

ECO-EFFICIENCY IN INDUSTRY AND SCIENCE

The Computational Structure of Life Cycle Assessment

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The Computational Structure of Life Cycle Assessment

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the term 'matrix' in this book refers to a rigid mathematical concept (see Appendix A), that is defined in a linear space and for which operations such as multiplication, transposition and inversion are defined. Thus, Graedel's (1998, p.100) concept of matrix as a table of 5×5 cells in which the user is supposed to enter an ordinal score between 0 ("highest impact") and 4 ("lowest impact") is outside the scope of the present book.

It will be assumed that the reader has a basic knowledge of the principles, framework and terminology of LCA. Useful texts at varying levels of depth are provided by Lindfors *et al.* (1995), Curran (1996), Weidema (1997), Jensen *et al.* (1997), Hauschild & Wenzel (1998), Wenzel *et al.* (1998), UNEP (1999), Guinée *et al.* (2002), and others. However, a short overview of the basic elements of LCA is discussed in the next section. We also will, as much as reasonably possible, adhere to the ISO-standards for LCA (ISO, 1997, 1998, 2000). At certain points, departures will be necessary, and at many places, new concepts must be introduced. When appropriate, such cases will be argued.

Throughout this book, it will be assumed that data availability is not a problem. In fact, the efforts and measurement, modeling and estimation techniques that are needed to obtain data is not discussed in this book. The central theme is how the data, once available, should be processed and combined to complete an LCA study. In the first few chapters, it will moreover be assumed that data are known exactly. This will allow us to present the basic structure in terms of deterministic equations. Chapter 6 discusses extensively the topic of perturbation theory, which includes the statistical processing of stochastic data.

1.1.2 Motivation

The main motivation for writing this book is that the computational structure is an important topic for which no reference book is available. Below, we first seek to explain that indeed the topic is underemphasised, and then will demonstrate its importance.

It is a remarkable fact that there is a large number of guidebooks for applying the LCA technique, but that the computational structure of LCA is hardly addressed in these books. To some extent, this is understandable: a person charged with carrying out an LCA study needs guidelines on which data to collect, which choices to make, and how to report assumptions and results. For the calculations, he or she will rely on LCA software, of which there is a large choice on the market (Siegenthaler *et al.*, 1997). But this alleged lack of direct utility is not a decisive argument, since most

guidebooks on LCA discuss the backgrounds of, say, models for ecotoxicity, even though these models are not used in an LCA, because it is only the tabulated characterisation factors that are derived from such models that are used. So, lack of direct utility when executing an LCA is not a valid reason for excluding material on the computational structure in guidebooks for LCA.

A further remarkable fact is that the computational structure is by and large overlooked by the theoretical literature on LCA as well. The equation which forms the basis for almost the entire book is

$$s = A^{-1}f \quad (1.1)$$

in which f is the final demand vector, A is the technology matrix (and A^{-1} its inverse), and s is the scaling vector; see Sections 2.1 and 2.2 for a full explanation. In the standard literature on LCA, this equation, as well as the terms final demand vector, technology matrix and scaling vector are missing entirely. And the few sources in which the computational structure is discussed are used in a rather limited way. An example may illustrate this. In 1994, one of the authors published a paper (Heijungs, 1994) that explicitly discussed some important elements of the computational structure of LCA. It introduced a matrix formalism towards the inventory analysis, and it gave a small example system with only four unit processes with a feedback loop that needed a matrix approach for a reliable solution. Six years later, in 2000, virtually all commercially available LCA programs were still unable to reproduce these results. Some of the programs refused to perform the calculation, others gave a totally wrong answer, and still others gave results that at best approximated the exact solution.

One might think that the computational structure of LCA is a too obvious issue to discuss in scientific publications. This is suggested by the formulation in the ISO-standard for inventory analysis: "Based on the flow chart and system boundaries, unit processes are interconnected to allow calculations on the complete system. This is accomplished by normalising the flows of all unit processes in the system to the functional unit. The calculation should result in all system input and output data being referenced to the functional unit." (ISO (1998, p.10)). The forerunner of the ISO-standard, SETAC's Code of Practice (Consoli *et al.* (1993)), provides some more information, but is still far from being exact and operational on that topic. Fecker (1992, p.4) writes in a book with the promising title *How to calculate an ecological balance?* that "the process parameters are

$$\mathbf{x} = (1 \ 2 \ 3)^T \text{ instead of } \mathbf{x} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

Chapter 2

The basic model for inventory analysis

In this chapter, the elementary formalism of the inventory analysis will be developed. It is based upon the simplifications that have been discussed by Guinée *et al.* (2002, p.III-15 *ff.*), *i.e.* a linear treatment of a steady-state situation. Approaches towards accounting for non-linearities and dynamic situations are discussed in Chapter 9. One could consider to start with the general model, and discuss the simplified model as a special case. This, however, would complicate the analytical treatment considerably, and it would moreover ignore that virtually all LCA studies, textbooks, software and databases are based on the simplified model. The general model is at present only an academic ideal, of which the practical applicability in concrete case studies is doubtful.

2.1 Representation of processes and flows

A first step in a formalised treatment is the construction of suitable system for the representation of quantified flows in connection with unit processes. For this, we introduce the notion of a linear space. A linear space is an abstract concept which allows us to uniquely represent a multidimensional data point as a simple vector with a definite value of each of the co-ordinates. See, *e.g.*, Apostol (1969) for an introduction into linear spaces.

For instance, consider a unit process (or process in short), say, production of electricity, which uses 2 litre of fuel to produce 10 kWh of electricity. Moreover, in doing so, it emits 1 kg of carbon dioxide and 0.1 kg of sulphur

dioxide. A linear space can now help us to describe this unit process in a very concise notation. We adopt the convention that the first dimension represents litre of fuel, that the second dimension represents kWh of electricity, that the third dimension represents kg of carbon dioxide and that the fourth dimension represents kg of sulphur dioxide. In term of linear spaces, the basis is

$$\begin{pmatrix} \text{litre of fuel} \\ \text{kWh of electricity} \\ \text{kg of carbon dioxide} \\ \text{kg of sulphur dioxide} \end{pmatrix} \quad (2.1)$$

Then the co-ordinates of the unit process production of electricity with respect to this basis is a simple vector

$$\mathbf{p} = \begin{pmatrix} -2 \\ 10 \\ 1 \\ 0.1 \end{pmatrix} \quad (2.2)$$

This will be referred to as the process vector for a particular unit process, in this case production of electricity.

Notice that we have written a minus sign in front of the 2 for the dimension that represents litre of fuel. The minus sign is a conventional indication for the direction of the flow. In Cartesian space, a negative x -co-ordinate indicates by convention a point at the left of the origin. Here, the negative co-ordinate indicates an input, while the other three positive co-ordinates indicate outputs. We emphasise the conventional nature of such a notation. In LCA, like in Cartesian geometry, a different choice leads to the same results when consistently followed.

Also notice that the vector that represents the unit process of electricity production has four co-ordinates in a definite order. We cannot interchange the elements of the vector, unless we change the order of the basis accordingly. Therefore, the order of the elements of the vector is fixed by convention as well. Again, this should be familiar from Cartesian geometry, where the first co-ordinate often represents the horizontal direction and the second the vertical direction.

A third type of convention is related to the choice of units. We might change the kg of carbon dioxide into a mg. Of course, we can only do this if we change the co-ordinate 1 in the third row of the process vector into a 1,000,000.

We will be involved with large systems comprising many different unit processes, like production of electricity, manufacturing of televisions, recycling of aluminium and transportation of tomatoes. A second step is therefore the representation of such a system of unit process. Let us consider a second unit process, say production of fuel. Suppose that for producing 100 litre of fuel, 50 litre of crude oil is needed, and that 10 kg of carbon dioxide and 2 kg of sulphur dioxide are emitted to the environment. A first thing to observe is that there is not yet an entry for crude oil in our four-dimensional linear space. A fifth dimension has therefore has to be added. Thus we change the basis into

$$\begin{pmatrix} \text{litre of fuel} \\ \text{kWh of electricity} \\ \text{kg of carbon dioxide} \\ \text{kg of sulphur dioxide} \\ \text{litre of crude oil} \end{pmatrix} \quad (2.3)$$

and have to adapt the process vector for electricity production accordingly into

$$\mathbf{p}_1 = \begin{pmatrix} -2 \\ 10 \\ 1 \\ 0.1 \\ 0 \end{pmatrix} \quad (2.4)$$

The co-ordinates of the additional unit process, production of fuel, is then

$$\mathbf{p}_2 = \begin{pmatrix} 100 \\ 0 \\ 10 \\ 2 \\ -50 \end{pmatrix} \quad (2.5)$$

A particularly concise notation for representing the resulting system of unit process is

$$\mathbf{P} = (\mathbf{p}_1 \mid \mathbf{p}_2) = \begin{pmatrix} -2 & 100 \\ 10 & 0 \\ 1 & 10 \\ 0.1 & 2 \\ 0 & -50 \end{pmatrix} \quad (2.6)$$

We will refer to this as the process matrix. Observe that a new convention is needed to express the fact that the first column represents the unit process

of production of electricity, while the second column represents the unit process of production of fuel. Column vectors will be indicated as p_1 , p_2 or p_j in general. An individual element of a process matrix can be referred to as $(P)_{ij}$ where i denotes the index of the row and j the index of the column. Observe that $(P)_{ij} = (p_j)_i = p_{ij}$. In the example, i runs from 1 to 5 and j from 1 to 2. The process matrix is then said to be of dimension 5×2 .

A third step is to partition the process matrix into two distinct parts: one representing the flows within the economic system, referred to as economic flows, and one representing the flows from and into the environment, referred to as environmental flows or environmental interventions or interventions for short. In the example, the first two rows, representing litre of fuel and kWh of electricity, are flows within the economic system, while the last three rows, representing kg of carbon dioxide, kg of sulphur dioxide and litre of crude oil are environmental flows. ISO (1997) speaks of product flows and elementary flows respectively, but the distinction between economic and environmental flows seems to be more popular. The partitioning leads to a partitioned matrix

$$P = \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} -2 & 100 \\ 10 & 0 \\ 1 & 10 \\ 0.1 & 2 \\ 0 & -50 \end{pmatrix} \quad (2.7)$$

Although this partitioning is not needed *per se* for the representation of unit process or entire systems of unit processes, it is a convenient step. Furthermore, it will turn out to be needed in the following steps. The matrix **A** that represents the flows within the economic systems will be referred to as the technology matrix. Matrix **B** will be called the intervention matrix, because it represents the environmental interventions of unit processes. Partitioning in this way may lead to matrices and with an unequal number of rows. The number of columns of **A** and **B** is equal, and it is also equal to that of the unpartitioned process matrix **P**.

A fourth step is more related to goal and scope definition than to inventory analysis. It involves the specification of the required performance of the system. In general, a reference flow ϕ will be determined as one way of fulfilling a functional unit that is quite arbitrarily chosen. For instance, a reference flow for this example could be 1000 kWh of electricity. The

vector

$$f = \begin{pmatrix} 0 \\ 1000 \end{pmatrix} \quad (2.8)$$

thus represents the set of economic flows that corresponds to this reference flow. Observe that we specify the complete set of economic flows, even though only one of these flows is the reference flow. The logic of using a co-ordinate system requires that we reserve an entry for every economic flow. In general, the only non-zero element of this vector, say the r th, is the reference flow:

$$f_i = \begin{cases} \phi & \text{if } i = r \\ 0 & \text{otherwise} \end{cases} \quad (2.9)$$

Vector **f** will be referred to as the final (or external) demand vector, because it is an exogenously defined set of economic flows of which we impose that the system produces exactly the given amount. Later on, in Section 3.4.2, we will discuss the case of comparing alternative products with more than one reference flow.

A final aspect of representation is the inventory table, *i.e.* the set of all environmental flows associated with the reference flow under consideration. How to find it will be the topic of the next section. For now, it suffices to discuss its notation. In the example co-ordinate system, we have three environmental flows. Even though some of these flows may be zero for a certain choice of **f**, we need to reserve vector elements for each of these flows. We will proceed to define

$$g = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix} \quad (2.10)$$

as a vector of environmental interventions, the inventory vector, where g_1 denotes the number of kg of carbon dioxide emitted by the total system, etc. The final demand vector and the inventory vector can be regarded as the aggregated external flows of the entire system. Stacking the two vectors

$$q = \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} 0 \\ 1000 \\ g_1 \\ g_2 \\ g_3 \end{pmatrix} \quad (2.11)$$

provides an easy reference to this system vector.

2.2 The inventory problem and its solution

So far, we have only discussed the representation of unit processes, systems of unit processes, reference flows, and so on. We did not calculate anything yet. In particular, we did not yet discuss how to obtain the values of g_1 , g_2 and g_3 . A treatment of this leads to a discussion of what we will call the inventory problem.

The two unit processes produce 10 kWh of electricity and 100 litre of fuel respectively. The reference flow is 1000 kWh of electricity. Reference flow and flows produced by the unit process do not match. We see that unit processes 1 and 2 produce 10 and 0 kWh of electricity, while the final demand is 1000 kWh. Obviously, we need to scale up unit process 1 by a factor of 100 in order to satisfy the 1000 kWh required. But it is equally obvious that the fuel requirement by that process will be scaled up by the same factor of 100, into 200 litre of fuel. This leads to an upscaling of the second unit process by a factor of 2, so that it produces 200 litre of fuel. This then matches exactly with the required 200 litre of fuel by the first unit process. There is no surplus nor a shortage, hence the system's flow of fuel is 0, precisely as was required by the final demand vector.

Apart from the fact upscaling a unit process affects the economic flows, it affects the environmental flows in the same way. For instance, the emission of carbon dioxide by the first unit process is upscaled from 1 kg into 100 kg. For the second unit process it is upscaled from 10 kg into 20 kg. A total system-wide emission of carbon dioxide of 120 kg is therefore found. In other words, the hitherto unknown g_1 is found to be 120. For the other two elements of the inventory vector, similar calculations yield $g_2 = 14$ and $g_3 = -100$. Recall that the minus sign indicates an input, in this case extraction of 100 litre of crude oil.

A more formal treatment can now be given. First, we introduce a vector with scaling factors, the scaling vector, as a generalisation of the factors of 100 and 2. We will indicate this vector by \mathbf{s} and write in the example case

$$\mathbf{s} = \begin{pmatrix} s_1 \\ s_2 \end{pmatrix} \quad (2.12)$$

For the first economic flow, fuel, a balance equation can be set up:

$$a_{11} \times s_1 + a_{12} \times s_2 = f_1 \quad (2.13)$$

In the concrete case, this amounts to

$$-2 \times s_1 + 100 \times s_2 = 0 \quad (2.14)$$

This equation cannot uniquely be solved for s_1 and s_2 . But there is a second balance equation available, for the second economic flow, electricity:

$$a_{21} \times s_1 + a_{22} \times s_2 = f_2 \quad (2.15)$$

or with the coefficients inserted,

$$10 \times s_1 + 0 \times s_2 = 1000 \quad (2.16)$$

Simultaneous solution of these two equations yields

$$\mathbf{s} = \begin{pmatrix} s_1 \\ s_2 \end{pmatrix} = \begin{pmatrix} 100 \\ 2 \end{pmatrix} \quad (2.17)$$

A final step towards a generally applicable treatment is in terms of matrix solution. The system of equations

$$\begin{cases} a_{11} \times s_1 + a_{12} \times s_2 = f_1 \\ a_{21} \times s_1 + a_{22} \times s_2 = f_2 \end{cases} \quad (2.18)$$

can be written as

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} s_1 \\ s_2 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \quad (2.19)$$

or even more concisely as

$$\mathbf{A}\mathbf{s} = \mathbf{f} \quad (2.20)$$

Given that the technology matrix \mathbf{A} is known and that the final demand vector \mathbf{f} is known, the balance equation can, under certain restrictions which are to be discussed in Section 2.4, be solved to yield the scaling vector \mathbf{s} :

$$\mathbf{s} = \mathbf{A}^{-1}\mathbf{f} \quad (2.21)$$

where \mathbf{A}^{-1} denotes the inverse matrix of the technology matrix \mathbf{A} . In the example case, we have

$$\mathbf{A} = \begin{pmatrix} -2 & 100 \\ 10 & 0 \end{pmatrix} \quad (2.22)$$

and

$$\mathbf{A}^{-1} = \begin{pmatrix} 0 & 0.1 \\ 0.01 & 0.002 \end{pmatrix} \quad (2.23)$$

Straightforward multiplication yields

$$\mathbf{s} = \mathbf{A}^{-1}\mathbf{f} = \begin{pmatrix} 0 & 0.1 \\ 0.01 & 0.002 \end{pmatrix} \begin{pmatrix} 0 \\ 1000 \end{pmatrix} = \begin{pmatrix} 100 \\ 2 \end{pmatrix} \quad (2.24)$$

So, we have found a recipe to calculate the scaling vector for the unit processes in a system, such that the system-wide aggregation of economic flows exactly agrees with the final demand vector that represents the pre-determined reference flow of the system. However, the inventory problem has not yet been solved completely, because the question was defined as to find the values of the system-wide aggregated environmental flows.

The scaling vector provides a direct clue to the final step in solving the inventory problem. We must recognise that scaling of a unit process affects both the economic flows and the environmental flows. For the first environmental flow, carbon dioxide, we have

$$g_1 = b_{11} \times s_1 + b_{12} \times s_2 \quad (2.25)$$

In the concrete case, this amounts to

$$g_1 = 1 \times s_1 + 10 \times s_2 \quad (2.26)$$

Inserting the values for s_1 and s_2 , we find for g_1

$$g_1 = 1 \times 100 + 10 \times 2 = 120 \quad (2.27)$$

More generally, we have

$$\begin{cases} g_1 = b_{11} \times s_1 + b_{12} \times s_2 \\ g_2 = b_{21} \times s_1 + b_{22} \times s_2 \\ g_3 = b_{31} \times s_1 + b_{32} \times s_2 \end{cases} \quad (2.28)$$

or in matrix notation

$$\mathbf{g} = \mathbf{B}\mathbf{s} \quad (2.29)$$

In the example case, we have

$$\mathbf{B} = \begin{pmatrix} 1 & 10 \\ 0.1 & 2 \\ 0 & -50 \end{pmatrix} \quad (2.30)$$

Matrix multiplication gives

$$\mathbf{g} = \mathbf{B}\mathbf{s} = \begin{pmatrix} 1 & 10 \\ 0.1 & 2 \\ 0 & -50 \end{pmatrix} \begin{pmatrix} 100 \\ 2 \end{pmatrix} = \begin{pmatrix} 120 \\ 14 \\ -100 \end{pmatrix} \quad (2.31)$$

In principle, the inventory problem is now solved. There is a rule ($\mathbf{s} = \mathbf{A}^{-1}\mathbf{f}$) that yields the scaling vector given a technology matrix and a final demand vector. And there is a second rule ($\mathbf{g} = \mathbf{B}\mathbf{s}$) that yields the inventory vector given the intervention matrix and the scaling vector.

In certain situations, it may be useful to provide explicit formulations without matrix algebra. This leads to the following formulae:

$$\forall i : \sum_j a_{ij}s_j = f_i \quad (2.32)$$

for the balance equation, and

$$\forall k : g_k = \sum_j b_{kj}s_j \quad (2.33)$$

for the elements of the inventory vector, *i.e.* for the environmental interventions g_k .

An interesting substitution of variables can now be made. If the expression for the scaling factors is inserted in the expression for the environmental interventions, we find

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f} \quad (2.34)$$

Matrix multiplication, like ordinary multiplication, is an associative operation, hence we may rewrite this as

$$\mathbf{g} = (\mathbf{B}\mathbf{A}^{-1})\mathbf{f} \quad (2.35)$$

which we will write as

$$\mathbf{g} = \mathbf{\Lambda}\mathbf{f} \quad (2.36)$$

where we have defined the intensity matrix $\mathbf{\Lambda}$ as

$$\mathbf{\Lambda} = \mathbf{B}\mathbf{A}^{-1} \quad (2.37)$$

This notation makes clear that the matrix $\mathbf{\Lambda}$ can be evaluated for a particular system of unit processes, and then be applied to any final demand vector, thus to any reference flow that emanates from the system. In the example we have

$$\mathbf{\Lambda} = \begin{pmatrix} 0.1 & 0.12 \\ 0.02 & 0.014 \\ -0.5 & -0.1 \end{pmatrix} \quad (2.38)$$

This matrix can, for instance, be applied to

$$\mathbf{f} = \begin{pmatrix} 0 \\ 1000 \end{pmatrix}; \mathbf{f} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \mathbf{f} = \begin{pmatrix} 10 \\ 0 \end{pmatrix}; \\ \mathbf{f} = \begin{pmatrix} 10 \\ 1000 \end{pmatrix}; \mathbf{f} = \begin{pmatrix} -10 \\ 0 \end{pmatrix}; \text{ etc.} \quad (2.39)$$

The meaning of these different types of final demand vectors will be discussed in Section 3.9. Using the matrix Λ implies that the scaling vector is not calculated. Even though the computation may be somewhat more efficient, knowledge of the intermediate results, in particular the scaling factors can provide a convenient tool for diagnosis of the results. Later on, in Section 2.6, we will also see that the scaling factors in some situations have a special meaning.

2.3 General formulation of the basic model for inventory analysis

The previous two sections have provided a view of the formalism and its rationale. But they have not provided a rigid formulation, and a scientific foundation is lacking anyway. This section provides such a general formulation. Readers interested in a more heuristical exposition of the computational structure of LCA may wish to defer the material in this section until they have gone through the other chapters, or they may decide to skip it all together.

The general formulation is based upon the principles of deductive logic: concepts are defined by formal definitions, *a priori* properties are assigned by axioms, and new properties are derived by lemmas or theorems, requiring a formal proof. Consequently, the following text is rather terse. Argumentations and illustrative examples are given in the previous sections.

We must first define the main objects of study, and postulate some of their properties. These include process vectors and matrices, the scaling vector, the final demand vector, as well as the property of linearity and additivity.

Definition 1 A process vector \mathbf{p} is a vector in a linear space of which the basis represents flows of goods, materials, services, wastes, substances, natural resources, land occupation, sound waves, and possibly other relevant items. The coefficients of this vector represent the amount of these items absorbed or produced by a particular unit process. A negative coefficient indicates an input of the process, a positive coefficient an output of the process, and a zero coefficient indicates that the item is not affected by the process. Two subsets of flows are distinguished: those which come from or go to another process (the economic flows), and those which come from or go to the environment (the environmental flows).

Definition 2 A process matrix \mathbf{P} is a set of process vectors, juxtaposed to one another. It may be partitioned into a technology matrix \mathbf{A} that represents the exchanges between processes, and an intervention matrix \mathbf{B} that represents the exchanges with the environment.

Axiom 1 Any process vector \mathbf{p}_j may be multiplied with an arbitrary constant s_j . In other words, processes represent linear technologies, and there are no effects of scale in production or consumption.

Note that this axiom can in its turn be presented as a theorem when higher-level axioms are postulated; see Theorem 3 in Heijungs (1998).

Definition 3 The constants s_j referred to in Axiom 1 may be stacked to form a scaling vector \mathbf{s} .

Axiom 2 Flows may be aggregated over various processes, paying respect to the sign.

Definition 4 A final demand vector \mathbf{f} is a vector of economic flows. The coefficients of this vector represent the amount of these items that a system under consideration should absorb or produce.

With these basis ingredients, the inventory problem can be formulated according to Lemma 1.

Lemma 1 Let \mathbf{A} be the technology matrix of a given system. In order to let the system absorb or produce a final demand vector \mathbf{f} , a scaling vector \mathbf{s} should be found such that the condition

$$\mathbf{A}\mathbf{s} = \mathbf{f} \quad (2.40)$$

is met.

Proof Applying a scaling vector \mathbf{s} to the system produces or absorbs a vector of economic flows $\tilde{\mathbf{f}}$. For one arbitrary economic flow i , we have, from Axiom 1 and Axiom 2,

$$\tilde{f}_i = a_{i1} \times s_1 + a_{i2} \times s_2 + \dots \quad (2.41)$$

As this applies for all economic flows, it follows that

$$\tilde{\mathbf{f}} = \mathbf{A}\mathbf{s} \quad (2.42)$$

The system thus produces or absorbs this amount. When it is imposed that the system produces or absorbs \mathbf{f} , one should find a scaling vector \mathbf{s} , such that

$$\tilde{\mathbf{f}} = \mathbf{f} \quad (2.43)$$

or equivalently

$$\mathbf{f} = \mathbf{A}\mathbf{s} \quad (2.44)$$

Q.E.D.

Theorem 1 *The condition $\mathbf{A}\mathbf{s} = \mathbf{f}$ referred to in Lemma 1, leads to a unique solution*

$$\mathbf{s} = \mathbf{A}^{-1}\mathbf{f} \quad (2.45)$$

provided that \mathbf{A} is square and non-singular.

Proof Substituting the expression (2.45) for \mathbf{s} into the condition (2.40) of Lemma 1, we have

$$\mathbf{A}\mathbf{s} = \mathbf{A}(\mathbf{A}^{-1}\mathbf{f}) = (\mathbf{A}\mathbf{A}^{-1})\mathbf{f} = \mathbf{f} \quad (2.46)$$

which shows that the expression for \mathbf{s} indeed is a solution. The appearance of the -1 to indicate inversion is allowed only if \mathbf{A} is square and non-singular. In that case, linear algebra teaches us that the solution is unique. Q.E.D.

Now, we proceed to define the inventory vector and the recipe how to find them.

Definition 5 *An inventory vector \mathbf{g} is a vector of environmental flows. The coefficients of this vector represent the amount of these items that a system under consideration absorbs or produces.*

Theorem 2 *Let \mathbf{B} be the intervention matrix of a given system. With a given scaling vector \mathbf{s} , the inventory vector \mathbf{g} is given by*

$$\mathbf{g} = \mathbf{B}\mathbf{s} \quad (2.47)$$

Proof For one arbitrary environmental flow k , we have, from Axiom 1 and Axiom 2,

$$g_k = b_{k1} \times s_1 + b_{k2} \times s_2 + \dots \quad (2.48)$$

As this applies for all environmental flows, Theorem 2 follows directly. Q.E.D.

This is, in fact, the entire axiomatic system for inventory analysis, at least for the basic case. Section 2.4 and Chapter 3 will discuss situations in which things are not so straightforward. In connection to Theorem 1, it may be noted that we have excluded the case that \mathbf{A} is non-square or singular. In that case, there are two possibilities: either there is a solution, be it or not unique, that can be found by a different method; or there is not a solution, although there may be approximate solutions.

2.4 Some notes on the basic model

The basic model and its solution have been presented above for a very simple example case and in a generalised form using matrix notation. The main idea has been the systematic construction of a set of linear balance equations, one for each economic flow, with a number of scaling factors, one for each unit process. Matrix inversion has been introduced as a way to solve such a system of linear equations. However, it is not the only way to find a solution; see Section 4.1. Moreover, matrix inversion is a time and memory consuming operation, that is not easily accessible to those with insufficient mathematical training. It may under certain conditions be an operation that is numerically unstable, producing incorrect results; see Sections 6.6 and 10.2. Finally, in many situations, it is not directly applicable to LCA. Matrix inversion requires that the technology matrix is square and invertible. This is not automatically the case in situations involving

- cut-off of economic flows;
- multifunctional unit processes;
- a choice between alternative processes;
- closed-loop recycling.

How to adapt the matrix approach is described in Chapter 3. Furthermore, the approach outlined above (and in Chapters 3 and 4) start from the assumption of complete certainty, whereas it is for sure that process data are often uncertain to some degree. The treatment of uncertainties is discussed in Chapter 6. Finally, the assumption of linear scaling of processes as well

heat from facility X and heat from facility Y has been built-in from the beginning. Denial of the 'no two brands' axiom thus means that hidden or implicit substitution-based allocation steps are made.

Of course, it also frequently happens that two brands are distinguished in a supply/use table. The system defined by

$$\mathbf{U} = \begin{pmatrix} 2 & 0 & 5 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ and } \mathbf{V}^T = \begin{pmatrix} 0 & 100 & 0 \\ 10 & 0 & 0 \\ 18 & 0 & 0 \\ 0 & 0 & 90 \end{pmatrix} \quad (4.56)$$

might also occur. In fact, the distinction of brands and multifunctionality is known to lead to rectangularity, and allocation-like procedures have been discussed at length in the theory of supply/use analysis (Konijn, 1994). Main schools are the following:

- the process-technology (or: industry-technology) model, in which every process is regarded as representing a unique technology to convert a bundle of inputs into a bundle of outputs;
- the commodity-technology model, in which every commodity (or: product) is assumed to be produced in a specific way, irrespective of the process where it is produced;
- the by-product technology model, in which a process's primary product is assumed to be produced in that particular way, and a process's non-primary product is assumed to be produced in the way according to the process that produces that product as its primary product.

The process-technology model does not solve the problem of rectangularity, unless a partitioning-like step is added. In many cases, this is done implicitly on an economic basis: outputs of co-products are all in monetary terms, so the inputs are distributed on the basis of the share in proceeds to the outputs. The commodity-technology model is clearly equivalent to the substitution method. The by-product technology model is a more sophisticated version of the commodity-technology model, along the lines that Weidema (2001) introduced in LCA.

Chapter 5

Relation with input-output analysis*

There is an interesting analogy between the technology matrix and the inventory problem on the one hand and an analytical tool for investigating industrial dependencies on the other hand. This latter type of analysis is called input-output analysis, or sometimes inter-industry analysis, and it has been introduced by Wassily Leontief around 1930. This chapter discusses the basic principles of input-output analysis (IOA) as originally introduced by Leontief, with an emphasis on its environmental extensions, and proceeds to discuss to important applications of IOA in relation to LCA: replacement of LCA by IOA, and combination of LCA and IOA. This chapter does not provide a comprehensive treatment of IOA; for this, the reader is referred to texts like Miller & Blair (1985) and Duchin & Steenge (1999).

5.1 Basics of input-output analysis and its environmental extension

In its original form, input-output analysis starts with a concept that is closely related to the technology matrix: the transactions matrix. This is a matrix of which a column represents the inputs of a process (or industry, or sector; although these terms occur frequently in the literature on IOA, we have here chosen to use the term process, to make the analogy with LCA as close as possible). But unlike the technology matrix, where the inputs of a process are formulated in terms of the flows of products (like fuel and electricity), the transactions matrix records the inputs in terms of the

other processes' outputs (like fuel production and electricity production). Another difference is that the technology matrix contains a process' inputs and outputs, distinguished by the sign, while the transactions matrix contains a process' inputs only; minus signs are not needed. The outputs of a process is by definition one single type of output, not steel or electricity but a plain process' output. It is not written as a matrix element in the column that represents that process, but it can be figured out by aggregating all processes' inputs of that process' output. A final element to notice is that IOA has been developed to analyse the structure of the economy, with an emphasis on the flows of money. The coefficients of the transactions matrix thus measure the inputs of the steel-producing process in terms of euro, dollar or yen, not in physical units like kg, kWh or km. Occasionally, one sees approaches in which the transactions matrix is measured in physical terms.

Let us for instance consider the transaction matrix

$$\mathbf{Z} = \begin{pmatrix} 2 & 10 \\ 4 & 2 \end{pmatrix} \quad (5.1)$$

in a linear space where the first row and the first column denote the process of production of fuel and the second row and the second column the process of production of electricity. The meaning of element z_{12} is that the second process needs 10 euro of the first process' output. It also needs 2 euro of its own output (z_{22}). In contrast to the technology matrix, the transactions matrix \mathbf{Z} is square by definition, as the rows and the columns refer to processes (sectors, industries).

To the transaction matrix \mathbf{Z} that indicates the inter-industry demands, we may append the demand by households as a vector \mathbf{y} . In the example below, the households exert a demand of 8 euro of the first process' output and 4 euro of the second process' output:

$$(\mathbf{Z} | \mathbf{y}) = \left(\begin{array}{cc|c} 2 & 10 & 8 \\ 4 & 2 & 4 \end{array} \right) \quad (5.2)$$

Thus, the first process' total output is $2 + 10 + 8 = 20$ euro, and the second process' total output $4 + 2 + 4 = 10$ euro. It is convenient to define a vector \mathbf{x} to indicate the total output:

$$(\mathbf{Z} | \mathbf{y} | \mathbf{x}) = \left(\begin{array}{cc|c|c} 2 & 10 & 8 & 20 \\ 4 & 2 & 4 & 10 \end{array} \right) \quad (5.3)$$

A next step in input-output analysis is the analysis of the economy-wide consequences of changes in household demand. For instance, what happens

when the demand of 8 euro of the first process' output is increased to 28 euro? This means that the first process' output is increased from 20 to 40 euro. Under the assumption of linear scaling, its input of the second process' output is then doubled from 4 to 8 euro. This on its turn implies an increased production volume of the second process, with a subsequent increase of this process' input of electricity. And so on.

It is convenient to define a matrix of technical coefficients $\tilde{\mathbf{Z}}$ by expressing each process' inputs as a fraction of its output

$$\tilde{\mathbf{Z}} = \begin{pmatrix} 2/20 & 10/10 \\ 4/20 & 2/10 \end{pmatrix} = \begin{pmatrix} 0.1 & 1 \\ 0.2 & 0.2 \end{pmatrix} \quad (5.4)$$

or more generally

$$\tilde{\mathbf{Z}} = \mathbf{Z}(\text{diag}(\mathbf{x}))^{-1} \quad (5.5)$$

where $\text{diag}(\mathbf{x})$ is the matrix that consists of the elements of \mathbf{x} at the diagonal and zeros at all off-diagonal places. The question is then to express the processes' new total output vector \mathbf{x}' as a function of the new households demand vector \mathbf{y}' . The expression is

$$\mathbf{x}' = (\mathbf{I} - \tilde{\mathbf{Z}})^{-1} \mathbf{y}' \quad (5.6)$$

where \mathbf{I} is the identity matrix of the same size as $\tilde{\mathbf{Z}}$. Here it is a 2×2 -matrix:

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (5.7)$$

Notice that we must distinguish here between the total output and households demand vectors \mathbf{x} and \mathbf{y} in the existing situation, and the same vectors \mathbf{x}' and \mathbf{y}' in a new situation. This allows us to calculate the effects of a change $\Delta \mathbf{y} = \mathbf{y}' - \mathbf{y}$ on $\Delta \mathbf{x} = \mathbf{x}' - \mathbf{x}$:

$$\Delta \mathbf{x} = (\mathbf{I} - \tilde{\mathbf{Z}})^{-1} \Delta \mathbf{y} \quad (5.8)$$

Without loss of generality, we may take the starting point as a reference situation, thus putting $\mathbf{x} = \mathbf{0}$, so that \mathbf{y}' coincides with $\Delta \mathbf{y}$. Inserting the unprimed symbols then yields the most usual form:

$$\mathbf{x} = (\mathbf{I} - \tilde{\mathbf{Z}})^{-1} \mathbf{y} \quad (5.9)$$

where the reinterpretation of \mathbf{y} as the households demand vector and \mathbf{x} as the total output vector can be made.

The term $(\mathbf{I} - \tilde{\mathbf{Z}})^{-1}$ is known as the Leontief inverse. In the example, it is

$$(\mathbf{I} - \tilde{\mathbf{Z}})^{-1} = \begin{pmatrix} 1.54 & 1.92 \\ 0.38 & 1.73 \end{pmatrix} \quad (5.10)$$

For a households demand

$$\mathbf{y} = \begin{pmatrix} 28 \\ 4 \end{pmatrix} \quad (5.11)$$

one then finds

$$\mathbf{x} = \begin{pmatrix} 50.78 \\ 17.69 \end{pmatrix} \quad (5.12)$$

for the processes' total output vector. Because \mathbf{Z} is square, the expression $\mathbf{I} - \tilde{\mathbf{Z}}$ represents a square matrix as well. Although it may still be singular in exceptional cases, there is no allocation step needed to transform a rectangular matrix into a square one as in LCA.

In LCA, the final demand vector normally consists of zeros at all but one place. Suppose that we in IOA make the special choice of zero households demand for all processes but one, and for that process a demand of 1 euro. Using this for \mathbf{y} , the resulting vector \mathbf{x} measures the output of all processes as a result of 1 euro demand from one particular process. The elements of \mathbf{x} are known as the Leontief multipliers.

Although primarily designed as a tool for the analysis of economic dependencies, IOA can serve environmental analyses as well when it is extended with so-called satellite accounts for the environmental flows. Below the transactions matrix, additional rows to account for carbon dioxide, sulphur dioxide, crude oil, etc. are added. The satellite matrix $\tilde{\mathbf{B}}$ is structurally identical to the intervention matrix \mathbf{B} of the inventory analysis. Environmental interventions associated with a certain households demand vector \mathbf{y} are then

$$\mathbf{g} = \tilde{\mathbf{B}} (\mathbf{I} - \tilde{\mathbf{Z}})^{-1} \mathbf{y} \quad (5.13)$$

Some care should be taken in directly comparing \mathbf{g} from LCA with from IOA, as well as using \mathbf{B} from LCA as $\tilde{\mathbf{B}}$ in IOA or the other way around, as there may be differences in the ordering or level of aggregation. Moreover, $\tilde{\mathbf{B}}$ is defined per euro of process output, while \mathbf{B} is, like \mathbf{A} , defined with respect to an arbitrary reference unit, such as 100,000 kg of steel or 1000 TV sets.

5.2 Comparison of LCA and IOA

The Leontief inverse plays a role that is comparable to the inverse of the technology matrix; see Table 5.1 for an overview of analogous concepts.

Table 5.1: Overview of analogous concepts in life cycle inventory analysis and input-output analysis.

life cycle inventory analysis	LCA	input-output analysis	IOA
product, economic flow (unit) process		commodity industry, sector, establish- ment	
technology matrix	\mathbf{A}	transactions matrix	\mathbf{Z}
final demand vector	\mathbf{f}	technical coefficients matrix	$\tilde{\mathbf{Z}}$
scaling vector	\mathbf{s}	households demand vector	\mathbf{y}
inverse of technology matrix	\mathbf{A}^{-1}	total output vector	\mathbf{x}
intervention matrix	\mathbf{B}	Leontief inverse	$(\mathbf{I} - \tilde{\mathbf{Z}})^{-1}$
equation for \mathbf{s}	$\mathbf{s} = \mathbf{A}^{-1}\mathbf{f}$	satellite matrix	$\tilde{\mathbf{B}}$
equation for \mathbf{g}	$\mathbf{g} = \mathbf{B}\mathbf{s}$	equation for \mathbf{x}	$\mathbf{x} = (\mathbf{I} - \tilde{\mathbf{Z}})^{-1} \mathbf{y}$
		equation for \mathbf{g}	$\mathbf{g} = \tilde{\mathbf{B}}\mathbf{x}$

Despite the similarities between LCA and IOA, there are some subtle differences. These ultimately relate to the difference in set-up of the matrices. The transactions matrix \mathbf{Z} of IOA is of the type process \times process (the most common terms for this are industry \times industry and sector \times sector). This means that the labels of rows and columns refer to processes (or industries, or sectors). The technology matrix \mathbf{A} of LCA is of the type commodity \times process, so that the labels of rows refer to commodities (or products, or economic flows) while the labels headers of columns refer to process (or industries, or sectors). Some important consequences are the following:

- The transactions matrix of IOA specifies the flow from one process to another process, without paying regard to the product that actually flows between these two processes. In LCA, the technology matrix specifies the flow of products to and from a process, without an explicit specification of the origin or destination of such flows.
- As we have seen in Section 3.2, an important problem in LCA is the fact that the technology matrix is often not square, so that matrix inversion cannot be applied, at least not directly. Allocation procedures must then be employed. The transactions matrix of IOA is always square, and the Leontief inverse can almost always be calculated.

- The diagonal of a transactions matrix has a special meaning: it represents the inputs of an industry to itself. An example could be electric power plants that use a part of their own electricity, for instance for pumping fuel into the combustors, and agriculture, where corn produced is partly used to feed cattle. In LCA the diagonal has no particular meaning. In fact, it is often not tractable, because the technology matrix is rectangular. Moreover, changing the ordering of industries in IOA has no influence on the interpretation of the diagonal as self-inputs as long as the order of the rows and columns is the same. In LCA, the order of processes and products may be changed independently, so that any suggestion of a special diagonal (as in Frischknecht & Kolm (1995)) is spurious. As a side remark, it may be noted that the interpretation of diagonal elements in IOA in terms of self-inputs is questionable as well; see Waugh (1950), who writes that the transactions matrix is a "hollow" matrix, *i.e.* with zero diagonal, Edey & Peacock (1959) who write down a "—" in the diagonal entries, and Georgescu-Roegen (1971, p.256 *ff.*) who devotes an entire discussion to the subject.
- The coefficients of a technical coefficients matrix have a limited range of 'intelligible' values: they lie between 0 and 1, and the sum over one column does not exceed 1. For technical coefficients matrices in physical units and for LCA's technology matrix, these restrictions do not hold or are weaker. However, as the majority of texts on IOA deal with monetary units, certain properties and theorems (see, *e.g.*, Section 4.2) cannot be applied to IOA in physical terms and LCA.
- The conventional degree of specificity differs to quite some extent between LCA and IOA. In IOA, the entire economy is categorised into a few hundred industries, covering many different processes, with typical names as "metal ores mining." In LCA, a much finer categorisation is attempted; distinguishing mining of copper ore, iron ore, bauxite, etc.

One can say that IOA on the basis of an process×process table contains no information on commodities. This is often not entirely clear from texts dealing with IOA. Thus, one often sees expressions like "the industry plastics materials," where the label "the industry plastics materials production" would be more appropriate. Moreover, one should recognise that the households demand vector is not a demand of commodities (products),

but a demand for industry's output. Demand is specified as "2 euro of plastics materials output," not as "2 euro of plastics materials."

As said, the exposition of IOA and the comparison with LCA are based on the original formulation of IOA. Original means here: on the basis of a process×process (or industry×industry) matrix. In the course of time modifications to this original scheme have been proposed, for instance leading to IOA on the basis of a commodity×process (or commodity×industry) matrix. For the purpose of the present book, we have chosen to categorise such formats as LCA, supply/use framework, or activity analysis (see Konijn (1994)). Here, the typical feature of IOA is regarded to be its process×process structure, leading to a square matrix by definition and the characteristic Leontief inverse with the $I - \tilde{Z}$.

5.3 IOA instead of LCA

A number of authors (*e.g.*, Lave *et al.* (1995), Hendrickson *et al.* (1998), Joshi (2000)) criticise LCA for being incomplete and approach the problem of finding environmental interventions associated with a certain external demand by switching to IOA. An important problem of traditional LCA is that process data must be collected for a very large number of processes, and that cut-offs (see Section 3.1) are needed at many places. Several decades of institutionalised compilation of IO-tables have resulted in a fairly complete and accurate picture of inter-industry flows. Thus, attempts have been made to replace the technology matrix by the input-output matrix. The approach is known as "economic input-output life-cycle analysis" or EIO-LCA in short.

Instead of the process-specific environmental coefficients, national emission tables like the US Toxics Release Inventory are coupled to the IO-matrix. Thus

$$g = BA^{-1}f \quad (5.14)$$

is replaced by

$$g = \tilde{B} (I - \tilde{Z})^{-1} y \quad (5.15)$$

Lenzen (2001) compares "conventional and input-output-based life-cycle inventories" and concludes that errors due to cut-off may be larger than the errors introduced by using IOA. Lave *et al.* (1995) show that indirect discharges by computer production exceed direct discharges by a factor of 26. On the other hand, several authors mentioned discuss limitations (see, *e.g.*, Nielsen & Pedersen Weidema (2001)). These include:

- the input-output tables themselves do not cover the entire life cycle; most prominently consumption processes and waste treatment are excluded;
- national IO-tables have separate entries for import and export, and hence tend to exclude interventions from production abroad;
- the industry classification of IO-tables is quite coarse, so that aggregation errors will be introduced.

In addition to the latter fact, we would like to point out that LCA is very often used to compare fairly similar products, such as bottles from polyethylene and bottles from polycarbonate, or in product design situations, where a designer wants to know the effects of changing materials. When these two materials are lumped together in one classification as “plastic materials,” the range of applications of LCA is seriously restricted. The crucial connecting element is that we must translate a reference flow in the final demand vector f into a households demand vector y . Whenever this is not possible, EIO-LCA is doomed to give up.

Several authors in the field of energy analysis discuss the use of input-output analysis, sometimes as opposed to the type of analysis that traditionally shows up in LCA, which is then called “process analysis” or “vertical analysis.” Boustead & Hancock (1979) and IFIAS (1974) are standard references in this respect. Miller & Blair (1985) also discuss “energy input-output analysis” and “environmental input-output analysis.” And pathbreaking studies on the relation between economic chains and the environment, such as Ayres & Kneese (1969) and Leontief (1970) are based on (process×process) IOA as well, as are newer applications, such as Perrings (1987). An exception that should be mentioned here is Victor (1972), who bases an economy-wide study on the commodity×process structure.

5.4 Hybrid analysis

As discussed above, LCA yields quite specific data but suffers from providing an incomplete picture. IOA, in contrast, yields a fairly complete system, but is in certain respects overly aggregated and hence unspecific. The result is for both approaches an increase of uncertainty. This observation leaded various efforts to combine the strengths of both, which are generally called hybrid analysis. In general, the IOA-based part in a tiered hybrid analysis provides relatively complete far upstream system boundaries while

the LCA-based part provides a much more specific near upstream system and the downstream boundaries (see Marheineke *et al.* (1998)).

For the purpose of analysis, we discuss in the next two sections two different approaches here under the names tiered hybrid analysis and internally solved hybrid analysis. The reader should acknowledge, however, that the connection of LCA and IOA in a hybrid analysis is a topic to which current much research is devoted. For a more comprehensive presentation, see Suh & Huppes (2002).

5.4.1 Tiered hybrid analysis

The concept of hybrid analysis appears from the 1970s in energy analysis. Bullard *et al.* (1978), Van Engelenburg *et al.* (1994) and Treloar (1997) combined process analysis based on flow charts with IOA to calculate net energy requirements of a product or an entire economy. The computational structure of tiered hybrid analysis can be formulated from the following phrases (Bullard *et al.*, 1978, p.281–282): “Some of the input materials may be typical products of I-O sectors ... Thus the only input materials requiring further process analysis are atypical products not easily classified in an I-O sector.” It is remarkable that, like in LCA, process analysis is not described in mathematical terms while input-output analysis is. A mathematical interpretation would be as follows:

$$g = g_{IOA} + g_{LCA} = \tilde{B} (I - \tilde{Z})^{-1} y + B A^{-1} f \quad (5.16)$$

Thus, y determines the IOA-based part of the hybrid analysis, while f determines the LCA-based part. There is no interaction between y and f , nor between \tilde{Z} and A ; this accounts for the qualification ‘tiered.’ It is up to the user to specify the separation between the IOA-based and the LCA-based demand in an appropriate way. Note that we may symbolically unify the two tiers as

$$g = \begin{pmatrix} \tilde{B} & B \end{pmatrix} \begin{pmatrix} I - \tilde{Z} & 0 \\ 0 & A \end{pmatrix}^{-1} \begin{pmatrix} y \\ f \end{pmatrix} \quad (5.17)$$

so that the general form employed in this book may be maintained (Suh & Huppes, 2001).

This presents just one approach towards partitioning the final demand into a commodity part, generated with an LCA-system, and a process part, generated with an IOA-system. There are two radically different choices possible for this partitioning. In LCA, we have seen the following choices