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Incorporating unit manufacturing process models into life cycle assessment workflows

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Abstract

Life cycle assessment (LCA) carries significant uncertainties and imprecision due to a number of factors, including the framework's linearity assumptions and the wide use of aggregate unit processes in practice. In this work, we exploit the unit manufacturing process (UMP) information model (ASTM E3012-16) to enable parametric environmental analysis of manufacturing systems without disrupting the traditional LCA workflow. We present a formal mapping of an extension of the ASTM E3012 data model and the ecoSpold2 data model. We then demonstrate the utility of this mapping by (1) generating life cycle inventory (LCI) data from an example UMP model representing a vertical milling process and (2) linking the results with an existing LCI database. To show value, we use the Brightway2 framework to process the LCI data and complete a LCA. We conclude by comparing LCA results generated from the parametric milling UMP model against LCA results of a similar milling unit process model from a commercial database.

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Keywords: Unit Manufacturing Process, Life Cycle Inventory Data, Life Cycle Assessment, Brightway2, Jupyter Notebooks, Ecoinvent, ASTM E3012

1. Introduction

Current life cycle assessment (LCA) practices carry significant uncertainty due to a lack of data and reusable parametric models as well as the presence of a number of critically flawed assumptions (e.g., models are linear to single inputs and are transferable across similar geographical locations) [20]. Life cycle inventory (LCI) database (*"pre-computed"*) models contain methods, e.g., the pedigree matrix, to deal with such uncertainties, yet the debate on their efficacy continues (see recent editorial from Heijungs et *al*. [10]). As a result, practitioners seeking more precise, scalable, and parametric LCI models spend significant effort in constructing their own models from scratch [7]. Without a standard model representation, it has become increasingly more difficult to properly exchange, reproduce, and explain LCA workflows. Leading researchers and practitioners have recognized these challenges through a recent LCA capability roadmap, stating that three of the most critical opportunities are *describing model contents*, *describing model structure*, and *collaborative use of models* [15]. In the LCA community, some have attempted to improve the transparency of their work by including supplemental material describing their models [5, 21]. However, manual reconstruction is still required to replicate these studies.

In response to these challenges, this paper leverages an existing standard for representing parametric manufacturing process models, i.e., unit manufacturing process (UMP) models as defined by ASTM E3012-16 [1], and links them to traditional LCA workflows. By generating LCI data from UMP models, we demonstrate a means for storing and exchanging parametric LCI models for manufacturing processes. Manufacturing processes present a key opportunity since existing manufacturing LCI models available in commercial databases do not commonly feature process-level parametric relationships to enable decision making in traditional manufacturing workflows. Instead, models rely on high-level aggregated assumptions that are not scalable to low-level manufacturing operations, e.g., distinguishing differences in milling slots or pockets of the same

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volume. For example, the ecoinvent database[1] scales all machining operations based on the weight of product produced or operation conducted. In other words, removing material in a complex manner to create a 1 kg sphere and cutting simpler shapes to create a 1 kg cube would share identical environmental impacts. Such an assumption is fundamentally flawed and causes significant uncertainty.

Motivated by such challenges, others have developed frameworks and tools to develop, curate, and deploy parametric process models to achieve more sustainable manufacturing [8, 9, 11, 13, 14, 19]. However, these solutions do not follow a strict standards-based approach and are hence difficult to integrate into traditional LCA workflows. Our approach is complementary to these efforts yet maintains a strong focus on standards throughout its design and implementation.

Both E3012-16 and ISO14048 [12] contain data representations for representing environmental impacts of manufacturing processes[2]. However, these representations are incompatible due to their differing purposes. E3012-16 is designed to communicate and formally characterize the performance of manufacturing processes through a common information model while the ecoSpold2 format was created to curate LCI datasets for LCAs in databases and conforms to ISO 14048, which defines requirements for LCA data formats [12]. Providing a model transformation from E3012 into LCA workflows allows for more accurate manufacturing process models to be considered when conducting an LCA. This would allow manufacturers to reuse their production models in LCAs and would allow LCA practitioners to better understand how a change at the production phase could ripple throughout the entire product lifecycle. This paper explores this model transformation by mapping an E3012 model[3] into ecoSpold2 and conducting an LCA using the Brightway2 framework [17]. Note that the E3012 model encodes *UseBounds* for each model input and output, facilitating record-keeping related to uncertainty quantification [2].

In this paper, we present (1) the development of a formal mapping between the UMP and ecoSpold2 information models, (2) the generation of LCI data demonstrated through a milling case study, and (3) guidance for the revision of E3012 to facilitate its utility in LCA workflows. We view this work as critical in (a) forming a bridge between previous efforts of curating parametric manufacturing models, such as the Cooperative Effort on Process Emissions in Manufacturing (CO2PE!) [7] and (b) presenting a cohesive vision for a UMP repository [3].

2. Methods and tools deployed

The main goal of this work is to develop a pipeline that ports data from the UMP representation into the traditional LCA workflow. Here, we assume that users are implementing the revised E3012 information model [2] to communicate and exchange UMP models. We also assume that LCA software in our

[1] We considered ecoinvent 3.4 (see: https://www.ecoinvent.org/)

[2] The LCA data format used in this paper is ecoSpold2

[3] We use the schema extension proposed in Bernstein et *al.*[2]. The extension has been proposed as a E3012 revision and is under ballot in ASTM E60.13.

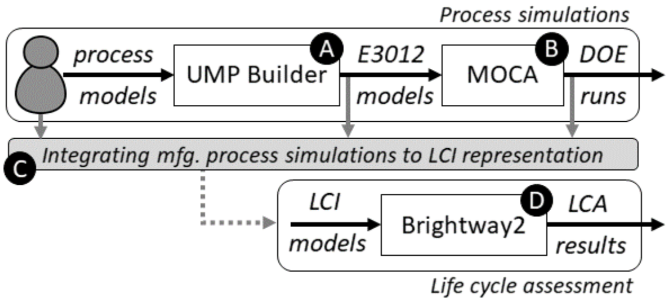

Fig. 1. Pipeline realized by mapping E3012 to ecoSpold2. Each labeled step (A-D) signifies a stage of data transformation or manipulation (A-D).

workflow accepts the ecoSpold2 information models as inputs. Based on prior experience, we also assume that user input is necessary due to the required domain expertise of selecting LCI models from traditional databases. Requirements for achieving the mapping between the UMP and ecoSpold2 formats in an open-source manner, include (1) an open tool that accepts and runs UMP models, (2) open LCA software that ports to LCI models, and (3) an interactive framework that prompts practitioners for domain expertise when needed.

Figure 1 presents the data pipeline for generating LCA results from parametric models curated as UMP models. To begin, a manufacturer or modeler contributes a parametric model representing a manufacturing process. In our work, ASTM E3012 is used to represent domain-specific data about the physical inputs, outputs, and resources, as well as mathematically defined transformations and product and process information [1]. We leverage the UMP Builder [2] (labeled as A in Fig. 1) to help manufacturers validate their conformance to the standard, share and reuse their UMP models, as well as interface with modeling, simulation, and analysis tools.

From the UMP model, we extract the structure and content to obtain operational code by using the **MO**del **C**omposition and **A**nalysis (MOCA) tool [16] (B in Fig. 1), outputting a Jupyter notebook[4]. This code contains control parameters set by the manufacturer and variable constraints that enable bounded simulations. The output code from MOCA can also be used for optimization, which could help improve a system with respect to a given metric of interest, e.g., cost or energy consumption. Executing the simulation generates a text file that stores all the values involved in each of the instances, e.g., control parameters, intermediate variables and metrics of interest.

Using both the parametric model and the simulation results, we perform a user-assisted mapping (C in Fig. 1) that yields an ecoSpold2 file compatible with Brightway2 (D in Fig. 1), an LCA framework. This file contains not only data describing the physical input and output of the manufacturing process in question but also links to other entries that provide inventory data of processes involved. This improves precision of results by covering the complete life cycle of the product. The generated ecoSpold2 file is then added to a dataset to be used by

[4] Used for evaluating the UMP models (see: http://jupyter.org/)

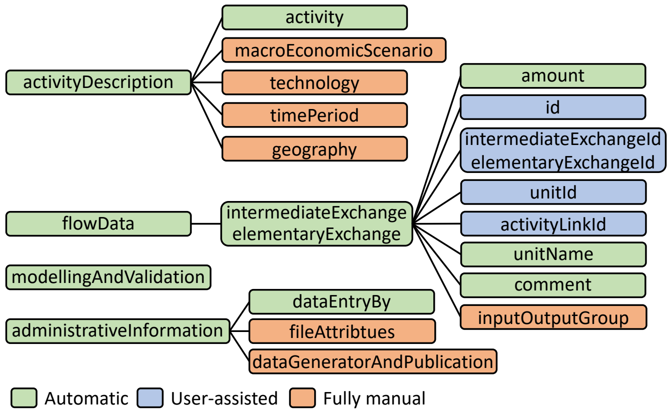

Fig. 2. Necessary fields for a generated ecoSpold file. Color of each field classifies how information is ported from UMP models in our implementation.

Brightway2 for performing LCA, assuming that the ecoSpold2 file has been appropriately generated.

To be clear, Fig. 1-[A, B, and D] represent steps that are generally applicable to other scenarios. The UMP Builder [2], can be used to generate models conforming to the revised E3012 schema. MOCA [16] can be used to graphically develop operational models using a domain-specific modeling language and Brightway2 [17] can be used to conduct LCAs. Our mapping (Fig. 1-C) facilitates the correlation between all three tools.

3. Mapping between the E3012 and ecoSpold2 data formats

Even though there are similarities between the E3012 and ecoSpold2 formats, we identified major differences that involved necessary steps for validation to successfully append the LCI database, e.g., *exchangeIds* and *unitIds*. Figure 2 classifies the mandatory fields for an ecoSpold2 file to be accepted by Brightway2 based on whether the information is available from the UMP model or additional support is required.

With the data provided by the UMP model and the simulations from MOCA, some of the required fields to generate valid ecoSpold2 files can be directly populated (Fig. 2, in green). However, in other cases, the system prompts the user to select an equivalent entry in the database (Fig. 2, in blue). For example, if the UMP model includes aluminum scrap as an output, the user must specify the appropriate option available in the LCI database, e.g., "treatment of aluminium scrap, post-consumer, prepared for recycling, at remelter" or "treatment of aluminium scrap, new, at remelter" as in ecoinvent. Linking inappropriate activities can significantly impact the LCA results. Data types shown in orange in Fig. 2 signify ecoSpold2-specific information not currently represented in E3012:

- *technology*, capturing characterizations of the technological domain of the activity, e.g., the relative modernity and significant peculiarities of the domain
- *macroEconomicScenario*, allowing for alternative macro-economic activities to be modelled and captured
- *dataGeneratorAndPublication*, containing information about who collected, compiled, or published the data, which may be the same person as under *dataEntryBy*
- *inputOutputGroup*, providing more details by classifying them into categories, such as materials/fuels, electricity/heat, services, or activities from the technosphere

For these instances, we added dummy data to meet ecoSpold2 requirements. These additions do not affect the LCA results.

To accomplish the mapping, the Mapping Module (MM) first extracts the input and output names and symbols (captured as MathML equations) from the E3012 model. For each input and output, a corresponding exchange in ecoSpold2 will be created. The MM uses the symbols to extract the input and output quantities computed by the MOCA simulation and maps them to the amount of the respective exchange.

To perform a LCA, each exchange needs to be linked to an activity. Inputs of the UMP model are linked to exchanges that are produced by an activity while outputs of the UMP model are linked to exchanges consumed by an activity. The exchange representing the reference product, i.e., the resulting product of the manufacturing process, does not need to be linked. Since the database could contain thousands of datasets, identifying the appropriate activity to link is user-assisted. For an exchange used as an input, the MM will provide activities that contain a "reference product" exchange matching with the name of the E3012 input. For an exchange used as an output (excluding the reference product), the MM is going to provide activities that consume the exchange as input from the technosphere, and match with the name of the E3012 output. The user must choose the appropriate activity from the prompted list.

Since E3012 does not currently handle a way to specify a reference product, the user is prompted to specify which output relates to the product generated. The reference product exchange is treated differently since it needs not to be linked to an existing activity. Once the appropriate activity has been chosen, the MM generates a *IntermediateExchangeId* and includes a *activityLinkId*, which represents the *id* of the entry to be linked.

For the rest of the fields (Fig. 2, in orange), the user manually adds information during mapping. For example, the *geography* field can be instantiated by finding the appropriate geographical location in the meta-data files, e.g., the *id* corresponding to United States. A similar approach can be used for *timePeriod*, *macroEconomicScenario*, *dataGeneratorAndPublication*, and *fileAttributes*. Some fields such as *technology* and *modellingAndValidation* are required in the ecoSpold2 schema. However, Brightway2 does not use their content. In other words, dummy values added for these fields do not affect LCA results.

In our implementation, we assume that all physical inputs and outputs of manufacturing processes are received from or generated to the technosphere, representing activities generated by human-driven economic processes. In future work, we plan to enable mapping to activities and flows to and from the ecosphere, representing flows that directly interface with ecological systems (e.g., waste water into a river from a coal burning plant). However, this requires more detailed and structured information about the inputs and outputs in the E3012 data model.

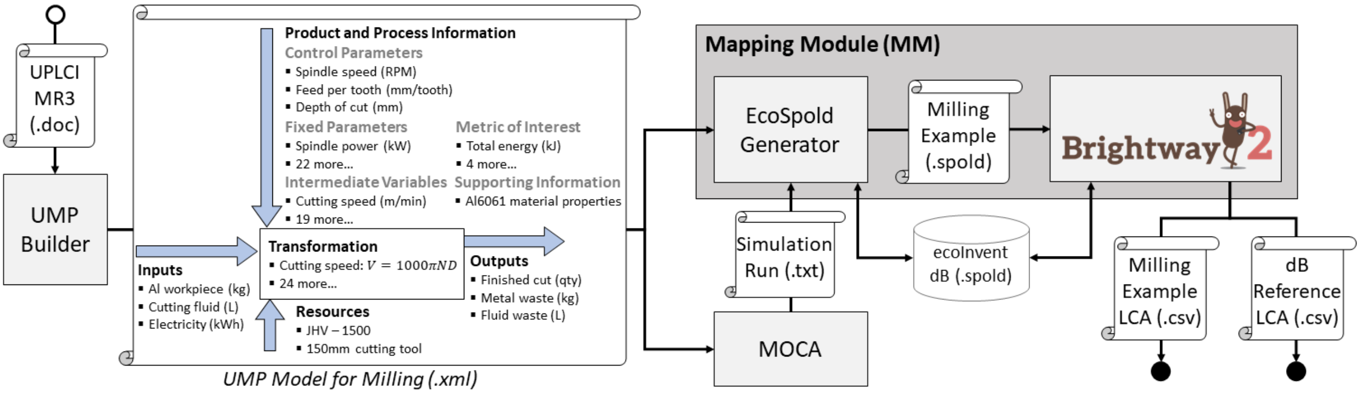

Fig. 3. Demonstration of the UMP-ecoSpold2 mapping through a milling case study.

4. Case study: integrating a milling UMP with ecoinvent

Figure 3 describes the data used and generated to demonstrate our UMP-ecoSpold2 mapping methodology. We borrow all assumptions and modeling procedures, including functional unit, scope, and system boundaries, from the milling example (code: MR3) reported by the Unit Process Life Cycle Inventory (UPLCI) team [18]. We built the model on the UMP Builder[5] and consulted the MR3 document as needed. Through the UMP Builder, an eXtensible Markup Language (XML) document was generated formally describing the parametric milling UMP model. This model consists of 25 transformation equations, 3 physical inputs, 3 physical outputs, 2 elements describing the manufacturing resources referenced in MR3, and a total of 52 entities describing product and process information. For every variable used in the transformation equations, an accompanying definition of its type, bound, and unit are captured under product and process information.

The semantic information describing each variable, equation, and the relationships between them is interpreted with the MOCA tool to generate operational code in the form of a Jupyter notebook. We used the MOCA-generated code to evaluate the UMP milling model. This case study presented the energy, waste, and time consumed for milling a straight cut of 90 000 mm^3 of prismatic aluminum (Al) workpiece. For the case study, the control parameters, depth of cut, spindle speed, and feed per tooth, were set to 3 mm, 255 rev/min, and 0.381 mm/tooth, respectively. We recognize that these settings are conservative; however, we aimed to conform exactly to the UPLCI model. All computed values were compared to the case study section of the UPLCI MR3 document to validate our milling model was created and evaluated appropriately.

To generate an ecoSpold2 file corresponding to the UMP model, the MM extracts semantic information from the milling XML document, including units, symbols, and names. The MM also obtains numerical data from the text file generated from MOCA, including values associated with metrics of interest (e.g., waste generated). Here, each representing metrics of interest, the computed energy consumption, cycle time, aluminum waste generated, and CO_2 emissions are 0.334 kWh, 90.3 s, 0.244 kg, and 0.196 kg CO_2, respectively. Through the use of the semantic data, the MM queries onto the ecoinvent database, a commercial LCI database, to link entities of the milling UMP, e.g., aluminum 6061, cutting fluid, and electricity, to database activities that either generates the UMP input or consumes the UMP outputs. This is necessary to perform a complete LCA. In the generated “MillingExample.spold” file, the functional unit of a single cut is set to a dimension of 90,000 mm^3 (or 0.24489 kg of Al). Energy consumed, waste generated, and cycle time were scaled based on the size of the cut. We rely on Brightway2 to evaluate the milling process’s environmental impacts using the Tool for Reduction and Assessment of Chemicals and other Environmental Impacts (TRACI) methods[6]. After verifying that the milling UMP can be used to generate LCA data, we conducted an initial validation study to test whether our model is producing realistic, feasible values as compared with commercial models present in the ecoinvent 3.4 database. In this use case, we compare the values generated by our milling UMP against *aluminum milling, small parts RoW*, which is an entry in the ecoinvent database, since the metadata description within the ecoinvent file seemed to match the intent of the UPLCI MR3 milling descriptions. While comparing to the dataset *aluminum milling, small parts*, there were some important considerations. The ecoinvent database selects the weight of the material cut from the part as a functional unit, making the initial shape of the part a fundamental consideration in the equation. In our test case, we use a single horizontal cut instead, allowing us to obtain a more precise and scalable measure.

To compare results between the TRACI impacts of the milling case study with the existing database (DB) entry, we conducted nine Monte Carlo (MC) simulations (50 000 runs each) with the Brightway2 framework using the uncertainty properties from the ecoSpold2 file of the DB entry. The main idea was to perturb each individual exchange of the *aluminum, small parts RoW* based on their individual uncertainty characteristics, fit a probability density function (PDF) to the results

[5] Public version of UMP Builder (see: https://umpbuilder.nist.gov/)

[6] TRACI was developed by the Environmental Protection Agency (EPA). See https://tinyurl.com/yde3bjno

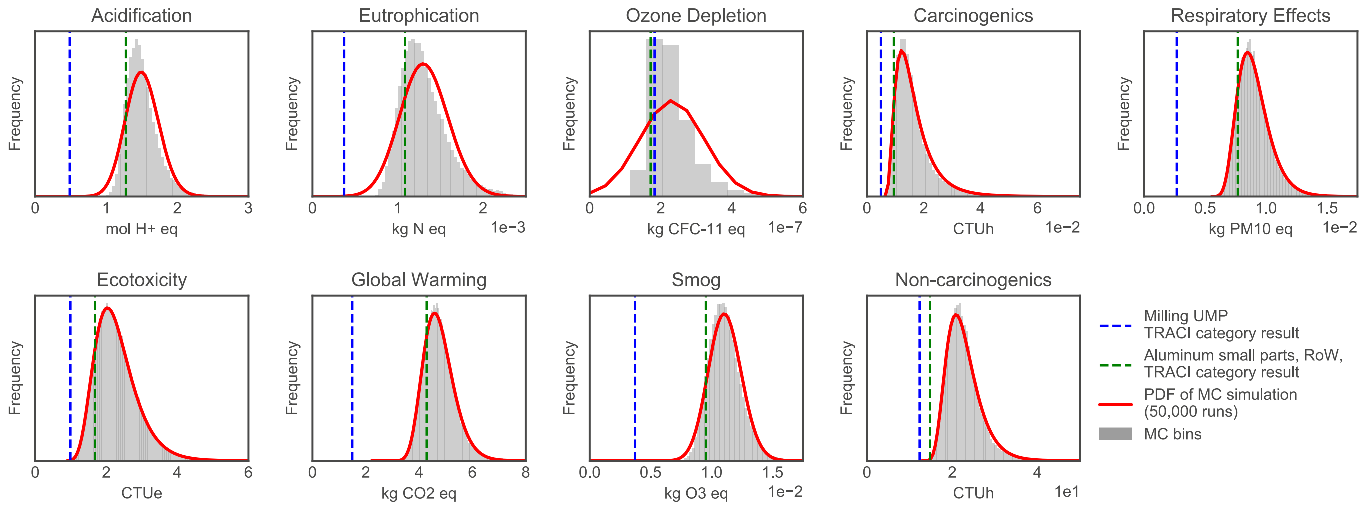

Fig. 4. Results of a Monte Carlo simulation (50,000 runs) of *aluminum, small parts RoW* with comparison of results to our Milling UMP (blue dotted line). The green dotted line signifies results of an LCA conducted with only the nominal values available in the DB entry.

Table 1. Our test case compared against similar activity in ecoinvent
*Refers to values from database entry, *aluminum milling, small parts RoW*

TRACI category (units)	DB*	CDF_{DB}*	UMP	CDF_{UMP}
acidification (mol H+ eq)	1.28	0.162	0.486	6.32e-7
ecotoxicity (CTUe)	1.68	0.132	0.990	8.53e-5
eutrophication (kg N eq)	1.10e-3	0.213	3.71e-4	2.22e-4
global warming (kg CO_2 eq)	4.29	0.214	1.49	**0.0**
ozone dep. (kg CFC-11 eq)	1.72e-7	0.251	1.83e-7	0.292
smog (kg O_3 eq)	9.53e-3	0.121	3.72e-3	5.41e-10
carcinogenics (CTUh)	9.47e-3	6.30e-2	4.91e-3	**0.0**
non-carcinogenics (CTUh)	14.8	3.39e-4	12.4	3.15e-14
resp. effects (kg PM10 eq)	7.68e-3	0.143	2.67e-3	**0.0**

based on the TRACI categories, and observe if our test case data falls within the bounds of the PDF. According to the DB entry, each exchange is modeled as a lognormal random variable. Here, we assume that the MC results can be approximated as a lognormal distribution. Though difficult to prove, it has been observed that linear combinations of lognomal random variables effectively approximate to a lognormal distribution [6].

Figure 4 summarizes the result of the nine MC simulation runs for each TRACI impact category. The PDFs fitted to the simulation data, the values of the milling UMP test case, and the values of the DB entry are shown in red, blue, and green, respectively. The values from the UMP results are considerably lower than those for the database entry, except for results for ozone depletion. To understand the degree of their difference, we evaluated the cumulative distribution function (CDF) at each value, as shown in Table 1. As seen in the CDF evaluation for the UMP values, with the exception of the ozone depletion result, the UMP results fall outside the uncertainty bounds of the database entry. In other words, the CDF evaluations are practically zero. In three cases, i.e., global warming, carcinogenics, and respiratory effects, the evaluation of the CDF was zero (shown in bold). Interestingly, the discrete values from the database entry seem to represent a rather liberal estimation of the results, falling to the left tail of the PDF.

Here, we offer an explanation for the differences observed. The complexity of both models are considerably different. The UMP milling example carries 6 exchanges while the database entry has 27 exchanges. If we were to include, for example, impacts associated with compressed air and other auxiliary manufacturing resources (similar to the ecoinvent entry), we would expect to obtain closer values. However, it is not clear which of the 9 resulting values (i.e., which impact category) would be most affected. These issues get to the center of the difference between a parametric approach and using "pre-computed" LCI data. The "pre-computed" data is heavily aggregated and incorporates effects from industry-wide exchanges regardless of whether the process utilizes every one. This is evident in the low CDF values of the database entry itself against the MC simulations. However, we recognize that parametric models built using the E3012 data model require more rigorous testing and validation than what was done for the milling UMP example. Characterizing the validation requirements of such UMP models to be as trusted as "pre-computed" LCI models is a necessary step to push this work forward.

5. Future directions and closing remarks

In this paper, we discussed the mapping of the E3012 and ecoSpold2 data models and demonstrated its utility in a traditional LCA workflow using Brightway2. Through this exercise, we informed the on-going revision of the E3012 standard. For example, we included units and bound equations for *Input* and *Output* entities in the UMP to ease the integration with LCA tools. We also identified an opportunity to integrate a definitive "functional unit" and clearer classifications of waste into the UMP information model. However, these concepts require additional research to be addressed properly.

Our work is not without its limitations. Our pipeline relies on significant human input for some of the mapping, as discussed in Section 3. Selecting appropriate database entries is an expert-driven exercise and, hence, is prone to human error. Another limitation is that we do not yet integrate the design of experiments simulations from MOCA with Brightway2. In other words, we do not fully leverage the rich information describing the control variables to simulate LCA data. If such integration was realized, relating LCA results to product design decisions would be feasible. Additionally, we assume in this work that a single UMP model maps in a one-to-one fashion to a single LCI database entry. We do not address pooling information from multiple UMP sources to a single LCI process.

Other limitations of this work relate to the E3012 information model and support around it. As of now, we have yet to demonstrate validation protocols for UMP models. To integrate information from several UMP models, consistency in model topography is critical, including considerations related to naming conventions, units, and shared content (e.g., equations). Developing a "master data" context similar to how ecoinvent handles this issue could be a reasonable research direction.

To conclude, we plan to relate the LCI data generation back to the control variables defined in the UMP to enable system-tradespace exploration. One of the key challenges with effectively making environmentally-efficient decisions at the design stage is having the appropriate data representations speak to one another. From that perspective, previous design tools and frameworks have not been ideal [4]. We envision that integrating the UMP information model will help realize a new suite of tools that can explore "what-if scenarios" tied to design decisions and how their effects propagate through the lifecycle. In other words, we will extend the pipeline to relate UMP models to parametric design attributes. For example, how does the number of teeth in a gear design change the machining strategy and what is its impact on the environment? Developing a automated pipeline to reflect on such questions would facilitate deeper design space exploration. We believe that such an achievement would demonstrate the impact and scalability of the UMP modeling approach.

Disclaimer

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