Proceedings of the ASME 2011 International Design Engineering Technical Conferences &
Computers and Information in Engineering Conference
IDETC/CIE 2011
August 28–31, 2011, Washington, DC, USA

DETC2011-48500

INTEGRATION OF LIFE CYCLE INVENTORIES INCORPORATING MANUFACTURING UNIT PROCESSES

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ABSTRACT

Sustainable manufacturing (SM) concerns the manufacture of products with regard to environmental, social, and economic impacts over the entire life cycle. With a primary focus on environmental concerns, life cycle assessment (LCA) can support SM practices. The life cycle inventory (LCI) is a key phase of LCA, and this paper considers the integration of manufacturing unit processes (MUPs) into system-level LCIs, which requires consideration of process flow diagrams at different levels of abstraction. Furthermore, uncertainty quantification is an important component of LCA interpretation, and this paper proposes a method to synthesize LCIs from the process-level to the system-level that consistently quantifies uncertainty in the inventories. The method can incorporate MUP data derived from measurements and/or modeling and simulation. Further development towards a complete methodology is discussed.

INTRODUCTION

A simple definition of a *sustainability* is “the capability to use a resource without permanently depleting it, thus preserving the resource for future use” [1]. Several facets of sustainability have been identified, the most important of which include environment, society, and economy. Despite the straightforward definition given above, the identification and validation of sustainable practices can be difficult given the complex interactions between environment, society, and economy, and the myriad uncertainties involved. Nevertheless, given the reality of limited resources, sustainable living is necessary to ensuring a reasonably sufficient and enduring quality of life.

Sustainable manufacturing (SM) refers to the provision of manufactured products in a sustainable manner, i.e., in a manner that does not permanently deplete environmental, social, and economic resources during the complete life cycle of the manufactured product. In SM practice, it is insufficient to design a product merely for function, manufacturability, and profit. Rather, a sustainable design also considers, for example, how the product can be manufactured in an energy efficient way, used in an environmentally and socially responsible manner, and recycled into the raw materials for the next generation of products. These additional considerations require a corresponding evolution of the supporting methodologies, techniques, and computational and information tools for life cycle engineering [2–5].[1]

SM subsumes traditional manufacturing (TM). Here, TM refers to widely adopted manufacturing principles and practices such as Lean Manufacturing and Total Quality Management, which are not concerned with environmental and social impacts. SM inherits numerous requirements and issues from TM, including customer satisfaction, geometric/functional tolerancing, material/component selection, supply chain management, manufac-

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[1] Methodologies are concerned with *what* to accomplish, while techniques are concerned with *how* to accomplish. Tools (such as computer software and data-collection sensors) implement the techniques that realize a given methodology.

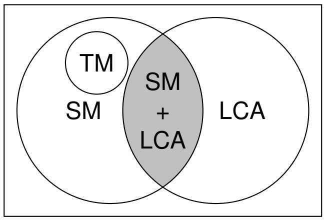

FIGURE 1. **The relationship between SM, TM, and LCA.**

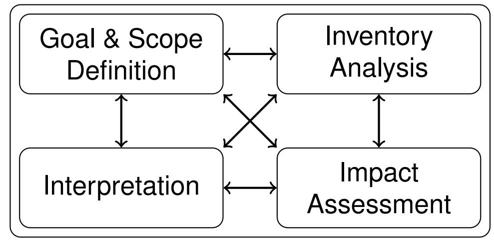

FIGURE 2. **The four interconnected phases of LCA.**

turing process issues, and cost/profitability constraints. In this paper, the term *manufacturing system* refers to the network of activities/processes whose purpose is the production of a given manufactured product, without specific consideration of later stages of the product's life cycle.[2]

The environmental impact over a manufactured product's life cycle is an important additional consideration in SM practice. Life cycle assessment (LCA) has been, and continues to be, developed as a *comprehensive* methodology for assessing *relative* environmental performance of product systems. A *product*[3] *system*, in LCA terminology, is a network of activities/processes that performs a given function to society, which includes *all* life cycle stages. Thus, an LCA product system for a function provided by a manufactured product includes the manufacturing system for that manufactured product. A comprehensive and properly conducted LCA avoids inadequate assessments arising from the choice of an overly narrow problem scope and prevents unaccounted "impact shifting" from, say, the usage stage of a product to the product's supply chain or end-of-life [6–10].

LCA is not without certain limitations [11, 12]. Nevertheless, LCA is a relatively mature and internationally standardized methodology [6, 7], thus deserving consideration in the support of evolving SM practices. However, in contrast to other international standards, such as the *Guide to the Expression of Uncertainty in Measurement* for metrology [13], computational implementations of the LCA methodology that include uncertainty quantification are not yet well standardized [14, 15]. Also, because LCA is also applied in areas outside manufacturing, such as the service and construction industries, LCA is not fully subsumed by SM (See Fig. 1).

In the standardized methodology [6,7], the four phases of an LCA are:

1. Goal and Scope Definition,
2. Inventory Analysis (a.k.a. Life Cycle Inventory, or LCI),
3. Impact Assessment (a.k.a. Life Cycle Impact Assessment, or LCIA), and
4. Interpretation.

The Goal and Scope Definition phase is critical at the outset of an LCA, identifying stakeholders viewpoints, applicable regulations and voluntary standards, time/budget constraints, etc., as well as establishing a consensus on the purpose and desired outcome(s) of the LCA. Once identified, the scope of the LCA guides the choice of environmental impact *indicators* that must be determined during the Life Cycle Impact Assessment (LCIA) phase of the LCA, as well as the *functional unit* and *system boundary*. These choices enable the Life Cycle Inventory (LCI) phase of the LCA to proceed, in which the product system is decomposed (over the entire life cycle, but within the system boundary) into the productions of the component products needed to realize the functional unit.[4] The resulting *product flows* in the *technosphere* of the system under study are related to the corresponding *elementary flows* effected in the *ecosphere* by the product flows' demand, relative to the chosen functional unit and system boundary. Once the elementary flows have been *compiled* into *inventories* for the entire system, they are used in the LCIA phase to determine the previously selected environmental impact indicators. Once these impacts have been assessed, the Interpretation phase can summarize and validate the LCA, determine its implications, and judge its success. In practice, an LCA is usually an iterative process, and the four phases are interconnected rather than executed in a strict progression (see Fig. 2).

SM and LCA share the concept of *unit processes* that transform inputs into outputs, however, the abstraction level with respect to what the unit process encompasses differs. Manufacturing unit processes (MUPs) have been defined in both TM and SM contexts [16–18], and examples include: an individual turning operation in a machining sequence, a casting or painting process, or a (sub)assembly sequence. Thus, higher-level manufacturing systems are composed of several interconnected, lower-level MUPs. In a similar fashion, the LCA methodology decomposes a product's entire life cycle into many interconnected unit processes [6, 7]. In an LCA model for a manufactured product, the manufacturing stage can be represented as a single unit pro-

[2]For future reference, the term *part* will be used to refer to an instance of a manufactured component or product.

[3]In LCA terminology, *product* may refer to any product or a service, not necessarily a manufactured product.

[4]For example, a functional unit could be specified as 100 miles driven at 65 mph on a level paved road by a climate controlled vehicle occupied by two adults and two children and meeting the regulatory standards necessary for legal operation in the state of California.

cess with specified inputs and outputs. A decomposition of this unit process typically reveals the manufacturing system with its underlying MUPs, as well as additional unit processes relevant to the LCA. At various levels of abstraction, unit processes can encompass widely different temporal, spatial, production, and other scales. Such *multi-resolution* issues can cause consistency and integration problems across the multiple scales.

In order to support SM practices, the integration of MUPs into LCAs must address several issues, including:

1. LCA models operate at coarse scales and typically rely upon considerable averaging (e.g., spatial, temporal, population), contrasting the finer scale physical models typically available for MUPs.
2. Often, data relevant to the environmental impact of MUPs is neither included in legacy information systems nor readily available for collection.
3. Uncertainty quantification for LCA is not well standardized and often omitted altogether [19].
4. Although LCAs are used for decision support, design and production optimization is not a primary consideration in a typical LCA.
5. The integration of methodologies, techniques, and tools for LCA and manufacturing is limited, as is the consideration of social and economic factors.

Fortunately, LCA is still evolving and SM efforts can and should influence this evolution so as to address some/all of the above issues. This paper specifically addresses the consistent integration of MUP data into the determination of LCIs for LCA, including uncertainty quantification. Data sources can include modeling, measurement, and simulation. This integration is key to the subsequent assessment of the relative environmental performance over the entire life cycle of a manufactured product using the standardized LCA methodology.

Multi-resolution LCI methodologies, techniques, and tools

The LCI is a key phase of LCA, associating elementary flows to/from the ecosphere with product flows demanded by the technosphere [14, 20]. The LCI phase usually requires considerable time, money, and effort for system modeling and data collection, as well as compilation of the unit-process level elementary flows into a single, system-level inventory. Multiple types of uncertainty exist in the LCI phase, including modeling and data uncertainty. Thus, uncertainty quantification in the LCI phase (and subsequent LCIA phase) is important for making LCA results transparent and LCA-based decisions justifiable.

A *process flow diagram* is a model of the product system that specifies the relationships between the involved unit processes (see Fig. 3). The functional unit of the product system determines the *system demand flow(s)*. The study described in this paper is restricted to LCAs with a single system demand flow (i.e., no useful co- or by-products requiring allocation in the LCI). The system demand flow determines the simultaneous product flows of all the interconnected unit processes, called *reference flows*, that are necessary to meet the demand for the functional unit.

Interconnection of unit processes in an LCA process flow diagram requires reconciliation of, among other things, the various units of measurement, temporal and spatial scales, system boundaries, available data, and averaging methods. The modeling usually involves a *steady-state* consumption/production assumption, which means that fluctuations in the flows during the timescale under consideration are not resulting from system transients, thus allowing more reliable determination and usage of average flows. Another common and important assumption is *linearity of technologies*. With this linearity assumption, a unit process's *benchmark*[5] *product and elementary flows* scale proportionally to the meet the demand of the given reference flow, and the system as a whole can be described mathematically as a linear system.

The validity of the above two assumptions requires that the resulting model is an adequate approximation of reality at the given level of model abstraction, or *resolution*. The highest level of abstraction in an LCA, here termed the *LCA-level*, is a *system-level* resolution that includes all stages of the product life cycle represented as unit processes (e.g, raw material extraction, manufacture, usage, recycling). A given unit process can itself be treated as a *process-level system* to be further resolved into a process flow diagram composed of more detailed unit processes. In particular, the manufacturing system is often represented by a single unit process in an LCA-level process flow diagram, and this unit process can be treated as a system with its own process flow diagram that incorporates MUPs.

While the methodology for compiling LCIs at a system-level or process-level may, in principle, be the same, the different resolutions typically require the application of different techniques and tools. For example, process-level discrete event simulation (DES) can provide part-level data using a model of a manufacturing system. Such data is too detailed for the LCA-level, and so the *average* environmental flows (and their corresponding uncertainties) for the process-level system must be compiled for representation as an LCA-level unit process. Likewise, uncertainties in average product flows are often not included in LCI datasets at the LCA-level, even though this information may be derivable from measurements or DES. Furthermore, allocation of elementary flows may be unavoidable at the process-level because, for example, a single manufacturing line/plant sometimes produces multiple products in parallel.

[5] The term *benchmark flow* used here is not part of the ISO LCA standard.

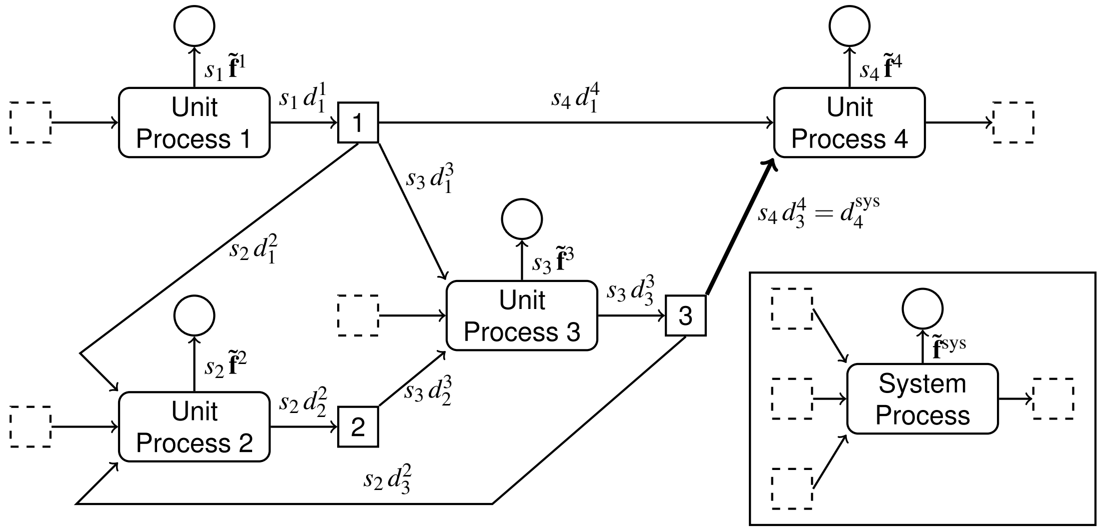

FIGURE 3. **Multi-resolution of process flow diagrams.** Process-level and system-level process flow diagrams represented by directed graphs. The inset picture represents the system-level view of the System Process composed of Unit Processes 1–4. Elementary flows to the ecosphere are denoted by an arrow to a circle and a square denotes a junction for a specific product flowing in the technosphere. Labeled arrows indicate reference flows, and the model has a single system demand flow, d_4^{sys}, represented by the thickened arrow. Scalars $s_1, \ldots, s_4$ denote respective benchmark production scalings for Unit Processes 1–4 required to produce the system demand flow. System-level inventories are compiled from the process-level elementary flows. Depending upon the system boundaries, flow diagrams can represent a gate-to-gate manufacturing process containing several MUPs, or a comprehensive product life cycle from cradle to grave/cradle. The input-only and output-only products (dashed squares) and their associated product flows would not appear in a cradle-to-grave/cradle LCA.

Paper outline

This paper is organized as follows: the next section discusses an integrated approach for the determination of LCIs at different levels of abstraction, including a consistent treatment of uncertainties and correlations using (co)variances. Two different techniques for LCI compilation, one at the LCA system-level and one at the manufacturing process-level, are described, and a specific process-level example is given of a manufacturing system involving a turning MUP. The Discussion section then discusses the present results as well as issues in the development of a complete methodology. Finally, the Conclusion section is followed by an appendix containing certain mathematical details.

AN INTEGRATED APPROACH TO THE DETERMINATION OF SYSTEM-LEVEL AND PROCESS-LEVEL LIFE CYCLE INVENTORIES

LCA validity relies, in part, upon the quality of the inventory compiled in the LCI phase. For a given unit process, many LCI datasets list a relevant set of *average* elementary and input product flows corresponding to a specific output product flow [21–23]. When uncertainty information for a particular elementary flow is included, it is typically given as a variance/standard deviation and considered to be stochastically independent of other flows, both within and between unit processes. The uncertainty analysis of the LCI compilation described here generalizes this variance-only situation, and the *variance-covariance matrix* of a system-level elementary flow vector is considered to be a sufficient description of the uncertainty in, and dependencies among, the compiled inventories.[6] Note that the (co)variances of the *state of knowledge of the average flows* of unit processes are considered throughout, not of the *population distribution* of these flows at steady-state production.

At the higher system-level, the compilation procedure accommodates covariance information about elementary flows both *within* and *between* unit processes. In the absence of variance and/or covariance information (i.e., some/all (co)variances are assumed zero), the analysis simplifies accordingly. Furthermore, when several unit processes are collected into an independent system, the variance-covariance matrix for the compiled, system-level flows allows consistent treatment of the system as an independent unit process in a higher-level process flow diagram. At the lower process-level, the compilation procedure for a manufacturing system converts part-level flow information into averages and (co)variances that can be used in the higher level compilation. The consistent integration of system-level and

[6]Standard deviations and correlation coefficients can be derived directly from the variance-covariance matrix.

process-level LCI compilations is a key consideration of the approach.

Higher-level LCI compilation

A method for higher-level LCI compilation is now described for systems such as the one represented by the cradle-to-grave/cradle process flow diagram depicted in Fig. 3. The method is broken down below into conceptual stages, with the mathematical details located in the Appendix.

Scaling production to meet system demand. As discussed above, a standard assumption for LCI compilation at the LCA-level is that unit processes scale linearly. Thus, the benchmark product flows of the various unit process (e.g., electricity, materials, transportation, etc.) must be appropriately scaled to become reference flows that satisfy the specified system demand flow. For the proper subsequent accounting of elementary flows, any unit process that consumes its *own* product, such as a parasitic load, should account for this internally. Balancing average product flow production with consumption across all unit processes and applying the system demand flow constraint leads to the following linear system, written in matrix-vector form, which models steady-state production in the technosphere:

$$\mathbf{D}\,\mathbf{s} = \mathbf{d}^{\mathrm{sys}}, \tag{1}$$

where $\mathbf{D}$ is the *technology matrix*, $\mathbf{s}$ is a *scaling factor vector*, and $\mathbf{d}^{\mathrm{sys}}$ is the *system demand vector*.[7] The linear system must be solved for the column-vector $\mathbf{s} = (s_1, \ldots, s_N)^{\mathrm{T}}$, which has one scalar entry for each of the N unit processes in the process flow diagram. The technology matrix represents the benchmark product flow requirements of the N unit processes, so that each column of $\mathbf{D}$ is derived from the demand vector for the corresponding unit process at a specified steady-state production level, i.e.,

$$\mathbf{D} := \left[\mathbf{d}^1 \cdots \mathbf{d}^N\right]. \tag{2}$$

For a well-formulated LCA model, the linear system (1) has at least one solution $\mathbf{s}$, otherwise the product system would not be feasible.[8] Note that the computation of $\mathbf{s}$ is deterministic.[9]

<u>**EXAMPLE 1**</u> The linear system (1) is derived here for the cradle-to-grave/cradle system whose process flow diagram appears in Fig. 3. Balancing the input flows with the output flows at each of the three product junctions (squares 1–3 and incident arrow labels in Fig. 3) gives the following linear system

$$\begin{aligned}
s_1 d_1^1 - s_2 d_1^2 - s_3 d_1^3 - s_4 d_1^4 &= 0,\\
s_2 d_2^2 - s_3 d_2^3 &= 0,\\
- s_2 d_3^2 + s_3 d_3^3 - s_4 d_3^4 &= 0,\\
s_4 d_3^4 &= d_4^{\mathrm{sys}},
\end{aligned}$$

where the last row is derived from the system demand flow constraint. Note that a sign convention corresponds to the product flow arrows.

Compiling scaled elementary flows. If there are M average elementary flows to/from the environment in an LCI (e.g., carbon dioxide, ozone, lead, etc., which are of concern for the subsequent LCIA), then these flows can be represented mathematically by a vector of length M, called an *elementary flow vector*. In order to incorporate uncertainty information in the *average* flows, the elementary flow vectors are *random* vectors. In a general setting, the elements of these vectors are random variables that are jointly distributed, both within and across unit processes. There is one random elementary flow vector for each of the N unit process, denoted $\tilde{\mathbf{f}}^1, \ldots, \tilde{\mathbf{f}}^N$,[10] which form the columns of the random *intervention matrix*, $\widetilde{\mathbf{F}}$, i.e.,

$$\widetilde{\mathbf{F}} := \left[\tilde{\mathbf{f}}^1 \cdots \tilde{\mathbf{f}}^N\right].$$

The system-level elementary flow vector $\tilde{\mathbf{f}}^{\mathrm{sys}}$ (also a random vector) is *compiled* by summing the scaled process-level elementary

[7] The matrix technique and terminology of [14] has been adopted here. However, some of the notational labels have been changed for clarity. The system demand vector, $\mathbf{d}^{\mathrm{sys}}$, is determined by the system demand flow(s) corresponding to the chosen functional unit. For a functional unit with only a single corresponding system demand flow, the system demand vector has a single, non-zero entry and allocation is unnecessary.

[8] The matrix $\mathbf{D}$ need not be square, and several factors influence its dimensions, such as multi-functionality of the product system and modeling choices for product-flow cutoff [14]. If $\mathbf{D}$ is square and invertible, then $\mathbf{s} = \mathbf{D}^{-1}\mathbf{d}^{\mathrm{sys}}$ is the unique solution. However, computing $\mathbf{D}^{-1}$ may not be the most computationally efficient way of solving the linear system. Furthermore, an important consideration is the sensitivity of a solution $\mathbf{s}$ to small changes in $\mathbf{D}$ or $\mathbf{d}^{\mathrm{sys}}$, which depends on the properties of $\mathbf{D}$ and reflects the sensitivity of the modeled system to perturbations [14].

[9] Demand-related uncertainties in the technosphere are outside the scope of the present work.

[10] An overset tilde ($\sim$) denotes a random quantity, e.g., $\tilde{a}$, $\tilde{\mathbf{a}}$, $\widetilde{\mathbf{A}}$ denote a random scalar, random vector, and random matrix, respectively. Expected values, vectors, and matrices are denoted by $\mu_{\tilde{a}} = \mathsf{E}[\tilde{a}]$, $\mu_{\tilde{\mathbf{a}}} = \mathsf{E}[\tilde{\mathbf{a}}]$, $\mu_{\widetilde{\mathbf{A}}} = \mathsf{E}\left[\widetilde{\mathbf{A}}\right]$, respectively. The variance of the random scalar $\tilde{a}$ is denoted by $\sigma_{\tilde{a}}^2 = \mathsf{V}[\tilde{a}] = \mathsf{E}\left[(\tilde{a} - \mu_{\tilde{a}})^2\right]$, the covariance of two random scalars $\tilde{a}_1$ and $\tilde{a}_2$ is denoted by $\sigma_{\tilde{a}_1,\tilde{a}_2} = \mathsf{C}[\tilde{a}_1, \tilde{a}_2] = \mathsf{E}\left[(\tilde{a}_1 - \mu_{\tilde{a}_1})(\tilde{a}_2 - \mu_{\tilde{a}_2})\right]$, and the variance-covariance matrix corresponding to the random vector $\tilde{\mathbf{a}}$ is denoted by $\Sigma_{\tilde{\mathbf{a}}} = \mathsf{E}\left[(\tilde{\mathbf{a}} - \mu_{\tilde{\mathbf{a}}})(\tilde{\mathbf{a}} - \mu_{\tilde{\mathbf{a}}})^{\mathrm{T}}\right]$. Note that $\sigma_{\tilde{a}}^2 = \sigma_{\tilde{a},\tilde{a}}$.

flow vectors, which can be compactly represented by a matrix-multiplication as follows:

$$\tilde{\mathbf{f}}^{\mathrm{sys}} = \sum_{n=1}^{N} s_n \tilde{\mathbf{f}}^n = \widetilde{\mathbf{F}}\mathbf{s}, \tag{3}$$

where $\mathbf{s} = (s_1, \ldots, s_N)^{\mathrm{T}}$ is a (deterministic) solution to system (1).[11] (Also see Fig. 3.)

Uncertainty quantification for elementary flows with dependencies. In general, the compilation of the system-level random elementary flow vector $\tilde{\mathbf{f}}^{\mathrm{sys}}$ in (3) requires computing the joint distribution of the component random variables. In practice, the expected value of $\tilde{\mathbf{f}}^{\mathrm{sys}}$, denoted $\mu_{\tilde{\mathbf{f}}^{\mathrm{sys}}}$, and the variance-covariance matrix for $\tilde{\mathbf{f}}^{\mathrm{sys}}$, denoted $\Sigma_{\tilde{\mathbf{f}}^{\mathrm{sys}}}$, can provide adequate information about $\tilde{\mathbf{f}}^{\mathrm{sys}}$. The diagonal and off-diagonal entries of the variance-covariance matrix describe uncertainties and correlations, respectively. The matrix-vector multiplication in (3) is somewhat nonstandard, because the matrix is random and the vector is deterministic, not vice versa. The appendix provides the computational details, starting with the general case in which the all the elements of $\widetilde{\mathbf{F}}$ are dependently distributed, and finishing with some special cases that use common independence assumptions.

Lower-level LCI compilation

Compiling the LCI of a lower-level system from its constituent unit processes can require different techniques and tools than the higher-level compilation. For example, characterization of the manufacturing stage of a product at the LCA-level involves consideration of lower-level manufacturing (and supporting) unit processes. MUPs are often modeled using specialized tools, such as DES software [2]. Furthermore, model simulations and process measurements can provide detailed information about individual instances of manufactured components or finished products. This information about a population of manufactured products must be compiled into average product and elementary flows that are consistent with the higher-level LCI compilation techniques described in the previous subsection.

Compilation of an LCI for a manufacturing system requires knowledge of the chosen LCIA indicators and a precise delineation of the system's boundary. The choice of indicators and boundary determines which flows will be considered as input products from the technosphere vs. elementary flows to/from the ecosphere. A single output product is assumed here, which requires all downstream technosphere by-products (such as used coolant) to be converted to environmental flows within the manufacturing system. The functional unit and corresponding system demand flow for the LCA-level process flow diagram indicates the order of magnitude of the system's production level. This production level provides a benchmark output product flow for the corresponding simulation/measurements of the manufacturing system.

Depending on the maturity of the product's design and manufacture, some combination of simulation and measurement can generate data that allows determination of the average input product flows and average elementary flows for the given production level, as well as the necessary (co)variance information. Because of internal and external variabilities, repeated samples of the flows for the desired production level are necessary to provide uncertainty information. Some level of statistical correlation in the flows is expected, arising from manufacturing systems comprised of interconnected MUPs.

Let $\tilde{\mathbf{f}}^{\mathrm{man}}$ denote the (random) elementary flow vector to be compiled for a manufacturing system (i.e., the average elementary flows, with uncertainty, at a given steady-state production level), and let $\mathbf{f}^{\mathrm{man}_1}, \ldots, \mathbf{f}^{\mathrm{man}_Q}$ denote the Q independently sampled elementary flow vectors. An estimator for the expected value of $\tilde{\mathbf{f}}^{\mathrm{man}}$, denoted by $\widehat{\mu}_{\tilde{\mathbf{f}}^{\mathrm{man}}}$, is given by the sample mean $\bar{\mathbf{f}}^{\mathrm{man}}$, i.e.,

$$\mu_{\tilde{\mathbf{f}}^{\mathrm{man}}} \approx \widehat{\mu}_{\tilde{\mathbf{f}}^{\mathrm{man}}} := \bar{\mathbf{f}}^{\mathrm{man}} = \frac{1}{Q} \sum_{q=1}^{Q} \mathbf{f}^{\mathrm{man}_q}.$$

Likewise, an estimator for the variance-covariance matrix $\Sigma_{\tilde{\mathbf{f}}^{\mathrm{man}}}$, denoted by $\widehat{\Sigma}_{\tilde{\mathbf{f}}^{\mathrm{man}}}$, can be obtained from the sample variance-covariance matrix of the mean. In particular, the $(j,k)^{\mathrm{th}}$ element of $\Sigma_{\tilde{\mathbf{f}}^{\mathrm{man}}}$ is reasonably approximated by

$$\begin{aligned}\sigma_{\tilde{f}_j^{\mathrm{man}}, \tilde{f}_k^{\mathrm{man}}} &\approx \widehat{\sigma}_{\tilde{f}_j^{\mathrm{man}}, \tilde{f}_k^{\mathrm{man}}} := S_{jk}^{\mathrm{man}} \\ &= \frac{1}{Q(Q-1)} \sum_{q=1}^{Q} \left(f_j^{\mathrm{man}_q} - \bar{f}_j^{\mathrm{man}} \right) \left(f_k^{\mathrm{man}_q} - \bar{f}_k^{\mathrm{man}} \right),\end{aligned}$$

where $f_j^{\mathrm{man}_q}$ denotes the j^{th} component of the q^{th} sample vector. These estimators are unbiased, improving as the sample size Q increases. Furthermore, for small Q and/or skewed data, this estimator can significantly underestimate the actual variance. Correction factors for normal and other common distributions are given in [24].[12]

Note that using a *validated* model/simulation for independent sampling may be more efficient than taking repeated measurements. However, many model/simulation parameters

[11] If multiple solutions exist, then an opportunity exists to choose $\mathbf{s}$ in a manner that optimizes the elementary flows (expected values and/or uncertainties). This interesting stochastic optimization problem is not addressed here.

[12] For normally distributed data, variances are multiplied by the correction factor $\frac{Q-1}{Q-3}$ [24]. Note that $\frac{Q-1}{Q-3} \approx 1$ for sufficiently large Q.

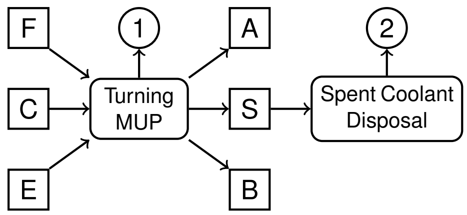

FIGURE 4. **Process flow diagram for an example manufacturing system.** Squares represent individual product flows (F: feedstock, C: coolant, E: electricity, A: part A, S: spent coolant, B: part B). Circles represent elementary flow vectors for the two unit processes. The Turning MUP contributes lost oil and lost water to flow 1, and the Spent Coolant Disposal contributes spent oil and spent water to flow 2.

may have to be based *initially* on prior experience or expert judgement, for example, because a product is in a design/pre-production stage.

The product inputs and output (technosphere demands) for the manufacturing system can be compiled in a similar manner as the elementary flows, i.e., by aggregating the part-level data for the specified number of units of output product produced. The average values of these input product flows over the Q simulations/measurements are used as the (signed) entries in the column of the deterministic technology matrix (2) that corresponds to the manufacturing system of the LCA-level process flow diagram.[13]

EXAMPLE 2 A simple DES model of a manufacturing system was created for the purpose of evaluating the proposed method for process-level LCI compilation. The model consisted of a turning process that manufactured two fictional products: part A and part B. To manufacture either part, the process used part specific feedstock, coolant (cutting fluid composed of an oil/water mixture), and electricity as inputs from the technosphere. For purposes of illustration, the abridged set of elementary flows to the ecosphere were lost coolant oil, lost coolant water, spent coolant oil, and spent coolant water. For simplicity, waste feedstock material, building overhead, capital equipment, etc., were omitted. See Fig. 4.

The turning machine was fed from an upstream buffer that held feedstock for the two product types. Coolant was consumed during the cutting process and maintenance was performed at regular intervals, causing short interruptions in production. Stochastic functions determined the model's processing times, feedstock replenishment, and maintenance duration time. The randomized processing time of each product together with

[13]The incorporation of uncertainties in product flows is currently being researched. Larger sample sizes also reduce the estimation error in the average product flows.

TABLE 1. **Parameters for simulation example.** The notation $\mathrm{N}(\mu, \sigma)$ indicates that a random number is drawn from a normal distribution with mean μ and standard deviation σ. Similarly, the notation $\mathrm{T}(a, b, c)$ indicates that a random number is drawn from a triangular distribution with lower limit a, upper limit b, and mode c. In both cases new numbers are drawn for each production cycle.

Machine related data [unit]	**Value**	
Processing power [kW]	12	
Idle power [kW]	4.5	
Maintenance frequency [hr]	2	
Maintenance time [s]	N(900,100)	
Coolant flow [mL/min]	17	
% Coolant lost per cycle [-]	T(2,8,5)	
% Coolant oil volume [-]	30	
% Coolant water volume [-]	70	
Part specific data [unit]	**Part A**	**Part B**
Inter arrival time [s]	N(126,11)	N(144,11)
Processing time [s]	N(42,1)	N(72,1)
Parts produced [-]	1000	1000

the deterministic coolant flow and energy consumption determined the per-part resource usage. The simulation model was run to produce one thousand parts of each product with fifty replications ($Q = 50$ samples). The DES was first allowed to reach steady state and then the electricity usage and the coolant usage/loss were logged for each part produced (with parts A and B tracked separately). Water and oil were assumed to be lost in the same proportion as their volume fractions in the coolant. For machine idle time due to maintenance or starvation, the corresponding idle electricity consumption was attributed to the subsequent part produced. See Table 1.

For part A, the input product flows and elementary flows for individually produced parts were summed into total values for each production simulation. Average input product flows (feedstock, electricity, and coolant) and elementary flow vectors (lost oil/water and spent oil/water) were computed from these totals, the (symmetric) variance-covariance matrix computed for the elementary flow vector.[14] From this information the coefficient of variation vector was computed. Spent oil and spent water showed a positive covariance, this was attributed to the fact that they both varied linearly with the processing time. Lost oil and spent oil displayed a negative covariance, this was most likely because the

[14]The data distribution was verified to be approximately symmetric. However, for simplicity, no correction factor was applied to the computed (co)variances.

lost oil was removed from what would otherwise have become spent oil. The same was true for lost water and spent water. See Fig. 5.

DISCUSSION

In this section, we discuss the usefulness of the above application of LCA to SM practice, as well as issues to be considered in the further development of a complete methodology.

Towards a methodological application of LCA to SM

Manufacturers are often interested in branding their products as sustainable [25]. However, for this purpose, a manufacturer may merely conduct a cradle/gate-to-gate environmental impact assessment of a product's manufacture with respect to a very limited number of customer-recognized indicators (such as carbon footprint). Furthermore, such assessments may be non-standard, unvalidated, and/or fail to quantify uncertainties, and thus be subject to significant dispute. Adherence to a standardized LCA methodology to assess relative environmental performance can avoid certain inadequacies in SM practice, such as those from overly restricted scope or boundary selection. Furthermore, the environmental impact management of a product requires a combined understanding of both the low/high impact contributors and the low/high uncertainty contributors (e.g., via sensitivity analysis). Transparent methods and techniques for LCI compilation that include uncertainty quantification, such as those proposed in this paper, are key enablers of LCA-supported, validated, and optimized SM practices that make robust decisions. However, this work does not address issues related to the LCIA phase of LCA (or other environmental impact assessments), such as the standardization of indicators, metrics, and indices used for regulatory compliance or branding purposes. Furthermore, this work could benefit from harmonization with other relevant developing standards, such as ISO 14955 and ISO 20140 [26, 27].

The methods we propose for LCI compilation at the LCA-level (system-level) and for the manufacturing system (process-level) incorporate uncertainty analysis for the elementary flows to/from the ecosphere, represented consistently at different levels by variances in the average elementary flows. Inclusion of covariances enables the examination of the importance of correlations in LCA interpretations. For example, consideration of stochastic independence can help guide boundary selection for unit processes and inform the choice of stochastic optimization criteria for environmental impact management (possibly across unit process boundaries and across multiple levels of resolution). The verified importance of correlations, enabled by the methods presented here, would also have implications on LCI information systems and data formats, which would have to be adapted to handle jointly distributed random product/elementary flows.

Process-level LCI compilation using tools such as DES to model MUPs enables precise and transparent allocations of LCIs among multiple products from the same manufacturing facility, and can reveal large uncertainty contributors and stochastic dependencies both among and between product flows and elementary flows. Lower level modeling/simulation can improve environmental-impact decision making with regards to both the design of, and manufacturing process for, a product. Even in a cradle/gate-to-gate assessment, the output product can be designed to mitigate downstream environmental impacts (i.e., through performance/longevity) while satisfying customer needs/desires and, possibly, to further reduce costs by facilitating product remanufacturing/recycling. In a gate-to-gate assessment, the input product flow(s) may be optimized to reduce cost and/or mitigate upstream environmental impacts.

Issues with the proposed method

The mathematical method for LCI compilation proposed here uses variance-covariance information to characterize uncertainties in individual average elementary flows and correlations between these flows. The simplified treatment of average product flows (i.e., technosphere demands) as deterministic quantities, combined with the linearity assumption, makes the variance-covariance information sufficient for consistency in the approach between different levels of abstraction. This considerably simplifies the computational procedure and underlying data requirements, because a more complete characterization of jointly distributed random vectors is not necessary. There are potential issues, however, with treating product flows deterministically. For example, measurements and DES models of a manufacturing system could reveal significant statistical uncertainties in the required *input product flows* (such as variance in the average energy usage due to machine starvation and maintenance in EXAMPLE 2 above). In many cases, these uncertain input product flows correspond directly to upstream environmental flows. Furthermore, within a unit process, the product flows can be jointly distributed with the elementary flows.

One alternative is to include some/all of the upstream technosphere unit processes in the process flow diagram of the lower-level system, so as to properly account for the upstream effects. However, this encapsulation may inhibit LCA-level optimization involving technosphere resources (such as electricity) that may be common to multiple unit processes. A second alternative is to treat product flows universally as random variables that are, in general, jointly distributed with the elementary flows. However, the corresponding computational and data requirements become significantly more demanding. By incorporating fully characterized, jointly distributed flows, this comprehensive approach would have additional system information. In principle, such information can improve LCI compilations and their subsequent use in (possibly nonlinear) models in the LCIA phase of an LCA.

Lastly, it is worth noting that validation remains a key com-

$$\text{Avg. feedstock} = 500 \text{ kg}, \quad \text{Avg. coolant} = 11.9 \text{ L}, \quad \text{Avg. electricity} = 144 \text{ kW}\cdot\text{h}, \qquad \widehat{\mu}_{\tilde{\mathbf{f}}^{\text{man}}} = \begin{bmatrix} \text{Avg. lost oil (L)} \\ \text{Avg. lost water (L)} \\ \text{Avg. spent oil (L)} \\ \text{Avg. spent water (L)} \end{bmatrix} = \begin{bmatrix} 0.18 \\ 0.42 \\ 3.40 \\ 7.92 \end{bmatrix},$$

$$\widehat{\Sigma}_{\tilde{\mathbf{f}}^{\text{man}}} = \begin{bmatrix} 6.18E-08 & 1.44E-07 & -3.33E-08 & -7.78E-08 \\ 1.44E-07 & 3.36E-07 & -7.78E-08 & -1.81E-07 \\ -3.33E-08 & -7.78E-08 & 1.32E-07 & 3.09E-07 \\ -7.78E-08 & -1.81E-07 & 3.09E-07 & 7.21E-07 \end{bmatrix}, \quad \%\ \text{C.V.} = \begin{bmatrix} 0.139 \\ 0.139 \\ 0.011 \\ 0.011 \end{bmatrix}.$$

FIGURE 5. **Average flows, variance-covariance matrix, and coefficients of variation vector for the DES example with 50 simulation runs.**

ponent of LCA modeling, which occurs across various levels of abstraction. When some combination of process measurements and simulation are used to support an LCA, the corresponding validation should be transparent and well-documented. Standards can play an important role in validation, especially as a product moves from design to production and as manufacturing processes evolve and mature. Additional research is necessary to ensure that model validation at lower levels successfully translates into confidence in model interpretation at the LCA-level.

CONCLUSION

By describing how to integrate MUPs into system-level LCIs, this paper proposes a method by which LCA can better support SM practices. Specifically, the method synthesizes LCIs from the process-level to the system-level while consistently quantifying uncertainty in the inventories and correlations among elementary flows. By way of an example DES model of a manufacturing system, the method is shown to generate simulation-based MUP LCI data that can be integrated at higher levels. Because uncertainty quantification is key to robust LCA interpretation, the proposed method incorporates inventory uncertainties, while product flow uncertainties were identified among the important issues for further research.

Well-integrated LCI compilation with uncertainty quantification is a necessary precursor to robust life cycle and environmental impact assessments/decisions in SM, which are important for advancing standardization efforts related to regulatory compliance and product branding. Testing and validation in a real industry setting would be useful to further refine and advance the approach described here, and would also present an opportunity to investigate and provide recommendations concerning the appropriate combination of measurement and simulation techniques and tools. Furthermore, it would enable better evaluation of multi-resolution and dependency issues in, as well as the relative importance of, uncertainty quantification in LCIs.

Appendix: Higher-Level LCI Compilation Details

Recall system (3) for the compilation of a higher-level LCI, repeated here:

$$\tilde{\mathbf{f}}^{\text{sys}} = \sum_{n=1}^{N} s_n \tilde{\mathbf{f}}^n = \widetilde{\mathbf{F}}\mathbf{s}.$$

The expected value of the system-level average elementary flow, $\mu_{\tilde{\mathbf{f}}^{\text{sys}}}$ (a deterministic vector), is given by

$$\mu_{\tilde{\mathbf{f}}^{\text{sys}}} = \mu_{\widetilde{\mathbf{F}}}\mathbf{s}, \tag{4}$$

where $\mu_{\widetilde{\mathbf{F}}}$ (a deterministic matrix) is the expected value of the random matrix $\widetilde{\mathbf{F}}$. In particular, for M elementary flows and N unit processes, the $(m,n)^{\text{th}}$ entry of the matrix $\widetilde{\mathbf{F}}$ is the m^{th} component of the n^{th} elementary flow vector, denoted by $\widetilde{F}_{mn} := \tilde{f}^n_m$. It follows that the m^{th} component of $\tilde{\mathbf{f}}^{\text{sys}}$ is given by

$$\tilde{f}^{\text{sys}}_m = \sum_{n=1}^{N} s_n \widetilde{F}_{mn}, \quad m = 1, \ldots, M. \tag{5}$$

In general, the components $\tilde{f}^{\text{sys}}_m$ are jointly distributed, so that the $M \times M$ variance-covariance matrix

$$\Sigma_{\tilde{\mathbf{f}}^{\text{sys}}} := \mathsf{E}\left[\left(\tilde{\mathbf{f}}^{\text{sys}} - \mu_{\tilde{\mathbf{f}}^{\text{sys}}}\right)\left(\tilde{\mathbf{f}}^{\text{sys}} - \mu_{\tilde{\mathbf{f}}^{\text{sys}}}\right)^{\text{T}}\right]$$

describes the uncertainty in, and dependencies among, the compiled system-level elementary flows. Computation of the full variance-covariance matrix is necessary to incorporate the system as an stochastically independent unit process in a higher-level process flow diagram. The variances and pairwise covariances of the entries of $\widetilde{\mathbf{F}}$ (assumed to be known) are sufficient for the computation of $\Sigma_{\widetilde{\mathbf{f}}^{\mathrm{sys}}}$, as shown next.

Without loss of generality, consider the computation of an arbitrary element of the variance-covariance matrix $\Sigma_{\widetilde{\mathbf{f}}^{\mathrm{sys}}}$, denoted $\sigma_{\widetilde{f}_j^{\mathrm{sys}},\widetilde{f}_k^{\mathrm{sys}}}$.[15] The direct computation of $\sigma_{\widetilde{f}_j^{\mathrm{sys}},\widetilde{f}_k^{\mathrm{sys}}}$ gives

$$\begin{aligned}\sigma_{\widetilde{f}_j^{\mathrm{sys}},\widetilde{f}_k^{\mathrm{sys}}} &= \mathsf{E}\left[\left(\widetilde{f}_j^{\mathrm{sys}} - \mu_{\widetilde{f}_j^{\mathrm{sys}}}\right)\left(\widetilde{f}_k^{\mathrm{sys}} - \mu_{\widetilde{f}_k^{\mathrm{sys}}}\right)\right] \\ &= \mathsf{E}\left[\widetilde{f}_j^{\mathrm{sys}} \cdot \widetilde{f}_k^{\mathrm{sys}}\right] - \mu_{\widetilde{f}_j^{\mathrm{sys}}} \cdot \mu_{\widetilde{f}_k^{\mathrm{sys}}}.\end{aligned}$$

The factors in the second term $\mu_{\widetilde{f}_j^{\mathrm{sys}}} \cdot \mu_{\widetilde{f}_k^{\mathrm{sys}}}$ are computed in system (4), or, equivalently, by taking the expected values of equations in (5). Because the scalars s_{n_*} are deterministic constants, the computation of the first term

$$\mathsf{E}\left[\widetilde{f}_j^{\mathrm{sys}} \cdot \widetilde{f}_k^{\mathrm{sys}}\right] = \mathsf{E}\left[\sum_{n_1=1}^{N} s_{n_1}\widetilde{F}_{jn_1} \cdot \sum_{n_2=1}^{N} s_{n_2}\widetilde{F}_{kn_2}\right]$$

ultimately requires the computation of

$$\mathsf{E}\left[\widetilde{F}_{jn_1} \cdot \widetilde{F}_{kn_2}\right] = \sigma_{\widetilde{F}_{jn_1},\widetilde{F}_{kn_2}} + \mu_{\widetilde{F}_{jn_1}} \cdot \mu_{\widetilde{F}_{kn_2}},$$

for all combinations of $n_1 = 1,\ldots,N$ and $n_2 = 1,\ldots,N$. This follows from the (co)variance relationship

$$\begin{aligned}\sigma_{\widetilde{F}_{jn_1},\widetilde{F}_{kn_2}} &= \mathsf{E}\left[\left(\widetilde{F}_{jn_1} - \mu_{\widetilde{F}_{jn_1}}\right)\left(\widetilde{F}_{kn_2} - \mu_{\widetilde{F}_{kn_2}}\right)\right] \\ &= \mathsf{E}\left[\widetilde{F}_{jn_1} \cdot \widetilde{F}_{kn_2}\right] - \mu_{\widetilde{F}_{jn_1}} \cdot \mu_{\widetilde{F}_{kn_2}},\end{aligned}$$

in which $\sigma_{\widetilde{F}_{jn_1},\widetilde{F}_{kn_2}}$ is assumed to be known and $\mu_{\widetilde{F}_{jn_1}}$ and $\mu_{\widetilde{F}_{kn_2}}$ are computed entries in the matrix $\mu_{\widetilde{\mathbf{F}}}$.

Two special cases are notable. First, if elementary flows between two different unit processes are probabilistically independent (or merely uncorrelated), then $\sigma_{\widetilde{F}_{jn_1},\widetilde{F}_{kn_2}} = 0$ for $n_1 \neq n_2$, and

$$\mathsf{E}\left[\widetilde{F}_{jn_1} \cdot \widetilde{F}_{kn_2}\right] = \mu_{\widetilde{F}_{jn_1}} \cdot \mu_{\widetilde{F}_{kn_2}}.$$

Second, if two elementary flows within a single unit process are probabilistically independent (or merely uncorrelated), then $\sigma_{\widetilde{F}_{jn},\widetilde{F}_{kn}} = 0$ for $j \neq k$, and

$$\mathsf{E}\left[\widetilde{F}_{jn} \cdot \widetilde{F}_{kn}\right] = \mu_{\widetilde{F}_{jn}} \cdot \mu_{\widetilde{F}_{kn}}.$$

In practice, a common situation occurs when elementary flows between unit processes are independent, but elementary flows within individual unit processes are not, in which case the elements of the variance-covariance matrix $\Sigma_{\widetilde{\mathbf{f}}^{\mathrm{sys}}}$ are given by

$$\sigma_{\widetilde{f}_j^{\mathrm{sys}},\widetilde{f}_k^{\mathrm{sys}}} = \sum_{n=1}^{N} s_n^2\, \sigma_{\widetilde{F}_{jn},\widetilde{F}_{kn}}.$$

In particular, the variances on the diagonal are sums of squares, i.e.,

$$\sigma^2_{\widetilde{f}_m^{\mathrm{sys}}} = \sum_{n=1}^{N} s_n^2\, \sigma^2_{\widetilde{F}_{mn}}, \qquad m = 1,\ldots,M.$$

If, in addition, the elementary flows within all unit processes are all mutually independent, then the variance-covariance matrix is diagonal, i.e.,

$$\Sigma_{\widetilde{\mathbf{f}}^{\mathrm{sys}}} = \begin{bmatrix} \sigma^2_{\widetilde{f}_1^{\mathrm{sys}}} & 0 & \cdots & 0 \\ 0 & \sigma^2_{\widetilde{f}_2^{\mathrm{sys}}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^2_{\widetilde{f}_M^{\mathrm{sys}}} \end{bmatrix}.$$

[15]Note that $\sigma_{\widetilde{f}_j^{\mathrm{sys}},\widetilde{f}_j^{\mathrm{sys}}} = \sigma^2_{\widetilde{f}_j^{\mathrm{sys}}}$ on the diagonal of $\Sigma_{\widetilde{\mathbf{f}}^{\mathrm{sys}}}$.

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