

Systematic Review of Engineering Simulation Models for Life Cycle Assessment

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Abstract: Manufacturing companies increasingly integrate the strive towards sustainability into product engineering to reduce resource consumption and environmental impacts. A substantial share of a product's environmental performance is determined during engineering. Early assessments rely on generic data, which is gradually replaced by more concrete simulation and primary data as product maturity increases. The effective use of engineering simulation models for Life Cycle Assessment (LCA) therefore remains a central challenge under heterogeneous, distributed and rapidly evolving data. This article presents a systematic review of product engineering approaches for integrating simulation models into LCA. A seven-step research approach is applied to identify, categorize and evaluate existing approaches across CAx tools. Relevant simulation parameters for sustainability assessment, including material properties, process descriptors, consumables and waste streams, are identified and analyzed. Based on identified data characteristics, the potential of Data Science and Artificial Intelligence methods for LCA data preparation is assessed. A conceptual knowledge-graph-based decision support approach is derived to enable structured integration, traceability and reuse of simulation data for sustainability assessment. The approach is evaluated using criteria from literature. Structured integration of simulation data improves early-stage data quality and supports decision-making in sustainable product engineering.

Keywords:

Product Engineering, Simulation Model, Sustainability, Life Cycle Assessment

1 Motivation

Leading companies are progressively engineering their products to reduce resource consumption and environmental impact. A significant amount of a product's environmental impact is determined during engineering. Maximizing the scope for design in engineering necessitates making valid estimations about the product's sustainability throughout the entire life cycle [1]. This assessment requires consolidating a wide variety of information and data from different IT-systems. In Life Cycle Assessment (LCA), generic database values are used to make initial estimates within the product life. These values are gradually replaced by more concrete simulation and primary data as the product matures. Primary data consists of real data from production processes and other sources. Due to high volume, diversity and distribution across different IT-systems, applicability of the data is limited. Using simulation data carries the potential to improve the quality of sustainability assessments at an early stage. Simulations currently used for sustainability assessments primarily describe the environmental impacts of processes involved in product life. Integrating existing engineering simulation models into tools such as Computer-Aided Design (CAD), Computer-Aided Engineering (CAE), Computer-Aided Manufacturing (CAM) and Finite Element Analysis (FEA) improves the quality of LCA and utilization of simulation for hybrid decision making in sustainable product creation (see Figure 1).

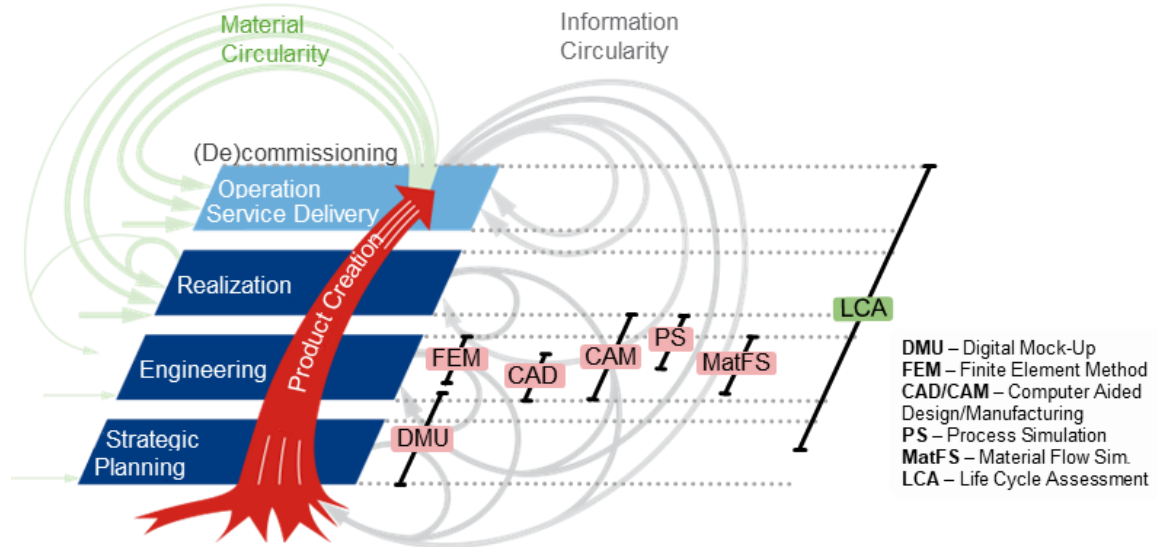


Figure 1: Potentials of simulation models in product engineering for dynamic Life Cycle Assessment in accordance with [2]

Current considerations of dynamic LCA in product engineering only marginally consider established simulation models, but focus on individual models and consider exemplary model elements. Established reviews prioritize process simulations over analysis of engineering simulation models. Current approaches have not yet been sufficiently adapted to recent technologies, such as Data Science and Artificial Intelligence (DS/AI), which offer enhanced potential to handle data for sustainability assessments. Considering these limitations, a review of approaches for integrating simulation models into LCA is conducted, analyzing data regarding sustainability and the potential of established DS/AI approaches. Two research questions (RQ) are formulated:

RQ1: Which product engineering approaches exist for integrating simulation models into LCA?

RQ2: Which existing DS/AI methods can potentially be utilized for data preparation for LCA?

The aim of this paper is to systematically compare existing approaches for integrating simulation models into LCA. Therefore, a conceptual approach for their implementation is derived and initially validated in an experimental laboratory environment. Section 2 presents the applied research approach. This is followed in section 3 by a state-of-the-art review. Section 4 describes the systematic analysis, evaluation and synthesis of identified approaches. Based on this analysis, parameters from existing methods are identified and a new conceptual approach for integrating simulation data into LCA is developed.

2 Scientific approach

The scientific approach is based on the Design Research Methodology (DRM) and focuses on descriptive research [3]. A seven-step process, derived from the DRM's four phases, is used to systematically analyze the integration of simulation data into LCA. As part of the research project Decide4ECO funded by the German Federal Ministry of Economy and Energy (BMWE) relevant decision points and success factors are identified (1). Based on the PRISMA scheme [4], a systematic literature review is conducted to identify approaches in which simulation model results are used for LCA (2). The identified approaches are analyzed regarding integration of engineering simulation models into LCA (3) and concerned parameters (4). Based on characterizations of data and information, potentials for using DS/AI methods are examined (5). A conceptual implementation of a knowledge graph for structuring data is carried out in a production laboratory environment (6). Based on this preparation, the resulting new conceptual approach is validated (7).

3 State of the art

This section introduces key concepts and principles of sustainable product engineering, with focus on simulation models across the product life cycle, data science and data space. Manufacturing companies increasingly account for ecological sustainability alongside functional and economic requirements in product engineering [5]. Early engineering decisions define key product characteristics. These decisions largely determine life-cycle environmental performance [5,6]. **Sustainability integration into product engineering** is supported by methods such as LCA. These methods enable the evaluation of environmental performance and circularity despite limited data availability [7]. As early design decisions largely determine a product's environmental footprint, systematic and quantitative assessment methods are required to evaluate sustainability impacts [6]. According to the ISO 14044, **LCA** is a standardized method for environmental sustainability assessment across the product life cycle [8,9]. This structured procedure ensures a transparent, consistent and reproducible assessment of environmental impacts. Potential environmental impacts are calculated based on life cycle inventory (LCI) data describing emissions and resource consumption. This enables engineers to make informed decisions regarding sustainable products [10]. Reliable LCA results depend on trustworthy, high-quality **LCI data**. Such data requires preparation involving complex transformations and quality checks. Availability of such data is currently limited by confidentiality and heterogeneous formats [11]. Within the LCA domain, data encompasses heterogeneous forms ranging from primary, site-specific measurements to aggregated secondary datasets, processed data products and non-standard outputs such as analysis protocols or software tools. **Data spaces** provide a viable approach to address challenges regarding inventory data. The technology is a key enabler of secure, sovereign and interoperable data exchange across manufacturing and supply-chain networks, helping to overcome fragmented and siloed data structures [12]. Integrating secure, sovereign data transfer enables collaborative LCA calculations across value creation networks [13]. **Simulation models** in tools like CAD, CAE, CAM, CAPP (Computer-Aided Process Planning) extend modeling and simulation to support sustainable product engineering. Customization and sustainability variables are integrated into design and process planning within these tools, enabling assessment of manufacturing energy use, emissions, waste generation and production flexibility. Knowledge-based software extensions increase interoperability among CAX tools to optimize engineering times and enable manufacturing decisions that consider LCA results [14]. **DS/AI approaches** offer practical means to improve accuracy and completeness of LCA. Method selection depends on study objective, data type and available volume [15]. DS/AI improve product engineering decisions while maintaining resource use. DS forms the basis for machine learning (ML) and ontology-based reasoning. AI systems display intelligent behavior, analyze environments, take actions with autonomy and achieve specific goals [16].

4 Systematic review of engineering simulation models

In this section, a systematic analysis is presented of the relevant approaches for implementing simulation models in sustainable product engineering. A conceptual model is developed based on an analysis of the approaches regarding the relevant aspects and parameters used.

4.1 Derivation of relevant engineering decision points

The analysis of relevant approaches is based on the collection and evaluation of user perspectives. Key engineering decisions are recorded for transfer to specific engineering processes [17]. These decision points are characterized by specific features such as relevant roles, key figures and questions and serve as a reference point for the integration of simulation models [18]. The decision points were identified in workshops with application partners from the automotive and consumer goods sectors. Based on an analysis of existing engineering processes, relevant decision points regarding sustainability of products

are identified. The identified characteristics of the decision points include: requirements change, solution principle change, material change, geometry change, production process change and supplier change. These points describe core artifacts and characteristics of sustainable product engineering and are further subdivided according to the respective decision-making situation.

4.2 Identification of relevant approaches using simulation models for LCA

To identify relevant approaches for the use of simulation models in LCA, a systematic literature review is conducted in accordance with the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) guidelines. The objective of the present study is to identify existing approaches for integrating simulation models into LCA-related applications. The basis for this study is a structured screening of the scientific databases Scopus and Web of Science. These databases provide quality-controlled literature sources. In addition, Google Scholar offers a way to check for completeness. Topic-specific search terms are derived from the research objective and combined into search strings using Boolean operators. The search strings are applied to the databases and bibliometric data of all retrieved publications are extracted for further analysis. The classification of existing tools providing engineering simulation models from ROMERO et al. [14] forms the basis for derivation of search terms. Each search string comprises three conceptual components: keywords related to product engineering, Life Cycle Assessment and the respective simulation approach (see Figure 2).

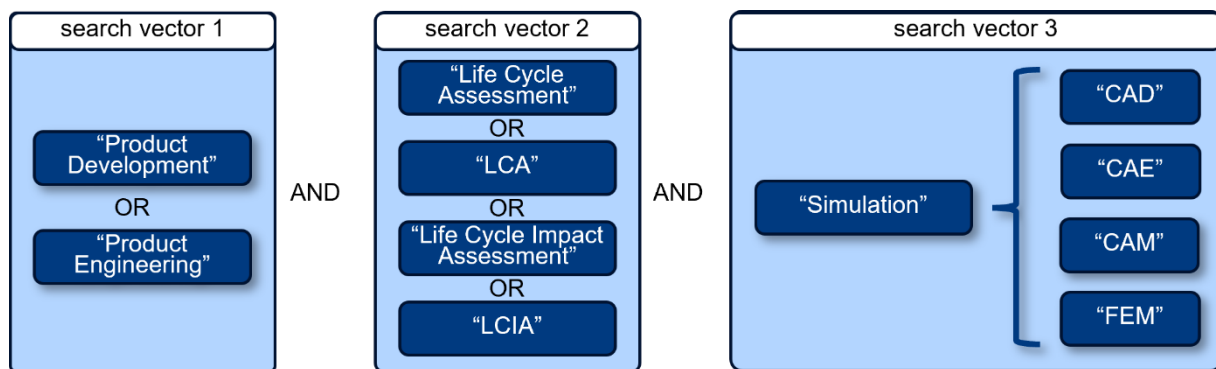


Figure 2: Search string formulation on three term vectors for identifying simulation approaches for LCA in product engineering

Results of the study are presented in Table 1. In database search, 738 publications are identified, of which 681 remain after removing duplicates. Following a screening process involving the evaluation of titles and abstracts, publications are selected based on their relevance to enhance the quality of LCA data through the integration of LCA with simulation tools, as well as the identification of simulation-based parameters relevant to LCA. This process resulted in the selection of 110 publications for a full-text assessment. Following the full-text analysis according to the same criteria, 22 publications are selected. Due to thematic overlap among the search strings, individual publications are retrieved multiple times and therefore identified as duplicates and included only once.

Table 1: Results of the systematic literature review

PRISMA Phase → tool category	CAD	CAE	CAM	FEM	Total
Total records	385	97	85	171	738
Total records (without duplicates)	370	81	79	151	681
Literature assessed for eligibility	36	13	13	48	110
Studies included in review	7	1	5	9	22

4.3 Categorization of relevant approaches

Identified approaches are analyzed regarding implementation of simulation models into sustainable product engineering. Analysis of the articles reveals three recurring characteristics of implementation approaches. The approaches are classified into engineering-level, process-level and tool-embedded model integration, as shown in Table 2 (RQ1).

Table 2: Categorization of included studies according to level of integration mentioned

(E) ngineering-level	(P) rocess-level	(T) ool-embedded
[8–10,14,19–31]	[9,19,21,25,27,32,33]	[8,10,14,23,28,33–36]

Engineering-level integration involves mapping product and process properties. Relevant data is extracted, harmonized and imported from simulation software into an LCI database. Therefore, LCI values are available for use in LCA software for sustainability calculations. CHEN, TAO and YU [20] propose a feature-based paradigm in which product features are systematically mapped to operational features. This allows CAD geometry and associated attributes to be translated into part- and process-level LCI entries. In ASNAFI et al. approach [19] translation of data provided by simulation tools is performed by a "Lifecycle data integrator" for LCI. The software tool collects relevant product and production attributes from heterogeneous sources, aligns the data in a unified data model and transfers it to LCA software. The approach further includes a "Life Cycle Analyzer" that enables feedback of sustainability data from impact assessment into simulation software. Complementary enterprise-level patterns include Product Lifecycle Management (PLM)- and mechanical Bill of Material (mBOM)-driven workflows. These workflows transition mBOM to Sphera LCA for Experts, which are used for systematic mapping of materials and processes [22,23]. Life-cycle engineering tools for additive manufacturing are enhanced to automate LCI generation from CAD/slicer outputs when mass/volume and material data are provided [21]. **Process level** integration links real or simulated manufacturing operations such as CAM and Computerized Numerical Control (CNC) outputs to environmental analysis. ANDRIANKAJA et al. [32] describe STEP-NC and ANGEL approaches in which toolpaths, cutting parameters and execution traces are used to compute operation level energy and material flows. These approaches are combined with discrete event simulation or Petri net models to generate temporally resolved machine state and power demand series for use in LCA. GAHA et al. [24] build on data extraction from simulation software and present a CAD/CAPP integration providing real time scenarios. LCI entries are assigned to product features, provide scenarios from CAD and CAPP and translate LCA results into the knowledge context of engineers. **Tool-embedded implementations** involve native integration into simulation tools. Native CAD plugins and cloud LCA services are used to provide engineers with environmental feedback inside modeling environments. MATHIEUX et al. [23] and SCHILLING et al. [34] publish examples such as SolidWorks Sustainability and Siemens NX Sustainability, in which environmental indicators are imported directly into CAD tools. BLIBECH [8] presents a One Click LCA integration with Building Information Modeling (BIM).

4.4 Evaluation of relevant approaches regarding decision making in engineering

For systematic review, product engineering approaches for integration of simulation models into LCA are evaluated with respect to their capacity to support decision making across engineering activities by enhancing data quality at initial stages. Evaluation criteria are established to assess these approaches into a structured manner. The criteria include support for common simulation tools within engineering workflows, interoperable export of simulation outputs for LCI ingestion, dynamic updating of LCI databases during engineering decisions, interpretable feedback for engineers and mapping of metadata and features to ensure consistency and traceability of simulation data. Table 3 summarizes how integration approaches identified in literature meet decision-relevant criteria. The categorization of these

approaches remains consistent with the classification established in Table 2. A black circle indicates fulfilled, a half-black/half-white circle partially fulfilled and a white circle not fulfilled.

Table 3: Results of evaluation relevant approaches regarding decision making

Category	Author	Approach	common simulation tools	export to LCI	dynamic LCI update	actionable feedback	metadata / feature mapping
E	MATHIEUX et al. [23]	CAD-based LCI extraction	●	●	◐	◐	●
E	BLIBECH [8]	Feature-based BIM–LCA	◐	●	◐	◐	◐
E	KO et al. [22]	PLM-driven mapping	●	●	◐	◐	●
E / P	FAVI et al. [21]	Additive manufacturing automated LCI	●	●	◐	●	●
E / T	CHEN et al. [20]	Feature-based CAD integration	●	●	◐	◐	●
P	ANDRIANKAJA et al. [32]	CAM/CNC integration with dynamic LCA	●	●	●	●	◐
P	ANDRIANKAJA et al. [32]	Machine simulation LCA	●	●	●	●	◐
T	MATHIEUX et al. [23]	Native CAD plugin	●	●	○	◐	◐
T	SCHILLING et al. [34]	Native CAD plugin	●	●	○	◐	◐
T	SCHILLING et al. [34]	Cloud-based LCA service	○	●	◐	◐	◐

● = fulfilled ◐ = partially fulfilled ○ = not fulfilled

The following examples illustrate typical approaches and link to the limitations identified for the three integration categories. **Engineering-level** integration remains limited by incomplete lifecycle information in early CAD models, as discussed by MATHIEUX et al. and BLIBECH [8,23]. Critical attributes such as use-phase energy, service life and detailed material inventories are often unavailable and are approximated using proxies, which reduces result robustness [8,23]. Feature-based CAD–LCA approaches proposed by CHEN et al. and GAHA et al. mitigate this limitation by explicitly mapping geometric and semantic features to process-relevant parameters and LCI flows [20,24]. These mappings improve traceability and enable systematic population of foreground inventories. Additional modelling effort is required for novel materials when database entries are missing, as shown in multiscale and material-focused studies by MIO et al. and BIANCHI et al. [9,31]. **Process-level** integration enables temporally resolved and operation-specific assessment but requires detailed CAM/CNC machine or simulation data and standardized translation mechanisms [30,32]. The ANGEL project mentioned by ANDRIANKAJA et al. exemplifies a strong operational approach by converting machine-state and power time series into process LCI entries, which supports iterative process planning with environmental metrics [32]. High data requirements and limited industrial adoption of enabling standards such as STEP-NC remain main constraints on scalability [30,32]. **Tool-embedded** model-level integration yields rapid model-level feedback inside CAD, BIM or PLM environments but often reports simplified indicators rather than full cradle-to-grave inventories [23,36]. Absence of continuous synchronization

with background LCA databases limits consistency in iterative design [8,36]. Best practice combines native in-tool indicators with PLM-driven mBOM exports and strict metadata governance to improve interpretability and reduce manual reconciliation across iterations [22,34].

4.5 Identification of relevant parameters

Based on the analyzed approaches, relevant parameters of simulation models are identified to enable a comparison across studies. Table 4 represents a summary of these parameters, including typical units and data sources, to ensure consistent and reproducible characterization.

Table 4: Identified relevant parameter

Parameter	Suggested unit	Typical source	References
geometry and mass	kg; mm ³ or m ³	CAD, mBOM, AM slicer, Parametric CAE	[21–23,26,27]
material properties	material ID; kg·m ⁻³	CAD metadata, PLM, multiscale / molecular dynamics, material database	[9,20,22,31]
mechanical material parameters	GPa; dimensionless	atomistic and multiscale simulations	[26,31]
process descriptors	G-code/vector; m·min ⁻¹ ; mm·rev ⁻¹ ; mm	CAM output, STEP-NC, NC simulation	[20,32]
temporal and energy profiles	s or h; kW	machine simulation, DES logs, machine control traces	[9,21,32]
consumables and waste streams	L; g or kg; cycles/parts	process simulation, shopfloor data, CAM / AM slicer, tool-life models	[22,32]
lifetime and use-phase variables	h; cycles; %; timestamped logs	durability simulation, monitoring, digital twin, in-service sensors	[9,21,33]
end-of-life and circularity parameters	%; categorical	PLM, EoL modelling	[9,27]

Geometry and mass metrics include part mass, nominal volume, additive manufacturing support volume and topology variants. They represent primary drivers of material flows and are extracted from CAD systems, mBOM structures and slicer or topology-optimization outputs. Material properties are required to match components to background inventories. Material properties derived from multiscale and molecular dynamics simulations are an alternative when suitable database records are unavailable. Mechanical material parameters, such as elastic modulus and Poisson's ratio, are necessary to support robust material substitution decisions. Process descriptors, including toolpath geometry, cutting speed, feed rate and depth of cut, combined with temporal and energy profiles, enable conversion of machine behavior into kWh and other LCI entries. Consumables and waste streams, such as coolant, lubricant, chips, support structures and tool wear, are captured for waste accounting and end-of-life modelling. Lifetime and use-phase variables, including service life, duty cycles and remaining useful life, are required to allocate use-phase impacts. End-of-life and circularity parameters further support modelling of recycling rates, recovery scenarios and circularity pathways. Support for handling data is essential for managing LCI data, particularly when using simulation and primary data.

4.6 Potentials of Data Science and Artificial Intelligence

Product engineering faces multiple challenges for LCA. These challenges can be grouped into three categories: data availability and quality (missing data, low-quality measurements, costly LCI data collection), data heterogeneity and scale (large volumes, redundant simulation outputs, inconsistent formats and units, fragmented sources) and integration and mapping issues (poor interoperability, domain-specific taxonomy and unit mismatches, mapping simulation outputs to LCI properties) [15,16]. DS/AI methods address distinct stages of LCI data preparation. Data architecture tools, blockchain, data

mining and data engineering support data collection, transfer and storage. Theoretical models and conceptual frameworks support regionalization of impacts, dynamic LCA and handling of big data. ML techniques can be applied to predict LCA results, decision support and benchmarking [15]. Knowledge graphs are positioned within both data architecture and conceptual frameworks due to incorporate structural data modelling and formalized ontologies [18]. ML is the most studied DS approach for LCA and is most applied to predict LCA results [15]. Typical targets include characterization factors, LCI entries and unit process inventories. The method commonly appears under the label “surrogate LCA” and is applied when new products or systems lack measured inventory data. Studies employ models that range from linear regressions to advanced neural networks. Model choice depends on available training data, feature complexity and required interpretability [15]. DS/AI methods increase availability, consistency and usability of LCI data, enable rapid scenario analysis and prediction of LCA results into early engineering stages and support automated decision-making and reducing uncertainty (RQ2).

4.7 Conceptual approach for simulation models in sustainable product engineering

A conceptual model for integrating simulation data into sustainability assessments is presented, which is based on analysis of existing approaches and necessary parameters derived from them. Building on preliminary work relating to impact analysis like model-Based Effect-Chain Analysis (MECA) for Complex Systems [37] and associated data models, this approach involves transferring identified simulation models to a knowledge graph [18]. The knowledge graph serves as a central representation that integrates all information relevant to assess the environmental impact of technical products. Based on the semantic model in form of an ontology, heterogeneous and extensive datasets can be integrated, analyzed and interpreted into the knowledge graph. The existing published model is supplemented by parameters listed in Table 4. These parameters enable assessments of LCAs based on realistic simulation data integrated in early stages of product engineering.

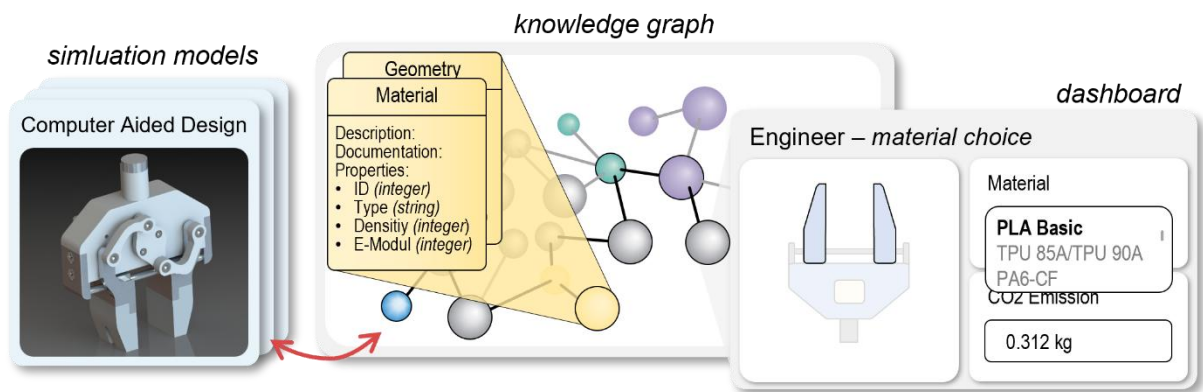


Figure 3: Knowledge Graph for implementation of simulation models for sustainable product engineering

Technically, the knowledge graph is implemented in Neo4J. A defined data model allows parameters from different source systems to be integrated, contributing to the harmonization of diverse data formats. Importing data via generic CSV tables allows for efficient integration of large, diverse datasets. The implementation is demonstrated using the example of a decision point for a material change. Based on a geometry created in CAD, relevant information on the component geometry and composition can be derived. Combining this information with other data stored in the knowledge graph, such as emission factors or energy consumption from additional simulation models, allows for initial conclusions to be drawn about the resulting environmental impacts. Role-specific dashboards provide corresponding calculations, such as CO₂ equivalents, using queries formulated in Cypher. These dashboards enable engineers to evaluate engineering decisions, such as material selection, based on concrete simulation data and immediately determine their environmental impact (see Figure 3). Integrating all relevant life cycle parameters (see Table 4) enables conclusions to be drawn regarding the entire product life cycle.

5 Discussion

The seven-step approach enables systematic and comprehensible analysis of existing methods and development of a conceptual model for incorporating simulation data into sustainability assessments. While the combination of structured literature analysis, parameter-based evaluation and conceptual implementation provides a methodologically consistent basis. In relation to the previously defined assessment criteria, the knowledge graph-based approach offers advantages in terms of interoperability integrating heterogeneous simulation data and consistently mapping metadata to ensure traceability. While dynamic updating of LCI-relevant information during technical decision-making processes is conceptually possible, practical implementation depends on additional interfaces and degrees of automation. Support for common simulation tools is not native; existing engineering workflows can only be integrated to a limited extent via standardized exports. The semantic structure of the knowledge graph simultaneously allows transparent and interpretable feedback on the results for engineers. The approach meets key criteria in conceptual terms but has limitations in terms of practical scalability.

6 Conclusion

The article presents a systematic analysis of existing engineering simulation models for sustainable product design. Using a seven-step research approach, the relevant approaches are identified, categorized and analyzed based on simulation parameters relevant to sustainability assessment, such as mechanical material parameters, process descriptors, consumables and waste streams. Based on this categorization, the potential use of DS/AI is identified and a conceptual model for a knowledge graph based decision support is developed. Relevant parameters are implemented into a knowledge graph to serve as a central representation integrating information for assessing environmental impact of technical products. The approach is validated using previously identified criteria. The approach enables early improvement of data quality using simulation data. Identified data and information can be systematically transferred to sustainability assessment, providing engineers with a solid foundation for making hybrid decisions regarding engineering sustainable products.

7 Acknowledgements

The authors gratefully acknowledge funding of the project Decide4ECO (13MX002G) by the German Federal Ministry of Economy and Energy (BMWE) from the European Union – NextGenerationEU. The results are solely those of the authors and do not necessarily reflect the views of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them. Results are reflected by the scope of DFG SPP2443 (coordination, PN521148212).

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