A or I -A: unifying the computational structures of process- and IO-based LCA for clarity and consistency

Heijungs, R.; Yang, Y.; Park, H.S.

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EDUCATION

A or I-A? Unifying the computational structures of process- and IO-based LCA for clarity and consistency

Reinout Heijungs[1,2] | Yi Yang[3,4] | Hung-Suck Park[4]

[1]Department of Operations Analytics, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands

[2]Institute of Environmental Sciences, Leiden University, Leiden, The Netherlands

[3]Key Laboratory of the Three Gorges Reservoir Region's Eco-Environment, Ministry of Education, Chongqing University, Chongqing, China

[4]Department of Civil and Environmental Engineering, University of Ulsan, Ulsan, Republic of Korea

Correspondence
Yi Yang, Key Laboratory of the Three Gorges Reservoir Region's Eco-Environment, Ministry of Education, Chongqing University, Chongqing 400045, China.
Email: yi.yang@cqu.edu.cn
Hung-Suck Park, Department of Civil and Environmental Engineering, College of Engineering, University of Ulsan, 93 Dehakro, Ulsan 680-749, Republic of Korea.
parkhs@ulsan.ac.kr

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Abstract

Why are both $\mathbf{A}^{-1}$ and $(\mathbf{I}-\mathbf{A})^{-1}$ used in life cycle assessment (LCA) matrix computations? This is a question that, in our experience of teaching LCA, students often wonder about and struggle with. A brief survey of the literature suggests that the question can also confuse experienced LCA practitioners. Here, we seek to unify the computational structures of the two LCA approaches to achieve greater clarity and consistency, especially to make them easier to teach. We first show how small but crucial differences in the set-up of the two approaches lead to the use of $\mathbf{A}$ versus $\mathbf{I}-\mathbf{A}$. Then, we discuss the options to unify the presentations in a coherent way. We do not prescribe one way or the other. A larger point we hope to stress is the importance of unification, which may have both pedagogical and methodological benefits.

KEYWORDS
education and training, hybrid life cycle assessment, IO-based life cycle assessment, life cycle assessment, process-based life cycle assessment, process analysis

1 | INTRODUCTION

There are two main approaches to life cycle assessment (LCA): process-based and input–output-based modeling (abbreviated as PLCA and IO-LCA hereafter). Both approaches are widely applied in LCA studies. Over the past two decades, many studies have examined the strengths and weaknesses of each approach (Junnila, 2006; Majeau-Bettez et al., 2011; Yang et al., 2017) and sought to integrate the two strands into hybrid LCA, attempting to combine the strengths of both (Lenzen, 2002; Suh et al., 2004; Yu & Wiedmann, 2018). Different from previous studies, here we focus on the difference in the computational structures of the two approaches.

Neglecting the precise meaning of the symbols, many documents on PLCA use (Heijungs & Suh, 2002):

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f} \tag{1}$$

while IO-LCA invariably uses (Hauschild et al., 2018):

$$\mathbf{g} = \mathbf{B}(\mathbf{I}-\mathbf{A})^{-1}\mathbf{f} \tag{2}$$

The difference is visually small, but numerically fundamental. We seek to explicate why **A** is often used in PLCA and **I** − **A** is used in IO-LCA and show that they can be presented in a unified format for greater clarity and consistency. Before we do this, we emphasize that our notation as in Equations (1) and (2) follows a tradition that associates $\mathbf{A}^{-1}$ with PLCA and $(\mathbf{I}-\mathbf{A})^{-1}$ with IO-LCA, as reflected in several textbooks and review papers over the past two decades, like Heijungs and Suh (2002), Suh and Huppes (2005), Islam et al. (2016), and Crawford et al. (2018). As communicated by Strømman (2021), however, several research groups and university classes have also been applying the $(\mathbf{I}-\mathbf{A})^{-1}$ form to implement PLCA (see, Hawkins et al., 2013).

The motivation for our attempt at unification is that in our experience of teaching LCA methods, this is the part students often struggle with the most. They are confused about which equation to apply, and even if they have memorized one for process-based modeling and the other for IO-based modeling, they leave without a clear understanding of why.

Further, a brief survey of the LCA literature shows that the computational differences appear also to confuse some experienced LCA practitioners. For instance, Mutel et al. (2012) cite Heijungs and Suh (2002) as a PLCA method, but then present the formula for IO-LCA. Jolliet et al. (2016) provide a presentation that agrees for 90% with PLCA, but then finish the last 10% with an IO-LCA formula. The documentation of the ecoinvent database (Weidema et al., 2013) is contradicting the factual structure of the datafiles: if you import the XML-files, you obtain a structure that should be processed with $\mathbf{A}^{-1}$, but the document suggests that $(\mathbf{I}-\mathbf{A})^{-1}$ is to be used. Nakamura and Nansai (2016) writes that "the matrix $(\mathbf{I}-\mathbf{A})$ corresponds to the technology matrix in PLCA" but does not inform the reader what this correspondence entails. A final example is provided by Agez et al. (2020), who write $\mathbf{B}^{\mathrm{lca}}(\mathbf{I}-\mathbf{A}^{\mathrm{lca}})^{-1}$, adding a footnote on the conversion from the conventional LCA-form **T** to their preferred from, creating $\mathbf{T}=\mathbf{I}-\mathbf{A}^{\mathrm{lca}}$, so effectively using $\mathbf{B}^{\mathrm{lca}}(\mathbf{I}-(\mathbf{I}-\mathbf{T}))^{-1}=\mathbf{B}^{\mathrm{lca}}\mathbf{T}^{-1}$. These examples suggest that the confusion may be more pervasive than only classrooms, and a unification of the two approaches may be helpful.

A previous attempt to create clarity in this matter (Islam et al., 2016) does not achieve enough, because it uses different notations for all concepts (e.g., $\beta = BA^{-1}\alpha$ for (1) and $r = E_{dir}(I-C)^{-1}d$ for (2)), with the result that these authors do not observe the similarity themselves. And a review of PLCA, IO-LCA, and hybrid LCA by Crawford et al. (2018) presents the formulas, but without any derivation, proof, or comment on the reasons behind the subtle differences. The *LCA Compendium* series features a chapter on *Algorithms of Life Cycle Inventory Analysis* (Srocka & Montiel, 2021), which also contrasts PLCA and IO-LCA. Overall, the comparison entails in the end little more than "the matrix **I** − **A** is analogous to the technology matrix for a product system in which each unit process produces one unit of output" (notation adapted), which does not resolve the enigma. Finally, we mention the paper by Suh et al. (2010), which discusses a harmonization of the procedures for co-product allocation in PLCA and IO-LCA, but does not go into the question of **A** versus **I** − **A**.

Here, we set three targets. First, we will discuss, side by side, the two different forms, PLCA and IO-LCA, in precise terms and using a harmonized notation, such that the bifurcations into Equations (1) and (2) are understandable. In doing so, we will put the emphasis on the differences between PLCA and IO-LCA, rather than on their similarities (which are numerous). Next, we discuss their unification and integration in hybrid LCA. Third, we discuss some of the advantages and disadvantages of the forms of (1) and (2), demonstrating that either form can be used to unify the two approaches.

2 | PRESENTATION OF THE TWO LCA-FORMS

Below, we present both forms, PLCA and IO-LCA, using a uniform notation. We will focus on matrix-based presentations. For IO-LCA, there is no other presentation, and virtually every textbook on input–output analysis (IOA) presents the basics more or less in this form. We refer to Miller and Blair (2009) and Leontief (1986) for basic references.

For PLCA, the situation is somewhat different. Most textbooks on LCA do not present the mathematical model. For instance, the recent textbook by Hauschild et al. (2018) only says that the "issue is commonly solved by matrix inversion," without providing any formula or detailing any matrix. Surprisingly, a later chapter of the same book presents the full algebraic details of the IO-LCA model, including (2). So, even a textbook that focuses on PLCA presents no mathematical treatment of PLCA, while it does present the mathematics of IO-LCA. The discrepancy between the level of mathematical treatment is even older than LCA. Bullard et al. (1978) are perhaps the first authors contrasting process-based and IO-based approaches, for energy analysis. These authors present the IO-part in matrix form, but the process-part is only shown in a heuristic way. We speculate that the presence of the IO-form in process-based texts may be one cause of the confusion.

In addition to matrix-based PLCA, there are also approaches to PLCA that do not employ matrix algebra, but, for instance, Petri nets (Schmidt & Häuslein, 1997). However, as our task is to contrast Equations (1) and (2), we will further focus on matrix-based PLCA.

2.1 | Process-based LCA (PLCA)

A standard reference for matrix-based PLCA is Heijungs and Suh (2002). The approach is based on the following principles:

- unit processes are activities that transform a bundle of inputs into a bundle of outputs;

- there are two types of inputs and outputs: intermediate flows (products, materials, electricity, waste to be treated, etc.) and elementary flows (emissions of CO_2, heavy metals, pesticides, etc.; extraction of ores, water, etc.);
- the amount of input (use) or output (supply) of intermediate flow i to or from unit process j is indicated by a_{ij}, where $a_{ij} < 0$ for inputs and $a_{ij} > 0$ for outputs;
- the amount of input (extraction) or output (emission) of elementary flow k to or from unit process j is indicated by b_{kj}, where $b_{kj} < 0$ for inputs and $b_{kj} > 0$ for outputs;
- a unit process j can be scaled linearly, with a scaling factor s_j, such that its inputs and outputs become $s_j a_{ij}$ and $s_j b_{kj}$;
- the functional unit of an LCA expresses an external demand for an amount of product(s);
- these amounts of products are organized as numbers f_i, where i indicates the intermediate flow;
- the system-wide environmental burdens of a product are expressed as numbers g_k, where k indicates the elementary flow;
- a balance of intermediate flows holds: the system must produce exactly the amount of intermediate products that are required to satisfy the functional unit.

With these principles, we can arrange a PLCA database in two matrices:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{3}$$

and

$$\mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \cdots \\ b_{21} & b_{22} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{4}$$

The first matrix is sometimes called the technology matrix or technosphere matrix, the second one the intervention matrix, ecosphere matrix, or environmental matrix. Both matrices can be square or non-square, and they can vary in size from study to study.

Further a case study specific external demand vector **f** contains the demand for products:

$$\mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \\ \cdots \end{pmatrix} \tag{5}$$

and a case study specific inventory vector contains the system-wide environmental burdens:

$$\mathbf{g} = \begin{pmatrix} g_1 \\ g_2 \\ \cdots \end{pmatrix} \tag{6}$$

The balancing principle, together with the linear scaling assumption now implies that

$$\begin{cases} a_{11}s_1 + a_{12}s_2 + \cdots & = f_1 \\ a_{21}s_1 + a_{22}s_2 + \cdots & = f_2 \\ \cdots \end{cases} \tag{7}$$

or in matrix notation

$$\mathbf{As} = \mathbf{f} \tag{8}$$

where we have defined the vector of scaling factors

$$\mathbf{s} = \begin{pmatrix} s_1 \\ s_2 \\ \cdots \end{pmatrix} \tag{9}$$

When **A** is square and invertible, this yields a unique solution

$$\mathbf{s} = \mathbf{A}^{-1}\,\mathbf{f} \tag{10}$$

When **A** is not square or when it is non-invertible, tricks may be needed (Heijungs & Frischknecht, 1998). When the scaling factors work on **A**, they also work on **B**. Hence, we have

$$\begin{cases} g_1 = b_{11}\,s_1 + b_{12}s_2 + \cdots \\ g_2 = b_{21}\,s_1 + b_{22}s_2 + \cdots \\ \qquad \cdots \end{cases} \tag{11}$$

In matrix terms, this is

$$\mathbf{g} = \mathbf{Bs} \tag{12}$$

Given **s**, the inventory vector **g** is found. The intermediate result for the scaling vectors can be inserted in this equation:

$$\mathbf{g} = \mathbf{BA}^{-1}\mathbf{f} \tag{13}$$

This is the basic equation for PLCA (at least, for its inventory part).

As an illustration, we use the example from Heijungs and Suh (2002). In this example, the first unit process ($j = 1$) is electricity production. It needs 2 L of fuel ($i = 1$) to produce 10 kWh of electricity ($i = 2$). Hence, $a_{11} = -2$ (L) and $a_{21} = 10$ (kWh). The second unit process is ($j = 2$) is fuel production. It needs no intermediate flows to produce 100 L of fuel; hence $a_{21} = 100$ (L) and $a_{22} = 0$ (kWh). Altogether,

$$\mathbf{A} = \begin{pmatrix} -2 & 100 \\ 10 & 0 \end{pmatrix} \tag{14}$$

For the environmental part, the electricity production process ($j = 1$) emits 1 kg CO_2 ($k = 1$) and 0.1 kg SO_2 ($k = 2$). And fuel production ($j = 2$) emits 10 kg CO_2 ($k = 1$) and 2 kg SO_2 ($k = 2$) and it extracts 50 L of crude oil ($k = 3$). So,

$$\mathbf{B} = \begin{pmatrix} 1 & 10 \\ 0.1 & 2 \\ 0 & -50 \end{pmatrix} \tag{15}$$

Observe the minus sign in front of the number 50 for crude oil. In some texts (Heijungs & Suh, 2002), the convention to indicate inputs with a negative number in **A** is also carried to **B**. In other texts (Jolliet et al., 2016), resource extractions are understood to be inputs and no negative sign is introduced. As long as this is done consistently, there is no difference in the results.

When the functional unit is 1000 kWh electricity ($j = 2$), the final demand vector is

$$\mathbf{f} = \begin{pmatrix} 0 \\ 1000 \end{pmatrix} \tag{16}$$

The matrix equations then give for the scaling factors

$$\mathbf{s} = \begin{pmatrix} -2 & 100 \\ 10 & 0 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ 1000 \end{pmatrix} = \begin{pmatrix} 0 & 0.1 \\ 0.01 & 0.002 \end{pmatrix} \begin{pmatrix} 0 \\ 1000 \end{pmatrix} = \begin{pmatrix} 100 \\ 2 \end{pmatrix} \tag{17}$$

and for the inventory vector

$$\mathbf{g} = \begin{pmatrix} 1 & 10 \\ 0.1 & 2 \\ 0 & -50 \end{pmatrix} \begin{pmatrix} 100 \\ 2 \end{pmatrix} = \begin{pmatrix} 120 \\ 14 \\ -100 \end{pmatrix} \tag{18}$$

This is interpreted as a system-wide emission of 120 kg CO_2 and 14 kg SO_2, and an extraction of 100 L crude oil.

We draw the reader's attention to the fact that the numbers in **A** and **B** in general have a dimension, and therefore a unit. In the example, a_{11} has the unit L, a_{22} has the unit kWh, and b_{12} has the unit kg. As argued by Heijungs (1998), we may alternatively interpret the coefficients of **A** and **B** as flows, for instance L/s, kWh/s, and kg/s. In that case, the scaling factors **s** will have a time unit (s). One of the reviewers suggested that one may also consider the coefficients of **A** and **B** to be expressed per unit of output. That would give L/kWh for a_{11}, kWh/L for a_{22}, and kg/L for b_{21}. This convention has, however, the weakness that for some processes it is not clear what the denominator is. For instance, the input of a combined heat power plant that uses 30 L of fuel to produce 10 kWh of electricity and 5 MJ of heat could then be written as 3 L/kWh, 6 L/MJ, or perhaps even 2 L/whatever. There is no requirement in the PLCA system that each process should have exactly one output. Cases may occur where a process has multiple outputs, or where a process may have no output at all, like in the case of waste-treatment process (Guinée & Heijungs, 2021).

2.2 IO-based LCA (IO-LCA)

For the IO-LCA, there is less standardization than for PLCA, but we can partly build on the principles of economic IOA, as presented by Miller and Blair (2009). In IOA, the basis of the data is provided by a pair of supply–use tables, which are then converted into an IO-table (IOT). This paper starts with the IOT, which is a square matrix that contains the transactions between the components of an economy. There are two distinct formats of IOT:

- product-by-product (P × P, aka commodity-by-commodity);
- industry-by-industry (I × I, aka sector-by-sector).

Below, we will elaborate the I × I format. In an I × I table, the principles are as follows:

- the input structure of industry *j* is represented by column *j*;
- its input from industry *i* is recorded as z_{ij} (a positive number);
- the output of industry *j* is indicated in a separate data structure as x_j.

These principles yield the organization of the data in two data structures: the transaction matrix **Z**:

$$\mathbf{Z} = \begin{pmatrix} z_{11} & z_{12} & \cdots \\ z_{21} & z_{22} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{19}$$

and the output vector **x**:

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \cdots \end{pmatrix} \tag{20}$$

Usually, but not necessarily, the matrix **Z** and the vector **x** contain observed data for one year for a demarcated region, for instance, the United States in the year 2015. Part of the observed situation is a final demand for the products of the industries by final users (households, governments, exports, etc.). Let us denote the final demand for the products of industry *i* by f_i. Then we can organize the final demands for the products of all industries in vector **f**:

$$\mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \\ \cdots \end{pmatrix} \tag{21}$$

Now, the transaction matrix is converted into a coefficient matrix, **A**, by re-expressing all inputs of industry *j* in relation to the output of industry *j*. More precisely:

$$a_{ij} = \frac{z_{ij}}{x_j} \quad (\forall i, j) \tag{22}$$

This defines a new matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{23}$$

In matrix notation, the conversion of ($\mathbf{Z}$, $\mathbf{x}$) into $\mathbf{A}$ takes place through

$$\mathbf{A} = \mathbf{Z}(\hat{\mathbf{x}})^{-1} \tag{24}$$

where the hat denotes diagonalization of a vector into a square matrix:

$$\hat{\mathbf{x}} = \begin{pmatrix} x_1 & 0 & \cdots \\ 0 & x_2 & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{25}$$

and therefore

$$(\hat{\mathbf{x}})^{-1} = \begin{pmatrix} \frac{1}{x_1} & 0 & \cdots \\ 0 & \frac{1}{x_2} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{26}$$

As a decision support tool, IOA is primarily used to model the effects of a new, changed, final demand (Miller & Blair, 2009). If the new final demand is given by vector $\mathbf{f}'$, this induces an output level for industry i, given by the direct demand for industry i's products (f_i') and the intermediate demand for industry i's products ($\sum_j a_{ij} x_j'$), where x_j' is the new output of industry j. Therefore, the new output of industry i is given by

$$x_i' = f_i' + \sum_j a_{ij} x_j' \quad (\forall i) \tag{27}$$

This can be written in matrix form as

$$\mathbf{x}' = \mathbf{f}' + \mathbf{A}\mathbf{x}' \tag{28}$$

which can be rearranged as

$$\mathbf{f}' = \mathbf{x}' - \mathbf{A}\,\mathbf{x}' = (\mathbf{I} - \mathbf{A})\;\mathbf{x}' \tag{29}$$

where $\mathbf{I}$ is the identity matrix:

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \cdots \\ 0 & 1 & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{30}$$

In this equation, $\mathbf{x}'$ is unknown, but $\mathbf{f}'$ and $\mathbf{A}$ are known. So we solve for $\mathbf{x}'$ as follows:

$$\mathbf{x}' = (\mathbf{I} - \mathbf{A})^{-1}\,\mathbf{f}' \tag{31}$$

Because $\mathbf{A}$ is based on an industry-by-industry format, it has the same number of rows and columns, it is square.

In the original situation, with transaction matrix $\mathbf{Z}$, industry output $\mathbf{x}$ and final demand $\mathbf{f}$, an environmental satellite can be added. The principles are as follows:

- the observed amount of input (extraction) or output (emission) of elementary flow k to or from industry j is indicated by r_{kj}, where $r_{kj} < 0$ for inputs and $r_{kj} > 0$ for outputs.

The elements r_{kj} can be organized in the satellite matrix R:

$$\mathbf{R} = \begin{pmatrix} r_{11} & r_{12} & \cdots \\ r_{21} & r_{22} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \tag{32}$$

Like the transaction matrix **Z** was converted into a coefficient form **A** through $\mathbf{A} = \mathbf{Z}(\hat{\mathbf{x}})^{-1}$, the satellite matrix **R** is converted to coefficient **B** form as well:

$$\mathbf{B} = \mathbf{R}(\hat{\mathbf{x}})^{-1} \tag{33}$$

In the situation of the new demand $\mathbf{f}'$, the new output is $\mathbf{x}'$. As a result, the new environmental burdens become

$$\mathbf{g}' = \mathbf{B}\mathbf{x}' \tag{34}$$

Together, we therefore find

$$\mathbf{g}' = \mathbf{B}(\mathbf{I} - \mathbf{A})^{-1}\mathbf{f}' \tag{35}$$

as the basic equation of IO-LCA. It should be noted that PLCA can also be formulated as above, that is., modeling the economic and environmental consequences of new demand. It is arguably how the model is intended to be used given the consequential or change-oriented nature of LCA. However, this topic is beyond the scope of this study: the interested reader may refer to Yang and Heijungs (2018) for a detailed discussion.

Let us also do a small example here. We have two industries: electricity production and fuel production. The transaction table in a particular study area and year are as follows:

$$\mathbf{Z} = \begin{pmatrix} 500 & 0 \\ 1000 & 2000 \end{pmatrix} \tag{36}$$

the final demand is

$$\mathbf{f} = \begin{pmatrix} 10000 \\ 5000 \end{pmatrix} \tag{37}$$

and the production volume is therefore

$$\mathbf{x} = \begin{pmatrix} 10500 \\ 8000 \end{pmatrix} \tag{38}$$

The environmental satellite is

$$\mathbf{R} = \begin{pmatrix} 1000 & 1200 \\ 100 & 240 \\ 0 & -6000 \end{pmatrix} \tag{39}$$

Again, observe the minus sign, which we have introduced here for consistency with the PLCA presentation. In IO-LCA, it is more usual to suppress this minus sign.

The above yields coefficient matrices

$$\mathbf{A} = \begin{pmatrix} 0.0476 & 0 \\ 0.0952 & 0.2500 \end{pmatrix} \tag{40}$$

TABLE 1 Overview of the differences between $\mathbf{A}_P$ and $\mathbf{A}_{IO}$

Aspect	PLCA (A_P)	IO-LCA (A_{IO})
Format (row × column)	Intermediate flow × unit process	Industry × industry
Size	Not necessarily square	Square
Coverage	Product system, with predefined system boundaries	Economy-wide, no predefined system boundaries
Ordering of rows and columns	Arbitrary	Symmetric (i.e., the same order of industries is used for rows and columns)
Coefficients	Inputs (< 0) and outputs (> 0)	Inputs (> 0)
Diagonal	No special meaning	Self-inputs
Self-inputs (the use of its own product)	Consolidated through net output	Recorded on diagonal
Output	In matrix as positive coefficient	Implicit, in **I**, so 1
Unit of coefficients	Same as unit of intermediate flow	Dimensionless for diagonal coefficients, unit of row industry/unit of column industry for off-diagonal coefficients

and

$$\mathbf{B} = \begin{pmatrix} 0.0952 & 0.1500 \\ 0.0095 & 0.0300 \\ 0 & -0.7500 \end{pmatrix} \tag{41}$$

Let us now impose a new final demand

$$\mathbf{f}' = \begin{pmatrix} 1000 \\ 0 \end{pmatrix} \tag{42}$$

Then we find for the outputs

$$\mathbf{x}' = \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 0.0476 & 0 \\ 0.0952 & 0.2500 \end{pmatrix} \right)^{-1} \begin{pmatrix} 1000 \\ 0 \end{pmatrix} = \begin{pmatrix} 1050.00 \\ 133.33 \end{pmatrix} \tag{43}$$

and for the environmental burdens

$$\mathbf{g}' = \begin{pmatrix} 0.0952 & 0.1500 \\ 0.0095 & 0.0300 \\ 0 & -0.7500 \end{pmatrix} \begin{pmatrix} 1050.00 \\ 133.33 \end{pmatrix} = \begin{pmatrix} 120 \\ 14 \\ -100 \end{pmatrix} \tag{44}$$

Finally, let us have a look at the dimensions. Usually, the transaction matrix **Z** and the output vector **x** are specified in monetary terms, say $ (or $/yr). Then the coefficient matrix **A** contains dimensionless numbers, and **B** contains numbers with units such as kg/$ and L/$. But in a physical IOT, the transaction table may also have been specified in mass units or other units. To facilitate the comparison with the PLCA model, we have here expressed electricity in kWh and fuel in liter. Therefore, the diagonal coefficients of **A**, a_{11}, and a_{22} are dimensionless, and the off-diagonal elements have a dimension: kWh/L for a_{12} and L/kWh for a_{21}. Likewise, the coefficient in **B** have units, such as kg/kWh and kg/L for b_{11} and b_{21}.

2.3 | A comparison

At first sight, the result seems surprising. How can a formula with **A** suddenly turn up with **I** − **A**, and still give identical results? One part of the answer is that we have carefully chosen the data in **Z** and **x** such that a consistent result appeared. The result is that the matrix **A** and **B** look very different in both representations. To be able to distinguish the two, we will add subscripts P and IO, thus writing $\mathbf{A}_P$, $\mathbf{A}_{IO}$, $\mathbf{B}_P$, and $\mathbf{B}_{IO}$.

In the construction of these matrices, and the subsequent derivation of the operational formulas, a number of subtle differences can be detected. Tables 1 and 2 give an overview.

TABLE 2 Overview of the differences between $\mathbf{B}_P$ and $\mathbf{B}_{IO}$

Aspect	PLCA ($\mathbf{B}_P$)	IO-LCA ($\mathbf{B}_{IO}$)
Format (row × column)	Elementary flow × unit process	Elementary flow × industry
Size	Usually not square	Usually not square
Ordering of rows and columns	Arbitrary (but columns must agree with those of $\mathbf{A}_P$)	Arbitrary (but columns must agree with those of $\mathbf{A}_{IO}$)
Coefficients	Inputs (<0) and outputs (>0)	Inputs (<0) and outputs (>0)
Diagonal	No special meaning	No special meaning
Unit of coefficients	Same as unit of elementary flow	Unit of elementary flow/unit of column industry

Some comments are needed. The coefficient matrix $\mathbf{A}_{IO}$ of IO-LCA contains, despite the suggestion from the term IO, inputs only, as positive numbers. The output is implicitly understood to be 1. Because the matrix is symmetric, all these implicit outputs of 1 are in the computations represented in the identity matrix $\mathbf{I}$. For PLCA, the corresponding matrix $\mathbf{A}_P$ contains the inputs, with a minus sign. The output (or outputs) is also part of the matrix, as a positive number. Because it is explicit, it need not be 1, but it can have any (positive) value, such as 10 and 100 in the numerical example. For the same reason, it need not reside on the diagonal, but can be anywhere. As a consequence, there is no necessary correspondence between the ordering of intermediate flows (rows) and unit processes (columns).

IO-LCA allows for self-inputs. For instance, the fuel industry uses some of its own products. In PLCA, the self-inputs are assumed to be consolidated. For instance, if a unit process needs 1 unit of its own product to produce 10 units of product, it effectively produces 9 units of products. The absence of self-inputs in PLCA leads to simpler expressions ($\mathbf{A}^{-1}$ instead of $(\mathbf{I}-\mathbf{A})^{-1}$), but on the expense of some loss of information.

2.4 | Provenance

Above, we connected the mathematical expressions to the way the data is organized. This is done for the following reasons.

The transaction matrix $\mathbf{Z}$ of IOA contains inputs only, and so does the coefficient matrix $\mathbf{A}$. To account for the fact that each sector produces something as well, the output must be added explicitly, through $\mathbf{I}$. This format has been developed by Leontief (1976), and it continues to be the standard presentation (Miller & Blair, 2009), also in environmental IOA (Hawkins & Matthews, 2009; Joshi, 1999; Wiedmann et al., 2015). It is based on an economic idea that goes back to Walras (1977): a production function which specifies the inputs needed to produce something valuable.

By contrast, the first mathematical treatment of LCA (Heijungs, 1994), as well as many follow-ups (Heijungs & Suh, 2002; Srocka & Montiel, 2021) choose to record inputs (negative) and outputs (positive) in the matrix $\mathbf{A}$. This set-up is more neutral in considering a process not as producing something from inputs, but as describing a process as the conversion of a bundle on inputs into a bundle of outputs. This idea goes back to activity analysis and linear programming (Koopmans, 1951), as well as to the more physically oriented analyses (Georgescu-Roegen, 1971).

We briefly discuss how the form with $\mathbf{I}-\mathbf{A}$ has certain computational properties that can be employed to speed up calculations and that can enrich the interpretation.[1] We further provide a historical account how the $\mathbf{I}-\mathbf{A}$ form entered the PLCA discussion.[2]

We believe that an understanding of the differences in provenance will help to understand the differences in mathematical details, even when ultimately a unified structure is chosen. Observe that the IO-LCA matrix $\mathbf{A}$ contains inputs only, despite its name, input–output.

3 | UNIFICATION OF PLCA AND IO-LCA

As argued for the theory of ecology by Lehman et al. (2020), a unified presentation has great pedagogical advantages. In this section, we will investigate a few options for this, taking lessons from hybrid LCA. The present article does not aim to further develop hybrid LCA; we refer to Suh et al. (2004) and Crawford et al. (2018) for theoretical treatises and to Suh (2004) for an illustrative example. Rather, we present a few aspects of hybrid LCA to study how PLCA and IO-LCA can be unified.

In hybrid LCA, the PLCA-form $\mathbf{A}_P$ and the IO-LCA-form $\mathbf{A}_{IO}$ are combined, in one matrix that we will denote as $\mathbf{A}_H$, using two connecting matrices, that are often referred to as upstream and downstream cut-off matrices, $\mathbf{C}_U$ and $\mathbf{C}_D$. We distinguish two presentations in the next two subsections.

3.1 | Unification under A

Suh (2004) defines the hybrid matrix as

$$\mathbf{A}_H = \begin{pmatrix} \mathbf{A}_P & -\mathbf{C}_D \\ -\mathbf{C}_U & \mathbf{I}-\mathbf{A}_{IO} \end{pmatrix} \tag{45}$$

and by similarly defining

$$\mathbf{B_H} = \begin{pmatrix} \mathbf{B_P} & \mathbf{B_{IO}} \end{pmatrix} \tag{46}$$

and

$$\mathbf{f_H} = \begin{pmatrix} \mathbf{f_P} \\ \mathbf{f_{IO}} \end{pmatrix} \tag{47}$$

he uses it in the "**A**-form":

$$\mathbf{g} = \mathbf{B_H} \mathbf{A_H^{-1}} \mathbf{f_H} \tag{48}$$

This form is also used by, among others, Suh and Huppes (2005), Heijungs et al. (2006), Lenzen and Crawfors (2009), Acquaye et al. (2011), Nakamura and Nansai (2016), Yang et al. (2017), Yu and Wiedmann (2018), and Crawford et al. (2018). A special mention is deserved by Perkins and Suh (2019), who write

$$\mathbf{A_H} = \begin{pmatrix} \mathbf{I} - \mathbf{A_P} & -\mathbf{C_D} \\ -\mathbf{C_U} & \mathbf{I} - \mathbf{A_{IO}} \end{pmatrix} \tag{49}$$

which they then use in an $\mathbf{A_H^{-1}}$ way.

3.2 | Unification under I − A

The opposite approach starts by defining

$$\mathbf{A_H} = \begin{pmatrix} \mathbf{I} - \mathbf{A_P} & \mathbf{C_D} \\ \mathbf{C_U} & \mathbf{A_{IO}} \end{pmatrix} \tag{50}$$

which is next used in an "**I** − **A**-form":

$$\mathbf{g} = \mathbf{B_H} (\mathbf{I} - \mathbf{A_H})^{-1} \mathbf{f_H} \tag{51}$$

This format is used by Agez et al. (2020). Strømman et al. (2006) and Strømman et al. (2009) combine the matrices in a way that we could write here as

$$\mathbf{A_H} = \begin{pmatrix} \mathbf{A_P} & \mathbf{C_D} \\ \mathbf{C_U} & \mathbf{A_{IO}} \end{pmatrix} \tag{52}$$

which they next use in the $(\mathbf{I} - \mathbf{A_H})^{-1}$ way. Probably, these authors have already written $\mathbf{A_P}$ as $\mathbf{I} - \mathbf{A_P}$ right from the start. This logic is followed more explicitly by Jakobs et al. (2021), who write that their matrix "is given in the input-output convention," deviating from "the standard LCA convention."

3.3 | A comparison

Mathematically speaking, the diverging presentations are a minor issue. Any square matrix **X** can be rewritten as **I** − **Y** using the trivial relationships

$$\mathbf{X} = \mathbf{I} - \mathbf{Y} \Leftrightarrow \mathbf{Y} = \mathbf{I} - \mathbf{X} \tag{53}$$

Effectively, this is what Agez et al. (2020) write in their footnote 7.

The evidence above shows that most authors prefer a unification under **A**. In addition, we point to Suh and Heijungs (2007), who discuss various complications in using **I** − **A**. For instance, there is not necessarily a correspondence between rows and columns, and the data is not necessarily normalized per unit of output. Additional transformations, described in the appendix of Peters (2007), as well as by Suh and Heijungs (2007) may be needed before the $\mathbf{I}-\mathbf{A}$ becomes meaningful.

4 | CONCLUSIONS

The formulas for process-based LCA and IO-based LCA are highly similar, this similarity conceals that there are a number of crucial differences between the two formats. We have shown how the two formulas follow from quite different principles. We have also explored how they can be combined in hybrid LCA, and we saw that both viewpoints (process based and IO based) have been used to actually build a hybrid formula. However, we have also demonstrated that the IO-format assumes more pre-processing steps than the process-format does. For instance, in process-based LCA, there need not be a correspondence between rows and columns of $\mathbf{A}$, and the data need not be normalized per unit of output. For this reason, a unification in the direction of the process-based formats is much easier than in the direction of the IO-format.

That being said, the purpose of our paper is not to "peddle" one form of unification over the other form. For example, teachers at NTNU have preferred $\mathbf{I}-\mathbf{A}$ to $\mathbf{A}$, applying $\mathbf{I}-\mathbf{A}$ to PLCA studies through redefining the PLCA matrix as if it is an IO-LCA matrix (see 3.2), and they have been teaching this way of unification to students over the past two decades (Strømman, 2021). Precisely, our purpose is to highlight the importance of unification, given the challenge the two formulas present to LCA students and the confusion they may cause to even experienced LCA researchers. We strongly suggest that a unified format is taught for greater clarity and consistency. Our paper can be used as teaching material to help students better understand why the two approaches differ in their computational structure and how they can be unified in consistent formats, one way or the other. It is the choice of the student (or the reader) as to which format they prefer to use in their own research.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

ORCID

Reinout Heijungs https://orcid.org/0000-0002-0724-5962

Yi Yang https://orcid.org/0000-0002-0600-602X

Hung-Suck Park https://orcid.org/0000-0002-5523-7633

[1] **Power series expansion in lieu of inversion:** In a period when only a few scientists had access to computers, Waugh (1950) proposed to speed up the IOA computations using a trick. The trick consisted on rewriting $(\mathbf{I}-\mathbf{A})^{-1}$ as $\mathbf{I}+\mathbf{A}+\mathbf{A}^2+\mathbf{A}^3+\cdots$, and then resorting to the much easier process of multiplying and adding matrices. In the current computer age, this power series trick seems to have become obsolete, as is shown by the fact that a modern handbook on IOA (Ten Raa, 2017) does not mention it.

In the context of LCA, this trick has been revived by Peters (2007). But, as discussed by Suh and Heijungs (2007), its rests on quite a few assumptions. First, the steps outlined above (reordering rows and columns to create a one-to-one correspondence, normalization per unit of output) must be carried out. But even that is typically not enough, because the power series only make sense when it converges (i.e., does not go to infinity with high powers). As outlined by Suh and Heijungs (2007), this may also require a rescaling of rows, such that the norm or eigenvalues of $\mathbf{A}$ satisfy certain conditions. In the field of economics, the validity of the Hawkins-Simon conditions (Hawkins & Simon, 1949) is still of major concern. The process-based format is much more flexible in that respect, as long as no power series are used. This may have repercussions for the validity and applicability of structural path analysis for LCA (Suh & Heijungs, 2007).

[2] **The source of I - A in PLCA:** In Section 1, we observed that some authors discuss PLCA, but then provide the IO-LCA form instead. In fact, we can trace this idea back to Frischknecht et al. (2004). It is worth quoting this text to some extent, where we have changed their notation a bit to streamline their symbols with ours: "Matrix $\mathbf{A}$ can be rewritten as $\mathbf{A} = \mathbf{I}-\mathbf{W}$ … The inverse can be written as … $\mathbf{A}^{-1} = (\mathbf{I}-\mathbf{W})^{-1} = \sum_{k=0}^{\infty} \mathbf{W}^k$ …. For the numerical implementation of the matrix inversion direct methods are usually applied that make use of publicly available source code libraries." So, apparently these authors decide to rewrite $\mathbf{A}^{-1}$ as $(\mathbf{I}-(\mathbf{I}-\mathbf{A}))^{-1}$ and then as $\sum_{k=0}^{\infty}(\mathbf{I}-\mathbf{A})^k$, but not for the purpose of using the power expansion trick (Waugh, 1950) in computing, but for no obvious reason at all. After all, they just invert $\mathbf{A}$ directly, without the use of $\mathbf{I}-\mathbf{A}$.

Despite the fact that this text seems to fulfil no function, it has been quite influential, probably because it was written in connection to the ecoinvent database (https://www.ecoinvent.org/), which is the most widely-used LCA database on the market. We think that the advent of $\mathbf{B}(\mathbf{I}-\mathbf{A})^{-1}$ in PLCA is sometimes motivated from an IO-background (Agez et al., 2020) and sometimes from an ecoinvent background (Jolliet et al., 2016).

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