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Automated LCA through semantic integration of design and process data

Till Tschiltschke^{a,*}, Sebastian Wehking^a, Theresa Riedelsheimer^a,
Kai Lindow^a^aFraunhofer Institute for Production Systems and Design Technology IPK, Pascalstraße 8-9, 10587 Berlin, Germany* Corresponding author. Tel.: +49 30 39006-374; E-mail address: till.tschiltschke@ipk.fraunhofer.de**Abstract**

Global challenges including climate crisis, resource scarcity and regulations are forcing companies to accelerate their sustainable transformation. This paper introduces a digital solution for sustainable design to assess and optimize the environmental impact of products. An approach for automated LCA based on design data is proposed to overcome the limitations of heterogeneous data formats and IT systems. The main results are the semantic mapping of product and LCA process data and its integration into a functional architecture. An implementation in the use case of fuel cell production is described. Moreover, the main challenges and next steps are discussed.

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Keywords: Design for Sustainability; Automated LCA; Semantics in Design, Digital Integration**1. Introduction**

Global challenges such as climate change, resource scarcity, and regulatory developments are fundamental drivers for assessing and minimizing the ecological impact of products [1]. To unlock ecological optimization potentials, it is essential to integrate ecological assessment into product design as early as possible [2]. The evaluation of a product's ecological impact is standardized within the framework of lifecycle assessment (LCA) [3]. Core activities are the collection of all relevant lifecycle (LC) processes and data as part of the lifecycle inventory and the subsequent quantification of impact during the lifecycle impact assessment (LCIA). Therefore, computational approaches are required to streamline the time-intensive process of data collection from various IT systems [2,4]. The gap between the designers perspective focusing on functional design characteristics (e.g. requirements, geometry) and the process oriented view of LCA hinders the identification of ecological optimization potentials during the design phase [2,5]. As 80% of design contributes to variant or adaptive

design, reusing of the LCA process knowledge is a promising approach for the efficient integration of LCA into product design [6]. Additionally, LC data is often directly dependent on technical resources (e.g. machines, transportation vehicle). Therefore, formalized representation of design characteristics and their relation to LC processes and data is fundamental for the automated processing in the context of LCA-based product design.

Nomenclature

BONSAI Big Open Network for Sus. Assessment Information	
CAD	Computer Aided Design
CPM	Core Product Model
LCA	Lifecycle Assessment
LCD	Lifecycle Design
LCIA	Lifecycle Impact Assessment
OAM	Open Assembly Model
OWL	Ontology Web Language
PLM	Product Lifecycle Management

2. State of the Art

2.1. Semantic knowledge capturing

The main goal of developments in the field of semantic web technologies is expressing information in a formal way, so that it can be processed by computational applications. Ontologies represent a formalized description of commonly agreed upon domain knowledge [7]. Gruber defines an ontology as “an explicit specification of a conceptualization” [8]. Here, conceptualization refers to the representation of domain knowledge through a formal description of objects and relations among them. Key elements of an ontology are a taxonomy (vocabulary) of concepts and descriptive inference rules [7]. Relevant applications are sharing of a common understanding of information, reusing domain knowledge, making domain assumptions explicit and analyzing domain knowledge [9]. In particular, the inferring of implicit information based on expressed rules (reasoning) and queries for information extraction or integration are beneficial capabilities for automation purposes [7,10]. Therefore, the semantic integration of design and process data in the LCA context within an ontology is explored.

2.2. Current approaches

The semantic mapping of design characteristics to LCA processes is addressed by various approaches. Faneye and Anderl [11] present an architecture of an information model that implements functional relationships between product properties and LC processes. However, a standardized specification of the product and LCA process domain is not provided. This approach gets extended through the work of Jianjun et al. [12] by referencing the core product model (CPM) as a standardized representation of product data. Nevertheless, the functional relations between product and LCA process data are not specified and an integration of technical resources as reasonable source of LC data is missing. The feature-based approach of Zhou and Tao [13] focusses on integration of design and manufacturing. A conceptual LC data model is presented which links product data to operational process data. The schematic integration of data from enterprise tools is mentioned. A generic specification of product data, LCA processes and the functional relations is not provided. Kuczynski et al. propose three different software implementations for transforming BOM data into a product system model which gets processed through an LCA software [14]. In this context, the product system model or LCA model represents the sequence of LC processes connected through in- and output flows. Although, the approaches match the requirements of comprehensive LCA schemas, the linking to product characteristics is not realized. Zhang et al. [10] describe an ontology for LCA focusing on the integration of process data along the entire product LC. Comprehensive rule sets and reasoning capabilities enable automated data extraction. However, the representation of product information is limited to generic assembly structures. Furthermore, technical resources and their relation to LC data are not

considered. Further approaches realizing automated LCA based on product data are reviewed by Tschiltshcke et al. [15].

2.3. Research goal

The literature exemplifies the following gaps regarding the research context:

- Lack of comprehensive representation and semantic linking of product and LCA process data in a standardized information model
- Missing integration of technical resource as reasonable source of LC data
- Focus on downstream integration of product data into LCA without tracing back LCIA results to initial design characteristics

Therefore, the goal of this paper is developing a generic ontology for the integration of product and LCA process data as a basis for the implementation into a framework for automated LCA. The following research questions are derived. RQ1: Which generic elements are required for the representation and semantic linking of product and LCA process data? RQ2: How can a functional implementation of the semantic schema be realized in the context of automated LCA?

3. Methodical Approach

3.1. Use case description

The use case comprises a fully automated process chain for the production of a simplified fuel cell. The setup is divided into three layers (s. Fig. 1). During configuration an order is received, which specifies the product (desired capacity, material). The respective product configuration is automatically created through a parametric CAD model according to a predefined rule set. A prospective LCA is conducted based on local process knowledge and the provided process data. The orchestration starts with the generation of a process model representing the sequence of process steps connected through product flows as well as the involved

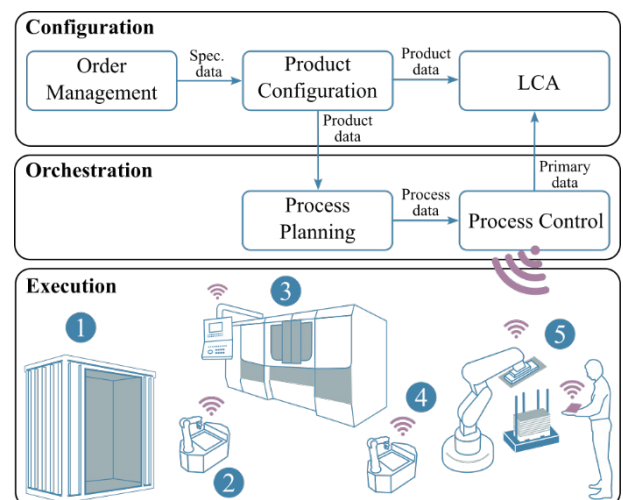


Figure 1: Use case of automated fuel cell production.

technical resources. Subsequently, the process model is used for orchestrating the production line through a communication interface.

The execution starts with an AGV picking up raw material from the warehouse (1) and transporting it to the milling machine (2). At the milling machine, the configuration-specific milling pattern is produced (3). Afterwards, the milled plates are transported to the assembly station (4), where the final stacking of the fuel cell stack is conducted by a worker and a supporting robot (5). During the process, primary data (e.g. process time, energy consumption) is collected and transferred to the orchestrating process model. When the execution is finished, the primary data is processed within a retrospective LCA. The described setup and functionalities are used for the subsequent definition of key elements for a semantic integration of product and process data in the context of LCA.

3.2. Ontology development

The description of elements and steps of ontology development is based on the established OWL convention [16]. The most relevant entities are classes, properties and individuals. Classes are sets of individuals, which represent objects from the domain of interest. The connections of individuals and literals (data values) are defined through properties. Additionally, OWL provides capabilities for contextualization of data through class expressions and axioms. These specify class-dependent conditions of properties and general statements about interdependencies in the domain. Individuals that satisfy certain conditions are referred to as instances of the respective expression. Further inferences can be implemented through rule-based languages (e.g. SWRL) [17]. Information extraction and data incorporation is realized through graph-based query languages (e.g. SPARQL) [18].

The ontology is developed according to the procedure described by Noy and McGuinness [9]. As part of this study, the first five steps are carried out. After, defining the domain and scope of the ontology existing information models are incorporated. Based on the use case analysis, important terms for subsequent definition of the class hierarchy are identified. Finally, relevant relations are implemented through properties. The instantiation and implementation of detailed rule sets will be part of future developments.

4. Results

4.1. Domain and scope definition

The goal of the development is defined through the specification of several aspects including the considered domain and application, the reasonable information and desired stakeholders for usage and maintenance (s. Tab. 1). Generally, the key objective is the integration of a LC perspective into product design. Therefore, the term lifecycle design (LCD) ontology is introduced.

Table 1: Domain and scope of the LCD ontology.

Topic	Answer
Domain	Product design data with dependencies to generic LC processes and technical resources in the context of LCA
Application	Automation of LCA through computational process and data aggregation based on design data
Information	Relations of explicit design characteristics to certain LC processes and technical resources: functional = functional dependencies quantified = quantification of LC data
User	Design engineer, process planner, LCA expert
Maintenance	Domain experts

4.2. Identification of key elements and information models

The standardized PPR approach is chosen as the fundamental framework for integrating product, process and technical resource information [19]. Accordingly, a process consists of input and output flows that are transformed through an operator. Representative flows are products (e.g. material), energy (e.g. electricity) and information (e.g. signal). Additionally, operators use technical resources for transformation activities.

Based on the use case analysis, key elements of the ontology are identified and grouped according to the PPR clusters (s. Fig. 2). Relevant information in the product domain is mainly provided by the order-related requirements (e.g. fuel cell capacity) and a parametric CAD model representing the physical product structure (e.g. groove pattern of bipolar plates). The common distinction of assembly and parts gets extended by features as functional sub-elements representing distinct design characteristics. Therefore, generic classes of features are incorporated as defined by Favi et al. [20]. Additionally, artifacts of early design stages (functional and logical) are added to complete the product definition [21].

The process domain contains specific foreground processes of the considered process chain (e.g. transport of material), which generate primary LC data (e.g. energy consumption). Linked to the foreground system are generic background processes (e.g. electricity production) that are based on secondary data provided by databases. A sequence of processes (e.g. transport and milling) is generated through connections of

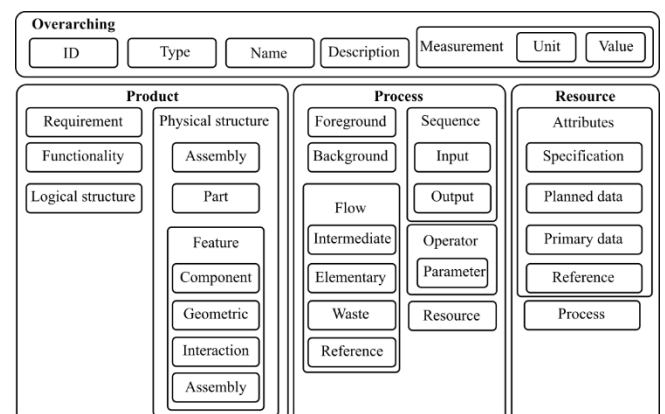


Figure 2: Key domain elements identified through use case analysis.

input and output flows. Operators are defined in accordance with the PPR framework, including parameters for the quantification of performed transformations. Additional elements, such as certain flow categories and references, are incorporated as defined in the ISO standard [3].

Artifacts of technical resource are grouped into related processes and attributes. Attributes include specification data (e.g. fuel cell capacity of AGV) that is used for the calculation of required LC data (e.g. energy consumption). Furthermore, a distinction is made between planned data and primary data, representing the prospective and retrospective application of LCA. Finally, overarching aspects that belong to more than one cluster are grouped separately, including ID structures, type definitions and measurements.

Beside the PPR model, further information models have to be considered to ensure compatibility of the system under development with existing structures and vocabulary [9]. Therefore, established information models for the domains of product representation and LCA processes are incorporated. The CPM developed at the NIST represents comprehensive design information including geometry, function, form, behavior, material and various decompositions and relationships between these aspects [22]. The CPM gets extended through the open assembly model (OAM) with further classes and properties for the inclusion of assembly structures. The models are compatible with the standard for the exchange of product model data (STEP), ensuring a high level of interoperability [23]. Furthermore, the integration in the aspired development is enabled through an OWL-based implementation [24].

The BONSAI ontology provides a top-level representation of LCA process knowledge [25]. It combines aspects of different ontologies in the LCA domain to provide an interoperable framework for LCA data exchange and storage. Furthermore, established ontologies for measurement and provenance data are incorporated. The applicability is validated through the extraction of datasets from two different databases and subsequent transformation in a uniform representation format. In addition to the classes required for flows, processes, values and references, agents are also introduced as entities that correspond to the presented concept of technical resources. The

extension for parameters of agents respective to a certain process is proposed, but not specified. Overall, the BONSAI ontology offers a promising approach for integrating LCA data into the planned PPR framework.

4.3. Extension of ontology

The LCD ontology is presented by focusing on the most relevant classes and properties for the representation and interaction of the PPR domains. Further details are provided in the respective approaches [23,25]. The naming convention has been harmonized, eliminating underlines from the CPM model names. For simplification inverse properties are not illustrated separately. The underlying data model was highlighted by a prefix and color code (s. Fig. 3).

In the CPM a product is represented through the class *Artifact* and its subclasses *Part* and *Assembly*. The superordinate class *Specification* allows for the incorporation of conceptual product descriptions through requirements, functions and logical structures. Functional sub-elements of an *Artifact* are grouped within the class *Feature*. The definition of relevant features must be implemented accordingly to functional dependencies within individual LC phases (e.g. *MillingFeature*). This level of granularity is required, as many LC processes and corresponding LC data correspond to attributes of distinct product features. Representative attributes are *Geometry* and *Material* connected to the *Form* class. Further attributes related to assembly features are contained in the OAM, but not illustrated.

In the BONSAI ontology LCA processes are represented through entities of the class *Activity*, which are linked to quantitative input and output entities of the *Flow* class. An *Activity* is performed by an *Agent*. Furthermore, the class *AgentAttribute* is incorporated to capture relevant resource-specific attributes affecting the quantification of LC data.

The interconnection between the product and LCA domain is realized through the concept of operators. As proposed in the PPR framework entities of the *Operator* class represent the logical transformation of quantitative flows within defined processes (e.g. *MillingOperator*). This concept is extended by considering transformations of LCA flows depending on product characteristics. Generic transformation logics are

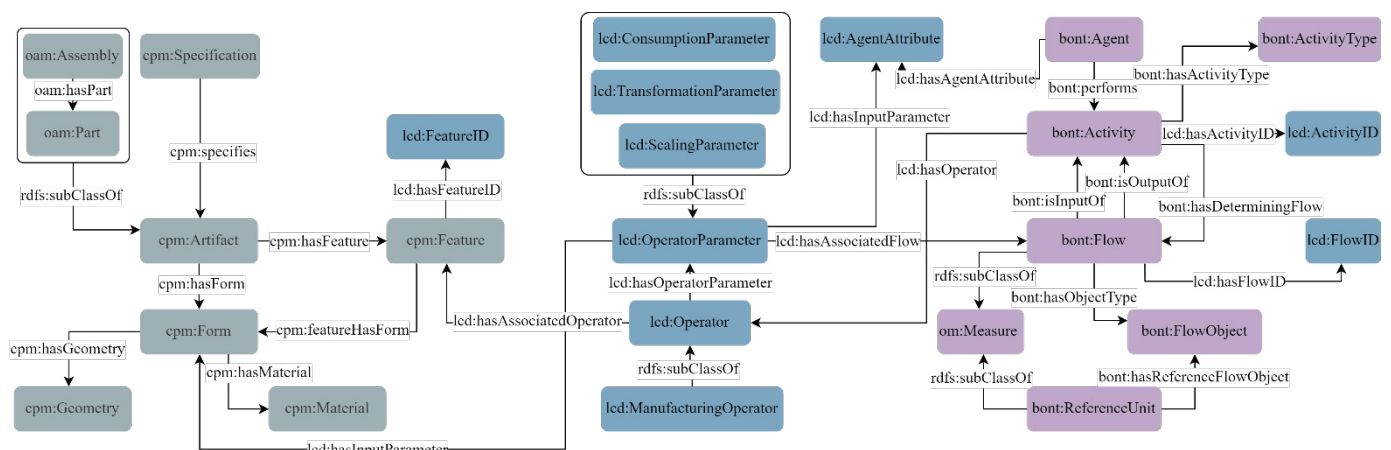


Figure 3: Diagrammatic representation of LCD ontology with entities of the CPM/OAM domain (grey), the BONSAI ontology (purple) and new ones (blue).

implemented through entities of the class *OperatorParameter*, which are assigned to certain *Operator* entities. Different subclasses of *OperatorParameter* group relevant transformation logics. The introduced parameters are *ScalingParameter* (e.g. scaling of resource-specific LC data in proportion to a product parameter), *TransformationParameter* (e.g. geometrical transformation during manufacturing) and *ConsumptionParameter* (e.g. electricity consumption resulting from electro-technical specification). This selection is based on the use case analysis carried out. Further parameters can be added in the defined schema. Relevant input data for the definition of an *OperatorParameter* is referenced through relations to the product domain (e.g. *Form* class) and the LCA domain (e.g. *Agent* class). Mathematical transformation of LC data related to an *OperatorParameter* is implemented through operator-specific rule sets. Results of the logical transformation are converted into the quantification of an associated *Flow*. This ensures the product-specific adaptation of LCA data.

In the context of future implementation, an organization-specific knowledge base will be created by instantiating reusable data related to products, processes and technical resources. An exemplary workflow for the integration of product data in the automated assessment of a milling process is derived from the use case. Relevant product information is provided through a CAD model of the fuel cell *Assembly* structure. The *Part* bipolar plate contains a geometrical *Feature* representing the groove pattern of the flow field. The *Feature* is categorized as an instance of the subclass *MillingFeature* by the inference of geometrical and material related attributes. The subclass *MillingFeature* is associated to a *MillingOperator*, which has a *TransformationParameter* assigned to it. Predefined input parameters are input condition (geometrical bounding box of feature), output condition (pocket pattern as modelled), axial/radial depth and specific *AgentAttributes* of a certain milling machine affecting the process time and energy consumption (e.g. standard cutting speed, feed rate).

The affected *Flows* of the *LCA Activity* are energy consumption (input flow) and waste material (output flows). The quantification of these *Flows* is automatically carried out by executing the predefined rule set of the assigned *TransformationParameter*. Therefore, geometrical and resource-specific attributes are extracted from their semantic representation and converted to *Flow* values. The generated process data is incorporated in an LCA model for conducting the impact assessment by referencing the data through the integrated *ID* structure. Finally, the implemented semantic connection allows for tracing back the impact results to the initial design feature.

4.4. Functional integration

The systematic integration of the presented semantic approach into an functional architecture is based on the elements proposed by Zhang et al. [10]. Fundamental extensions are related to the integration of PLM data and the explicit linking of product and LCA process data through reasoning and mapping functionalities. The architecture includes four functional modules (s. Fig. 4). The first module is provided by the developed LCD knowledge base. It contains

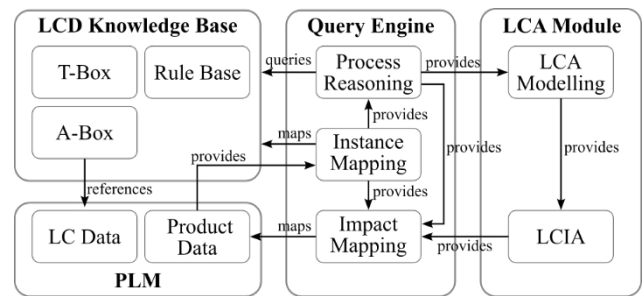


Figure 4: Functional integration of design and LCA process data.

the general terminology through the defined class hierarchy and properties (T-Box) and assertions through instantiation of product, process and technical resource data (A-Box). Additionally, a rule base is implemented formalizing the required logic for reasoning. Instead of generating duplicates of LC data stored in various PLM systems, the A-Box should have an interface allowing for referencing of relevant data endpoints. In this way, persistent data management is ensured in the second module of PLM systems. Furthermore, the PLM module manages product data (e.g. requirements, specifications and information of the physical product), which is provided to the query engine. This central module contains three major functionalities for reasoning and data mapping. During instance mapping the provided product data is mapped onto the defined structure of the LCD knowledge base. The identified features are then provided to the process reasoning. Reasoning for related processes and LC data is conducted through the described concept of interlinking operators and integration of technical resource data. Extracted process data is provided for executing LCA modelling in the last module through an interface to an appropriate LCA tool. The results of the impact assessment are fed back to the impact mapping in the query engine. Additionally, results of instance mapping and process reasoning are provided, representing the required relations between process-oriented LCIA results and product-oriented instances. Thereby, the LCIA results are mapped back onto the initial design data.

5. Discussion

The presented approach enables bidirectional support for the integration of LCA into product development. The underlying requirements definition regarding core entities of the LCD ontology is based on a simplified use case in a laboratory environment. The resulting limitations are partially overcome by the incorporated, highly generalized domain models. However, validation in an industrial environment is required. Automated reasoning for process data based on design data and integrated LCA modelling significantly accelerates the time, knowledge and labor-intensive process of data collection and model generation. This effectively supports LCA experts regarding monitoring and reporting activities. The definition of suitable rule sets and queries is part of future work. This may result in modifications to the class and property structure, which corresponds to the highly iterative process of ontology development [9]. Additionally, designers are assisted through the automated mapping of LCIA results onto explicit design features. The semantic linking realized through the LCD

ontology bridges the gap between the process-oriented perspective of LCA and the product-oriented view of designers. This enables the reliable identification of ecological optimization potentials in an existing design. The integration of conceptual design entities (e.g. requirements, functionalities) ensures traceability through the entire design phase. Identified optimization potential can therefore be considered as early as possible in the development of future product generations. Fundamental to this is the creation of a knowledge base with regard to organization-specific product features and processes. Automated extraction and import functions must be provided for this in order to keep the initial effort for implementation as low as possible. In addition, the continuous expansion of the knowledge base must be ensured by identifying and integrating new entities. Simultaneously, the approach focuses on recurring content so that long-term time and cost savings can be expected. The integration of technical resources also supports process planners in the ecological design of LC processes and the selection of appropriate technical resources. However, this also increases the complexity of referencing LC data from different IT systems. Standardized interfaces must be developed for this by incorporating existing concepts (e.g. asset administration shell, open services for lifecycle collaboration).

6. Conclusion

A new approach to the semantic linking of design characteristics with lifecycle processes and data was developed as part of the PPR framework. The described LCD ontology contains generic models from the domains of product description and LCA process representation. The implementation in the context of automated LCA was described by introducing a functional architecture. Future work includes the development of comprehensive reasoning capabilities. This involves validating the classes and property structure developed with regard to the automated derivation of LCA process data from a design description with subsequent mapping of LCIA results to design characteristics. Furthermore, implementation into an industrial use case is intended for development of a technical architecture transferable to different IT environments.

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