frontiers | Frontiers in Sustainability

TYPE General Commentary
PUBLISHED 13 February 2023
DOI 10.3389/frsus.2023.1076475

OPEN ACCESS

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SPECIALTY SECTION
This article was submitted to Quantitative Sustainability Assessment, a section of the journal Frontiers in Sustainability

RECEIVED 21 October 2022
ACCEPTED 19 January 2023
PUBLISHED 13 February 2023

CITATION
Schaubroeck T (2023) Response to Commentary: Further clarifications on a more basic modeling framework for life cycle methods. *Front. Sustain.* 4:1076475. doi: 10.3389/frsus.2023.1076475

Response to Commentary: Further clarifications on a more basic modeling framework for life cycle methods

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KEYWORDS

LCA, life cycle assessment, life cycle modeling, dynamics, life cycle inventories (LCI), life cycle sustainability assessment

Response to Commentary on
Non-linearity in LCA—What are we talking about?

by Heijungs, R., and Suh, S. (2022). *Front. Sustain.* 3:1049362. doi: 10.3389/frsus.2022.1049362

In response to the commentary of Heijungs and Suh (2022), some further clarifications are provided concerning the more basic modeling framework brought forward in a previous article published in this journal (Schaubroeck, 2022a). Since Heijungs and Suh (2022) do not highlight clearcut errors, as will be made apparent, the main messages and content of the particular work (Schaubroeck, 2022a) still stand and hold, but its content could benefit from further explanation. Detailed replies to the comments of Heijungs and Suh (2022) are presented in the Supplementary Table 1. Replies to comments related to the book by Heijungs and Suh (2002) are restricted to the latter. Clarifications concerning the modeling framework and its relevance are presented in the following three points. Note that a preprint version of this article has been uploaded online (Schaubroeck, 2022b).

First, it is good that Heijungs and Suh (2022) again bring forward that the matrix inversion approach (Linear inverse modeling) is not the only computational structure/framework for LCA. Hence, other or more basic modeling frameworks, such as the one presented by Schaubroeck (2022a), can be brought forward and can be of relevance.

Second, when it comes to the notation style of the formula of Equation (3) in the work of Schaubroeck (2022a), Heijungs and Suh (2022) question having a function with a set of output variables and a set of input variables, but some references point out this possibility, for example.[1] In fact, one needs to rather consider the particular function as p_p: $\mathrm{V}^{\mathrm{n}} \rightarrow W^m$ (considering V^n and W^m are co-domains with n and m type of elements), for which a unique set of input variable amounts will provide a unique set of outcome variable amounts. Yet, indeed, the formulation of the equation in question is somewhat of an uncommon way of formulating things, especially in the field of LCA. To further clarify, the following two alternative versions of the equation are presented (using parameters as specified in the original work):

$$\{F_x, F_v, \ldots\} = \left\{p_x\left(\left\{F_y, F_z, \ldots\right\}, t, OC\right), p_v\left(\left\{F_y, F_z, \ldots\right\}, t, OC\right), \ldots\right\} \quad (1)$$

In this equation, each parameter F_i has a corresponding function p_i that only has this parameter as a single output variable, which is more conventional. One can also just write it as a collection:

1 https://www.khanacademy.org/math/multivariable-calculus/thinking-about-multivariable-function/ways-to-represent-multivariable-functions/a/multivariable-functions

$$\begin{cases} F_x = p_x\left(\left\{F_y, F_z, \ldots\right\}, t, OC\right) \\ F_v = p_v\left(\left\{F_y, F_z, \ldots\right\}, t, OC\right) \\ \cdots \end{cases} \quad (2)$$

When it comes to the type brackets and their order, namely, $f(\ldots\{\ldots\})$, this is also somewhat unconventional. The second set of brackets "{…}" is strictly speaking redundant, but it was used to distinguish the set of flows separately from time and other conditions.

Moreover, an example is presented for further clarification, as also advised by Heijungs and Suh (2022). Consider the case related to Figure 1 on heat and electricity in the original work (Schaubroeck, 2022a). That figure depicts industrial processes, but there is, in fact, also the implicit process of energy supply selection, which represents dynamics and is more interesting to study. Using Equation (3) from the original work (Schaubroeck, 2022a), one can derive the following formula:

$$\{electricityfromgrid, heatfromboiler, electricitycfromCHP, heatfromCHP\} = energysupplyselectionprocess_p\left(\{electricity, heat\}, timepoint\right) \quad (3)$$

If we consider a simplistic version where one can readily switch between the energy sources and there is no restriction due to fixed ratios of the Combined Heat and Power generator (CHP), the following oversimplified mathematical expression can be obtained for each *timepoint*:

$$\begin{cases} electricity > 0 \bigwedge heat > 0 \rightarrow electricityfromCHP = electricity \\ \qquad\qquad \bigwedge heatfromCHP = heat \\ electricity = 0 \bigvee heat = 0 \rightarrow electricityfromgrid = electricity \\ \qquad\qquad \bigwedge heatfromboiler = heat \end{cases} \quad (4)$$

To put it simply, only if both heat and electricity are simultaneously asked, the CHP is used, otherwise, electricity is obtained from the grid and heat from a boiler.

Third, the main advantage of the presented framework in the original work (Schaubroeck, 2022a) is its openness to further developments, including non-linear developments. The value of the associated abstractness seems questioned by Heijungs and Suh (2022), but it is the abstractness that makes it general and open. Also note that, in the original work (Schaubroeck, 2022a), it is not claimed to have introduced new specific non-linear frameworks, and alternatively, reference is made to many. Moreover, many other advantages of the original work (Schaubroeck, 2022a) have also been overlooked. To further emphasize and clarify this, some benefits/novelties of the original work (Schaubroeck, 2022a) are listed here:

- An expression in mathematical terms of an open and general framework in the context of LCA, allowing to guide further users and developers to be more free in modeling development.
- Specification of how this computational framework is aligned with a more basic and open framework for LCA, as recently specified by Schaubroeck et al. (2022), and can be specifically applied for attributional and consequential LCA.
- An elaboration on dynamic effects beyond a specification over time, and how this is limited in the matrix inversion approach. In fact, this aspect is the most elaborated and novel.
- A specification of a case on co-product dynamics is illustrated in Figure 1 of the original work (Schaubroeck, 2022a).
- Pointing out further possibilities to improve the frameworks of DyPLCA (Pigné et al., 2020) and Temporalis (Cardellini et al., 2018): "For non-linear modeling, process equations could be readily changed, possibly grouped by types of processes to facilitate execution. In the case of dynamics, specifically for graph-based search tools, dynamic graphs could be considered that can alter over time (Holme, 2015; Vernet et al., 2022)". In the original work, it has been forgotten to mention that these frameworks also include a complete temporal differentiation, with a complete temporal database for a version of ecoinvent 3.2 in the case of DyPLCA. This benefit should be considered when evaluating the extent of limited practical flow coverage with the given computational power.

Overall, with these further clarifications, I hope to have addressed the points raised by Heijungs and Suh (2022) concerning the framework.

Author contributions

The author confirms being the sole contributor of this work and has approved it for publication.

Acknowledgments

A preprint version of this article has been uploaded online (Schaubroeck, 2022b).

Conflict of interest

The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/frsus.2023.1076475/full#supplementary-material

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