Footprint</i>
GHG	<i>Greenhouse Gas</i>
IM	<i>Injection Molding</i>
IMT	<i>Injection Molding Technology</i>
LCA	<i>Life Cycle Assessment</i>
PLA	<i>Polylactic Acid</i>
PP	<i>Polypropylene</i>
PowCo	<i>Power Coefficient</i>
ProCo	<i>Production Coefficient</i>
TD-ABC	<i>Time-Driven Activity-Based Costing</i>
UoM	<i>Unit of Measurement</i>
uCFP	<i>Unit-Carbon Footprint</i>

1. Introduction

Background

It was already recognized at the end of the last century that the natural resources and environmental media (supplies of air or water) are not infinite, and they should be used more effectively and efficiently and equitably among the world's population; if not, an environmental crisis is imminent due to the increasing global human population (Schaltegger & Burritt, 2000). Fossil fuel combustion related to human activities increased emissions of Greenhouse Gases (GHGs) by 50% over the last 30 years; the energy and heat production sectors accounted for 34%, and industries for 24% of global GHG emissions in 2019 (IPCC, 2022). The plastic production industry is also a significant emitter within the industry. The plastic production industry is also a significant emitter within the industry. The plastic production industry is a relevant contributor to the industry emissions. Out of the global GHG emissions in 2019, the OECD reported 3.3% of emissions, which translates to 14% of the industry's global GHG emissions (Ritchie & Roser, 2023). The plastic production industry, as per Ribeiro et al. (2012), is one of the most widely used processes in plastic injection molding (IM), which enables the rapid and efficient production of large quantities. These parts are used by many industries, such as aerospace, automotive, consumer, and medical products.

The GHG emissions are attributed to the energy requirements of the particular industry sectors, and hence, in order to reduce these emissions, first, the energy consumption (EC) of these sectors should be reduced. The International Energy Agency indicated that in 2024 the industrial sector used 37% of the global energy, and 65% of this energy use was fossil fuels (IEA, 2024). Globally, the energy saving is becoming more and more significant because the reduction of energy used can have a positive impact on the current environmental issues, and in addition, it can lower the costs of the finished products. Plastic IM is quite a clean process and, therefore, not very energy-intensive; however, when it is produced on an industrial scale all over the world. Even a small drop in energy use can save a lot of power (Cardeal, 2016) and indirectly lower the GHG emissions of certain industries.

The first step toward EC and GHG reduction is their measurement and reporting. In recent years, countries have implied stricter corporate sustainability rules to conform with their national sustainable development goals and with the global sustainability standards (R. He et al., 2021). For enterprises that have to report their GHG emissions, the internationally

accepted GHG Protocol provides accounting and reporting standards and tools to help them achieve a low-emission economy (GHG Protocol, 2011). These standards are essential for the implementation of more sustainable manufacturing practices (Komoto et al., 2020).

Problem Statement

According to Hazaea et al. (2023), the transition toward a green economy from the traditional economy is one of the most important challenges for organizations, and this transition requires high-quality administrative work. The new regulations about the GHG emission measurement and reporting put a high demand on the GHG accounting for the organizations, especially the plastic manufacturing industry, which has a high contribution to the global GHG emissions. The existing information management systems are effective for the traditional management and accounting tasks, but they lack the functionalities for proper GHG emission accounting in complex environments like the IM technology in the plastic production industry. The actual sustainability performance assessment of the product's life cycle is predominantly based on the weight of the product, without considering other manufacturing factors (Madan et al., 2015). An exemplary case is an MIT study about the EC of the injection molding technology (IMT) on an industry level by Thiriez & Gutowski (2006), which will be discussed subsequently.

There are limited studies that investigated the GHG accounting from an economic and financial perspective, and this provides an area for future studies, which should expand the use of theories related to carbon accounting to get better results and understanding of the accounting role in GHG emission reduction (Hazaea et al., 2023). For the sustainability-relevant but less researched area is the integration of sustainability assessment into the existing systems, according to Maas et al. (2016, p. 237): “(...) *how companies can and do integrate sustainability assessment, management accounting, management control, and reporting?*” The existing research in this area dealt with specific methods in mostly an isolated manner, but “(...) *only a few papers investigate the integration and interplay of accounting, management control, and reporting approaches*” (Maas et al., 2016, p. 238).

For that very reason, the aim of this master's thesis is the specification—including the conceptual and operational design—and implementation of an Activity-based GHG Accounting model, which extends the existing ERP systems with sustainability assessment. The Activity-Based Life-Cycle Accounting methodology is applied to design the GHG Accounting model for the plastic industry when the production process involves multiple

activities and equipment, like in the IMT. To address this aim, the following research questions (RQs) are formulated to guide the development and implementation of the Activity-based GHG Accounting model:

RQ1: How can the modelling language for the AB-LC-ACC methodology be specified, and how can the IM-specific domain knowledge be modelled with this language on a conceptual level?

RQ2: How can the mathematical model of the IM domain be translated into an operational model that is aligned with the conceptual language?

RQ3: How can the operational model defined by the AB-LC-ACC methodology be implemented using a data science-capable programming language?

Research Objectives

To realize the aim of this thesis, a primary research objective is defined, which is the specification and implementation of the proposed Activity-based GHG Accounting model by setting up a digital system that extends the existing Enterprise Resource Planning (ERP) system with a sustainability assessment in the form of GHG Accounting. The ‘Activity-Based Life-Cycle Accounting (AB-LC-ACC) methodology’ (Alaoui & Schwaiger, 2024) provides the framework for the development and implementation of the model. It is based on the principles of ‘Domain Engineering’ (DE) (Arango, 1989), which defines the process via three steps, i.e., 1) domain analysis, 2) infrastructure specification, and 3) infrastructure implementation. The actual steps after applying this methodology to the GHG Accounting model development are as follows: 1) the application domain is analyzed, and the terminology is defined in order to create the conceptual model of the GHG Accounting Model, 2) the conceptualized model is operationalized by defining the calculation metric and extending the model with all the information, which is relevant for the implementation, 3) the operationalized model is implemented by coding the GHG Accounting Model, including the functionalities in a data science-capable programming language.

In order to develop a comprehensive GHG Accounting model, the system boundary, which is the scope of the GHG emission assessment object, has to be defined. For this thesis, the system boundary is the ‘cradle-to-gate,’ which covers all the activities from the raw material extraction until the end of the production of the Finished Good (FG), including the transportation of the material and the secondary activities of the production, like the heating of the production facility.

Significance of the Study

For long-term survival, both economic and environmental stability are required. Schaltegger & Burritt (2000, p. 371) aptly expressed this idea: *“It is a dictum for most businesses that short-run and long-run survival depend on income and cash flow; it is equally as simple and important for business management to recognize that without the environment and without ecological biodiversity there is no society, without society there is no economy and without an economy there is no opportunity for win–win business situations.”*

Since this statement was made in 2000, environmental awareness has grown significantly among different stakeholders, including legislators, academics, and customers (Hazaea et al., 2023). Furthermore, the continually increasing energy costs and the growing need to comply with the environmental regulations and standards imposed significant economic and environmental pressures on manufacturing industries (B. He et al., 2023). Saving energy is, however, an issue of much concern, as the industrial sector consumes a lot of energy, and reducing the EC can help in lowering the costs and also play a part in mitigating climate change (Cardeal, 2016).

In order to remain globally competitive, improved production systems and reduced environmental impact are needed for the manufacturers, which they can achieve by switching from experience-based manufacturing practices to science-based modeling, decision-making, and production (Mani et al., 2014). According to M. Tang & Ge (2018), the primary contributor to the increase in carbon emissions is the manufacturing of goods and services. GHG accounting is beneficial because it provides a mechanism to measure and quantify the GHG emissions, so the organizations will know their status (Hazaea et al., 2023). GHG Accounting and disclosure are important, because recently they became one of the important factor influencing the strategic decisions of the organisations (Alsaifi et al., 2020). Among the many GHG reporting ways, the most significant are the annual corporate reports and sustainability reports (R. He et al., 2021).

GHG Accounting offers multiple practical benefits; it can lead to a competitive advantage with the legislative requirements, which can foster enhanced sustainability practices. It can also enhance the information collection and dissemination as well as provide an overview of the current status and performance of the companies. Furthermore, it positively influences the financial performance of the companies and can result in possible cost reductions (Hazaea et al., 2023).

Structure

The structure of this paper is as follows. The next chapter gives a theoretical overview of the topics that are discussed in this master's thesis. It includes the Activity-Based GHG Accounting as the calculation foundation, the AB-LC-ACC methodology as the methodological framework for the model development, and the IMT as the application field of the developed model. The next chapter presents the conceptual design of the model, including the understanding of the domain knowledge, the discussion of the modeling language, and the creation of the conceptual domain model as a merge of the previous sections. The following chapter discusses the operational design of the model by defining the mathematical modeling language and subsequently developing the operational domain model to extend the conceptual model with relevant information for the implementation. At the end of this chapter, the calculation parameters and their relationships are specified, and the corresponding functions are created. Next, the prototypical implementation of the model with a use case is demonstrated, where the implementation steps for the production of two specific plastic bowls are explained, and the results of this use case are discussed. Lastly, the paper is concluded with a brief outlook.

2. Theoretical overview

The following chapter provides a comprehensive overview of the key concepts applied in the master's thesis. These concepts are important to have a solid theoretical foundation on which the model can be specified and implemented. Figure 1 illustrates these concepts and their interrelationships. Starting with the core concept of the GHG Accounting model, the accounting in the form of the 'Activity-Based Costing' (*ABC*)—to have a precise cost allocation—is one of the cornerstones of the model. It is extended with the other core concept of the sustainability assessment in the form of the GHG emission assessment (*GHG*)—to evaluate the environmental aspects and potential impacts of the product, process, or service. The combination of these concepts results in the *Activity-Based GHG Accounting*, which enables the sustainability impact assessment on the accounting fundamentals.

In order to do the GHG accounting in a structured manner and enable the integration into the information system of the organizations, specifically the ERP system of plastic manufacturers, the *AB-GHG Accounting* is extended with the *Domain Engineering* principles and the *ERP-Control Domain*; this combination is called the *AB-LC-ACC methodology* (Alaoui & Schwaiger, 2024). In order to specify and implement the model precisely, the *ERP-Control Domain* is needed, which provides the domain knowledge for the precise specification and implementation of the model for the plastic manufacturing industry.

The following sections explain the building elements of the *AB-LC-ACC* model, in the first instance the *ABC*, then the *AB-GHG Accounting*, next the *DE* principles, then the *ERP-Control Domain* and finally, *IMT* is explained in detail.

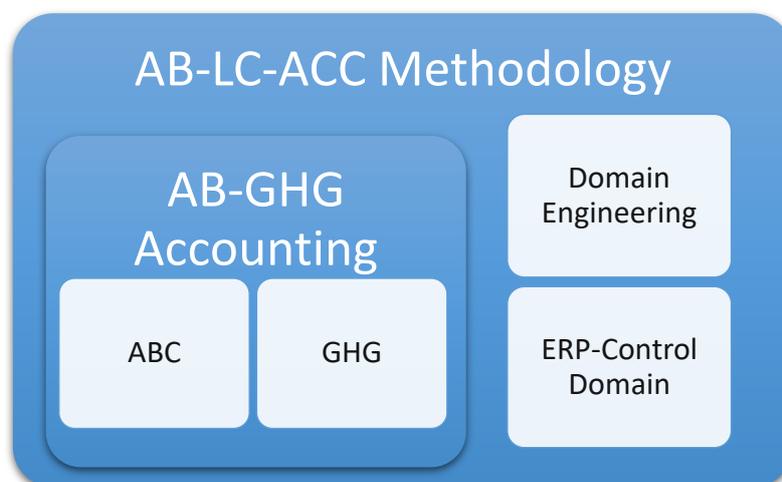


Figure 1 Schematic Overview of key concepts and their interrelationships in the Activity-Based Life-Cycle Accounting Methodology (own figure)

2.1 Activity-Based GHG Accounting

Activity-Based Cost Accounting

The traditional costing model was developed before the 1980s for mass production of some standardized products and was not adequate for manufacturing environments of the 1980s (Kaplan, 1984). Because of conventional costing systems, such as the inaccurate allocation of the overhead costs, there is a need for a new costing system, called ABC in advanced manufacturing, in order to provide more accurate and useful information for decision-making and planning. ABC is an alternative to the conventional costing systems. It was designed by Harvard Business School professors R. Cooper and R. Kaplan in the United States (Cooper & Kaplan, 1991). The new costing approach was necessary because traditional cost accounting could no longer fully meet existing needs.

ABC analyzes in greater depth the activities required to produce a product and the proportional resources spent. The ABC suggests a consumption-dependent approach for allocating overhead expenses based on consumption levels, and it generates a more precise analysis of the consumed costs within an organization. In the first step, resources are assigned to activities using resource drivers (e.g., time, kWh), and in the second step, activities are assigned to products using activity drivers (e.g., number of repetitions, number of spare parts) (Everaert et al., 2008). The system's goal is to utilize and analyze all information with the objective of eliminating excess costs from the value chain (Hooshang, 2004).

An additional benefit of the ABC is the dual view of costs from process and product perspectives (Turney, 1991). It can be utilized to determine product costs and to optimize the processes (Emblemsvåg & Bras, 2001). Besides the benefits, ABC had some challenges, and in time many companies abandoned ABC because it did not capture the complexity of actual operations in complex and dynamic environments, the implementation took too long, and it was too expensive to maintain. To solve these problems, Kaplan & Anderson (2004) introduced the concept of 'Time-Driven Activity-Based Costing' (TD-ABC). It is the simplification of the original ABC methodology; it uses solely time as a resource driver, and it offers the ability to identify complex transactions in a simple way using time equations (Bruggeman et al., 2005). TD-ABC simplifies the costing process by eliminating the time-consuming interview and survey processes for employees to assign resource costs to activities (Kaplan & Anderson, 2007). Based on literature studies from 56 journals, TD-ABC has been applied in three different areas. Healthcare accounts for 66%, followed by industry with 23% and libraries with 11% (Areena & Abu, 2019).

AB-GHG Accounting: Standards

The United Nations Framework Convention on Climate Change (UNFCCC) took the first step towards GHG emission reduction in 1994, setting the objective to “*stabilize greenhouse gas concentrations in the atmosphere at a level that would prevent dangerous anthropogenic interference with the climate system*” (United Nations, 1992). The Kyoto Protocol extended the UNFCCC in 1997 by establishing binding objectives for GHG emissions for Annex I Parties, which include industrialized nations and economies in transition listed in Annex I of the Kyoto Protocol (United Nations, 1997). It entered into force in 2005 and introduced the concept of Emission Trading, allowing nations to trade emission credits among themselves (United Nations, 1997).

The GHG Protocol, a collaboration between the World Resources Institute (WRI) and the World Business Council for Sustainable Development (WBCSD), established standardized emission reporting in the late 1990s (GHG Protocol, 2004). The *Corporate Standard*, released in 2001 and revised in 2004, defines Scope 1, Scope 2, and Scope 3 emissions (GHG Protocol, 2004). The *Product Life Cycle Accounting and Reporting Standard* (GHG Protocol, 2011) proposes the methodology for calculating the product Carbon Footprint (CFP) GHG inventory of particular products.

In the European Union, the *Non-Financial Reporting Directive* established the legislative basis for obligatory sustainability reporting for enterprises (European Commission, 2013). As the successor of the *Non-Financial Reporting Directive*, the *Corporate Sustainability Reporting Directive (CSRD)*, introduced in 2022, aims to improve transparency in corporate sustainability practices. Corporates classified as ‘public interest’ have to measure their GHG emissions, report on actual emissions, report on aimed reductions, and monitor the accomplishment of the reduction goals over time. It requires approximately 50,000 European companies to apply these new reporting standards from the financial year 2024 onward for reports issued in 2025 (European Commission, 2021).

The *European Sustainability Reporting Standards (ESRS)* are a group of separate rules that cover governance, social issues, and the environment. These rules come in the form of ‘topical standards’ and ‘cross-cutting’ reporting requirements. Addressing climate change – known as the ‘climate-first’ doctrine – has become the priority in politics. Consequently, the

standard ESRS-E1 ‘on climate change’ (ESRS-E1-Draft, 2023) is the most prominent reporting standard. For measurement and reporting of the GHG emissions, the ESRS-E1 standard refers to the methodology proposed in the established *GHG Protocol* (GHG Protocol, 2004), and for product-specific measurements of GHG emissions, it refers to the *GHG Protocol’s Product Standard* (GHG Protocol, 2011).

The majority of enterprises that perform GHG reporting rely on the *GHG Protocol* (Kaplan & Ramanna, 2021), and in 2023, 97% of disclosing *S&P 500* companies (the biggest 500 companies in the USA) reported their GHG emissions using the *GHG Protocol* (GHG Protocol, n.d.). It is not required by the *GHG Protocol* to fully report all of the emissions; the minimum requirement is that emissions for *Scope 1* and *2* are reported, thereby granting flexibility on *Scope 3* (GHG Protocol, 2004). This flexibility in the reporting is critical, as it introduces variability in the data types used and distinguishes between different uncertainties. Regarding the data types, primary and secondary data are distinguished in the *GHG Protocol*; primary data is considered supplier-specific data with higher quality, while the secondary data is described as industry-average with lower quality, which leads to lower uncertainties in the accounting and reporting process (GHG Protocol, 2011).

Regarding the uncertainties, three different types are defined: (1) Parameter, (2) Scenario and (3) Model uncertainty. (1) “*Parameter uncertainty is the uncertainty regarding whether a value used in the inventory accurately represents the process or activity in the product’s life cycle.*” (GHG Protocol, 2011, p. 80), this can be derived from the used activity or emission factor data. (2) “*(...) scenario uncertainty refers to variation in results due to methodological choices.*” (GHG Protocol, 2011, p. 81), it refers to the different assumptions made about the product life. (3) “*Model uncertainty arises from limitations in the ability of the modeling approaches used to reflect the real world.*” (GHG Protocol, 2011, p. 82), some inaccuracies always arise by simplifying the real world to numerical models.

The aim of the *GHG Protocol* is to capture a wide scope of emissions to achieve absolute precision in the data; thus, it allows exclusion based on significance when insufficient data is available, and it does not require the inclusion of non-attributable processes, but it encourages their inclusion when they are relevant (GHG Protocol, 2011). Using the *GHG Protocol* for GHG emission reporting has many benefits; according to Olausson (2020), it works well for internal purposes, when the aim is to increase the knowledge about one's own GHG emissions

or to compare one's emissions with previous years, while for external purposes, some challenges can arise when presenting the GHG emissions or comparing the emission results with other companies. However, alternative frameworks for GHG reporting exist, like the *ISO 14000* series or the *PAS 2050*, which is issued by the British Standards Institution, and they can offer other additional tools and perspectives for companies seeking to improve their GHG reporting practices.

AB-GHG Accounting: Process

According to Schaltegger & Burritt (2000), for most companies, accounting serves as the central information management system, which sources the information and forms the basis for integrated planning. This integrated planning is essential for an effective and efficient control-based environmental management system. In order to establish this environmental management system and improve the eco-efficiency of the companies, an explicit integration of economic information from traditional accounting with environmental information derived from ecological accounting is necessary. Internal stakeholders are interested in specific ecological values, while external stakeholders primarily focus on overall corporate performance. Consequently, for internal actors, mostly specific data and indicators are relevant, while the external accounting and reporting focus mostly on general and aggregated data and indicators. General indicators reflect the overall performance of a company, while specific indicators provide detailed information about processes, products, or operation sites (Schaltegger & Burritt, 2000). This master's thesis deals with economic (unit-time) and ecologic (EC, unit-Carbon Footprint (uCFP)) indicators, and the focus lies on the specific indicator of uCFP at the product level, which later can be aggregated to a general indicator at the company level.

To effectively calculate the uCFP of a specific object, carbon accounting can be applied, which is a system that employs accounting procedures and methodologies to document, collect, and analyze climate change data, validate information, and report on the fundamental elements of assets, liabilities, expenses, and revenues that are interconnected (Q. Tang, 2017). Carbon accounting is an integral part of sustainability accounting (Nartey, 2018), and it is an emerging field, which attracts researchers to examine the topic from its various aspects, especially its connection to the environmental changes (Le Breton & Aggeri, 2018). The researchers can show the importance of carbon accounting by stating facts and statistics, but the actual work to reduce the GHG emissions is dependent on political and societal decisions (Knutti & Rogelj, 2015). It is proven by the fact that the GHG accounting practices originated

from regulations and protocols in many countries, including Australia, China, and the European Union countries (Hazaea et al., 2023).

One of these GHG accounting practices is the Life Cycle Assessment (LCA), which is “*a process of evaluating the effects that a product has on the environment over the entire period of its life, thereby increasing resource-use efficiency and decreasing liabilities. It can be used to study the environmental impact of either a product or the function the product is designed to perform.*” (European Environmental Agency, 2025). Industries employ LCA to assess the sustainability performance of a product’s life cycle; they are predominantly based on the weight of the product (Madan et al., 2015). This approach is relatively simple, as it provides only a single and generic parameter for the estimation of the CFP (Matarrese et al., 2017). To improve the quality of the sustainability assessment and the GHG accounting, a more detailed method that considers multiple parameters is necessary.

To overcome this limitation and achieve a more precise and comprehensive assessment of environmental impacts, employing ABC methods for GHG accounting offers significant benefits. The *GHG Protocol* emphasizes the usage of activity data as a foundation for emission reporting practices (GHG Protocol, 2004). Kaplan & Ramanna (2021) highlighted the benefits of integrating the ABC methods as a fundamental principle for GHG accounting in their renowned work ‘Accounting for Climate Change’.

The beneficial connection between activity-based cost accounting and environmental accounting was initially shown by Stuart et al. (1998), who compared the traditional volume-based method with the activity-based method for waste allocation. This was further developed by Emblemsvåg & Bras (2001), by highlighting the ABC framework, which can cover other resource consumption alongside the financial aspects, like EC and waste management. This integration streamlines accounting procedures and improves financial accounting competence.

Emblemsvåg and Bras, along with Stuart et al., emphasize an intraorganizational perspective, while several publications use an interorganizational perspective, considering sustainability aspects for the whole life cycle and for the complete value chain. This approach has different names, like green activity-based management, Activity-based Life Cycle Costing or Activity-based Life Cycle Assessment:

- Kayrbekova et al. (2011) presents a methodology for activity-based life cycle costing that could be used for the planning of manufacturing facilities, calculating costs associated with environmental factors within the life cycle.
- Yang (2018) quantifies the carbon footprint of green energy supply and offers a tool for analyzing the carbon footprint per kilowatt-hour supplied. The EC life cycle has four phases: pre-construction, construction, operating, and decommissioning phases.
- Durán & Afonso (2020) present ‘Activity-based Life Cycle Costing’ for the management of spare component logistics, focusing on non-repairable spare parts. This method improved logistics cost allocation due to the activity-based approach, and it is further refined as ‘Time-Driven Activity-Based Life-Cycle Costing’ for maintenance (Durán et al., 2020). The revised model streamlines calculations by prioritizing time as the primary resource driver, consistent with Kaplan & Anderson (2004).
- Jourdain et al. (2021) present a comprehensive methodology for activity-life cycle costing and LCA, streamlining LCA criteria and assigning activities to products. They offer comprehensive guidance and present a case study for the integration of ABC-LCA.

According to Schaltegger & Burritt (2000), three practical issues have to be addressed about the conversion of existing accounting and reporting systems to environmental accounting:

- (1) Evaluation of the existing accounting and reporting system needs to be conducted.
- (2) Support must be provided to the operators and users of existing accounting and reporting systems during the transition to an updated framework of environmental accounting and reporting.
- (3) The existing accounting and reporting system must be redesigned and later implemented.

The *GHG Protocol* defines in total three different scopes for the emissions: *Scope 1*, which are the direct GHG emissions resulting from the combustion of oil, gas, and other fossil fuels within the organizational boundaries; *Scope 2*, which are the GHG emissions related to the consumed electric energy by the organization (GHG Protocol, 2004). The last one is *Scope 3*, which are the indirect GHG emissions originating outside the organizational boundaries, either as downstream within the value chain or as upstream due to business activities, and they can be divided into 15 distinct categories (GHG Protocol, 2011).

Kaplan & Ramanna (2021) introduce the ‘Environmental-Liability’ concept, which suggests that every transaction between a supplier and its customers should incorporate a carbon balance referred to as an E-liability. This E-liability represents the emissions emitted into the product up to that point. When the customer uses inputs from suppliers to generate product outputs, it assigns its own direct net emissions and the emissions embedded in those inputs to its products. This allows E-liabilities to accumulate along the supply chain and accumulate in a final carbon footprint handed over to the end consumer. Therefore, the reporting organization must track only the carbon emissions of their direct suppliers regardless of the suppliers field of activity. Thereafter, the reporting organization integrates its direct emissions with the supply chain emissions to allocate the total E-Liabilities to its customers.

According to Emblemståg & Bras (2001), an activity-based emission measurement helps not only to identify the relevant levers to reduce the overall emissions but also supports the integration of the financial and non-financial information. Additionally, this activity-based emission accounting approach can contribute to the improvement of the environmental performance of the reporting organization (Baumüller & Schwaiger, 2023; Emblemståg & Bras, 2001; Kaplan & Ramanna, 2021).

2.2 Activity-Based Life Cycle-Accounting (AB-LC-ACC) Methodology

Domain Engineering (DE)

For a smooth integration of the AB-GHG Accounting into the ERP systems of the manufacturing companies, a methodology is required that defines the integration process and principles. This methodology, known as DE (Arango, 1989), defines the process in three steps:

- 1) domain analysis,
- 2) infrastructure specification and
- 3) infrastructure implementation.

According to Arango (1989), in the 1) ‘domain analysis’ step, the reusable information of the problem domain has to be identified, acquired, and evolved for the software specification and construction. In the 2) ‘infrastructure specification’ step, the reusable information has to be selected and organized in order to fit the reuse patterns of the environment, and the architecture for reusable information has to be created. In the 3) ‘infrastructure implementation’ step, the results of the specification process have to be designed and encoded using specific representations required by the technology of the reusers.

Additional academic works extended the DE knowledge; Falbo et al. (2002) provide guidelines for transitioning from ontologies to object-oriented infrastructure definition. They propose a systematic approach that contains directives, design patterns, and transformation rules. Benevides & Guizzardi (2009) introduce 'OntoUML,' a model-based tool for conceptual modeling and domain ontology engineering, which extends the traditional Unified Modeling Language (UML) by incorporating metaphysical attributes. Henderson-Sellers & Gonzalez-Perez (2013) study the mathematical foundations of ontologies and modeling languages within the context of DE methodology. Their main focus is on the necessity to understand the fundamentals of the models, meta-models, ontologies, and modeling languages and how they work together. DE methodology is a holistic approach of combining domain and IT expertise. This approach is crucial in the ‘Domain Driven Design (DDD)’ methodology of Evans (2004) that deploys iterative refinement of the domain model to enhance software system alignment. Additionally, terminology and responsibilities have to be drawn from the model, and for the implementation, software development tools have to be used that are consistent with the modeling paradigm, such as object-oriented programming.

AB-LC-ACC Methodology

The application of the DE methodology to AB-GHG Accounting facilitates the development of the ‘Activity-Based Life Cycle Accounting (AB-LC-ACC) Methodology’. This methodology originates from the ‘3-Levers of Emission Control (3-LoEC) model’ (Baumüller & Schwaiger, 2023) and its associated modeling framework (Alaoui et al., 2024). It is founded on the general activity-based emission measurement logic, and it is built upon three constituting coefficients, i.e., the production (ProCo), the power (PowCo), and the emission coefficient (EmCo). These coefficients serve as 'decarbonization levers' for controlling the GHG emissions of the activity, and this is the origin of the model’s name. The 3-LoEC model is compliant with the GHG reporting requirements established by the *CSRD/ESRS-E1* regulation. The compliance is assured (Baumüller & Schwaiger, 2023) as they fulfill the requirements from the *GHG Protocol’s Corporate Standard* and *Product Standard* as well as the disclosure requirements from the *ESRS-E1* on Climate Change concerning the specification of emission control levers and the measurement of EC in the Unit of Measurement (UoM) of kWh.

The 3-LoEC modeling framework has been renamed the AB-LC-ACC methodology, providing an alternative to the ISO-LCA methodology (Alaoui & Schwaiger, 2024). This AB-LC-ACC methodology relates to the AB-GHG accounting systems and encompasses three fundamental characteristics of such accounting systems (Alaoui & Schwaiger, 2024, p. 264), namely:

- *“Alignment of the GHG accounting metrics’ computational logic with the 1-stage activity-based (AB) standard cost accounting methodology, where all activities are considered in relation to their inputs and outputs of resources.*
- *Application of the computational metrics to the life-cycle (LC) accounting of GHG emission impacts—according to the GHG Protocol’s requirements—from enterprise internal activities in the form of Scope 1 and 2 emissions and enterprise external (i.e., value-chain upstream and downstream) activities in the form of Scope 3 emissions.*
- *Integration of the computational logic and information into an enterprise information system (EIS) for establishing an integrated cost and GHG accounting system.”*

The DE, along with the AB-LC-ACC methodology, covers the whole spectrum from domain analysis to the infrastructure implementation, providing a holistic meta-perspective that combines the domain expertise with the IT expertise (Alaoui & Schwaiger, 2024). To express

this holistic meta-perspective, the authors referred to John Godfrey Saxe’s philosophical metaphor ‘The Blind Men and the Elephant’¹ in Figure 2. This metaphor well illustrates the need for a holistic view, from which the whole process can be seen, and by combining the different observations of the blind men, at the end the participants can see the elephant. By applying it to the AB-LC-ACC methodology, the DE Process can provide this holistic view that helps the participants of the different steps—conceptualization, operationalization, and implementation—to see the solution they are working on as a whole and be able to coordinate their efforts accordingly to the aim of the given project.

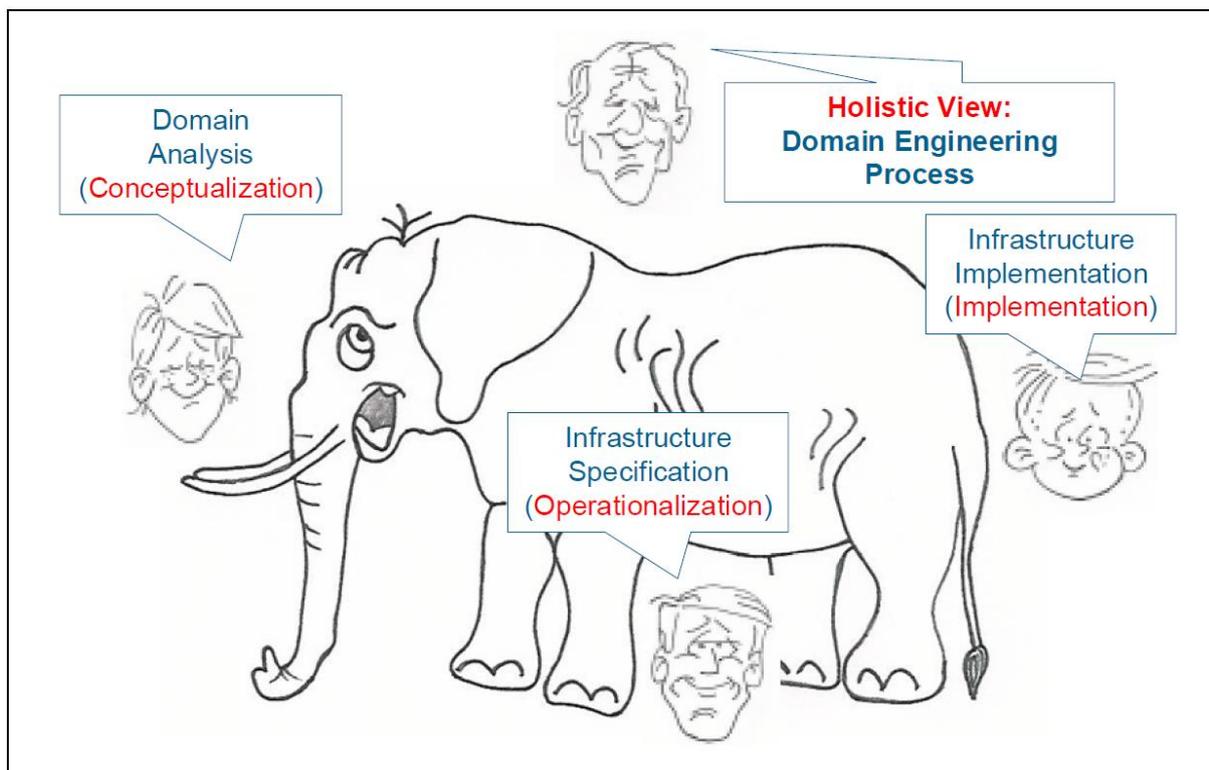


Figure 2 The Blind Men and the Elephant - Unifying an elephant (Alaoui & Schwaiger, 2024, p. 266)

Eric Evans (2004) emphasizes the significance of this comprehensive meta-perspective and underlines the importance of having correct language spoken in all three steps of the DE process. According to him, domain modeling should not separate concepts from implementation, because it provides a ‘ubiquitous language’ that ties domain experts and technologists together.

The actual steps of applying the AB-LC-ACC methodology for the topic of this master’s thesis follow the steps described in scientific work by Alaoui & Schwaiger (2024, p. 264):

¹ <https://allpoetry.com/The-Blind-Man-And-The-Elephant>

1. *“In the conceptualization (domain analysis) step of the domain engineering process the AB-LC-ACC language is used to specify the conceptual model of the AB-LC-ACC domain. For considering implementation issues in the conceptual modeling the formal modeling language UML is used to specify the AB-LC-ACC model.*
2. *In the operationalization (infrastructure specification) step the metrics for calculating the GHG emissions related to internal and external activities are specified. This provides the insight into the computational and informational requirements needed for calculating GHG emissions of the enterprise internal and external activities. With this insight the conceptual AB-LC-ACC model gets operationalized by adding the needed attributes and functionalities to the UML classes defined in the conceptual model.*
3. *In the implementation (infrastructure implementation) step the operationalized AB-LC-ACC model is implemented by coding the model’s information system and its related functionalities in a programming language. The most consistent way is the usage of object-oriented programming languages that support the UML’s object-oriented modeling paradigm used for the conceptual and operational AB-LC-ACC modeling.”*

In the first step, the authors distinguish between ‘concept’ and ‘pattern’ to clearly identify the origin of them; while the first one refers to the underlying domain, e.g., internal or external emission accounting, the second one refers to the UML language of the IT domain, e.g., entity class and event class. For the implementation step, the authors propose the use of R-Tidyverse (Wickham et al., 2023), and they reason their choice in this way (Alaoui & Schwaiger, 2024, p. 264):

1. *“R-Tidyverse is a solid open-source platform with excellent functionalities in statistical and data science-based programming,*
2. *it is an up-to-date programming platform that has many advantages compared to traditional spreadsheet platforms,*
3. *it can be extended by including additional libraries for the object-oriented programming paradigm and*
4. *it can be extended by including the R-Shiny library for building graphical user interfaces.”*

ERP-Control Domain

GHG emission measurement and management is a complex task for multinational corporations, and information systems are developed to support these efforts (Corbett, 2013). The aim of these information systems has to be the creation of purpose-oriented knowledge that enables regular and systematic corporate eco-efficiency information, and to achieve this, these systems have to be integrated with corporate environmental management systems (Schaltegger & Burritt, 2000). These information systems fulfill three key functions for the organization's operations: 1) they can automate existing business processes, by replacing human labor 2) they can inform the senior management and their employees, by providing data to them and 3) they can transform operations, by reshaping processes and industry relationships (Rush et al., 2015).

According to Alaoui & Schwaiger (2024), one such information system that illustrates these functions is the ERP-Control EIS, which combines the information bases of ERP systems and Production Control systems in accordance with *ISO's ECSI Standard* (IEC-ECSI, 2013). The advantage of this ISO-standardized ERP-Control system is that it can be utilized without dependence on a specific proprietary ERP and Production Control system, and additionally, in contrast to the traditional ERP systems, it is defined in a formal modeling language (UML), and due to this UML language, it can be used as a ubiquitous language.

The underlying theoretical foundation of the ERP-Control system is shown in Figure 3, as a conceptual domain model based on the *ISO's ECSI Standard* (2013). This domain model focuses only on the cost accounting aspect of the ERP-Control system; the extension with the GHG accounting concepts will be discussed in Chapter 3.

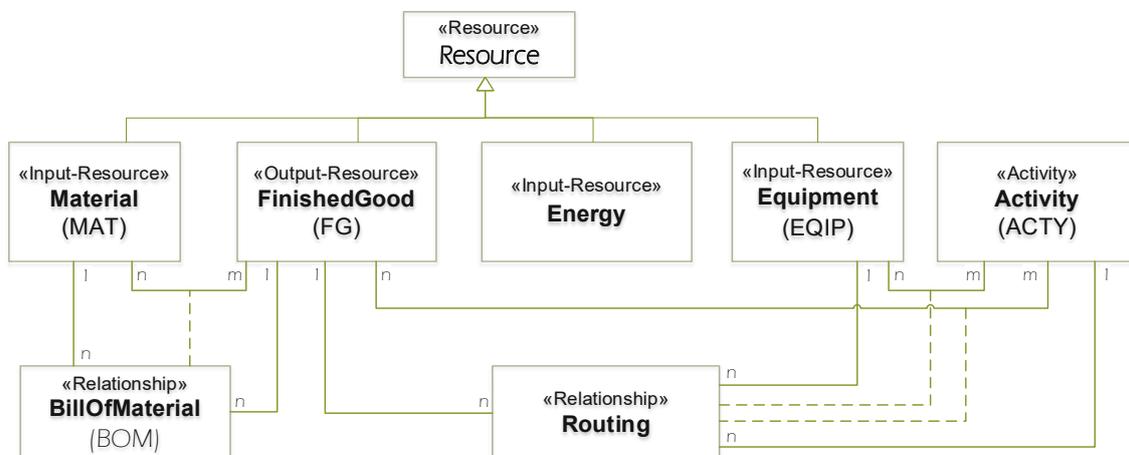


Figure 3 ERP-Control System - Conceptual cost accounting domain model (own figure based on the ECSI standard, 2013)

The core element of the conceptual domain model is the *Resource* class, which categorizes the different types of resources utilized in the ERP-Control system. According to the ECSI-specification, the *Material (MAT)*, *Energy*, and *Equipment (EQIP)* are categorized as «Input-Resources» whereas *FinishedGood (FG)* is an «Output-Resource». With this input-output categorization, the ERP-Control system is founded on a ‘production theoretical’ framework, whereby input resources are converted to output resources through various activities. The *Material* class represents the raw material or the components needed as input for the production process; the *Energy* class indicates the consumed energy resources during the production process; the *Equipment* class represents machinery or tools involved in the production process; and *FinishedGood* represents the final product or output of the production process. *Activity* class represent tasks or operations executed within the production process.

BillOfMaterial (BOM) and *Routing* are concepts that help to specify relationships between various resources. The *BOM* «Relationship» class links the *Material* with the *FinishedGood* classes through defining the material hierarchical structure and their quantities needed for the FGs. The *Routing* «Relationship» class links the *Equipment*, *Activity*, and *FinishedGood* classes by linking the process flow or sequence of operations with the required resources to complete the activities.

The conceptual domain model also contains the cardinalities of the relationships, which support the understanding of the dependencies and multiplicities between the resources, activities, and outputs. Two types of relationships are modeled in the conceptual domain model: ‘one-to-many (1-n)’ and ‘many-to-many (m-n)’. One-to-many is when each instance of Entity A can be related to one or more instances of Entity B but each instance of Entity B is related to only one instance of Entity A. Many-to-many is when each instance of Entity A may be related to several instances of Entity B and vice versa.

As described by Alaoui & Schwaiger (2024), the ERP-Control domain is the foundation of the AB-LC-ACC domain, covering the financial and production concepts in IT patterns. It integrates into the ERP-Control domain by aligning the GHG accounting concepts with the ABC accounting concepts. The idea of the AB-LC-ACC domain model originates from Emblemsvåg & Bras (2001), who developed an integrated methodology for assessing the life-cycle cost and environmental impacts of finished products. Further developing their concepts, Alaoui and Schwaiger emphasized the environmental impact in terms of GHG emissions and integrated it with the ERP-Control domain model, which resulted in the AB-LC-ACC domain model.

2.3 Plastic Industry and Injection Molding (IM)

Plastic is widely used in several industry sectors, and in 2000 it was estimated that 42% of produced toys consisted of plastic, 38% of the monitoring and control systems were composed of plastic, and 33% of small house appliances were made up of plastic (Fisher et al., 2005).

Among the plastic industry, IM is the most important because it can mass produce complex technical articles fast, with tight tolerances and with low or no finishing operations (Matarrese et al., 2017). The short cycle time indicates high throughputs, and easy automation is possible through constant and repeatable production (Thiriez, 2006). Around one third of the plastics by weight are produced with IM technology (Kanungo & Swan, 2008) and nearly all industries use IM plastics (Matarrese et al., 2017).

IM Equipment

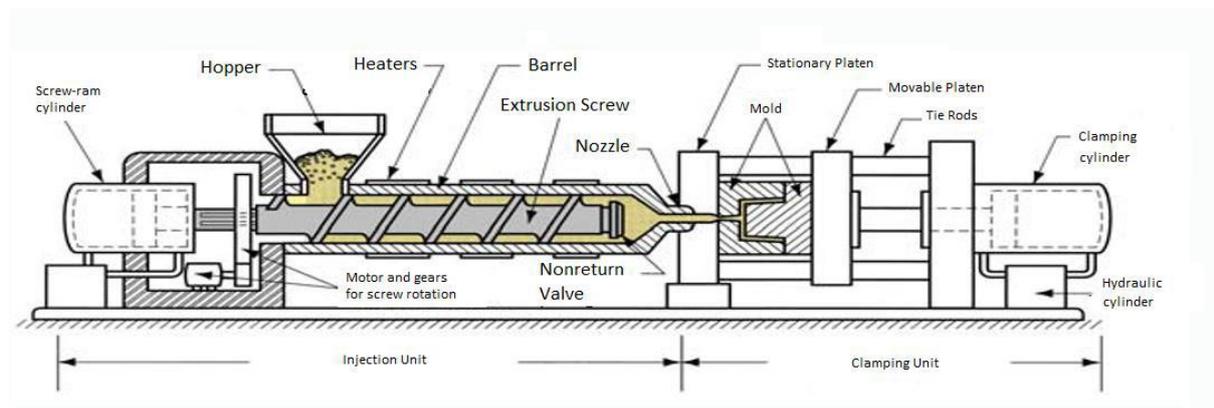


Figure 4 Schematics of a typical IM machine (Cardeal, 2016)

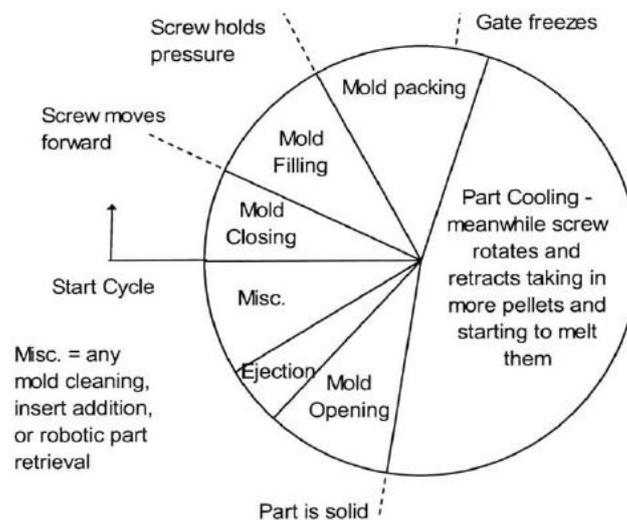


Figure 5 Representation of an IM cycle (Thiriez, 2006)

In order to understand the IMT, Figure 4 shows the schematics of typical IM equipment, and Figure 5 portrays a typical molding cycle, which consists of these steps, according to Thiriez's (2006, p. 16) description:

“The injection molding cycle starts when the mold platens (i) close, forming the negative of the part to be molded. It must be mentioned that the mold basically consists of a sprue, a runner system, a gate, and a mold cavity. The sprue transports the molten polymer from the injection nozzle to the runner system. The runner consists of flow channels that distribute the molten polymer to several gates in a complex part, or to multiple connected parts in a multi-part die. In the case of a simple one-part mold, runners are generally not needed. A gate is the interface right before the molten polymer enters the mold cavity.

Once the mold is closed, the molten polymer (g) is ready to be injected. The screw (e) advances forcing the melt into the mold. Since the melt decreases in volume as it solidifies, the screw must hold a substantial pressure after injection to ensure that the mold is completely full.

Once the mold has been packed, the gate (h) freezes and the molten polymer inside the mold is left to cool. If substantial cooling is needed, the mold might incorporate water channels to improve the heat transfer rate. While the melt is cooling, the screw retracts and rotates in order to start melting the next batch of pellets. As the pellets are fed, pressure starts building next to the nozzle.

Once the polymer in the mold has solidified, the mold opens and the part is ejected. In some instances, push rods are used to help eject the part. In the case of intricate geometries, the mold might need side-pulls in order for the part to be released. A side pull is a section of the mold opening in a direction perpendicular to injection.”

As indicated in Figure 4, the IM equipment primarily consists of two main parts: the *injection unit* and the *clamping unit*. According to Thiriez (2006), the *injection unit* is responsible for feeding, melting, and injecting the polymer into the mold, while the *clamping unit* opens and closes the mold and provides sufficient pressure during injection so no molten polymer can escape from the mold. These equipment units perform various functions to complete the IM cycle (Thiriez, 2006, p. 16-17):

- “1.) *Clamp open and close (and any further adjustment in the case of toggle clamps).*
- 2.) *Screw forward and retract (injection & screw decompression)*
- 3.) *Screw rotation (screw recharge)*
- 4.) *Ejection pins forward & retract (Part eject)*
- 5.) *Any side pull mold movement.”*

These functions need drives and energy sources; in case multiple functions need to be used at the same time, then more energy sources are needed, which can be motor-driving pumps, accumulators, or electric motor-driving gearing (Thiriez, 2006).

IM History

In 1872, John and Isiah Hyatt developed the first IM machine (Rubin, 1972). This machine used an arbor press to drive a plunger through a heated polymer barrel into a mold. This process produced precise, repeatable, and three-dimensional plastic parts (Muccio, 1994). They evolved into what is known as plunger IM machines.

Due to shortage of metals and rubber after the second world war, many industries shifted to thermoplastics as they could meet the market requirements at low costs. James Watson Hendry invented the reciprocating screw IM machine in 1946, and the rotating screw revolutionized plastic IM (Brydson, 1990). The rotating screw provided better management of the production process and thus an improvement of the quality of the injection-molded products. Since the 1970s, this design has prevailed (Rubin, 1972).

In 1985, the first all-electric IM machine was invented in Japan. It replaced the AC induction motors and accumulators with electric servomotors for each function of the machine, which provided the benefits of an independent pump machine without the idling inefficiencies. Due to these efficiency improvements, the energy-saving potential was increased in the range of 50-75% compared to the hydraulic alternatives (Thiriez, 2006).

Three different types of injection machines use the screw system, each of them with different energy profiles (Thiriez, 2006). Hydraulic machines are the most common, and their EC is the most significant, due to the large movements of oil with the hydraulic pumps. They consume a significant amount of energy while idle, which reduces the overall efficiency. Their primary benefits of the hydraulic machines are the large capacity and clamping force that they can generate (Cardeal, 2016). Hybrid injection machines represent a compromise between the

hydraulic and full-electric ones; they are mixes of them. The injection unit is either electric or hydraulic, whereas the clamping unit is the opposite of the injection unit. Some hybrids have both drives in the same unit, and the predominant variant of hybrid has an all-electric injection unit with a hydraulic clamp unit (Thiriez, 2006). The last type is all-electric powered machines, which use servo motors to power the mechanical drives. Three to five servo motors are used for all of the aforementioned functions (1-5 on pages 29-30), as recommended by Thiriez (2006).

Besides the energy-saving potential and the flexibility of having a motor for each function, all-electric systems have other advantages (Thiriez, 2006). Shortening of the cycle time, due to the capability of running multiple functions simultaneously. Cleaner production environments and possible cleanroom manufacturing (healthcare, electronics, automotive) by eliminating the necessity for oil and using a closed-loop liquid cooling system. The absence of hydraulic oil implies better labor and environmental conditions by lowering the risks of oil-related spills, employee falls, fire hazards, and fugitive oil mist. Reduced air conditioning because of the reduced EC and waste energy production. Lower noise level by elimination of the hydraulic pumps. All-electric systems have a quick startup and setup, and they provide high molding quality, increased efficiency, and repeatability without the operator's involvement. On the other hand, they offer mixed economic incentives, with a higher initial capital investment than hydraulic equipment. In cases when higher molding pressure is required, the hydraulic clamps are more precise and reliable for pressure control (Thiriez, 2006).

3. AB-LC-GHG-Accounting:

Conceptual design

In the following chapter, the conceptual design of the AB-LC-GHG-Accounting model will be discussed, with the aim of defining the terminology of the GHG accounting model based on the first step of the AB-LC-ACC methodology (conceptualization). According to Schaltegger & Burritt (2000), the integration of the financial and ecological accounting systems has to be started at the conceptual level. To illustrate this conceptual design process, the ‘Triptych of conceptual modelling’ by Mayr & Thalheim (2021) is utilized, as shown in Figure 6, which contains three dimensions: the *encyclopedic*, the *linguistic*, and the *conceptual model*.

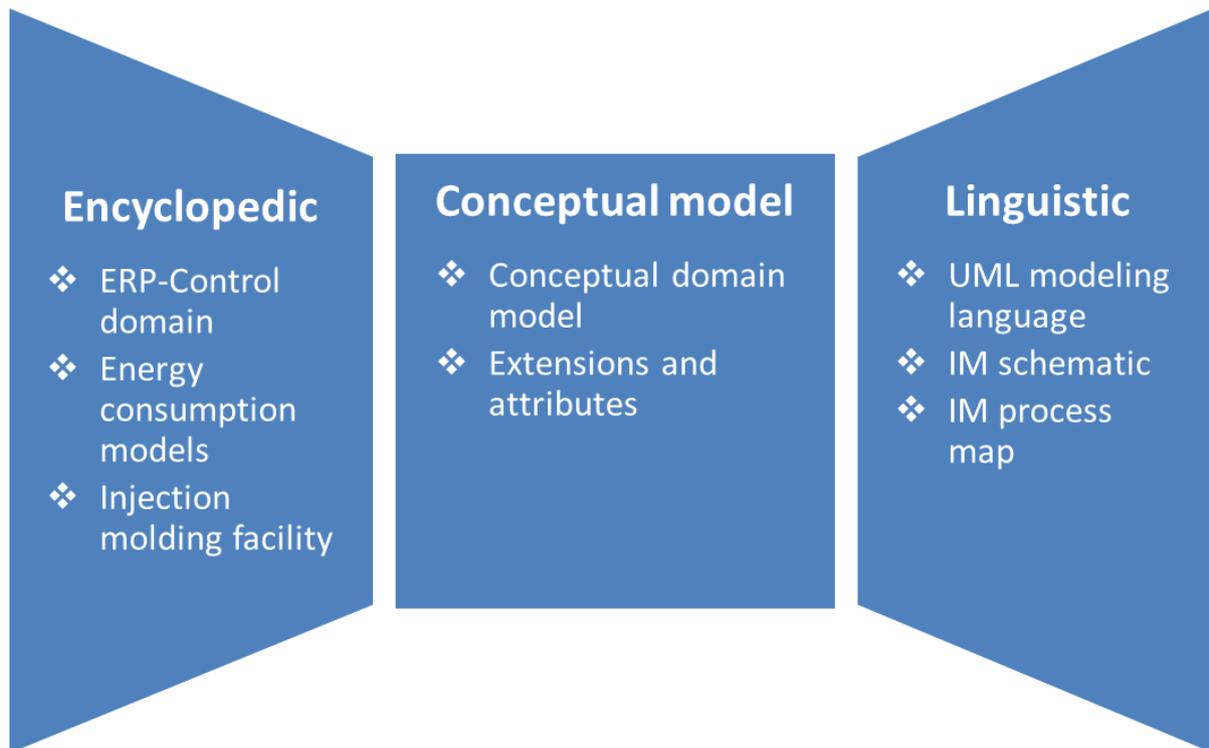


Figure 6 Triptych of the GHG accounting model (own figure, based on Mayr and Thalheim's (2020) work)

The *encyclopedic* dimension focuses on the knowledge of the specific domain by containing all the domain-relevant knowledge and expressing it through linguistic terms. For the master's thesis, this encyclopedia includes the ERP-Control application domain, which specifies the application domain for the GHG accounting model for the IMT. The foundation of the GHG accounting model is the EC and its mathematical modeling, which is expressed by the EC

models. Lastly, the IM facility describes the stages with their relevant components of the IM manufacturing facility.

The *linguistic* dimension emphasizes the modeling of the domain through a language, which is generally accepted in the community and semantically based on the understanding of the community members (Mayr & Thalheim, 2021). The modeling language of the master's thesis is the UML, which meets the criteria established in the 'Triptych of the conceptual modeling', and it was referenced as an example in that work. This UML is employed for the conceptual and operational modeling in this thesis, and this modeling starts with the schematic of the IM process, which illustrates the participating processes and equipment and their interrelationships. This schematic, with the help of the domain knowledge, will be further specified into a process map, which describes the whole IM manufacturing process, considering the order of the processes and the different scenarios.

The *conceptual model* dimension connects the two other dimensions, with the aim of establishing a structured view of the domain knowledge with the modeling language by selecting, using, reconsidering, ordering, and integrating their domain knowledge and modeling language elements (Mayr & Thalheim, 2021). The concepts from the initial two dimensions are transferred into the conceptual model, and this conceptual model is extended with relevant extensions and attributes, which enables to accordingly model the GHG emissions of the IM process.

3.1 Injection Molding Technology (IMT) domain

Domain selection: ERP-Control Domain

In the ‘Triptych of the conceptual modeling’ (Mayr & Thalheim, 2021), the encyclopedic dimension emphasizes the general knowledge of the specific domain in the form of concepts, notions, and terms. The authors of the ‘Triptych...’ stated that in natural or technical sciences, unlike in other disciplines, the conceptualization is the initial step, and based on it, one or more languages are defined for representing the elements and relationships of the domain of interest. The first step of the AB-LC-ACC methodology is the conceptualization with the aim of specifying the conceptual model of the domain with the AB-LC-ACC language (Alaoui & Schwaiger, 2024). According to Reinhartz-Berger et al. (2013, p. ix.): *“Before any system can be collaboratively developed, used, and maintained, it is necessary to study and understand the domain of discourse. This is commonly done by developing a conceptual model.”* To be able to develop a conceptual model, first the application domain has to be selected, which is where the conceptual model will be developed. In our digital age, the multinational corporations have already implemented an EIS to manage and support the core business processes, information flows, reporting, and data analytics within an organization. This information system has different domains, depending on the functions that have to be fulfilled. As outlined in Chapter 2.2, the modeling of the GHG emissions is a complex task, and it relates to the accounting and production domain, which are managed by the ERP and the Production Planning and Control (Control) systems. This ERP-Control domain is in accordance with the *ISO/IEC Standardization* of the ‘Enterprise Control System Integration’ (IEC-ECSI, 2013), which provides a suitable specification of the domain to be used for the analysis. In their research, Komoto & Furukawa (2022) employed the same IEC standard to model the context information for the digitalization of the environmental performance evaluation of the manufacturing systems.

Energy consumption

After understanding the application domain, the next step is to comprehend the IM process, including its workings and the relationships between activities and equipment within the hierarchical structure, in order to conceptually model them. In the AB-LC-ACC methodology, the GHG emission calculations are activity-based, and they utilize the EC of the activities as a fundamental element of the emission calculations (Alaoui & Schwaiger, 2024). In chapter 2.3, the IM cycle and equipment were discussed, but in order to calculate the GHG emissions of the IM activities, the EC of the IM cycle has to be analyzed. To further understand the EC of

the IM process, Thiriez (2006) conducted a study that measured and analyzed the energy use of hybrid and all-electric equipment. The findings are shown in Figure 7.

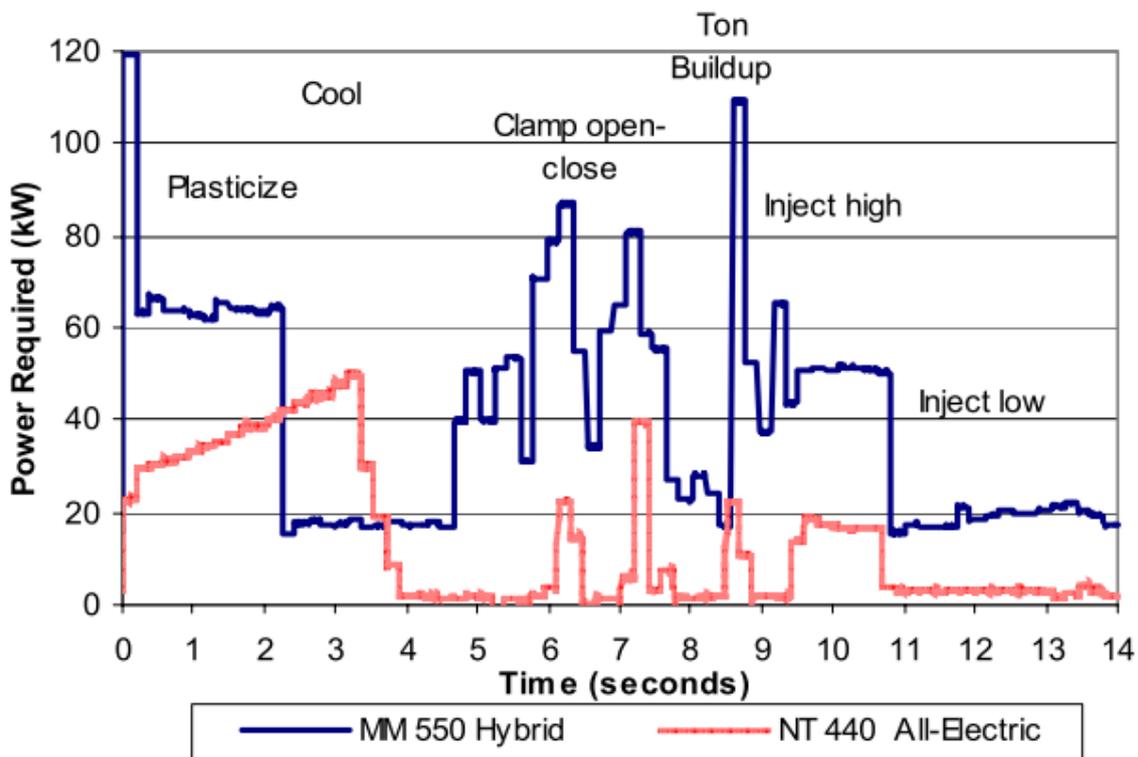


Figure 7 EC of an IM cycle for hybrid and all-electric equipment (Thiriez, 2006)

The EC of the IM process was described as follows (Thiriez, 2006, p. 24-25):

“The cycle starts with the heaters on and the screw rotating ‘plasticize’. The screw rotates shearing the plastic pellets, increasing their temperature to melt temperature. The heaters provide additional heat.

Once the polymer melts and is sufficiently mixed the screw turns off and just the heaters are kept on to maintain the polymer molten. This is portrayed in the above figures as the sharp drop right after plasticizing. The heaters are kept on waiting for the part from the previous cycle to cool.

When the part from the previous cycle is ready to be ejected the mold opens and secondary devices such as ejector pins are activated. This requires peaks of power but for a short time. The mold then closes and the tonnage builds up.

When the required mold pressure is achieved, the mold is then ready for injection. The screw advances pushing the melt into the mold. This is labeled in the figures as ‘inject high’.

After 'inject high', the melt in the mold solidifies and shrinks. A lower injection pressure, or packing pressure, must be applied in order to compensate for all the volume loss to shrinkage. After the injection stage the parts starts cooling and the screw recedes and starts rotating to melt the next batch."

In the recent years, multiple studies were conducted on EC prediction for different industrial processes, and they can be divided into three main categories (Cardeal, 2016):

1. Specific Energy Consumption (SEC) Models—these models aim to link the EC of a particular process to one of its attributes.
2. Process Based Models (PBM)—these models aim to estimate the EC based on the most relevant characteristics and aspects of the particular process.
3. Empirical Models—these models estimate the EC by mathematical formulations grounded on the physical and chemical features of the process. Experimental data is used for their development.

The SEC was defined by Thiriez & Gutowski (2006, p. 196) as “*specific energy consumption or energy consumption per kg of polymer processed*”, which indicates that the EC is dependent only on the weight of the processed polymer. They examined more than a hundred measurements and calculations to define the SEC for the three equipment types (hydraulic, hybrid, and all-electric).

SEC models are widely and frequently used for EC modeling, and this is due to some advantages: they are relatively simple and cost-effective to develop, as they can be evaluated with small datasets; for one company, calculated values can be applied for other company calculations with acceptable precision; quick and straightforward estimations can be obtained with them, especially when they are applied within the same company (Cardeal, 2016). The biggest disadvantage of the model lies in its simplicity, by considering only the weight and ignoring other important factors to the EC, like the size and geometry of the FG. Although SEC models are widely applied in the industry, due to the aforementioned fact, their application for IM is limited (Cardeal, 2016).

Process Based Models solve this one-factor dependency by considering a larger set of inputs. A PBM was developed by Ribeiro et al. (2012) to estimate the EC of the IM process, and it considered characteristics like the geometry of the injected product, the cycle time, and equipment properties. The specific coefficients of the model can be adjusted according to the processing conditions, type of material, and geometry of the part. For the model development,

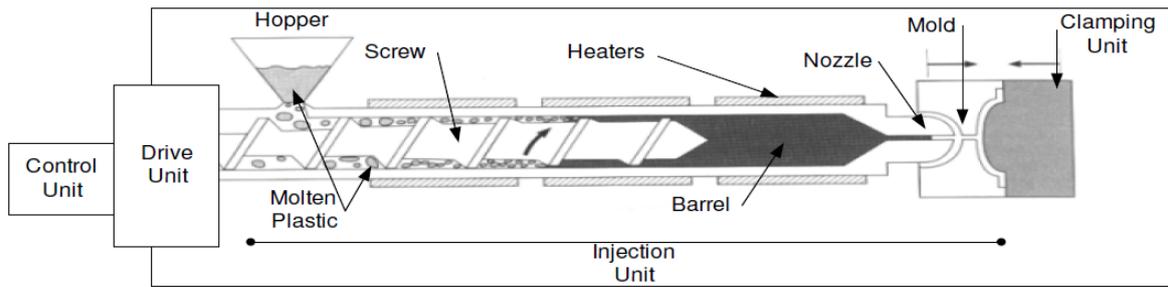
empirical relations and an experimental dataset were utilized. The benefits of the process-based approach include high-precision EC estimation when it is based on the right dataset, the potential for in-depth insights into specific processes and individual products, and a clear conceptual framework. On the other hand, precision has its price: the time-consuming, labor-intensive, and costly data collection; the extensive data requirements, which might render large-scale and multi-product analysis more difficult (GHG Protocol, 2011). Another categorization of studies about manufacturing EC measurement and improvement was made by Madan et al. (2015), who made these four categories:

1. Industry level, with the aim to find total and average EC
2. Plant level, with the aim to improve the plant's energy efficiency
3. Machine level, with the aim to understand the different machine types and tools
4. Process level, with the aim to study the effects of the required process energy

On the industry level, in their study, Thiriez & Gutowski (2006) considered the entire IM process as one activity with one piece of equipment and performed an industry-wide energy analysis. They defined an *Overall System Diagram*, where for each stage of the IM process, the average, low, and high SEC values were ordered and the average SEC value for the all-electric IM equipment was defined as 0.41 kWh/kg.

On the machine level, Kanungo & Swan (2008) investigated the EC of all-electric and hydraulic IM equipment. Based on their experimental research, they defined a range for the average SEC value for an all-electric machine as 0.11-0.37 kWh/kg, where the upper bound of the range is relatively close to the MIT study by Thiriez & Gutowski (2006). They considered various aspects that affect EC, like costs, EC, process parameters, and throughput. For the IM equipment, they defined four key parts: the injection unit, clamping unit, drive unit, and control unit, as shown in Figure 8.

The *injection unit* is responsible for the injection of the *molten plastic* into the *mold*; the *clamping unit* operates the mechanism to close, clamp, and open the *mold*; the *drive unit* powers the *electric servo motors* (and displacement pumps in case of the hydraulic equipment); and the *control unit* regulates the barrel temperatures, flow rates, and clamping forces (and oil for hydraulic equipment) (Kanungo & Swan, 2008).



Source: <http://www.cheresources.com/injectionzz.shtml>

Figure 8 IM equipment with the relevant parts according to Kanungo & Swan (2008)

On the process level, Madan et al. (2013) proposed a science-based guideline for the EC prediction of the IM process. They defined the relevant activities of melting, injecting, cooling, and resetting (which is the collection of the mold opening, ejecting, and mold closing activities). In addition to them, they also defined two activities, the control and the base load, which are running parallel to the IM cycle in the background. They did not differentiate among the various components of the IM equipment. More details about their guideline will be discussed in Chapter 4.1.

IM Facility

The IM process is only part of the whole IM manufacturing facility, which contains four stages, as shown in Figure 9: *Drying*, *Blending and dosing*, *Injection molding*, and *Regrinding* (Madan et al., 2015). In the *Drying* phase, the plastic beads and reusable scrap are fed into the dryer, with the aim of removing or reducing the moisture of the material to an acceptable level. In the next stage, the dried material is additionally mixed with colorants or additives. The third phase is the *Injection molding*, when the plastic mixture is melted and transformed into a solid part. The last phase is the *Regrinding*, where runners, gates, and other extraneous plastic are removed from the part and processed into granules suitable for adding to the virgin mix. This thesis focuses only on the drying and IM phase because they are energy intensive, while the other two phases can be neglected regarding the EC of the process.

According to Stan (2020), polymeric plastic materials contain a certain amount of water, and in order to have high-quality injection-molded FGs, these plastic materials have to be dehumidified or dried before the processing. The reason for drying the polymeric materials is to mitigate or eliminate the complications arising from excessive moisture content in plastic materials, and the possible impact of the complications depends on the type of polymeric resin, the drying time, and the technology applied. Some of the problems caused by the moisture that affect the product quality are not always visible; they can be identified using

appropriate analytical methods, primarily via destructive testing. Stan (2020) also discusses various dryer types used in the plastic industry, like hot-air dryers, desiccant dryers, compressed-air dryers, and vacuum dryers. The hot-air dryers are the oldest and simplest ones, the desiccant dryers are the most popular ones, with around 80% market share, while vacuum dryers are the most energy-efficient ones because of the absence of heating energy.

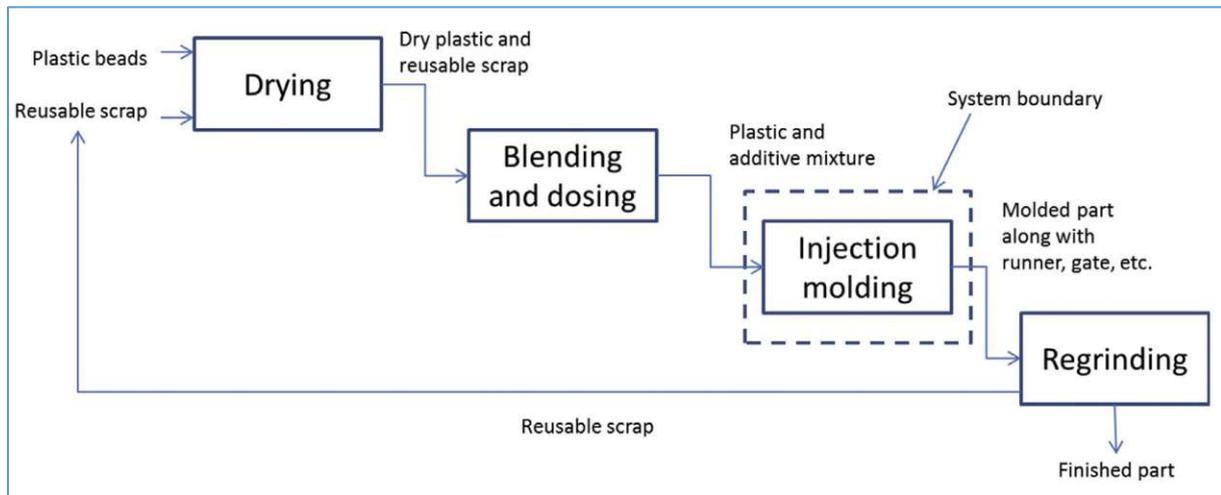


Figure 9 Stages of an IM manufacturing facility (Madan et al., 2015)

3.2 IMT domain modeling: UML modeling language

Common language

The integration of the business information (domain knowledge) into the EIS is a complex process that requires different perspectives and expertise from the participants. These experts have different backgrounds (domain or IT), and they may employ their own terminology (modeling language) during the integration steps, thereby complicating the communication and hindering the overall project progress. To overcome these hurdles, a common language is needed, one with which all the experts from different backgrounds are familiar. The solution for the common language is provided by the DDD methodology (Evans, 2004). This methodology, similar to DE, adopts a holistic meta-perspective, which covers the domain and IT expertise and provides a ‘ubiquitous language’ for the participants, which ensures clear and consistent communication among all stakeholders on components of the project. This ubiquitous language is employed in all three steps of the AB-LC-ACC methodology: 1) During the conceptualization (domain analysis) phase to specify the conceptual model. This specification is done by defining the concepts and patterns of the domain and modeling them with the UML formal modeling language. The concepts refer to the domain knowledge, while the patterns relate to the IT knowledge. 2) During the operationalization (infrastructure specification) phase to specify the calculation metrics related to the GHG emission measurement and operationalize the conceptual model by defining the computational and informational requirements necessary for the GHG calculations. 3) During the implementation (infrastructure implementation) phase to code the operationalized GHG Accounting model using an object-oriented programming language that supports the UML object-oriented modeling paradigm.

UML modeling basics

The UML is an object-oriented modeling language standard, which consists of a collection of notions for modeling systems from several perspectives and at different levels of abstraction (France et al., 1998). It provides a conceptual framework with abstract elements such as activity, attribute, class, relation, and state for defining domains of interest (Mayr & Thalheim, 2021). UML was established to model the architecture of software systems, and it has rapidly become the standard modeling language for software systems design (Eriksson & Penker, 2000).

IBM distinguishes between UML models and diagrams, defining models as an abstract representation of the system and diagrams as a concrete representation of the system (IBM, 2025). These models may exhibit different levels of detail, and they can be utilized for different purposes, such as defining the application domain for an analysis model during the system analysis phase or refining the application domain for a design model during the design phase. France et al. (1998) assert that UML offers one of the best modeling experiences, and its usefulness is already proven in practice. UML diagrams graphically represent the quantifiable aspects of a system, including class diagrams that illustrate the system's structure and activity diagrams to document the activity flow. They have a wide range of uses, like to visualize an entire system or project by high-level architects or managers, or to specify, visualize, and document applications by system developers (IBM, 2025).

Madan's scientific guide schematic

Once the relevant activities and equipment parts have been identified in Chapters 2.3 and 3.1, the next step is to match them accordingly. Considering that IM manufacturing is a complex system (Jung et al., 2021), process characterization is essential for understanding its complexity and is useful for evaluating sustainability performance (Mani et al., 2014). In their work, Madan et al. (2015) developed a schematic to delineate the relationships between the unit manufacturing processes (IM activities) and manufacturing equipment. This thesis creates a comparable *schematic*, illustrated in Figure 10, where the activities are based on the science-based guideline by Madan et al. (2013), and the equipment is derived from the research conducted by Kanungo & Swan (2008).

The *schematic* has two dimensions, namely the *Process* and the *Equipment*. The *Process* dimension represents the *Injection molding process* as the *Unit-manufacturing process*, including its six *Sub-processes*, which are the activities of the IM process outlined in the science-based guideline by Madan et al. (2013). In the *Equipment* dimension, the *Injection molding equipment* classified as *Manufacturing equipment* has four *Sub-systems*, similarly to Figure 8. According to Madan et al. (2015), due to the complexity of the IM process, in reality the functionalities of the sub-systems are dependent on each other, but for the sake of simplicity in their work, they are assumed to be independent. The relationships between them are represented by the lines, and while the original schematic (Madan et al., 2015) exhibits many-to-many (n-to-m) cardinalities, this thesis simplifies them to one-to-many (1-to-n).

In Figure 10, these one-to-many relationships between the sub-systems are depicted with the solid line, whereas the dashed lines illustrate the potential many-to-many relationships. Each activity is performed by one piece of equipment; however, the *Clamp unit* oversees two activities, specifically the *Cooling* and *Resetting*, while the *Base Load* activity is directly done by the *Injection molding equipment*. This level of complexity strikes an ideal balance between realistic presentation and modeling abstraction, making it well-suited for the purpose of the thesis. Figure 45 in the Appendix shows the schematic with the simple one-to-many relationship, which is utilized for the subsequent design step of the model.

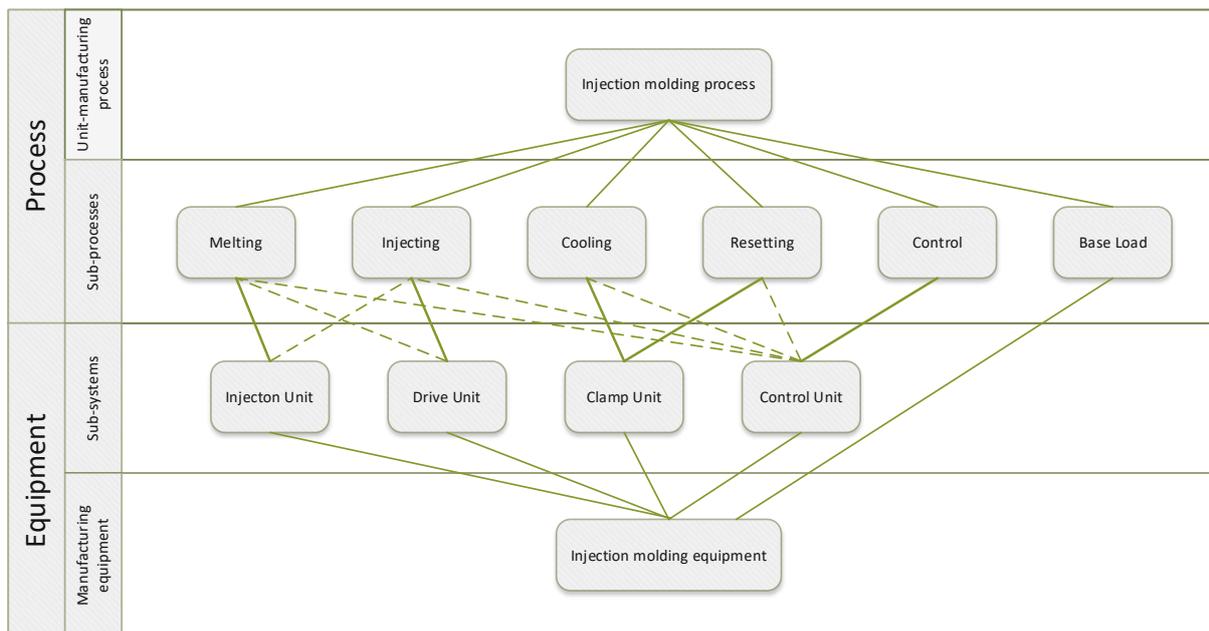


Figure 10 A schematic of the manufacturing process and the IM Equipment with a) one-to-many relationships (only continuous lines) and b) many-to-many relationships (all lines) (own figure, based on the work by Madan et al. (2015))

Upon understanding the vertical or structural dependencies of the IM manufacturing facility, the next step is to define the horizontal or sequential relationships of the activities, expressed as a process map in a UML activity diagram notation, shown in Figure 11.

The process map delineates just the two manufacturing activities of the IM facility in their own lanes, namely the *Drying* and the *Injection Molding Process*; the former is quite straightforward, whilst the latter is more complex. This complexity lies in the nature of the IM process, wherein certain activities, such as *Cool* and *Reset*, executed in parallel with the *Melt* activity.

This is due to the process characteristic of melting the next shot during the cooling and resetting of the current shot, as outlined in the IM cycle in Chapter 3.1. The *Control* and *Base*

Load activities are running parallel and continuously alongside the core IM activity, and when the number of required parts n is reached, then the process ends.

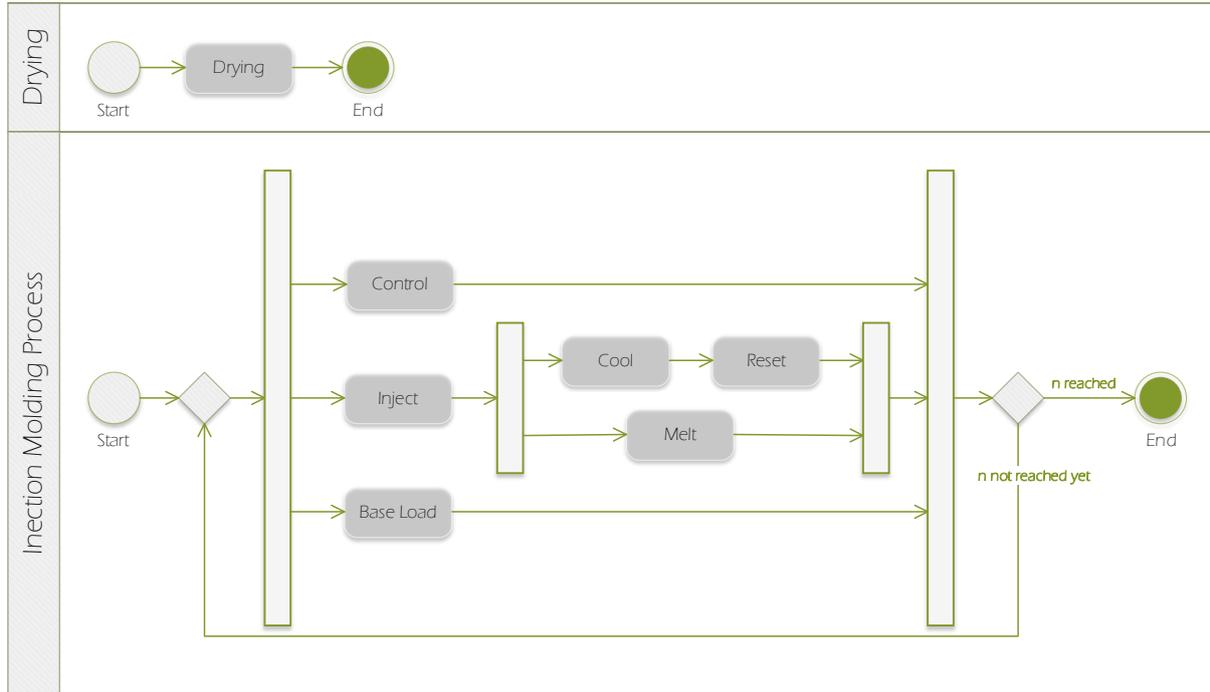


Figure 11 Process map of the IM Manufacturing Facility in UML notation (own figure)

actyName	Dryer	Injection Unit	Drive Unit	Clamp Unit	Control Unit	IM Equipment	Gas Heater	Truck
Drying	1	0	0	0	0	0	0	0
Melting	0	1	0	0	0	0	0	0
Injecting	0	0	1	0	0	0	0	0
Cooling	0	0	0	1	0	0	0	0
Resetting	0	0	0	1	0	0	0	0
Control	0	0	0	0	1	0	0	0
BaseLoad	0	0	0	0	0	1	0	0
Injection Molding	0	0	0	0	0	1	0	0
Heating	0	0	0	0	0	0	1	0
Transport	0	0	0	0	0	0	0	1

Table 1 Activity-Equipment Matrix for the Injection Molding Facility

To consider all the activities necessary for the production of an injection-molded part, the Table 1 *Activity-Equipment Matrix* for the IM facility is created, encompassing all the activities with their relevant equipment. The rows list the activities, while the columns list the

equipment; the *Injection Molding* activity is divided into its sub-activities according to the schematic in Figure 10, and the *Equipment* columns contain the equipment from the same schematic. Two secondary or support activities are added: the *Heating*, which represents the thermal regulation of the IM facility with its corresponding *Gas Heater* equipment, and the *Transport* activity, which symbolizes all the outbound logistics of raw material facilitated by the corresponding *Truck* equipment. In the matrix, the ‘1’ values represent an existing connection among the elements, while the ‘0’ values indicate the absence of a connection. This matrix is beneficial for the subsequent operationalization and implementation steps by transforming the visual representation of the process map into a structured data format.

3.3 IMT domain modeling: Conceptual domain model

Conceptual modeling

The central part of the ‘Triptych of conceptual modelling’ (Mayr & Thalheim, 2021) is the conceptual model, which is constructed upon the encyclopedic and linguistic “wing” or dimension; refer to Figure 6. The encyclopedic dimension was covered by the domain knowledge in Chapter 3.1, while the linguistic dimension was covered by the UML modeling in Chapter 3.2. By merging the two dimensions, the conceptual model of the AB-LC-GHG-Accounting model is created, which integrates the elements of the knowledge and modeling space and provides a structured view of the knowledge space (Mayr & Thalheim, 2021).

According to Reinhartz-Berger et al. (2013, p. ix.): *“The main purposes of conceptual models are: (1) supporting communications between different types of stakeholders and especially between developers and users; (2) helping analysts understand the domain of interest, its terminology, and rules; (3) providing input for the next development phases, namely top level and detailed design; and (4) documenting the requirements that originate from the real world for maintenance purposes and future reference.”*

By translating the Process map of the IM manufacturing facility (refer to Figure 11) into a conceptual domain model, the communication among stakeholders is supported (1), the terminology and relations of the elements (rules) are set (2), and in the next development phase of operationalization (infrastructure specification), this conceptual domain model is operationalized (3). Mani et al. (2014, p. 5903) state that *“Process models can either be activity models or information models. Activity models describe the dataflow and precedence in manufacturing processes. (...) Information models of manufacturing processes define entities and their relationships. The dataflow in activity models can be entities in information models.”* The information from the activity model (process map in Figure 11) has to be translated and integrated into the ERP-Control domain in the form of an information model (conceptual domain model) in order to model the hierarchical structure of the IM process with multiple activities and equipment parts. This model only achieves a conceptual status when the meaning of terms is explained in the conceptual space (Mayr & Thalheim, 2021). The objective is to systematically document the relevant information of the various IM process elements, such as the materials consumed, the equipment utilized, and the FG produced. This information is organized using the elements of the activity model, as referenced in the previous citation.

ERP-Control model extension

The conceptual model of the ERP-Control domain based on the ISO’s ECSI standard for accounting was presented in Chapter 2.2, and in order to model the GHG emissions, this conceptual model requires an extension. The refinement of the concepts by Alaoui & Schwaiger (2024) emphasized the environmental impact in terms of GHG emissions, resulting in the AB-LC-ACC domain model. Building on their work, this model has been further developed and extended to meet the unique needs of the plastic industry. Figure 12 shows the adapted conceptual domain model, with its GHG accounting extensions and related coefficients.

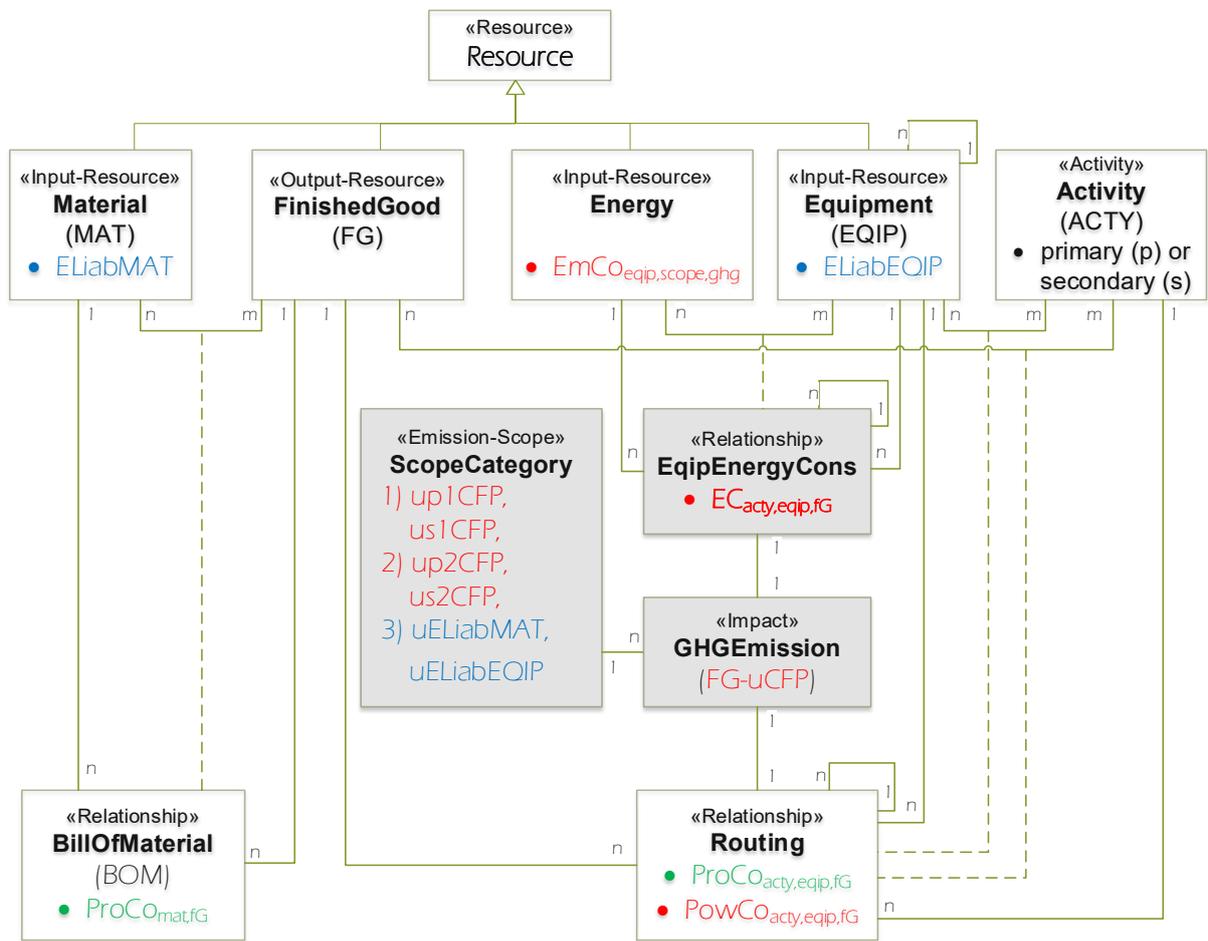


Figure 12 Conceptual domain model of the GHG Accounting in the ERP-Control system modeled in a UML class diagram (own figure based on Alaoui & Schwaiger (2024))

The AB-LC-GHG-Accounting model is based on the production theoretic input-output foundation, via the *Energy*, *Equipment*, and *Material* «Input-Resource» classes and the *FinishedGood* «Output-Resource» class, together with their connections to the *Activity* class (Alaoui & Schwaiger, 2024). The concept of production coefficients (*ProCo*) (indicated below the class names) was developed by the Nobel Prize laureate economist, Wassily

Leontief (1986), which specifies the required amount of input for one unit of output. Accordingly, the *BOM* and *Routing* «Relationship» classes have *ProCos* (*ProCo_mat,fG* and *ProCo_acty,eqip,fG*), and with their sub-indices—for *BOM*, the *mat* and *fG* and for *Routing* the *acty*, *eqip*, and *fG*—they indicate the elements involved in their respective *BOM* or *Routing* relationships. The *ProCo_mat,fG* specifies the material’s input per unit of output of the FG, whereas the *ProCo_acty,eqip,fG* specifies the activities and equipment input per unit of output of the FG. This information is crucial for activity-based systems, namely the standard cost accounting and standard GHG accounting, as they rely on a ‘standard value’ for the ProCo, and by employing this ProCo standard, a ‘parametric model-based’ cost and GHG-accounting system is created (Schwaiger, 2013). Such a system is essential for the forward-looking cost and GHG planning and management control systems.

Besides the aforementioned ProCos, there are additional coefficients, such as the *PowCo* (*PowCo_acty,eqip,fG*) for the *Routing* class, which is derived using the same logic as the ProCo, but it indicates the power of the given equipment that is used to execute the given activity for the given FG. The *EmCo* (*EmCo_eqip,scope,ghg*) indicates the rate of the GHG emission (in the unit of measure ‘kgCO₂e/kWh’) for the given equipment regarding the scope and GHG emission category. In addition to the coefficients, the emission liabilities (*ELiabMAT* and *ELiabEQIP*), addressed in Chapter 2.1, are included in the *Material* and *Equipment* classes. They specify the embedded external GHG emissions of the given material or equipment, which are accumulated from the raw material extraction until the beginning of the consumption of the material or the use of the equipment (Kaplan & Ramanna, 2021). The colors of the coefficients signify specific meanings: the green ProCo represents the unit time, which is associated with the standard cost accounting system; the blue emission liabilities indicate external emissions, while the red coefficients in general are related to the GHG accounting system.

The extension of the cost accounting domain model with the GHG accounting model on a conceptual level involves the inclusion of additional computational artifacts and information. The main objective of the extension is the integration of the GHG emission information represented as the product’s unit-carbon footprint (*FG-uCFP*) into the existing accounting system. The *FG-uCFP* contains all the ‘cradle-to-gate’ emissions, both internal and external, that occurred during the whole life cycle of the product until the end of the production activity, and it is stored in the computational artifact *GHGEmission*. This «Impact» class is linked to the two additional computational artifacts, the *EquipEnergyCons* and *ScopeCategory*

classes. The former one provides the information about the internal activity's EC ($EC_{acty,eqip,fG}$), while the latter one provides the necessary information for categorizing the various components of the $FG-uCFP$.

The calculation logic for internal activities' EC and GHG emissions is provided by the 3-LoEC metric from the AB-LC-ACC modeling framework (Alaoui & Schwaiger, 2024):

- The internal activity's 'unit-energy consumption', defined as the EC for one unit of the FG ($EC_{acty,eqip,fG}$ in $EquipEnergyCons$), is calculated by multiplying the production coefficient ($ProCo_{acty,eqip,fG}$ from $Routing$) with the PowCo ($PowCo_{acty,eqip,fG}$ from $Routing$).
- The internal activity's 'unit-GHG emission', or carbon footprint for one unit of the FG ($uCFP_{acty,eqip,fG}$ in $GHGEmission$), is calculated by multiplying its EC by the EmCo ($EmCo_{eqip,scope,ghg}$ from $Energy$).

The calculation logic for external upstream GHG emissions is provided by the Emission Liability (ELiab) metric:

- The 'unit-emission liability' ($uELiabMAT_{acty,eqip,fG}$) for the material 'consumed' in the activity is calculated by multiplying the material's ProCo ($ProCo_{mat,fG}$ from $BillofMaterial$) by the material's ELiab ($ELiabMAT$ from $Material$).
- For the equipment 'used' in the activity, the corresponding unit-ELiab ($uELiabEQIP_{acty,eqip,fG}$) is calculated by multiplying the equipment's ProCo ($ProCo_{acty,eqip,fG}$ from $Routing$) by the ELiab per capacity unit of the equipment (proportion of $ELiabEQIP$ from $Equipment$).

In the conceptual domain model, the relationships among the entities are also specified. The $EquipEnergyCons$ exhibits a one-to-many relationship cardinality to the «Input-Resource» classes of $Energy$ and $Equipment$, while it has a one-to-one relationship towards the $GHGEmission$ class, indicating that an equipment may possess several EC values, while each EC value corresponds to a singular GHG emission value. The $GHGEmission$ class exhibits a one-to-many relationship with the $ScopeCategory$, whereby each GHG emission value may correspond to a single scope category, but a single scope category may appear multiple times in the $GHGEmission$ table.

There are three recursive relationships in the conceptual domain model for the «Input-Resource» class $Equipment$ and «Relationship» classes $EquipEnergyCons$ and $Routing$. "A recursive (or unary) relationship is defined as an association between instances as they take

on roles within the same entity. Roles play an important part in the examination of structural validity, especially for recursive relationships. (...) Examining these roles allows us to classify all recursive relationships into symmetric or asymmetric associations while further classifying asymmetric relationship types into hierarchical, circular, and mirrored associations." (Dullea & Song, 1999, p. 388). These recursive relationships are represented by the loops with the one-to-many (1-n) cardinalities, indicating the hierarchical relationship among the entities. The recursive relationship of the «Input-Resource» class *Equipment* is essential for compact function programming because different parameters relate to distinct equipment parts, and without this parent-child relationship, the data retrieval would be complicated, resulting in a more complex coding structure. The recursive relationships for the «Relationship» classes *EquipEnergyCons* and *Routing* are essential for recursively summarizing the different children to their parents, and by applying this pattern, the relevant elements for the summation can be selected; for example, not all activities are relevant for calculating the cycle time of the IM process (see Figure 11), whereas all activities are relevant for the EC calculation of the IM Equipment.

4. AB-LC-GHG-Accounting: Operational design

In the following chapter, the operational design of the AB-LC-GHG-Accounting model will be discussed, focusing on specifying the calculation metrics and developing the operational domain model by incorporating the needed attributes and functionalities into the previously specified conceptual model, in accordance with the second step of the AB-LC-ACC methodology (operationalization). Analogous to the ‘Triptych of the conceptual modeling’, shown in Figure 6, the operational design encompasses three dimensions: the knowledge, the modeling, and the combined dimensions.

In the knowledge dimension, the mathematical model is defined based on a pre-existing science-based guideline (Madan et al., 2013). Initially, the model is defined for any type of activity, and subsequently, it is specifically tailored for the melting process. In the modeling dimension, the operational domain model is created by extending the conceptual domain model with the requisite operational information, e.g., concepts, patterns, and functionalities. The combination of the metrics and the operational domain model results in the parameter and function system, which describes these attributes and their storage location. These parameters are also harmonized with the practical knowledge in a comparison table in order to facilitate the implementation.

4.1 IMT domain modeling: Mathematical modeling language

The industry employs LCA to assess the sustainability performance of a product's life cycle, and they are predominantly based on the weight of the product (Madan et al., 2015). Similar to the MIT study (Thiriez & Gutowski, 2006), these LCA databases provide only a single and generic parameter for estimating the EC (Matarrese et al., 2017), without considering other manufacturing factors, such as the material, part geometry, equipment specifics, or the cycle time (Madan et al., 2013; Mani et al., 2014; Matarrese et al., 2017). In his master's thesis, Thiriez proposes further refinement of his analysis and requests more theoretical models for EC prediction, a necessity also emphasized by Cardeal (2016) in his master's thesis. These improvements can be achieved with more accurate EC estimation (Mani et al., 2014; Matarrese et al., 2017), which takes into account additional factors on a more granular level of the IM technology.

The GHG Protocol (2011) requires the activity-based approach to calculate improved EC, and, therefore, it is the most widely recognized approach in management sciences for process-level management (Jourdain et al., 2021). Madan et al. (2013) published a research paper that introduced a science-based guideline to characterize the EC for part manufacturing using the IM process. This novel approach is more comprehensive than the MIT (2006); it involves multiple activities, and it considers many factors of the IM process, like the characteristics of the material, the FG, and even the equipment. The 3-LoEC metric from the AB-LC-ACC methodology provides the general calculation framework for the EC and GHG calculations, as discussed in Chapter 3.3 and shown in Equation (1).

$$\begin{aligned} uCFP_{acty,fg} &= ec_{acty,res,fg} \cdot e_{res,scope,ghg} \\ &= a_{acty,res,fg} \cdot p_{acty,res,fg} \cdot e_{res,scope,ghg} \end{aligned} \quad (1)$$

where

uCFP ...	uCFP of the activity for the FG [kgCO ₂ e]
ec ...	EC of the resource for the activity for the FG [kWh]
e ...	EmCo of the resource [kgCO ₂ e/kWh]
a ...	ProCo of the activity for the resource for the FG [res. unit]
p ...	PowCo of the activity for the resource for the FG [kWh/unit]

To calculate the $uCFP$ of an activity associated with a specific FG, the EC has to be multiplied with the EmCo (e) of the activity. The EC (ec) is calculated by the multiplication of the ProCo (a) and the PowCo (p) of the specific activity. The ProCo, representing the unit input of the resources, is a key concept in both standard cost accounting and the GHG calculations. These coefficients (a , p , e) constitute the 3-LoEC metric, and by varying these levers, the $uCPF$ of the activity can be adjusted accordingly.

Equation (1) additionally contains the sub-indices of the parameters, highlighting the importance of the precise definition of the calculation metric, which will be relevant for the modeling steps. Each sub-index specifies the dependency of the given parameter, and for the EC calculations, the levers (a, p) are always dependent on the activity ($acty$), resource (res), and FG (fG) variables. Resource refers to the different types of equipment that are used for the execution of the activities.

The next step is to define the levers specifically for the IM activities. The original mathematical expressions from the scientific guideline are translated to the language of the AB-LC-ACC methodology by replacing the parameters with the corresponding expressions of the AB-LC-ACC methodology' and by specifying the sub-indices for each parameter. This is the first step toward the operationalization of the original equations.

The product EC is calculated by summing up the EC of the IM activities (specified in Fig. 10). In addition to the EC calculations, the cycle time of the IM process is defined by calculating the ProCo (unit-time) of each activity included in the IM cycle (inject, cool, reset).

This guideline aligns with the AB-LC-ACC methodology since it is activity-based, by defining the EC of the activities, and it is time-driven, by defining the unit-time for these activities. This science-based guideline consists of five steps and follows the chronological order of the implementation by defining the equations in a bottom-up manner. To demonstrate the guideline, an operational order is used by explaining the equations in a top-down way, starting with the last step. To determine the EC of a FG (ec_{fG}) that is produced by an all-electric IM equipment, according to Equation (29) in the Appendix, the EC of the IM process ($ec_{fG;shot}$), and the supporting processes ($ec_{fG;auxiliary}$) have to be divided by the number of the cavities (n_{fG}) of the IM equipment. This thesis considers the drying activity as an example for the supporting process, and the metric to calculate the EC of this activity is explained in the Appendix in Equations (27)-(28). For simplicity, the number of cavities (n_{fG}) is designated as 1, so the EC of a FG (ec_{fG}) equals the sum of the EC of the IM process

($ec_{fG;shot}$) and the auxiliary process ($ec_{fG;auxiliary}$). The EC for the IM process is calculated according to Equation (2):

$$ec_{fG;shot} = ec_{inj,driveU,fG} + ec_{cool,clampU,fG} + ec_{melt,injU,fG} + ec_{reset,clampU,fG} \quad (2) \\ + ec_{control,contrU,fG} + ec_{base\ load,IME,fG}$$

where

$ec_{fG;shot}$: energyCons ... EC for the FG [kWh]

ec_{acty} : energyCons ... EC of the sub-equipment for the activities for the FG [kWh]

The EC of the IM process is calculated by summing up the EC of all the IM process participating activities from Figure 10. Each EC of the activities is calculated in a different way, with various parameters related to the specific activity. Certain activities (*melt*, *inject*, *cool*, and *base load*) are calculated with equations; the remaining activities (*reset* and *control*) are estimated by approximation, relying on the previous activities. The time-driven-based calculation of the 3-LoEC metric is present for the *melt*, *inject*, and *base load* activities by multiplying the ProCo (a) with the PowCo (p) to get the EC (ec) of the activity. The detailed calculations of the ECs are elaborated in the first section of the Appendix.

Regarding the sub-indices, the first part before the semicolon always indicates the variables upon which the given parameter depends, while the second part after the semicolon further specifies the variable, when applicable. The second part of the parameter following the colon, highlighted with grey, represents the operationalized version of the coefficients or parameters, showing the transition from the conceptual to the operational, from the mathematical to the programming domain. These elements no longer contain sub-indices anymore; the dependencies are represented in other forms, e.g., in the data structure or the storage location.

To calculate the cycle time ($a_{IM,eqip,fG}$) of the IM process, the unit-times of the *inject*, *cool*, and *reset* activities have to be summed, according to Equation (3):

$$a_{IM,IME,fG} = a_{inj,driveU,fG} + a_{cool,clampU,fG} + a_{reset,clampU,fG} \quad (3)$$

where

$a_{IM,IME,fG}$: ProCo ... ProCo of the process for the IM equipment (IME) for the FG [s]

$a_{acty,eqip,fG}$: ProCo_acty ... ProCo of the activities for the sub-equipment for the FG [s]

The guide specifies the parameters for equipment and material selection by defining them and by explaining the calculation steps. Further details are in the first section of the Appendix.

To demonstrate a specific application of the guide, the EC calculation of the melting activity is demonstrated. In the guide, the EC of the melting activity is expressed as the last part of Equation (4), which is indirectly the multiplication of the production ($a_{melt,injU,FG}$) and power coefficients ($p_{melt,injU,FG}$).

$$ec_{melt,injU,FG} = a_{melt,injU,FG} \cdot p_{melt,injU,FG} = \frac{V_{fG;shot}}{Q_{melt,injU,FG;mat}} \cdot p_{melt,injU,FG} \quad (4)$$

where

ec : energyCons ...	EC of the melting activity of the sub-equipment ($injU$) for the FG [kWh]
a : ProCo_melt ...	ProCo of the melting activity for the sub-equipment ($injU$) for the FG [sec]
p : PowCo_melt ...	PowCo of the melting activity of the sub-equipment ($injU$) for the FG [kW]
V_{shot} : V_shot ...	volume of the IM shot of the FG [m ³]
Q_{mat} : Q_mat ...	maximum flow rate of the melting activity of the sub-equipment ($injU$) for the FG [m ³ /s]

To calculate the ProCo, the two variables ($V_{fG;shot}$) and ($Q_{melt,injU,FG;mat}$) have to be determined. The volume of the IM shot ($V_{fG;shot}$) is influenced by the parameters listed below Equation (5) and can be calculated according to Equation (5):

$$V_{fG;shot} = V_{fG} \cdot \left(1 + \frac{\varepsilon_{fG}}{100} + \frac{\Delta_{fG}}{100}\right) \cdot n_{fG} \quad (5)$$

where

V_{shot} : V_shot ...	volume of the IM shot of the FG [m ³]
V : V_FG ...	volume of the injection molded FG [m ³]
ε : Epsilon ...	shrinkage rate of the polymer of the FG [%]

Δ : **Delta** ... percentage of the part volume used for the gating system of the FG [%]

n : **n_cav** ... number of cavities related to the FG [1]

The material flow rate for the melting activity ($Q_{melt,eqip,fg;mat}$) is calculated according to Equation (6), and the list of influencing parameters is listed below the equation.

$$Q_{melt,eqip,fg;mat} = \frac{p_{eqip}}{pr_{fg}} = Q_{eqip,max} \cdot \frac{pr_{eqip,max}}{pr_{fg;rec}} \quad (6)$$

where

Q_{mat} : **Q_mat** ... material flow rate of the activity of the equipment for the FG [m³/s]

p : **P_EQIP** ... PowCo of the equipment [W]

pr_{rec} : **p_inj** ... recommended injection pressure of the FG [MPa]

Q_{max} : **Q_max** ... maximum flow rate of the equipment [m³/s]

pr_{max} : **p_max** ... maximum injection pressure of the equipment [MPa]

4.2 IMT domain modeling: Operational domain model

The main goal of the operational domain modeling is to translate the conceptual domain model in Figure 12 into its operational version, illustrated in Figure 13. This transition considers the GHG-accounting concepts as classes and clearly specifies their attributes and methods. The concepts of the cost and GHG accounting are modeled in the UML-class diagram language, and by utilizing the same modeling language for both conceptual and operational modeling, it ensures consistency between the two models. The key concepts in the conceptual modeling are expressed in the same visual modeling language, which is utilized by the IT domain's operational domain. The advantages include not just visual consistency but also terminological consistency between the two domains—accounting and IT—as well.

To represent the IT domain-related concepts, 'IT patterns' are used; one of those patterns is the Entity-Attribute-Value (EAV) pattern². It is used in the *ECSI Standardization* for the ERP-Control system, and it enables dynamically adding properties to the entity tables later, without changing the operational data model itself. It provides flexibility and scalability of the implemented IT application by separating the property and value classes for the *MAT*, *FG* and *EQIP* concepts (tables), as seen in Figure 13. All the calculation parameters are stored according to this pattern in the tables.

The various coefficients of the 3-LoEC metric are shown in the operation domain model in Figure 13; the production and power (*proCo*, *powCo*) are stored in the *Routing* class while the emission (*emCo*) is stored in the *Energy* class. Another important IT pattern is the 'primary key' (*PK*) and 'foreign key' (*FK*). The primary keys identify the table's instances, whereas the foreign keys link to the information specified by the sub-indices in Equation (1).

In addition to the keys, the tables contain supplementary information for the computation, like the attributes and the calculation functions as methods. These calculation functions are shown at the bottom of the *Routing*, *EquipEnergyCons*, and *GHGEmission* tables, and will be discussed further in the subsequent section. This representation is in alignment with the object-oriented design pattern from Evans (2004) DDD methodology. In the tables, certain attributes are shown with the slash (/) mark, which means they are derived from other tables.

² https://en.wikipedia.org/wiki/Entity-Entity-attribute-value_model

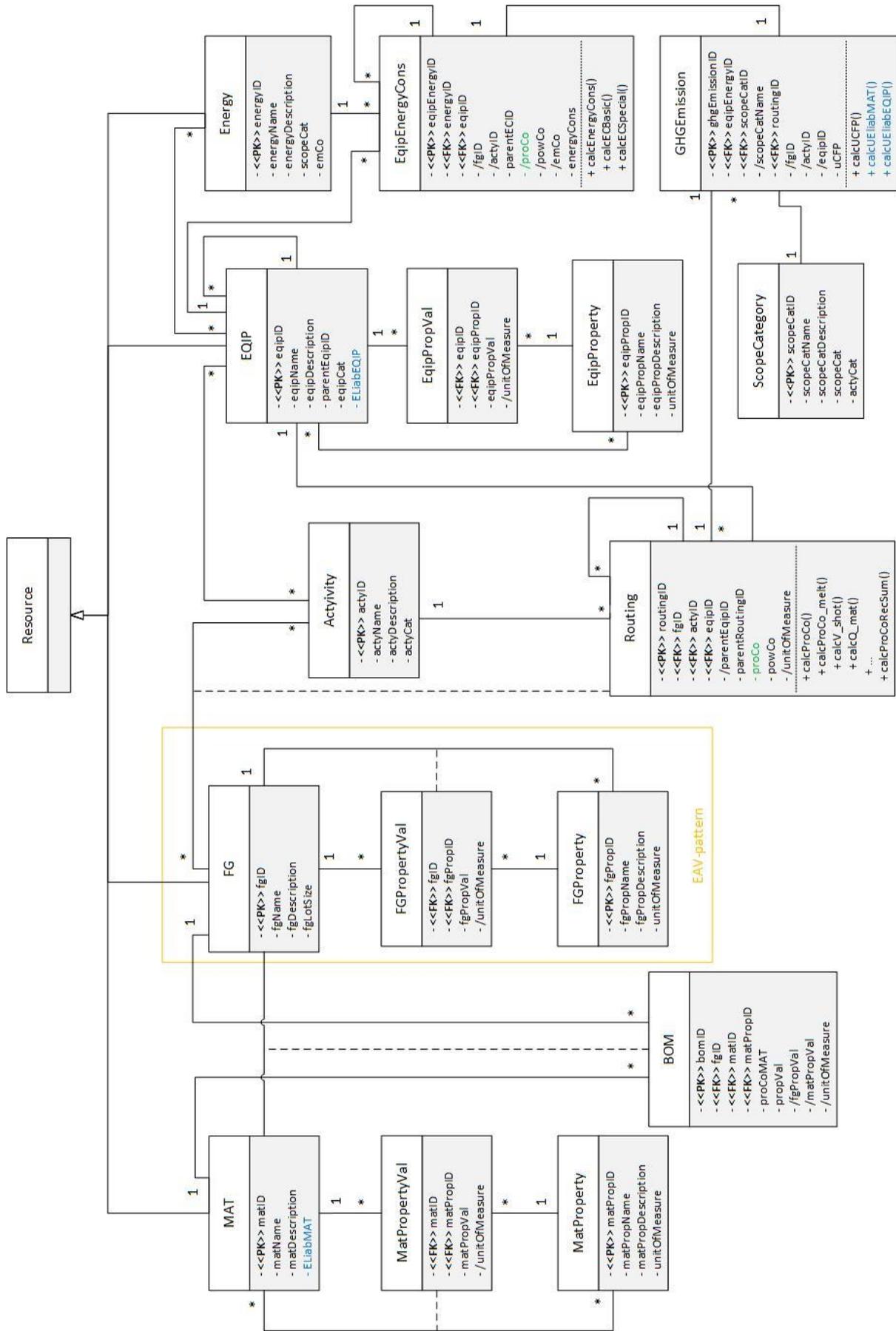


Figure 13 Operational domain model of the IM process in the ERP-Control system (own Figure)

4.3 IMT domain modeling: Relationship of parameters and functions

Key parameters to influence the EC

The operational domain model in Figure 13 shows the structure of the tables and their related attributes but did not specify the parameters that influence the EC of the IMT on a more granular level. It is a complex process; several different factors and parameters influence the EC (Weissman et al., 2010), and the relationship among these parameters is nonlinear (Jung et al., 2021). Numerous studies listed the parameters of the IM process (Matarrese et al., 2017); the two main influencing factors are the material (Muroyama et al., 2011) and the equipment (Weissman et al., 2010). Wu et al. (2023) further divided the parameters into the following categories:

- Temperature: temperature of the barrel and the temperature of the mold.
- Speed: injection speed.
- Time: injection holding time, cooling time, and cycle time.
- Pressure: holding pressure, maximum pressure.
- Stroke position: cushion position, V-P switch-over position.

Processing parameters are important because by optimizing them, the energy performance of the IM process can be improved (Li et al., 2015). An alternative approach is the physical improvement and upgrading of the IM equipment (Arisoy et al., 2015). According to Wu et al. (2023), optimizing the process parameters is more practical and feasible. Jung et al. (2021) stated that the most important parameters are the temperature (molding and hopper) and the time (injection and cycle).

The aforementioned categorization has a technical approach, and it is challenging to align with the concepts of the ERP-Control domain models. Ribeiro et al. (2012), in their study, proposed an alternative categorization for the key influencing factors of EC, and according to them, these are the installed power, cycle time, part maximum thickness, mass of injected material, and material properties. Built on their categorization, and for a better alignment with the ERP-Control domain models, this thesis follows this categorization of the key parameters listed in Table 2:

Category	Parameter	Mathematical	Operationalized
General	Production coefficient	-	proCo
	Power coefficient	-	powCo
	Emission coefficient	-	emCo
FG	Part volume	V	V_FG
	Recommended injection pressure	p_{inj}	p_inj
	Part depth	d	d_FG
	Number of cavities	n	n_cav
	Maximum wall thickness	h_{max}	h_max
	Part surface	A_{part}	A_FG
	Part weight	-	m_FG
	Material	Thermal diffusivity	α
Gating system volume		Δ	Delta
Shrinkage rate		ε	Epsilon
Heat capacity		C_p	C_p
Density		ρ	Rho
Heat fusion		H_f	H_f
Injection temperature		T_{inj}	T_inj
Polymer temperature		T_{pol}	T_pol
Mold temperature		T_m	T_m
Ejection temperature		T_x	T_eject
Emission Liability Material		-	ELiabMAT
Material volume		-	V_MAT
Material weight		M	m_MAT
Maximum moisture content		m	moisture
Travel distance		-	L_travel
Equipment		Maximum pressure	p_{max}
	Maximum flow rate	Q	Q_max
	Dry cycle time	t_d	t_d
	Clamp stroke	S	S_clamp
	Coefficient of performance	COP	COP
	Emission Liability Equipment	-	ELiabEQIP
	Power	P_i	P_EQIP
	Lifetime capacity	-	C_life
	Screw diameter	D	D_screw
	Injection capacity	$V_{injection\ capacity}$	V_inj_cap
	Clamping force	F_{clamp}	F_clamp
	Screw stroke	-	L_s
	Specific Moisture Evap. Rate	SMER	SMER
	Efficiency	η	eta

Table 2 List of key parameters used in the GHG Accounting model

In the *General* category, the *production* and *power coefficients* represent the cycle time and installed power of the equipment, while the last three categories align with the three entity tables from the ERP-Control domain models, namely the *Material*, *FinishedGood*, and *Equipment*. The *Emission Liabilities* in the *Material* and *Equipment* categories represent the external upstream emissions stemming from the material and equipment. The names of the parameters are derived from the scientific guide, and they are listed in the *Mathematical* column, while their operationalized versions are listed in the *Operational* column. The parameters listed in the *Mathematical* column are identical to the ones in the scientific guide (Madan et al., 2013), and the initial two coefficients (*proCo* and *powCo*) are indirectly dependent upon those parameters. The separation of the coefficients from the three parameter categories enables simplified modeling in case the required parameters are unavailable or a straightforward solution is needed.

The key parameters listed in Table 2 are required for the GHG emission calculations, and in order to execute the calculations in a systematic way, the parameters have to be stored in accordance with that system. Initially, they are stored in the ERP system's relevant table, then they are retrieved for the calculation functions to derive the (intermediate) results according to the equations based on the scientific guide, and finally the results of the calculations have to be stored back accordingly into the information system.

The first two coefficients from the *General* category are stored in the *Routing* table; however, their values are calculated using the calculation functions, which will be discussed later in this section. The *EmCo* is stored in the *Energy* table and constitutes external data used for the GHG calculations. The key parameters from the remaining three categories are stored in the *MAT*, *FG*, and *EQIP* 'xxxProperty' and 'xxxPropertyVal' tables according to the EAV pattern.

In Table 2, the *Operational* column represents progress towards practical implementation; however, when it comes to setting up the model with the actual data from the databanks or manufacturer of the equipment, it poses challenges, as each manufacturer may employ their own taxonomy with their preferred unit of measures (*UoM*), which often diverges from the standardized nomenclature and *UoM* of the variables. In order to show these differences and foster the synchronization of the model's data with the manufacturers data, Table 3 presents the science-based guide parameters along with their abbreviations and *UoMs*, mapped to the parameters from the manufacturers data sheet (Arburg, 2022), including their names and *UoMs*. In the Appendix the Figure 46 shows the original data sheet from the manufacturer.

Scientific guide (Madan et al., 2013)			Data sheet from manufacturer (Arburg)	
Name	Abbr.	UoM	Name	UoM
Maximum pressure	p_max	Mpa	Injection pressure	bar
Separating force	F_separating	MN	Ejector force	kN
Injection capacity	V_injection capacity	m^3	Calculated stroke volume	cm^3
Diameter of the screw	D	m	Screw diameter	mm
Injection stroke	S	m	Screw stroke	mm
Maximum flow rate	Q	m^3/s	Injection flow	cm^3/s
Dry cycle time	t_d	s	Dry cycle time	s
Clamp force	-	tf	Clamping force	kN
Clamp stroke	-	m	Opening stroke	mm
Shot volume	-	g	Shot weight	g
Plasticizing capacity	-	g/s	Material throughput	kg/h

Table 3 Conversion table of the scientific guide parameters to the data sheet of the equipment manufacturers

General and specific parameters and equations

In the previous section, the parameters have been operationalized; the next step towards the implementation is the operationalization of the equations. This entails translating them from the mathematical terminology to the computational terminology by leaving the sub-indices and using their operationalized version from Table 2. These sub-indices were previously transformed into the operational domain model through the data structure and linkages among the various tables in the model. The operationalized version of Equation (1) is shown in Equation (7), maintaining the same mathematical logic as Equation (1) but altering the nomenclature of the elements:

$$uCFP = energyCons \cdot emCo = proCo \cdot powCo \cdot emCo \quad (7)$$

where

$uCFP$... uCFP of the activity for the FG [kgCO₂e]

$energyCons$... EC of the resource for the activity related to the FG [kWh]

$emCo$... EmCo of the resource [kgCO₂e/kWh]

$proCo$... ProCo of the activity for the resource for the FG [res. unit]

powCo ... PowCo of the activity for the resource for the FG [kWh/unit]

In the operational domain model, the attributes of the concepts (tables) are consistently stored in lowercase as variables or coefficients, which also applies to the equations derived from them, exemplified by Equation (7), which is a general equation utilizing the general variables, such as *proCo* in the *Routing* table in Figure 13 or in Equation (7). In the calculation of variables for a given activity, the same variable may be represented with a capital letter, such as *ProCo_melt* in Equation (8).

To demonstrate the operationalization of the mathematical model, the specific calculations for the melting activity are shown in Equations (8)-(10). The calculation steps are based on the scientific guide by Madan et al. (2013), and they are further discussed in the first section of the Appendix.

$$ProCo_{melt} = \frac{V_{shot}}{Q_{mat}} \quad (8)$$

where

ProCo_melt ... ProCo of the melting activity for the sub-equipment (injU) for the FG [sec]

V_shot ... volume of the IM shot of the FG [m³]

Q_mat ... maximum flow rate of the melting activity of the sub-equipment (injU) for the FG [m³/s]

To calculate the ProCo for the melting activity, the volume of the IM shot (*V_shot*) has to be divided by the maximum flow rate of the melting activity (*Q_mat*). In the subsequent equations, these variables are specified, beginning with the shot volume in Equation (9):

$$V_{shot} = V_{FG} \cdot \left(1 + \frac{Epsilon}{100} + \frac{Delta.}{100}\right) \cdot n_{cav} \quad (9)$$

where

V_shot ... volume of the IM shot of the FG [m³]

V_FG ... volume of the injection molded FG [m³]

Epsilon ... shrinkage rate of the polymer of the FG [%]

Δ ... percentage of the part volume used for the gating system of the FG [%]

n_{cav} ... number of cavities related to the FG [1]

The variable of shot volume (V_{shot}) is calculated with the above-listed parameters of the melting activity, and the material flow rate is specified in Equation (10):

$$Q_{mat} = Q_{max} \cdot \frac{p_{max}}{p_{inj}} \quad (10)$$

where

Q_{mat} ... material flow rate of the activity of the equipment for the FG [m^3/s]

Q_{max} ... maximum flow rate of the equipment [m^3/s]

p_{max} ... maximum injection pressure of the equipment [MPa]

p_{inj} ... recommended injection pressure of the FG [MPa]

Calculation functions

The previous section addressed the operationalization of the mathematical formulas, but the IM is a complex process; it depends on several factors, and the science-based guide involves many variables and equations for the specific activities. A structured approach to handling its complexity is necessary. This structure is provided by the system of calculation functions, from which the main ones are depicted on the operational domain model in Figure 13. It constitutes a structure due to the presence of multiple levels of functions that are built upon each other and are stored in different locations (tables) to follow the calculation logic of the scientific guide.

Following the steps of the GHG emission calculation outlined in Equation (7), which is the operationalized form of Equation (1), the initial step involves determining the ProCo (*proCo*). In order to calculate the proCo for the entire IM process, all the different activities that are involved in the process have to be considered, as shown in Figure 14.

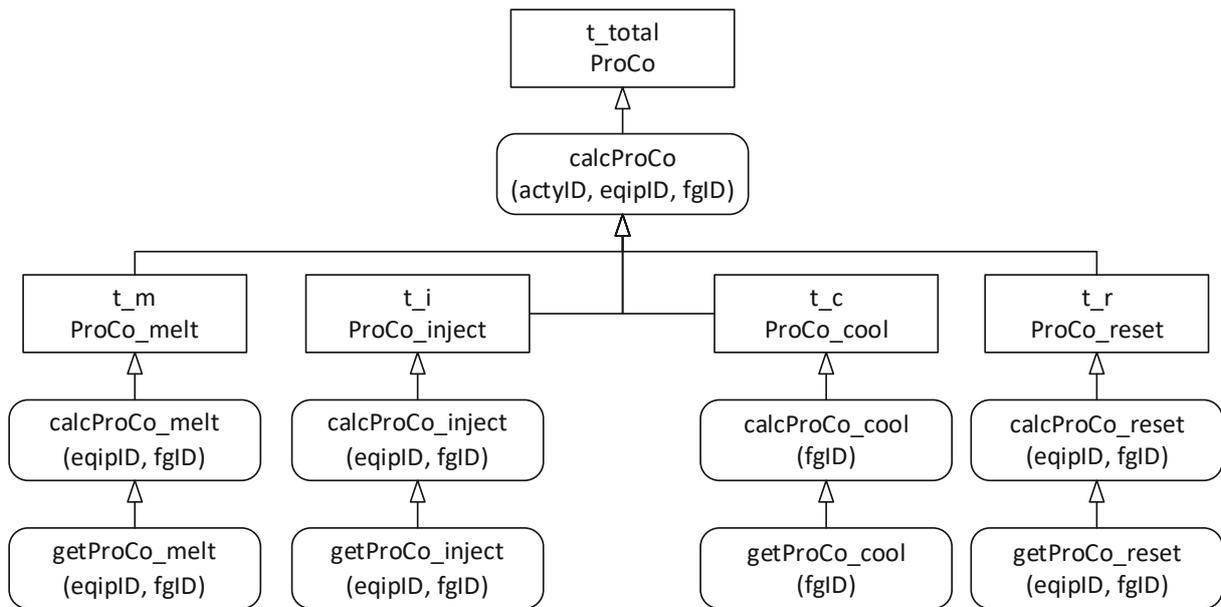


Figure 14 Structure of the calculation functions related to the ProCo of the IM process (own figure)

Figure 14 illustrates the structure of the calculation functions for the *ProCo*, with the rounded rectangles as the different functions and the standard rectangles as the output of the corresponding function and input of the higher-level function. In the rounded rectangles, the names of the functions are specified with all the dependent variables, for example, the *eqplD* and *fgID* for the *calcProCo_melt()* function. The standard rectangles specify the output of the related functions; in the first row, the mathematical name is derived from the scientific guide, while the second row already has the operationalized names. All four functions (*melt*, *inject*, *cool*, and *reset*) are distinct from each other due to the characteristics of the IM process. To demonstrate the lower levels of the *calcProCo()* function, the melting activity is chosen in accordance with the previous operationalization of the parameters and functions from the Equations (8)-(10).

Figure 15 displays the detailed structure of the calculation function of the melting activity. To calculate the *ProCo_melt*, first the *V_shot* and *Q_mat* have to be calculated with the relevant functions (*calcV_shot()* and *calcQ_mat()*). These lower-level functions are calculated using the input parameters connected to them on the bottom of Figure 15, for instance, the part volume for the *calcV_shot()* function, which is shown in the bottom left corner of the figure. The first row of the normal rectangle describes the mathematical names of the parameters according to the scientific guideline, while the second row specifies their operationalized name with the respective category of the parameter; in the case of the part volume '*V*' the operational name is *V_FG* and it belongs to the FG parameter category. The figure contains additional functions, namely the get functions (*getV_shot()*), which are relevant for the

implementation of the GHG calculation model, and they will be addressed accordingly in the subsequent chapter.

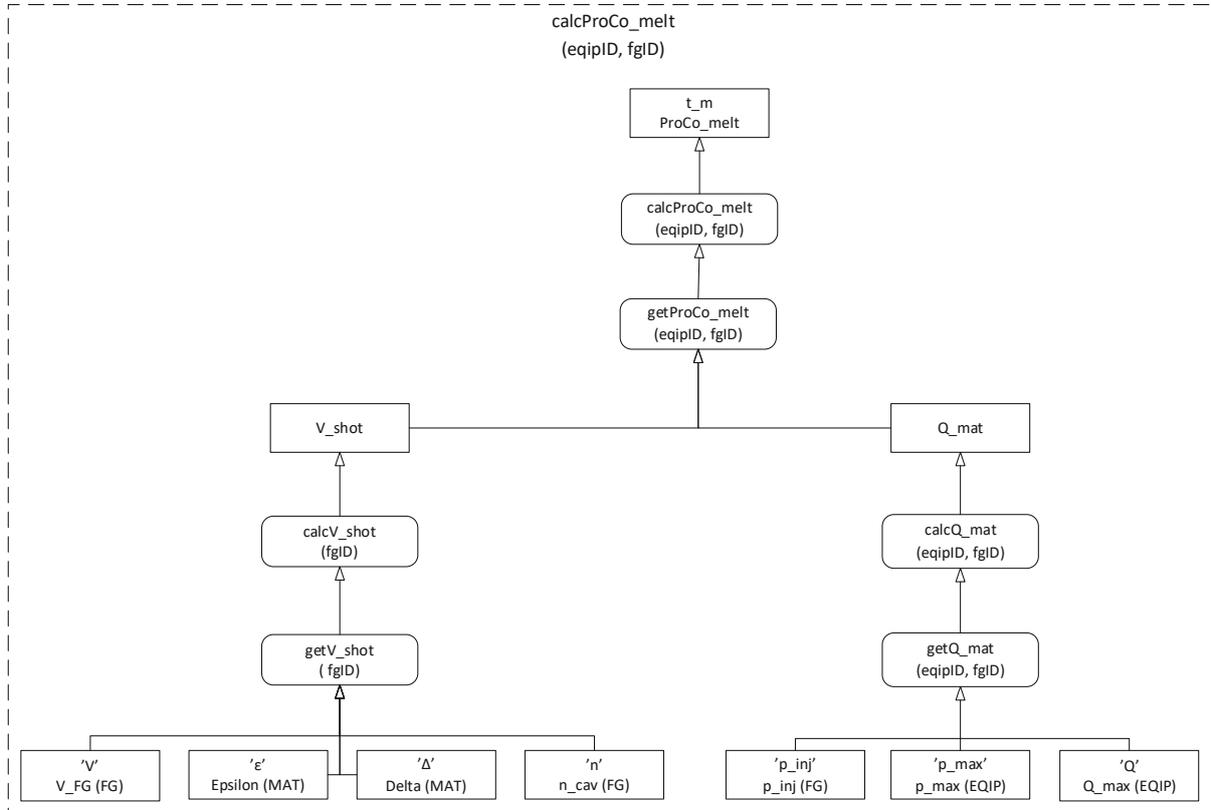


Figure 15 Detailed structure of the calculation function of the melting activity (*calcProCo_melt()*) with all the parameters (own figure)

The same calculation logic applies to the other ProCo calculation functions, except for *calcProCoRecSum()*, which is a recursive function designed to recursively add up the calculation functions for the ProCos of the IM activity. This will be examined in detail in the following chapter. The PowCo is calculated similarly to the ProCo; the sole distinction is that no recursive summation is necessary, as the different power values are equipment-specific and independent of each other. In the operational domain model depicted in Figure 13, the calculation functions for the production and power coefficients are connected to the *Routing* table, as the results of these functions are stored in that table.

Following the calculation logic outlined in Equation (7), the next step after defining the production and power coefficients is to calculate the EC associated with the various activities. The *calcEnergyCons()* function is defined for this purpose and linked to the *EquipEnergyCons* table, based on the same logic as the coefficients are connected to the *Routing* table. The *calcEnergyCons()* function comprises two sub-functions in order to distinguish between the basic calculations (*calcECBasic()*) and the specific ones (*calcECSpecial()*). The basic

function facilitates the normal multiplication of the relevant coefficients (*proCo* and *powCo*) for the different activities, while the special function addresses the unique cases that require special calculation logic to determine the EC of a given activity; further information regarding the special cases can be found in Appendix 8.1.

The last step of the GHG emission calculation following Equation (7) is to calculate the uCFP of the activities. These calculations are executed by the *calcUCFP()* function, which determines the uCFP for each internal activity through the multiplication of the ECs with the relevant EmCos. For the external upstream emission calculations, the *calcUEliabMAT()* and *calcUEliabEQIP()* functions are responsible, utilizing the E-Liability metric (described in Chapter 3.3), with the calculation logic detailed in Appendix 8.2. These calculation functions are linked to the *GHGEmission* table, as their results are stored accordingly in that table.

The system of the calculation functions is crucial, and to prepare for the implementation, a scientific approach is necessary to maintain structured and clean programming. This scientific approach is provided by the functional programming, which is defined as (Hu et al., 2015, p. 349): *“Functional programming is a style of programming: the main program is a function that is defined in terms of other functions, and the primary method of computation is the application of functions to arguments. Unlike traditional imperative programming, where computation is a sequence of transitions from states to states, functional programming has no implicit state and places its emphasis entirely on expressions (or terms).”*

The following IT patterns were applied in the implementation of the model (Chambers, 2014; Hudak, 1989):

- First-class and Higher-order functions: Functions can be assigned to variables, passed as arguments, and returned by other functions. Higher-order functions are functions that take other functions as parameters or return them as results.
- Pure functions: Functions that have no side effects; given the same input, they always return the same output.
- Immutability: Variables are assigned values only once and cannot be modified after their initial assignment.
- Function composition: A modular and reusable approach where complex functions are built by combining smaller ones.

5. AB-LC-GHG-Accounting: Prototypical Implementation

In the following chapter, the prototypical implementation of the AB-LC-GHG-Accounting model will be discussed, focusing on the implementation of the operationalized model by coding the model's information system and its functionalities in a programming language (implementation). For the implementation, an object-oriented programming language, 'R_Tidyverse' (Wickham et al., 2023), is used, which is capable of data science methodologies and supports the UML's object-oriented modelling paradigm. It is an open-source programming language based on R's statistical foundations and also allows consistent data selection, manipulation, and modeling tasks.

To demonstrate the implementation, a practical use case is employed, which will be described first. After this, the implementation steps will be discussed, starting with the entity and relationship table creation, followed by the translation of the functions from the operational design chapter. The application of these functions will be demonstrated on the use case, and the corresponding results will be presented and discussed. Different aspects of the GHG emissions will be illustrated with graphical figures to help the understanding and facilitate the comparison of the different scenarios.

5.1 Use Case definition: Plastic bowl production

The use case for this thesis is the serial production of two different types of plastic bowls with the IMT. Two distinct materials are used for the two types of bowls: polylactic acid (PLA) and polypropylene (PP).

PLA Material

PLA is a relatively new plastic type, in the early stages of its development, unlike the fossil-derived plastics, which have been produced for about a century (Carus, 2017). It is a thermoplastic derived from natural lactic acid, and corn starch, sugarcane, or tapioca roots are used as organic raw materials for the production. The properties of the PLA are similar to those of other polymers, leading to significant interest in its integration into the plastic industry as a feasible alternative to the petroleum-based thermoplastics. It is an eco-friendly thermoplastic distinguished by its biocompatibility, biodegradability, and compostability, which can be processed similar to other thermoplastics (Enemuoh et al., 2021).

PP Material

PP is a synthetic resin formed by the polymerization of propylene. As a significant family of polyolefin resins, it is molded or extruded into various plastic items that necessitate toughness, flexibility, light weight, and heat resistance³. It is a rather easy material for IM despite its semicrystalline characteristic, and it can be processed by nearly all thermoplastic-processing methods⁴.

Use case

The implementation is demonstrated by the serial production of two distinct plastic bowls seen in Figure 16. As proposed by Muroyama et al. (2011), the implementation has a systematic approach, taking into account the transportation of the material, the heating of the IM facility, and the upstream emissions associated with the material and equipment used for the IM process. Two different all-electric IM equipment are used for the demonstration because this machine type is the most energy efficient (Kanungo & Swan, 2008). The demonstration case is based on a previous study (Alaoui et al., 2024), incorporating an additional FG with updated material, FG, and equipment details.

³ <https://www.britannica.com/science/polypropylene>

⁴ <https://www.bpf.co.uk/plastipedia/polymers/PP.aspx>

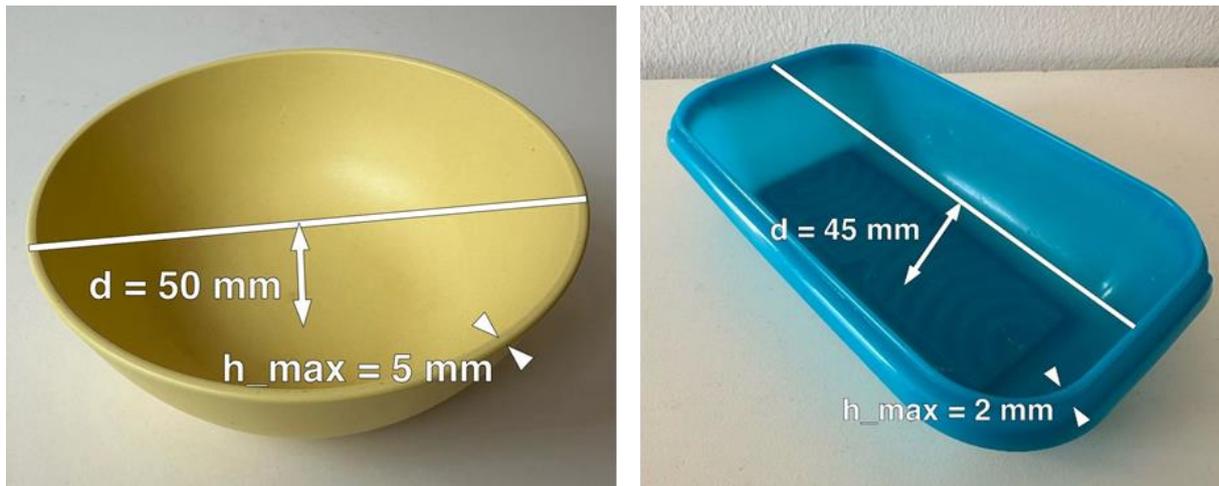


Figure 16 Demonstration plastic bowls (FG 1, FG 2) with the most relevant information for IM technology (d... depth, h_max... maximum wall thickness) (own figure)

The implementation steps will be demonstrated based on this use case information:

FG 1 specific information

- Plastic bowl consists of PLA plastic with the weight of 124 g/unit.
- Per lot, 100 pieces of the bowl are produced so that the lot weight is 12.4 kg.
- E-Liability of the PLA plastic is 0.5 kgCO_{2e}/kg.
- IM equipment is 'Arburg Allrounder 520E': 28 kW nominal power.
- E-Liability of the equipment 'Arburg Allrounder 520E' is 11,900 kgCO_{2e}/kg.
- PLA is transported 500 km via truck (Transport activity), which gives 6.2 ton-kilometers (t-km) for the transport activity.

FG 2 specific information

- Plastic bowl consists of PP plastic with the weight of 50 g/unit.
- Per lot, 100 pieces of the bowl are produced so that the lot weight is 5 kg.
- E-Liability of the PP plastic is 1.9 kgCO_{2e}/kg.
- IM equipment is 'Arburg Allrounder 470E': 21 kW nominal power.
- E-Liability of the equipment 'Arburg Allrounder 470E' is 9150 kgCO_{2e}/kg.
- PLA is transported 600 km via truck (Transport activity), which gives 3 ton-kilometers (t-km) for the transport activity.

General information

- Both materials are dried for 2 h with the Dryer equipment ‘Arburg Thermolift 100-3’.
- The space occupied for each IM equipment with the auxiliary equipment and storage space is 100 m², and the heating is calculated for that space as well.
- Heater equipment is ‘Master BLP 103 Direct Gas Fired Heater’ that operates with an average consumption of 0.28 m³/h natural gas with an energy of 10.73 kWh/m³ for heating the IM equipment’s located production shop.
- The weather conditions were considered for Central Europe’s climate conditions.
- Heater’s gas has an EmCo of 0.2 kgCO_{2e}/kWh.
- Transportation vehicle is operated with diesel, and the diesel consumption of the truck is 1.89 liters per 100 t-km.
- Diesel has an energy of 9.94 kWh/liter and an EmCo of 0.27 kgCO_{2e}/kWh.
- EmCo is the grid emission factor based on the Austrian energy mix for scope 2 emission and the year 2023, amounting to 76 gCO_{2e}/kWh.

5.2 IMT domain implementation: Entity and Relationship tables

The implementation starts with establishing the fundamentals, specifically the creation of the entity and relationship tables derived from the operational domain model. In order to store and organize the data in a structured way, a relational database in a table form is applied. In this table form, the rows denote the entities, while the columns indicate the specific attributes from the operational domain model. With the primary and foreign key pattern, defined in the operational section, relationships of the different tables can be established.

One category of these tables is the ‘entity tables’, which are utilized to represent and store information about entities. An entity is a distinct object or thing in the real world that can be uniquely identified and described. The entity tables include the *MAT*, *FG*, *EQIP*, *Energy*, or the *Activity*, which is shown in Figure 17.

actyID	actyName	actyDescription	actyCat
1	1001	Melting	Melting the polymer ... Primary
2	1002	Injecting	Injecting the molten ... Primary
3	1003	Cooling	Cooling the injected ... Primary
4	1004	Resetting	Resetting the equip... Primary
5	1005	Control	Control of the electr... Primary
6	1006	BaseLoad	Base load of the inje... Primary
7	1007	InjectionMolding	Injection molding st... Primary
8	1008	Drying	Drying the plastic be... Secondary
9	1009	Heating	The heating of the p... Secondary
10	1010	Transport	Transportation of go... Secondary

Figure 17 Activity table to store the activities accordingly

In the Activity table, all the activities are represented, which are involved in the IM production process. The *actyID* serves as a primary key, providing a unique identifier to the entities of the table in order to distinguish the instances of the table. The *actyName* and *actyDescription* attributes serve to name and describe the specific activity, while the *actyCat* is to categorize the activities into two groups: *Primary*, encompassing the main activities, which participate in the IM process, like the *Melting* or *Cooling* activities, and *Secondary*, comprising the auxiliary activities, which support the IM process, like the *Drying* or *Transport* activities.

Another entity table is the *FG*, as shown in Figure 18, which contains all the FGs for the use case: the *DecoBowl* with *fgID 9001* (referred as FG 1) and the *FoodBowl* with *fgID 9002* (referred as FG 2). Unlike the *Activity* table, the last attribute is the *fgLotSize*, which specifies the quantity of the produced FGs for the given FG for this use case.

fgID	fgName	fgDescription	fgLotsize
1	9001	DecoBowl	A small decorative bowl with a thin wall, ...
2	9002	Food Bowl	A food-grade polypropylene bowl, desig...

Figure 18 FG table as an entity table showing the EAV pattern

The previous tables illustrated several entity tables that store the entities without specifying their properties or attributes. According to the Entity-Attribute-Value (EAV) pattern, discussed in Chapter 4.2, in order to provide dynamic updates to the tables without changing the operational data structure, the attributes of the entities have to be stored in a separate table, like the *FGProperty* table in Figure 19.

fgPropID	fgPropName	fgPropDescription	unitOfMeasure
1	9107	p_inj	Recommended injection pressure for the material
2	9108	n_cav	Number of the used cavity for the injection molding

Figure 19 FGProperty table as an attribute table showing the EAV pattern

The *fgPropID* in this table uniquely identifies the various attributes of the FG entity, and similar to the *FG* table, the properties have a name and description. The *unitOfMeasure* is also specified for the table, according to the operational domain model in Figure 13. The entries in Figure 19 represent the required parameters (*p_inj* and *n_cav*) associated with the FG, essential for calculating the ProCo of the melting activity (*ProCo_melt*), as outlined in Equations (8)-(10). The *unitOfMeasure* for the number of cavities (*n_cav*) is NA, indicating that a numerical value is required for this parameter.

Another type of the relational database is the ‘relationship table’, utilized to manage many-to-many relationships between two entity tables. These tables constitute the Value tables from the EAV pattern, used to store the values for the entities’ attributes. They contain foreign keys from the tables they join and often include additional attributes that describe the relationship. An example of this is the *FGPropVal* relationship table shown in Figure 20.

fgPropValID	fgID	fgPropID	fgPropName	fgPropVal	unitOfMeasure
1	909107	9001	9107	p_inj	100 MPa
2	909108	9001	9108	n_cav	1 NA

Figure 20 FGPropVal table as a relationship table showing the EAV pattern

The *fgPropValID* serves as the identifier of the entries, but it is not designated as a primary key. The *fgID* and *fgPropID* serve the foreign keys according to the operational domain model in Figure 13, linking the corresponding tables to the *FGPropVal* table, as seen by the *fgPropValID* values; they are the combinations of the *FG* and *FGProperty* tables primary

keys (90xx and 91xx). The table contains the *fgPropName* for enhanced readability and the *fgPropVal* to store the actual values for the FG properties, namely 100 MPa for the injection pressure and 1 for the number of the cavities.

Following the same pattern, the property values are shown in Figure 21 for the *Material* and in Figure 22 for the *Equipment*. They have the same structure as the *FGPropVal* table, and in the snippets only the *ProCo_melt* relevant parameters are shown, *Epsilon* and *Delta* for the *Material* and *Q_max* and *p_max* for the *Equipment*.

	matPropValID	matID	matPropID	matPropName	matPropVal	unitOfMeasure
	All	All	All	All	All	All
1	202104	2001	2104	Epsilon	1	%
2	202105	2001	2105	Delta	15	%

Figure 21 MatPropVal table as a relationship table showing the EAV-concept

	equipPropValID	equipID	equipName	parentEquipID	equipPropID	equipPropName	equipPropVal	unitOfMeasure
	All	All	All	All	All	All	All	All
1	404111	4002	DriveUnit_01	4007	4109	Q_max	164	cm ³ /s
2	404112	4003	ClampUnit_01	4007	4110	p_max	200	MPa

Figure 22 EquipPropVal table as a relationship table showing the EAV-concept

Another important entity table is the *Energy* table from the operation domain model, as shown in Figure 13. It stores the relevant information about the energy sources, including their scope categories and the EmCos, which are essential for the GHG emission calculations. It has the *energyID* as the primary key, and similarly to the other entity tables, the next two attributes describe the entries of the table (*energyName* and *energyDescription*). The *scopeCat* is to specify the corresponding scope (~1, ~2, or ~3) for the energy source according to the *GHG Protocol* as discussed in Chapter 2.1. The *emCo* attribute defines the EmCo of the energy source based on the external source as elaborated in Chapter 3.3.

BOM

An important concept of the ERP-Control domain is the *BillOfMaterial*, which connects the *Material* with the *FG* entity tables, as discussed in Chapter 2.2. This *BOM* relationship table specifies the quantity of an input material required to produce a given FG as shown in Figure 23.

	bomID	fgID	matID	matPropID	matPropName	matPropVal	proCoMAT	propVal	unitOfMeasure
	All	All	All	All	All	All	All	All	All
1	902001	9001	2001	2102	m_MAT	1.0	0.124	0.124	kg
2	902002	9001	2001	2114	L_travel	100.0	5.000	500.000	km
3	902003	9001	2001	2115	ELiabMAT	0.5	0.124	0.062	kg CO2e

Figure 23 BOM relationship table

The *bomID* serves as a primary key that uniquely identifies the distinct entries in the table, since its values are derived from the combination of the *FG* and *MAT* tables (90xx and 20xx). The *fgID* and *matID* as foreign keys specify the relationship between the *FG* and *MAT*, while the *matPropID*, also a foreign key, indicates the specific property of this relationship for which the value is stored in the *matPropVal* column, sourced from the *MatPropertyVal* table. The *proCoMAT* specifies the material's input per unit of output of the *FG*, which ratio is quantified in the *propVal* column with its corresponding *unitOf Measures* in the last column. The first row indicates that the input material contains 1 kg of units for the *FG* 1 (9001), and to produce 1 unit of this *FG* 1, 0.124 unit of the input material is required. In the third row, the *ELiabMAT* for the input materials unit is 0.5 kg CO₂e per kg of the material, and 1 unit *FG* 1 from this material has the unit *ELiab* (*uELiabMAT*) of 0.062 kg CO₂e. In the full *BOM*, all relationships of this use case are specified for both *FGs*.

Routing

The *Routing* table is another important concept that, like the *BOM*, connects the *FG* but with the *Activity* and *Equipment* tables to define the sequence of operations with the required resources to complete the activities. The initial *Routing* relationship table is shown in Figure 24.

	routingID	fgID	actyID	equipID	parentEquipID	parentRoutingID	proCo	uomProCo	powCo
	All	All	All	All	All	All	All	All	All
1	901001	9001	1001	4001	4007	NA	NA	h	NA
2	901002	9001	1002	4002	4007	901007	NA	h	NA
3	901003	9001	1003	4003	4007	901007	NA	h	NA
4	901004	9001	1004	4003	4007	901007	NA	h	NA
5	901005	9001	1005	4004	4007	NA	NA	h	NA
6	901006	9001	1006	4007	NA	NA	NA	h	NA
7	901007	9001	1007	4007	NA	NA	NA	h	NA
8	901008	9001	1008	4008	NA	NA	NA	h	NA
9	901009	9001	1009	4009	NA	NA	NA	h	NA
10	901010	9001	1010	4010	NA	NA	NA	ton-km	NA

Figure 24 Routing relationship table

The *routingID* serves as the primary key uniquely identifying each entry of the table by the combination of the FG and Activity IDs (90xx and 10xx). By the connection of the foreign keys of *fgID*, *actyID*, and *equipID*, each activity executed by a specific equipment for a given FG is specified. To establish the recursive relationships of the *Equipment* and *Routing* tables described in Chapter 3.3, the *parentEquipID* and *parentRoutingID* columns are introduced; the former is derived from the *Equipment* table, while the latter is explicitly specified in the *Routing* table, as indicated in the operational domain model in Figure 13. These concepts are used to describe the hierarchical relationships of the equipment and activities, as illustrated in Figure 10. The initial five activities (1001-1005) are using the four sub-systems of the equipment (4001-4004), all of which are parts of the manufacturing equipment (4007). The *parentRoutingID* is essential because in the IM cycle only the three activities (1002-1004) are involved; the melting activity (1001) is running parallel to the IM cycle, as illustrated in Figure 11.

The ProCo specifies the activities and equipment input per unit of output of the FG, and the subsequently calculated results are stored in the *proCo* column, with the corresponding *UoM* as discussed in Chapter 3.3. The UoM (*uomProCo*) for the proCo is unit time (*hour*) except for the last activity (*transport*), which is not time-driven, like the previous activities, but rather resource consumption-driven with the *ton-km* as UoM.

The power coefficient (*powCo*) indicates the power of the given equipment that is used to execute the given activity for the given FG. Similarly to the *proCo*, it will be calculated later, and the results will be stored in the *proCo* column. The coefficient (*proCo* and *powCo*) columns are blank at the moment of the creation of the *Routing* table, and they will be computed by the calculation functions or specified by the user later.

5.3 IMT domain implementation: GHG Accounting functionalities

After establishing the fundamentals by creating the entity and relationship tables, the next step involves calculating the relevant coefficients using the corresponding parameters and calculation functions. For these calculations, the already established parameters and the operationalized equations are employed, and to maintain a systematic approach to the function creation, the IT patterns of the functional programming were followed from Chapter 4.3. To demonstrate the application of the calculation functions, similarly to the previous chapters, the ProCo for the melting activity (*ProCo_melt*) is calculated in two steps; initially, the intermediate results are calculated with the sub-functions, followed by the application of these sub-functions to calculate the final result of the ProCo.

In order to calculate the *ProCo_melt*, first the intermediate results of *V_shot* (shot volume) and *Q_mat* (material flow rate) have to be calculated according to Equation (8). Following the Function composition IT pattern from the functional programming patterns, the value for *Q_mat* is calculated in three steps: first, the requisite parameters are retrieved with a *getQ_mat()* function, shown in Figure 25; then these parameters are calculated with the *calcQ_mat()* function, shown in Figure 26; and finally, the results of the calculation are displayed with the *displayQ_mat()* function, as shown in Figure 27.

```

Function: getQ_mat (.GlobalEnv)
1 function(equipID, fgID) {
2   # Retrieve the parent equipment ID associated with the given equipID
3   parentEquipID <- EQIP.tbl %>%
4     filter(equipID == !!equipID) %>%
5     pull(parentEquipID) %>%
6     first()
7
8   # Use equipID if parentEquipID is NA
9   parentEquipID <- if (is.na(parentEquipID)) equipID else parentEquipID
10
11  # Retrieve the maximum flow rate using the parent equipment ID for injection
12  Q_max <- EquipPropVal.tbl %>%
13    filter(parentEquipID == !!parentEquipID, equipPropID == 4109) %>%
14    pull(equipPropVal) %>%
15    first()
16
17  # Retrieve maximum pressure using the parent equipment ID for clamping
18  p_max <- EquipPropVal.tbl %>%
19    filter(parentEquipID == !!parentEquipID, equipPropID == 4110) %>%
20    pull(equipPropVal) %>%
21    first()
22
23  # Retrieve injection pressure for the finished good
24  p_inj <- FGPropertyVal.tbl %>%
25    filter(fgID == !!fgID, fgPropID == 9107) %>%
26    pull(fgPropVal) %>%
27    first()
28
29  return(list(Q_max = Q_max, p_max = p_max, p_inj = p_inj))
30 }

```

Figure 25 *getQ_mat()* function – Parameter retrieving function for the calculation

To calculate the material flow (Q_{Mat}) defined in Equation (10), the initial step involves retrieving the input parameters. However, these input parameters are varied, not just because they relate to distinct entities (like FG or $EQIP$), but also because they can relate to different sub-entities (like sub-systems of the equipment). This is represented in this function, where the two equipment parameters, the maximum flow rate (Q_{max}) and the maximum pressure (p_{max}), correspond to different sub-systems of the equipment.

To implement this function with several input parameters would require additional lines of code, increase the complexity, and prolong the execution time. To solve the complex input parameter problem, the adjacency pattern is implemented in the form of the parent-children IDs, as demonstrated in the first part of the function. The *parentEquipID* is designated to identify the parent equipment of the sub-systems of the equipment, which the different parameters belong to. This solution renders the *parentEquipID* sufficient because, with the additional *equipPropID*, the required parameter can be effortlessly retrieved from the *EquipPropVal* table as shown in Figure 22.

The R-Tidyverse function `filter()` is utilized to subset rows from the data frame; in this case, the *equipID* and the `!!` operator are used to treat the value of the *equipID* as a variable rather than treating it as a column name. It is important because, without this operator, only the first matching value for the condition would be displayed. The R-Tidyverse function `pull()` is used to extract a single column from a data frame as a vector, whereas the `first()` function returns the first element of a vector or a list. This solution keeps the code more concise and comprehensible. At the end of the function, the retrieved parameters are stored in a list.

Upon retrieving the required input parameters for the Q_{mat} function from the database, the subsequent step is to calculate them accordingly. The `calcQ_mat()` function in Figure 26 shows this calculation step by taking the parameters from the previously created list and computing the results according to Equation (10). The result of the function is the Q_{Mat} .

```
Function: calcQ_mat (.GlobalEnv)
1 function(equipID, fgID) {
2   # Get the parameters
3   params <- getQ_mat(equipID, fgID)
4
5   # Calculate the adjusted material flow rate (Q_Mat)
6   Q_Mat <- params$Q_max * params$p_inj / params$p_max
7
8   return(Q_Mat)
9 }
```

Figure 26 `calcQ_mat()` function – Calculation function of the material flow rate (Q_{mat})

The `displayQ_mat()` function is called to present the results of the previously created functions, providing the intermediate results for the specified input parameters, as shown in Figure 27.

```
Finished Good ID: 9001
Maximum flow rate (Q_max): 164 cm3/s
Maximum pressure (p_max): 200 MPa
Injection pressure (p_inj): 100 MPa
Calculated material flow rate (Q_Mat): 82 cm3/s
```

Figure 27 `displayQ_mat()` function – Results of the display function for equipment and FG

Upon calculating the intermediate results for the `ProCo_melt`, the next step is to utilize them for the second calculation step. In this step, the `ProCo_melt` is computed by following the identical IT pattern as in the first step. First, the `getProCo_melt()` function is called, which returns the previous intermediate results as a list of input variables for the actual calculation. The High-order function IT pattern is applied for this case because other functions (e.g., `calcV_shot()`) were used to return the results of this function, as shown in Figure 28.

```
Function: getProCo_melt (.GlobalEnv)
1 function(equipID, fgID) {
2   # Retrieve the shot volume (V_shot) for the given FG
3   V_shot <- calcV_shot(fgID)
4
5   # Retrieve the material flow rate (Q_mat) for the given equipment and FG
6   Q_mat <- calcQ_mat(equipID, fgID)
7
8   return(list(V_shot = V_shot, Q_mat = Q_mat))
9 }
```

Figure 28 `getProCo_melt()` function – Parameter retrieving function for the calculation

Similarly to the `getProCo_melt()` function, the previously defined functions are utilized to calculate the results, and the code for this is shown in Figure 29.

```
Function: calcProCo_melt (.GlobalEnv)
1 function(equipID, fgID) {
2   # Calculate the ProCo_melt directly using V_shot and Q_mat
3   ProCo_melt <- calcV_shot(fgID) / calcQ_mat(equipID, fgID)
4   return(ProCo_melt)
5 }
```

Figure 29 `calcProCo_melt()` function – Calculation function of the ProCo for the melting activity

The displayed results for `ProCo_melt` are shown in Figure 30.

```
Finished Good ID: 9001
Shot volume (V_shot): 116 cm3
Material flow rate (Q_mat): 82 cm3/s
Calculated production coefficient for melting (ProCo_melt): 1.414634 s
```

Figure 30 `displayProCo_melt()` function – Results of the display function of the ProCo for melting activity

The results for the lower level (children) are calculated using these functions; however, they need to be summarized to obtain the results of the higher levels (parent). In case of multiple levels and multiple entities, the manual summation of the results can be demanding, making automation advantageous. A recursive summation function *calcProCoRecSum* is defined, which leverages the adjacency pattern with the *parentIDs*. Figure 31 displays this recursive summation function for *proCo*.

```

Function: calcProCoRecSum (.GlobalEnv)
1 function() {
2   # Extract unique parentRoutingIDs that are actually used and have children
3   parentIDs <- unique(Routing.tbl$parentRoutingID[
4     !is.na(Routing.tbl$parentRoutingID)])
5
6   # Function to update a single parent's proCo based on its children
7   updateParentProCo <- function(parentID) {
8     # Calculate the sum of proCo of children linked to this parent
9     childProCos <- sum(Routing.tbl$proCo[
10      Routing.tbl$parentRoutingID == parentID], na.rm = TRUE)
11
12    # Update the parent's proCo if the sum is greater than 0
13    if (childProCos > 0) {
14      Routing.tbl$proCo[Routing.tbl$routingID == parentID] <-< childProCos
15      # Check if this parent has its own parent and update recursively
16      grandParentID <- Routing.tbl$parentRoutingID[
17        Routing.tbl$routingID == parentID]
18      if (!is.na(grandParentID)) {
19        updateParentProCo(grandParentID)
20      }
21    }
22  }
23
24  # Apply the function to each parent ID
25  invisible(sapply(parentIDs, updateParentProCo))
26 }

```

Figure 31 *calcProCoRecSum()* function – Calculation function for the *ProCo* with recursive summation

The recursive summation function *calcProCoRecSum* works as follows:

- The function identifies all the unique *parentRoutingID* values from the *Routing.tbl* data frame into a list that are actually used, i.e., they are not NA.
- The helper function *updateParentProCo* is defined, which will be used to update the *ProCo* value of a parent based on the sum of the *ProCo* values of its children.
- The sum of the *ProCo* for all children of a specific parent, identified by *parentID* is calculated and stored in the variable *childProCos*.
- The *ProCo* value of a parent is updated if the sum of its children's *ProCo* is greater than 0.
- The next section checks whether the current parent (identified by *parentID*) has its own parent (i.e., it is a child of another parent). If it does, the function is called recursively to update the grandparent's *ProCo*.
- The last section applies the *updateParentProCo* function to each *parentID* in the list of *parentIDs*.

In certain cases, not all children values are relevant for the recursive summation; for example, the cycle time (*proCo*) of the IM activity comprises just three activities (inject, cool, and

reset), which must be summarized for the correct results as it was discussed in Chapter 5.2. By defining the *parentIDs* in the *Routing* table (*parentRoutingID*), the real-world scenario can be accurately modeled.

When all the coefficients are either calculated with the calculation functions or defined by the user, the results have to be saved appropriately. The *Routing* table serves this function, and the updated table reflecting the results of the use case is shown in Figure 32.

	routingID	fgID	actyID	eqplID	parentEqplID	parentRoutingID	proCo	uomProCo	powCo
	All	All	All	All	All	All	All	All	All
1	901001	9001	1001	4001	4007	NA	0.03929539	h	19.1260080
2	901002	9001	1002	4002	4007	901007	0.07859079	h	4.1000000
3	901003	9001	1003	4003	4007	901007	1.64587002	h	0.1463858
4	901004	9001	1004	4003	4007	901007	0.11778807	h	NA
5	901005	9001	1005	4004	4007	NA	1.84224888	h	NA
6	901006	9001	1006	4007	NA	NA	1.84224888	h	0.2000000
7	901007	9001	1007	4007	NA	NA	1.84224888	h	NA
8	901008	9001	1008	4008	NA	NA	2.00000000	h	NA
9	901009	9001	1009	4009	NA	NA	1.84224888	h	3.0000000
10	901010	9001	1010	4010	NA	NA	6.20000000	ton-km	0.1900000

Figure 32 Routing relationship table with the updated coefficients (ProCo and PowCo)

The ProCos are related to the entire lot (*fgLotSize*), as delineated in the *FG* table in Figure 18, in contrast to the result of the *ProCo_melt()* function, which was calculated only for a single FG. This distinction is irrelevant for the PowCo, as it is independent of the quantity of the produced FGs.

The initial four proCos for the activities are calculated with specific functions as shown in Figure 14. The IM cycle is defined by the three activities (1002-1004), where the *parentRoutingID* is not NA, and the cycle duration is calculated for the IM activity (1007) applying the recursive summation function (*calcProCoRecSum()*). The *Control* and *BaseLoad* activities (1005 and 1006) are executed parallel to the IM cycle, according to the *Process Map* shown in Figure 11, while the *Heating* activity (1009) has the same proCo as the IM cycle due to its relevance for the whole cycle. The *proCo* for the *Drying* activity (1008) is defined by the technology, but for the *Transport* activity (1010), it is defined by the user, based on the relevant information about the activity.

The powCos are calculated or defined for the activity, rendering them independent of the number of repetitions. The first three activities are calculated according to the scientific guide, while the remaining three activities are defined directly by the user. If the values are NA, the calculation of the ProCos is not applicable.

5.4 IMT domain implementation: Application of GHG Accounting functionalities

The coefficients for the EC are specified; the following step is to calculate the EC and, consequently, the associated GHG emissions. In order to calculate the GHG emission of an activity, it is essential to include not only the EC but also the type of this energy, because that can influence the GHG emissions depending on the EmCo (*emCo*) of the energy source. To properly categorize the different energy sources, the *Energy* table is created with the corresponding scope category and *emCo* as shown in Figure 33.

energyID	energyName	energyDescription	scopeCat	emCo	
1	5001	Electricity mix	Electricity generated from mixed sources	Scope 2	0.076
2	5002	Natural gas	Natural gas for energy generation	Scope 1	0.200
3	5003	Fuel	Fuel for transportation	Scope 1	0.270

Figure 33 Energy table with the corresponding scope category and *emCo*

The use case encompasses three distinct energy sources (*electricity*, *gas*, and *fuel*), which are categorized accordingly into scope categories; the EmCos for these are sourced from external databanks.

The *EquipEnergyCons* table is created by joining the *EQIP*, *Energy* and *Routing* tables to calculate the EC of the activities executed by different equipment as shown in Figure 34.

equipEnergyID	energyID	equipID	actyID	fgID	parentECID	parentEquipID	proCo	powCo	emCo	
1	405001	5001	4001	1001	9001	405007	4007	0.03929539	19.1260080	0.076
2	405002	5001	4002	1002	9001	405007	4007	0.07859079	4.1000000	0.076
3	405003	5001	4003	1003	9001	405007	4007	1.64587002	0.1463858	0.076
4	405004	5001	4003	1004	9001	405007	4007	0.11778807	NA	0.076
5	405005	5001	4004	1005	9001	405007	4007	1.84224888	NA	0.076
6	405006	5001	4007	1006	9001	405007	NA	1.84224888	0.2000000	0.076
7	405007	5001	4007	1007	9001	NA	NA	1.84224888	NA	0.076
8	405008	5001	4008	1008	9001	NA	NA	2.00000000	NA	0.076
9	405009	5002	4009	1009	9001	NA	NA	1.84224888	3.0000000	0.200
10	405010	5003	4010	1010	9001	NA	NA	6.20000000	0.1900000	0.270

Figure 34 EquipEnergyCons table with the different coefficients (Production, Power, and Emission) of the activities

The table has all the important attributes from the *Routing* table, and it is extended with:

- *energyID*, required for the further categorization of the emissions,
- *parentECID*, required for the summation of the EC of the sub-equipment,
- *emCo*, required for the EC calculations of the activities.

The *BaseLoad* (1006) activity has a *parentECID* but lacks a *parentEquipID*. The reason is that this activity is directly ordered to the main IM equipment and not to one of the sub-systems of the equipment.

To calculate the EC, two cases have to be distinguished, the basic and the special one. In the basic case, they are calculated by a simple multiplication of the *proCo* and *powCo*, and the UoM of the results is kWh. The calculation function for this case is shown in Figure 35.

```

Function: calcEnergyCons (.GlobalEnv)
1 function() {
2
3 # Function to calculate basic energy consumption with efficiency adjustment
4 calcECBasic <- function(proCo, powCo, parentEquipID, actyID) {
5   if (!is.na(proCo) && !is.na(powCo)) {
6     basic_energy <- proCo * powCo
7     # Adjust the basic energy based on efficiency and activity type
8     if (actyID %in% c(1001, 1002, 1003, 1006, 1009, 1010)) {
9       efficiency <- EquipPropVal.tbl %>%
10        filter(equipID == !!parentEquipID, equipPropID == 4126) %>%
11        pull(equipPropVal) %>%
12        first()
13      # Only adjust if efficiency is defined and greater than zero
14      if (!is.na(efficiency) && efficiency > 0) {
15        basic_energy <- basic_energy / efficiency
16      }
17    }
18    return(basic_energy)
19  } else {
20    return(NA) # Return NA if any coefficient is missing
21  }
22 }

```

Figure 35 *calcEnergyCons()* function – Basic EC calculation for the given activities

The *calcECBasic()* function works as follows:

- The function takes four parameters: *proCo*, *powCo*, *parentEquipID*, and *actyID*.
- It checks if both *proCo* and *powCo* parameters are present; if any are absent, it immediately returns NA.
- If both coefficients are present, then the basic EC is calculated using the formula: $basic_energy = proCo \times powCo$.
- Next, the basic energy is adjusted based on the efficiency and activity type. This happens only for these activities: {1001, 1002, 1003, 1006, 1009, 1010}.
- The efficiency value is retrieved from the *EquipPropVal* table with the *parentEquipID* and the *EquipPropID* of 4126.
- If efficiency is neither missing nor zero, then the basic energy is adjusted by dividing it with the efficiency to get the adjusted basic energy.
- Finally, the basic EC is returned; if any required coefficient is missing, then NA is returned.

Certain special cases render the *PowCo* inapplicable, like the *Resetting* (1004), the *Control* (1005), or the *Drying* (1008) activities. In these cases, Madan et al. (2013) suggest a percentage-based summation of the other activities EC; for example, the reset activity

accounts for 25% of the other three activities (1001-1003) EC. The control activity, similarly to the reset, is 20% of the previous four activities (1001-1004). The snippet of the calculation function of the special cases is shown in Figure 36.

```

24 # Function to calculate energy consumption for special cases
25 calcECSpecial <- function(actyID, equipID, fgID, parentEquipID, equipEnergyID) {
26
27 # Retrieve ProCo and PowCo for the given activity and equipment ID
28 proCo <- EquipEnergyCons.tbl %>%
29   filter(actyID == !!actyID, equipID == !!equipID, fgID == !!fgID) %>%
30   pull(proCo) %>%
31   first()
32
33 powCo <- EquipEnergyCons.tbl %>%
34   filter(actyID == !!actyID, equipID == !!equipID, fgID == !!fgID) %>%
35   pull(powCo) %>%
36   first()
37
38 # Special logic for Resetting activity (actyID 1004)
39 if (!is.na(actyID) && actyID == 1004) {
40   relevantActivities <- c(1001, 1002, 1003)
41   energyCons <- EquipEnergyCons.tbl %>%
42     filter(fgID == !!fgID, actyID %in% relevantActivities) %>%
43     summarise(totalEnergy = sum(energyCons, na.rm = TRUE)) %>%
44     mutate(E_reset = 0.25 * totalEnergy) %>%
45     # Calculate EC for resetting as 25% of total energy from previous ACTYs
46     pull(E_reset)
47   return(energyCons)
48 }

```

Figure 36 `calcECSpecial()` function – Special EC calculation for the given activities

The `calcECSpecial()` function for the *Resetting* activity (1004) works as follows:

- The function takes five input parameters: *actyID*, *equipID*, *fgID*, *parentEquipID*, and *equipEnergyID*.
- It retrieves the *proCo* and *powCo* for the given *actyID* and *equipID* from the *EquipEnergyCons* table.
- If *actyID* is present and equals 1004, the special energy calculation is applied.
- A predefined set of relevant activities {1001, 1002, 1003} is defined.
- The total energy consumed is calculated for the relevant activities for the given *fgID*.
- The resetting EC is computed as 25% of the total EC from these activities.

The other special cases are coded accordingly, and the calculation logic for the drying activity is detailed in the Appendix 8.1.

After applying the calculation functions, the output of the functions has to be saved; thus, the *EquipEnergyCons* table is extended with the *energyCons* column as shown in Figure 37. The EC is calculated for each activity using the `calcEnergyCons()` function, except the *InjectionMolding* activity (1007), which represents the whole IM activity, and to summarize it, the same recursive summation logic is applied, like for the *proCos* in the previous section.

For the recursive summation, the *parentECID* is utilized, and the result is stored accordingly in the same table, shown in Figure 37.

	equipEnergyID	energyID	actyID	equipID	fgID	parentECID	proCo	powCo	emCo	energyCons
	All	All	All	All	All	All	All	All	All	All
1	405001	5001	1001	4001	9001	405007	0.03929539	19.1260080	0.076	0.7515640
2	405002	5001	1002	4002	9001	405007	0.07859079	4.1000000	0.076	0.3222222
3	405003	5001	1003	4003	9001	405007	1.64587002	0.1463858	0.076	0.2409320
4	405004	5001	1004	4003	9001	405007	0.11778807	NA	0.076	0.3286796
5	405005	5001	1005	4004	9001	405007	1.84224888	NA	0.076	0.2629436
6	405006	5001	1006	4007	9001	405007	1.84224888	0.2000000	0.076	0.3684498
7	405007	5001	1007	4007	9001	NA	1.84224888	NA	0.076	2.2747912
8	405008	5001	1008	4008	9001	NA	2.00000000	NA	0.076	0.8611111
9	405009	5002	1009	4009	9001	NA	1.84224888	3.0000000	0.200	5.5267466
10	405010	5003	1010	4010	9001	NA	6.20000000	0.1900000	0.270	1.1780000

Figure 37 EquipEnergyCons table extended with the energyCons results

Direct GHG Emissions

To calculate the direct (Scope 1 and Scope 2) GHG emissions, the EC (*energyCons*) has to be multiplied with the *emCo*, which was specified for all energy source types in the *Energy* table in Figure 33. The results of the GHG emission calculations are referred to as the unit-Carbon Footprint (*uCFP*); they are stored in the *GHGEmission* table, which serves as the relationship table for the *Routing*, *EquipEnergyCons*, and *ScopeCategory* tables as shown in Figure 38.

	ghgEmissionID	equipEnergyID	equipID	fgID	actyID	energyCons	emCo	uCFP
	All	All	All	All	All	All	All	All
1	906001	405001	4001	9001	1001	0.7515640	0.076	0.05711886
2	906003	405002	4002	9001	1002	0.3222222	0.076	0.02448889
3	906005	405003	4003	9001	1003	0.2409320	0.076	0.01831083
4	906007	405004	4003	9001	1004	0.3286796	0.076	0.02497965
5	906009	405005	4004	9001	1005	0.2629436	0.076	0.01998372
6	906011	405006	4007	9001	1006	0.3684498	0.076	0.02800218
7	906013	405007	4007	9001	1007	2.2747912	0.076	0.17288413
8	906015	405008	4008	9001	1008	0.8611111	0.076	0.06544444
9	906017	405009	4009	9001	1009	5.5267466	0.200	1.10534933
10	906019	405010	4010	9001	1010	1.1780000	0.270	0.31806000

Figure 38 GHGEmission table of the direct (scope 1 and scope 2) emissions

The table has the *ghgEmissionID* as the primary key and *equipEnergyID* as one of the foreign keys. The *Routing* foreign key is split into the *actyID*, *equipID*, and *fgID* attributes for enhanced clarity; however, the *scopeCatID* is not shown in this snippet because it will be relevant to the categorization discussed subsequently. The *uCFP* represents the GHG emissions for the entire lot (100 pieces) with the UoM of kgCO₂e. All the activities are considered direct contributors to the GHG emissions. The EC and GHG emissions of the activities for a given FG are illustrated in the form of bar plots as shown in Figure 39.

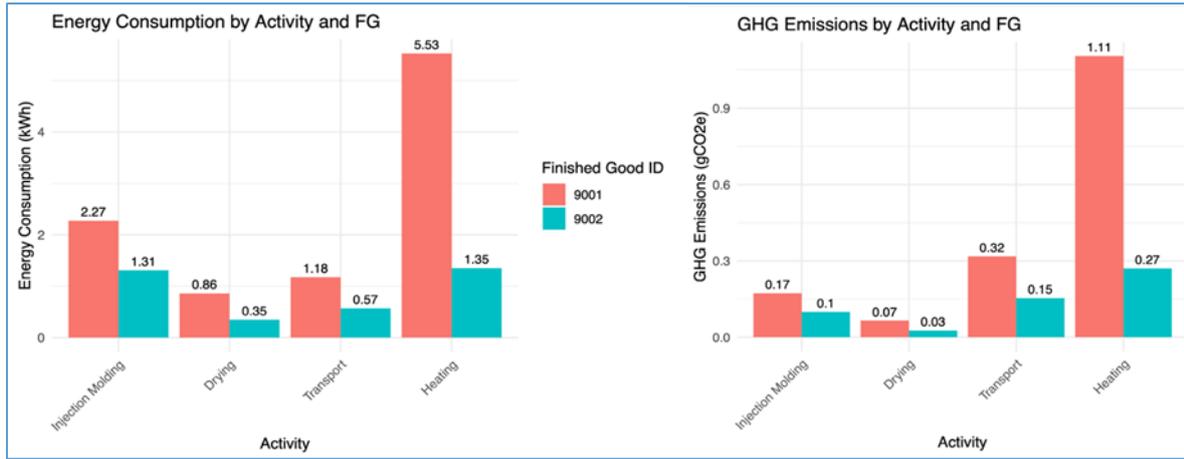


Figure 39 Bar plot of the EC and GHG emissions of the activities by FG (own figure)

This plot considers the IM sub-activities (1001-1006) as a singular main activity (1007), and it is extended with the additional activities (1008-1010). The left side displays the EC in kWh, while the right side shows the GHG emissions for both FGs (red or first for FG 9001, blue or second for FG 9002). The SEC value for the IM activity for FG 1 is calculated by dividing the EC (2.27 kWh) with the mass (0.124 kg) and the lot size (100 pieces) of FG 1, the result is 0.183 kWh/kg, which falls within the specified range for the all-electric IM equipment (0.11-0.37 kWh/kg), as established by Kanungo & Swan (2008). The SEC value for FG 2 is 0.262 kWh/kg, calculated by dividing 1.31 kWh by 0.05 kg and 100 pieces, and is within the specified range.

To enhance the comparability of the EC and GHG emission results, Figure 40 shows two pie charts derived from the previous figure, focusing only on the first FG (9001). The left pie chart represents the EC, with the biggest contribution from the *Heating* activity (~56%), followed by the *Injection Molding* activity at about 23%, and the combined contribution of the *Drying* and *Transport* activities totaling around 20%.

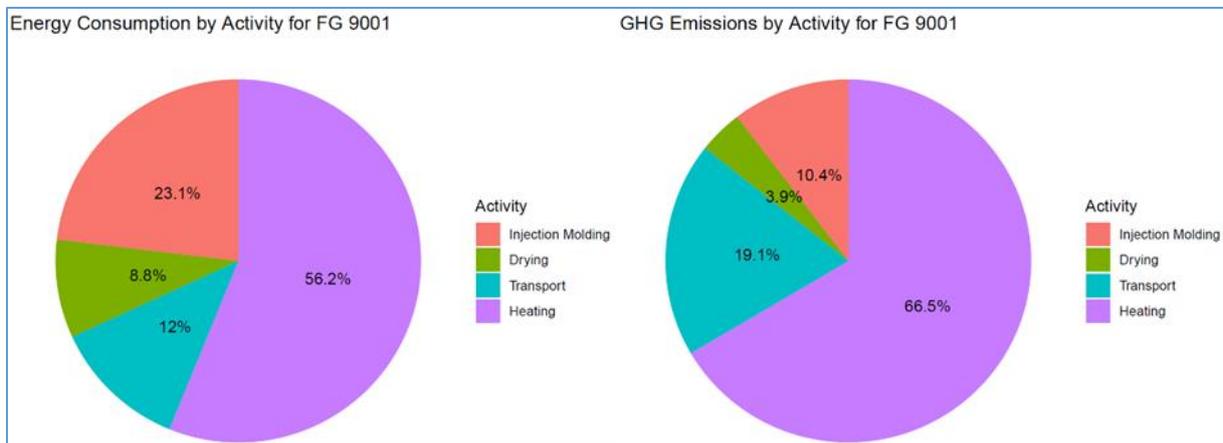


Figure 40 Pie charts of the EC and GHG emissions by activities for FG 9001 (own figure)

The right pie chart shows the GHG emissions, with *Heating* accounting for over two-thirds, *Transport* comprising nearly 20%, and the *Injection Molding* and *Drying* activities representing around 15%. The significant differences between the two charts results stem from the emCo, as heating exhibits almost three times and transport almost four times higher emCo compared to the other two activities (*Injection Molding* and *Drying*), which use electricity, in contrast to natural gas (*Heating*) and diesel (*Transport*).

A key advantage of the hierarchical structure of the IM process is the possibility to zoom in and analyze the activity on a more granular level. Figure 41 presents a detailed view of the IM activity at the sub-activity level for a specific FG using pie charts. Both sides show the EC for the different FGs, and the relatively huge differences in the *Cooling* and *Base Load* activities stem from the process characteristics.

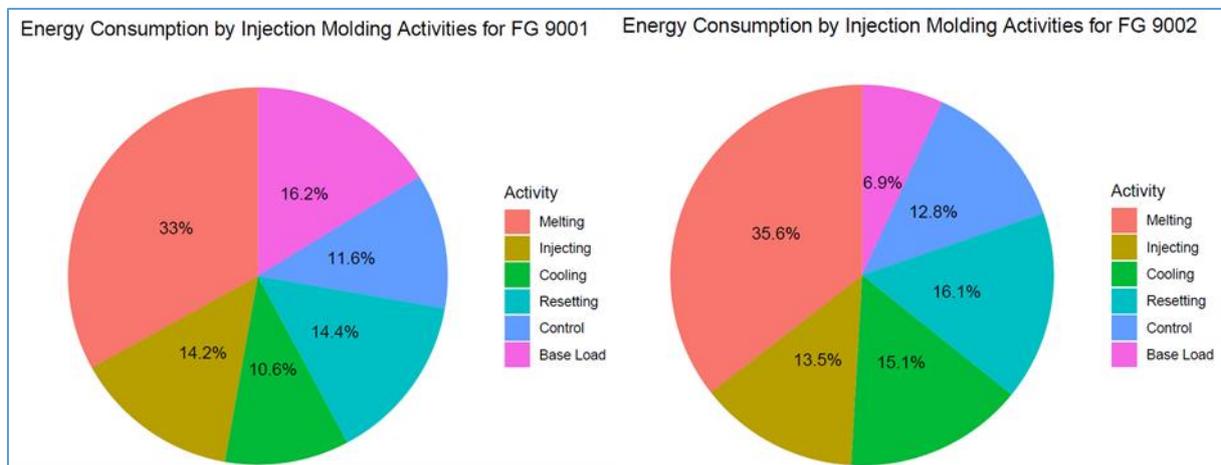


Figure 41 Pie charts of the detailed EC by activities for FG 9001 and FG 9002 (own figure)

Indirect GHG Emissions

The indirect (Scope 3) GHG emissions represent the embedded upstream emissions associated with the materials and equipment. Kaplan & Ramanna (2021) introduced the Environmental-Liabilities (E-Liabilities) concept to be able to track GHG emissions, which are accumulated during the whole life cycle of a product.

The E-Liabilities for the equipment are calculated based on the manufacturer's press release about the IM equipment carbon footprint (Arburg, 2022) and the ratio of the production time and lifetime capacity of the equipment. The E-Liabilities for the material are calculated based on its weight and Global Warming Potential (GWP) according to Morão & De Bie (2019). The E-Liability calculations are based on the methodology of Alaoui et al. (2024) while utilizing different input data; more details are available in Appendix 8.2.

So far, all the direct and indirect GHG emissions are calculated; however, for a detailed analysis, they have to be categorized as well. This categorization is based on the *ScopeCategory* table from the Operational Domain model in Figure 13, and it contains three main categories: the *primary*, *secondary*, and *Emission-Liability* CFPs, based on the activity types, which are further subdivided into specific scope categories as illustrated in Figure 42.

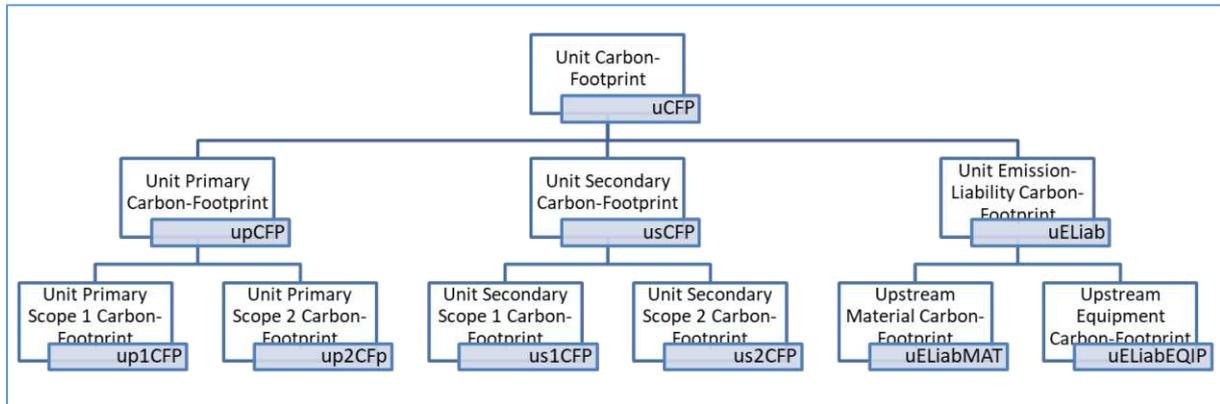


Figure 42 GHG emission categorization (own figure)

For the use case relevant categories are:

- Unit Primary Scope 1 Carbon-Footprint (*up1CFP*):
Scope 1 emissions of the primary activities for the given FG
- Unit Primary Scope 2 Carbon-Footprint (*up2CFP*):
Scope 2 emissions of the primary activities for the given FG
- Unit Secondary Scope 1 Carbon-Footprint (*us1CFP*):
Scope 1 emissions of the secondary activities for the given FG
- Unit Secondary Scope 2 Carbon-Footprint (*us2CFP*):
Scope 2 emissions of the secondary activities for the given FG
- Upstream Material Carbon-Footprint (*uELiabMAT*)
- Upstream Equipment Carbon-Footprint (*uELiabEQIP*)

To calculate the different *uCFP* values for the distinct categories, the *calcUCFP()* function is employed, which calculates the *uCFP* for the entire lot (100 pieces) as shown in Figure 43.

The *calcuCFP()* function for a given FG works as follows:

- The dataset from the *GHGEmission* table is filtered to extract relevant data for the specified *fgID*.
- The corresponding lot size value is retrieved from the *FG* table based on the *fgID*, using the *pull()* function.
- The *uCFP_value* is directly assigned from the dataset using the *mutate()* function.
- The activity hierarchy is considered to calculate the total *uCFP* for a given activity.
- The total *uCFP* value is returned for the entire lot for the given *fgID* in kgCO_{2e}.

```

Function: calcUCFP (.GlobalEnv)
1 ~ function(fgID) {
2   # Filter data for the given finished good ID
3   fg_data <- GHGEmission.tbl %>%
4     filter(fgID == !!fgID)
5
6   # Get the lot size
7   lot_size <- FG.tbl %>%
8     filter(fgID == !!fgID) %>%
9     pull(fgLotsize)
10
11  # Assign the uCFP value directly (in kgCO2e)
12  fg_data <- fg_data %>%
13    mutate(uCFP_value = uCFP)
14
15  # Calculate the total uCFP value considering the activity hierarchy
16  total_uCFP_value <- fg_data %>%
17    mutate(uCFP_value = ifelse(actyID %in% 1001:1006, 0, uCFP_value)) %>%
18    summarise(total_uCFP_value = sum(uCFP_value, na.rm = TRUE)) %>%
19    pull(total_uCFP_value)
20
21  # Return the value with units in kgCO2e
22  return(paste("The total carbon footprint for the finished good", fgID,
23    "is", round(total_uCFP_value, 2), "kgCO2e (not per unit)."))
24 ~ }
  
```

Figure 43 calcUCFP() function – uCFP calculation function for a given FG

Figure 44 presents the total uCFP for the entire IM facility. The left bar plot illustrates the *Total GHG emissions* for FG 1, including the upstream emissions of the material and equipment, while the right bar plot represents the previously described *calcuCFP()* function from Figure 43, with the different scope and activity categorizations based on the emission categorization in Figure 42.

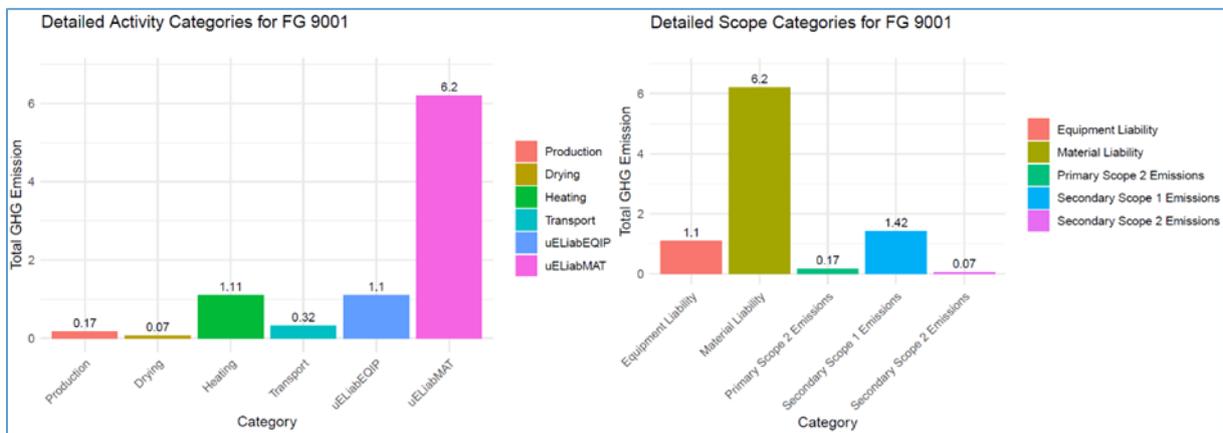


Figure 44 Bar plots of the detailed Activity and Scope categories for FG 9001 (own figure)

For FG 1, the primary contributor to GHG emissions is upstream emissions, with materials (*uELiabMAT*) accounting for around two-thirds of total emissions. The upstream equipment (*uELiabEQIP*) emission is similar to the *Heating* activity; both account for around 12%, while the combined emissions from *Production*, *Drying*, and *Transport* activities comprise in total around 6%.

6. Conclusion

Summary

The research objective of this master's thesis was “*specification and implementation of the proposed Activity-based GHG Accounting model by setting up a digital system that extends the existing ERP system with a sustainability assessment in the form of GHG Accounting.*”

To establish a methodological framework for the specification and implementation of the Activity-based GHG Accounting model, the AB-LC-ACC methodology was employed. The model development was segmented into three steps, each guided by distinct research questions (RQ). The first RQ focused on the specification of the modeling language and the conceptual domain modeling using the specified language:

RQ1: How can the modeling language for the AB-LC-ACC methodology be specified, and how can the IM-specific domain knowledge be modeled with this language on a conceptual level?

For the conceptual modeling, the ‘Tryptich of conceptual modeling’ was utilized, facilitating the specification of knowledge within the IM domain and the modeling language, thereby enabling the representation of this domain knowledge in accordance with the requirements of the conceptual model defined by the creators of the Tryptich.

The modeling language was specified based on the ERP-Control domain and the UML modeling language, and this notation was used to create a process map of the IMT, which was based on the domain knowledge of the IM technology. This modeling language was employed to create the conceptual domain model for the IMT by extending the ERP-Control domain model with the relevant attributes of the GHG emission modeling.

The next model development step was the operationalization of the conceptual model, for which the following research question was defined:

RQ2: How can the mathematical model of the IM domain be translated into an operational model that is aligned with the conceptual language?

The mathematical model specified in a scientific guide for calculating the EC in IMT was analyzed, and for the operationalization, relevant parameters and equations were translated into an operational language. The operational language was synchronized with the conceptual

model by using the same terminology from the conceptual model and by rephrasing the parameters into a format suitable for implementation.

Subsequently, the operational domain model was created by applying these formalities and defining the concepts relevant to the implementation of the operational model. These concepts include the key parameters and functions, which were defined in the operational language based on the mathematical model.

The final step of the model development is the implementation of the operationalized model, for which the following research question was defined:

RQ3: How can the operational model defined by the AB-LCA-ACC methodology be implemented using a data science-capable programming language?

The operational domain model was implemented by coding the AB-LC-GHG-Accounting model, including the functionalities in a data science-capable programming language. A use case was defined, which described the production of two different plastic bowls using IMT. The implementation started with the definition of the entity and relationship tables, which provide the fundamentals for the subsequent calculations and analysis. The content of these tables was created by the calculation functions, which specified all the relevant parameters and variables for the following steps. The EC and the GHG emissions were calculated by applying distinct calculation functions, and the results were categorized and visualized for proper analysis.

The scientific contribution of this master's thesis is twofold: on the one hand, it provides a comprehensive, ERP-Control domain based approach to the GHG emission modeling for the IMT by considering the multi-level structure of the activities and the manufacturing equipment. This more granular, process-oriented, and information system based approach provides additional information, which can be leveraged for multiple purposes: process optimization, sustainable manufacturing practices, and detailed sustainability management and reporting.

On the other hand, the extended life-cycle perspective on the manufacturing process, which considers the cradle-to-gate boundary, facilitates a holistic view for the whole life cycle of the product until the end of the production. It helps to identify the GHG emission-relevant stages of the life cycle, enabling the companies to focus on the serious emission sources and work on the optimization of these emitters.

Outlook

Possible directions for further research may involve the extension of the AB-LC-GHG-Accounting model to include the whole IM process, defined by the scientific guideline for IM technology, necessitating the addition of activities, materials, and equipment. With the extra activities, like blending and regrinding, the whole IM process can be covered, and these activities are not energy intensive, so they can add a new type of activity-equipment connection. Furthermore, the blending activity will necessitate the addition of new materials, such as colorants and adhesives. Another type of material can be the reused scrap from the regrinding activity, which would require new aspects for the modeling. The new materials would increase the material complexity and could require a multi-level BOM structure as well. Regarding the equipment, the forthcoming model version should have a many-to-many relationship for the activities and equipment, like the original scientific guide, as opposed to the current one-to-many relationship. With the extension of the model, the parameters could be extended as well; one possibility could be the shape of the FG as a parameter category because it has a great impact on the EC of the IM process.

Another direction for model extension could be the inclusion of additional life cycle stages after the production, like the use or disposal phase. These extensions would enable a more realistic modeling, with more details and a broader product portfolio. Upon analyzing the whole life cycle, the model could reach a higher level of complexity, hence aligning more effectively with corporate requirements through the cradle-to-gate boundary.

Although, the calculated SEC results for the all-electric IM equipment provide a validation for the GHG emission calculation model, however, further research on the same technology and a comparison with former calculation models could increase the validity and improve the accuracy of the model. Benchmarking against industry standards would be beneficial and could contribute to identify areas for further innovation.

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8. Appendix

8.1 IMT: Summary of Madan's guide for the EC of the IMT

In this section for the EC and GHG emission calculations, necessary parameters and equations will be demonstrated based on the science-based guideline developed by Madan et al. (2013).

This science-based guideline estimates the EC of the IM technology by defining the material and equipment-specific parameters for the calculations, and it consists of five steps (Madan et al. 2013):

1. Determine initial process parameters.
2. Define cavity details and determine other process parameters.
3. Select an IM machine.
4. Determine cycle time and theoretical minimum energy requirements.
5. Estimate EC.

In the first step, the IM process parameters, like the injection pressure (P_{inj}), injection temperature (T_{inj}), and mold temperature (T_m), are determined. These parameters are related to the material and, to some extent, to the geometry of the FG. The guideline provides recommended values for some thermoplastic materials; for different materials, additional data can be found at the IM equipment manufacturers and in online data banks.

The second step defines the cavity details like the volume of cavity (V_{cavity}) or the volume of the shot (V_{shot}) and determines other process parameters. Equations (11) and (12) show the cavity and shot volumes with the relevant parameters:

$$V_{fG;cav} = V_{fG} \cdot \left(1 + \frac{\varepsilon_{fG}}{100}\right) \quad (11)$$

where

- | | |
|-------------------|---|
| V_{cav} ... | volume of the cavity of the FG [m ³] |
| V ... | volume of the injection molded FG [m ³] |
| ε ... | shrinkage rate of the polymer of the FG [%] |

$$V_{fG;shot} = V_{fG} \cdot \left(1 + \frac{\varepsilon_{fG}}{100} + \frac{\Delta_{fG}}{100}\right) \cdot n_{fG} \quad (12)$$

where

V_{shot} ...	volume of the IM shot of the FG [m ³]
V ...	volume of the injection molded FG [m ³]
ε ...	shrinkage rate of the polymer of the FG [%]
Δ ...	percentage of the part volume used for the gating system of the FG [%]
n ...	number of cavities related to the FG [1]

Additional process parameters are the cavity projected area and the separating force, which are relevant for the equipment selection; more details about them are in the original guide (Madan et al. 2013).

In the third step, the IM equipment is selected based on the injection capacity, clamp force, plasticizing capacity, and clamp stroke parameters, which are defined in the original guide. The IM equipment selection is based on the aforementioned parameters and on the data sheet of the equipment, provided by the equipment manufacturers.

The fourth step determines the cycle times and the theoretical minimum energy requirements. The IM process cycle time consists of the injection time (t_i), cooling time (t_c), and mold resetting time (t_r), as shown in Figure 11. To calculate the injection time (t_i), first the average flow rate (Q_{mat}) shown in Equation (13) should be calculated, which is half of the maximum flow rate (Q_{avg}) as it is shown in Equation (14):

$$Q_{acty,eqip,fG;mat} = \frac{p_{eqip}}{pr_{fG}} = \frac{Q_{eqip;max} \cdot pr_{eqip;max}}{pr_{fG;rec}} \quad (13)$$

where

Q_{mat} ...	material flow rate of the activity of the equipment for the FG [m ³ /s]
p ...	PowCo of the equipment [W]
pr_{rec} ...	recommended injection pressure of the FG [MPa]
Q_{max} ...	maximum flow rate of the equipment [m ³ /s]

pr_{max} ... maximum injection pressure of the equipment [MPa]

$$Q_{acty,eqip,fg;avg} = 0.5 \cdot Q_{acty,eqip,fg;mat} \quad (14)$$

where

Q_{avg} ... average flow rate of the activity of the equipment for the FG [m³/s]

Q_{mat} ... material flow rate of the activity of the equipment for the FG [m³/s]

The injection time (a_{inj}) is defined in Equation (15):

$$a_{inj,eqip,fg} = \frac{V_{fg;shot}}{Q_{inj,eqip,fg;avg}} \quad (15)$$

where

a ... ProCo of the injection activity of the equipment for the FG [s]

V_{shot} ... volume of the IM shot related to the FG [m³]

Q_{avg} ... average flow rate of the activity of the equipment for the FG [m³/s]

The cooling time (a_{cool}) is the time needed for the solidification of the molten plastic in the mold. The original equation had a missing π from the logarithmic part, but in the newer version of the guide, this mistake was corrected (Madan et al., 2015), as it is shown in Equation (16):

$$a_{cool,eqip,fg} = \frac{(h_{fg,max})^2}{\pi^2 \cdot \alpha_{fg}} \cdot \ln\left(\frac{4}{\pi}\right) \cdot \left(\frac{T_{fg;inj} - T_{fg;mold}}{T_{fg;eject} - T_{fg;mold}}\right) \quad (16)$$

where

a ... ProCo of the cooling activity of the equipment for the FG [s]

h_{max} ... maximum wall thickness of the FG [mm]

α ... thermal diffusivity of the material related to the FG [cm²/s]

T_{inj} ... injection temperature of the material related to the FG [°C]

T_{mold} ... mold temperature of the material related to the FG [°C]

T_{eject} ... recommended part ejection temperature of the material related to the FG [°C]

The mold resetting time (t_{reset}) is the time to open and close the mold, and it is calculated according to Equation (17):

$$a_{reset,eqip,fg} = 1 + 1.75 \cdot t_{eqip;d} \sqrt{\frac{2 \cdot d_{fg} + 5}{S_{eqip}}} \quad (17)$$

where

a ... ProCo of the resetting activity of the equipment for the FG [s]

t_d ... dry cycle time of the equipment [s]

S ... maximum clamp stroke of the equipment [cm]

d ... depth of the FG [cm]

After the components of the cycle time for the IM are determined, the next step is to find the theoretical minimum energy required for each activity of the IM process. In their guideline, Madan et al. (2013) divide the IM process into (i) IM process energy and (ii) auxiliary operations energy. Before the injection, the polymer is heated and melted; for that, first the melting power (P_{melt}) has to be calculated according to Equation (18):

$$p_{melt,eqip,fg} = \rho_{fg} \cdot Q_{melt,eqip,fg;avg} \cdot C_{fg;p} \cdot (T_{fg;inj} - T_{fg;pol}) + \rho_{fg} \cdot Q_{melt,eqip,fg;avg} \cdot H_{fg;f} \quad (18)$$

where

p ... PowCo of the melting activity of the equipment for the FG [kW]

ρ ... specific density of the material related to the FG [kg/m³]

Q_{avg} ... average flow rate of the activity of the equipment for the FG [m³/s]

C_p ... heat capacity of the material related to the FG [J/kg°C]

T_{inj} ... injection temperature of the material related to the FG [°C]

T_{pol} ... initial temperature of the material related to the FG [°C]

H_f ... material heat of fusion related to the FG [J/kg]

The energy required to melt the plastic for one shot is calculated according to Equation (19):

$$ec_{melt,eqip,fg} = p_{melt,eqip,fg} \cdot \frac{V_{fg;shot}}{Q_{melt,eqip,fg,max}} \quad (19)$$

where

- ec ... EC of the melting activity of the equipment related to the FG [kWh]
 p ... PowCo of the melting activity of the equipment for the FG [kW]
 V_{cav} ... volume of the IM cavity of the FG [m³]
 Q_{max} ... maximum Flow rate of the activity of the equipment for the FG [m³/s]

The injection energy is calculated according to Equation (20):

$$ec_{inj,eqip,fg} = pr_{fg} \cdot V_{fg;shot} \cdot 10^3 \quad (20)$$

where

- ec ... EC of the injection activity of the equipment related to the FG [kWh]
 pr ... recommended injection pressure of the FG [MPa]
 V_{shot} ... volume of the IM shot of the FG [m³]

For the cooling energy, first the amount of heat to be taken out from the molded part (H_{cool}) has to be calculated according to Equation (21):

$$H_{cool,fg} = \rho_{fg} \cdot V_{fg;shot} \cdot C_{fg;p} \cdot (T_{fg;inj} - T_{fg;eject}) + \rho_{fg} \cdot V_{fg;shot} \cdot H_{fg,f} \quad (21)$$

where

- H_{cool} ... amount of heat to be taken out from the molded part (FG) [J]
 ρ ... specific density of the material related to the FG [kg/m³]
 V_{shot} ... volume of the IM shot of the FG [m³]
 C_p ... heat capacity of the material related to the FG [J/kg°C]
 T_{inj} ... injection temperature of the material related to the FG [°C]

T_{eject} ... ejection temperature of the material related to the FG [°C]

H_f ... material heat of fusion related to the FG [J/kg]

The cooling energy depends on the COP (coefficient of performance) of the cooling equipment, and it is calculated according to Equation (22):

$$ec_{cool,eqip,fg} = \frac{H_{cool,fg}}{COP_{eqip}} \cdot 10^{-3} \quad (22)$$

where

ec ... EC of the cooling activity of the equipment related to the FG [kWh]

H ... amount of heat to be taken out from the FG during the cooling activity [J]

COP ... coefficient of performance of the cooling equipment [1]

The energy for clamping, ejection, and opening/closing is approximately 25% of the process energy and calculated according to Equation (23):

$$ec_{reset,eqip,fg} = 0.25 \cdot (ec_{inj,eqip,fg} + ec_{cool,eqip,fg} + ec_{melt,eqip,fg}) \quad (23)$$

where

ec ... EC of the activities of the equipment related to the FG [kWh]

In the fifth step, the EC is estimated for the IM process, which is higher than the theoretical minimum energy requirements because of the energy loss during the transmission and at the drive unit. Due to the complexity of the IM process and the short cycle times, the demand on the drive and control systems is very high. For the all-electric IM equipment approximately 20% of the energy is used for control, besides that, the efficiency of the electric drives have to be considered, which in the original guideline is done for each sub-equipment (Equation (23)), but in this paper for the simplicity it is considered only one efficiency (η) value for all the sub-equipment of the IM equipment. Additionally to the process-related EC, the IM equipment has an EC for the basic equipment, like the display or the fan, which is running throughout the whole IM cycle; in this model, it depends on the basic power (P_b) and the cycle time (t_{cycle}). The energy required for a single shot is calculated according to Equation (24):

$$ec_{control,eqip,fg} = \quad (24)$$

$$\left(\frac{ec_{inj,eqip,fg} + ec_{cool,eqip,fg} + ec_{melt,eqip,fg} + ec_{reset,eqip,fg}}{\eta_{eqip}} \right) \cdot 0.2$$

where

$ec \dots$ EC of the activities of the equipment related to the FG [kWh]

$\eta \dots$ efficiency of the IM equipment [1]

$$ec_{basic,eqip,fg} = a_{IM,eqip,fg} \cdot p_{basic,eqip} \quad (25)$$

where

$ec \dots$ EC of the activities of the equipment related to the FG [kWh]

$a \dots$ ProCo of the IM process of the equipment for the FG [s]

$p \dots$ PowCo of the basic activity of the equipment for the FG [kW]

$$ec_{fg,shot} = \left(\frac{ec_{inj,eqip,fg} + ec_{cool,eqip,fg} + ec_{melt,eqip,fg} + ec_{reset,eqip,fg}}{\eta_{eqip}} \right) \cdot 1.2 \quad (26)$$

$$+ p_{basic,eqip} \cdot a_{IM,eqip,fg}$$

where

$ec_{shot} \dots$ EC of a single IM shot related to the FG [kWh]

$ec \dots$ EC of the activities of the equipment related to the FG [kWh]

$\eta \dots$ efficiency of the IM equipment [1]

$p \dots$ PowCo of the basic activity of the equipment for the FG [kW]

$a \dots$ ProCo of the IM process of the equipment for the FG [s]

Here comes the EC of the auxiliary process— the drying.

$$SMER_{dry,eqip,FG} = \frac{m_{dry,eqip,FG;w}}{ec_{evap,eqip,FG}} \quad (27)$$

where

SMER ... specific Moisture Evaporation Rate of the drying activity of the equipment related to the FG [kg/kJ]

m_w ... weight of the evaporated water of the drying activity of the equipment related to the FG [kg]

ec ... EC of the evaporation activity of the equipment related to the FG [kWh]

$$ec_{drying,eqip,FG} = \frac{(m_{FG;mat} \cdot x_{FG;m})}{SMER_{eqip}} \quad (28)$$

where

ec ... EC of the drying activity of the equipment related to the FG [kWh]

m_{mat} ... weight of the material loaded in the dryer related to the FG [kg]

x_m ... percentage of moisture in the material [%]

SMER ... Specific Moisture Evaporation Rate of the drying activity of the equipment related to the FG [kg/kJ]

The EC of a part is calculated by dividing the energy required for one shot (*E_{shot}*) by the number of cavities (*n*) in the equipment, which is calculated according to Equation (29):

$$ec_{FG} = \frac{ec_{FG;shot} + ec_{FG;auxiliary}}{n_{FG}} \quad (29)$$

where

ec ... EC of the activities related to the FG [kWh]

n ... number of cavities related to the FG [1]

8.2 Extended uCFP calculations: heating, transport, and E-Liabilities

The uCFP calculations of the secondary activities and E-Liabilities involve different approaches and metrics as discussed in Chapter 2.1. To calculate the uCFP of the heating activity, the time-driven approach is required because the EC, and based on it the uCFP, is dependent on the unit time of the activity.

On the other hand, the transport activity is not time-driven, e.g., unit-time dependent, but rather resource-consumption-driven (RCD), which means the EC of the activity is dependent on the amount of the input resource. This input resource for the transport activity is the tonne-km, which describes the weight and distance of the delivered good.

Material E-Liabilities are calculated based on weight, while equipment E-Liabilities are calculated by multiplying the equipment's capacity unit by its ProCo.

Heating activity: Construction and calibration of TD-AB-uCFP metric

First, the EC calculation and then the unit secondary scope 1 CFP ($us1CFP$) for the heating activity using the time-driven approach as shown in Equations (30) and (31):

$$e_{C_{heat,eqip,FG}} = a_{heat,eqip,FG} \cdot p_{heat,eqip,FG} \quad (30)$$

where

ec ... EC of the heating activity of the equipment related to the FG [kWh]

a ... ProCo of the heating activity of the equipment for the FG [s]

p ... PowCo of the heating activity of the equipment for the FG [kW]

$$us1CFP_{heat,FG} = e_{C_{heat,eqip,FG}} \cdot e_{eqip,1,ghg} \quad (31)$$

where

$us1CFP$... secondary (s) scope 1 unit (u) Carbon Footprint of the FG [kgCO₂e]

ec ... EC of the heating activity of the equipment related to the FG [kWh]

e ... scope 1 EmCo of the equipment [kgCO₂e/kWh]

Transportation activity: Calibration and validation of RCD-AB-uCFP metric

First, the EC calculation and then the unit primary scope 1 CFP ($up1CFP$) for the transport activity using the resource-consumption-driven approach as shown in Equations (32) and (33):

$$ec_{transp,res,FG} = a_{transp,res,FG} \cdot q_{transp,res,FG} \quad (32)$$

where

ec ... EC of the transport activity of the resource related to the FG [kWh]

a ... ProCo of the transport activity of the resource for the FG [s]

q ... PowCo of the transport activity of the equipment for the FG [kW]

$$up1CFP_{transp,res,FG} = ec_{transp,res,FG} \cdot e_{res,1,ghg} \quad (33)$$

where

$up1CFP$... primary (p) scope 1 unit (u) Carbon Footprint of the FG [kgCO₂e]

ec ... EC of the transport activity of the resource related to the FG [kWh]

e ... scope 1 EmCo of the resource [kgCO₂e/kWh]

Material's Emission Liability: Construction and Calibration of uELiabMAT metric

The ELiab is calculated according to Equation (34):

$$uELiabMAT_{mat,FG} = a_{mat,FG} \cdot ELiabMAT_{mat,3,ghg} \quad (34)$$

where

$uELiabMAT$... unit E-Liability of the material related to the FG [kgCO₂e]

a ... ProCo of the material related to the FG [kg]

$ELiabMAT$... scope 3 EmCo of the material [kgCO₂e/kWh]

Equipment's Emission Liability: Construction and Calibration of uELiabEQIP metric

First, the capacity unit of the equipment's E-Liability is calculated according to Equation (35):

$$cuELiabEQIP_{equip,3,FG} = ELiabEQIP_{equip,3,ghg} / LifetimeCapacity_{equip,FG} \quad (35)$$

where

cuELiabEQIP... capacity unit of the scope 3 E-Liability of the equipment related to the FG [kgCO₂e/h]

ELiabEQIP... scope 3 EmCo of the equipment [kgCO₂e]

LifetimeCapacity ... lifetime capacity of the equipment related to the FG[h]

Following, the unit-E-Liability calculation according to Equation (36):

$$uELiabEQIP_{acty,eqip,FG} = a_{acty,eqip,FG} \cdot cuELiabEQIP_{equip,3,FG} \quad (36)$$

where

uELiabEQIP... unit E-Liability of the activity of the equipment related to the FG [kgCO₂e]

a ... ProCo of the activity of the equipment related to the FG

cuELiabEQIP... capacity unit of the scope 3 E-Liability of the equipment related to the FG [kgCO₂e/h]

8.3 Rest of the appendix

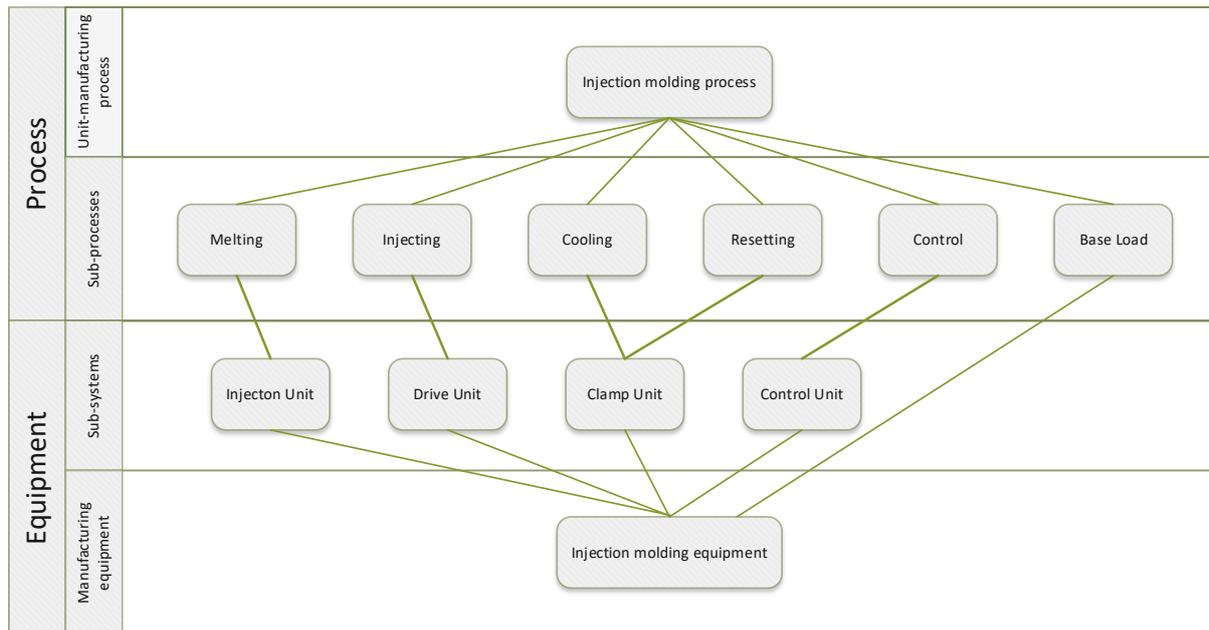


Figure 45 Schematic of the manufacturing process and the IM Equipment one-to-many relationship

Clamping unit		570 E GOLDEN ELECTRIC					
with clamping force	max. kN	2000					
Opening force stroke	max. kN mm	--- 450					
Mould height, fixed variable	min.-max. mm	--- 250-550					
Platen daylight fixed variable	max. mm	--- 700-1000					
Distance between tie bars (w x h)	mm	570 x 570					
Mould mounting platens (w x h)	max. mm	795 x 795					
Weight of movable mould half	max. kg	1300					
Ejector force stroke	max. kN mm	60 200					
Dry cycle time EUROMAP 2	min. s - mm	1,8 - 399					

Injection unit		400			800		
with screw diameter	mm	35	40	45	45	50	55
Effective screw length	LD	23	20	18	22	20	18
Screw stroke	max. mm	160			200		
Calculated stroke volume	max. cm ³	154	201	254	318	392	474
Shot weight	max. g PS	141	184	232	291	359	434
Material throughput	max. kg/h PS	25	29	35	46	53	59
	max. kg/h PA6.6	12,5	15	17,5	23	27	30
Injection pressure	max. bar	2500	2000	1580	2470	2000	1650
Holding pressure time	max. s - bar	300-2090	300-1600	300-1260	300-1970	300-1600	300-1320
Injection flow 2	max. cm ³ /s	126	164	208	174	216	260
	max. cm ³ /s	[162]	[214]	[270]	[228]	[282]	[340]
Injection speed 5	max. mm/s	130			110		
	max. mm/s	[170]			[140]		
Screw circumferential speed	max. m/min	27	31	35	28	31	34
Screw torque	max. Nm	480	550	610	900	1000	1100
Nozzle contact force retraction stroke	max. kN mm	60 300			70 400		
Heating capacity zones	kW	9,4 5			19,9 8		
Feed hopper	l	50			50		

Drive and connection			
with injection unit		400	800
Net weight of machine	kg	7800	8600
Sound press. level Insecurity 4	dB(A)	55 3	
Electrical connection 3	kW	30	47
	Total	A	80
	Machine	A	---
	Heating	A	---
Cooling water connection	max. °C	35	
	min. Δp bar	1,5 DN 25	

Figure 46 Snippet of the data sheet for the IM Equipment (Arburg Allrounder 570 E Golden electric, Source: Arburg)