# The Computational Structure of Life Cycle Assessment 

Reinout Heijungs and Sangwon Suh

THE COMPUTATIONAL STRUCTURE OF LIFE CYCLE ASSESSMENT

## ECO-EFFICIENCY IN INDUSTRY AND SCIENCE

VOLUME 11

Series Editor: Arnold Tukker, TNO-STB, Delft, The Netherlands

## Editorial Advisory Board:

Martin Charter, Centre for Sustainable Design, The Surrey Institute of Art \& Design, Farnham, United Kingdom
John Ehrenfeld, International Society for Industrial Ecology, New Haven, U.S.A.
Gjalt Huppes, Centre of Environmental Science, Leiden University, Leiden, The Netherlands
Reid Lifset, Yale University School of Forestry and Environmental Studies; New Haven, U.S.A.
Theo de Bruijn, Center for Clean Technology and Environmental Policy (CSTM), University of
Twente, Enschede, The Netherlands

# The Computational Structure of Life Cycle Assessment 

by

Reinout Heijungs<br>Centre of Environmental Science,<br>Leiden University, Leiden, The Netherlands

and
Sangwon Suh
Centre of Environmental Science,
Leiden University, Leiden, The Netherlands

A C.I.P. Catalogue record for this book is available from the Library of Congress.

ISBN 978-90-481-6041-9
ISBN 978-94-015-9900-9 (eBook)
DOI 10.1007/978-94-015-9900-9

Printed on acid-free paper

## All Rights Reserved

© 2002 Springer Science+Business Media Dordrecht
Originally published by Kluwer Academic Publishers in 2002
Softcover reprint of the hardcover 1st edition 2002
No part of this work may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without written permission from the Publisher, with the exception of any material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work.

## Preface

This books presents a complete overview of the computational aspects of life cycle assessment (LCA). Many books and articles have been written on LCA, including theoretical treatments of the entire concept, practical guidebooks to apply the technique, and concrete case studies in which LCA is applied to support decision-making with respect to environmental aspects of product alternatives. However, a good discussion of the computational structure of LCA is lacking. Knowledge is only partially documented, and what is documented is fragmented over diverse publications with mutual inconsistencies in approach, terminology and notation.

The book is the result of several years of research, along with the teaching of LCA at university classes and, not unimportantly, the development of software for LCA. This software has been designed to support the education of LCA, but it has been applied in real-world case studies as well. The name of the software is CMLCA, which is an abbreviation of Chain Management by Life Cycle Assessment. This program can easily be used to reanalyse and further explore the ideas that are outlined in this book. Another important source for this book relates to the work involved in connecting input-output analysis (IOA) to LCA. Software for this - MIET, an abbreviation of Missing Inventory Estimation Tool - is also available. Some of the basic routines have been implemented in Matlab script as well. All three pieces of software can be accessed, free of charge, through http://www.leidenuniv.nl/cml/ssp/software.html.

In developing the ideas that are written in this book, we have benefited from discussions during the last few years with Jeroen Guinée, Gjalt Huppes, René Kleijn and Ruben Huele at the Centre of Environmental Science, Leiden University, Rolf Frischknecht at ESU-services, ETH Zürich, Mark Huijbregts, formerly at the Interfaculty Department of Environmental Science, University of Amsterdam, now at the Department of Environmental Science, Nijmegen University and Wang Hongtao at Sichuan University. Igor Nikolić provided support in discovering the advanced features of type-
setting with $\mathrm{IAT}_{E} X$. The actual text, including possible omissions and errors, however, is our responsibility.

## Contents

Preface ..... v
1 Introduction ..... 1
1.1 Purpose of the book ..... 1
1.1.1 Aim ..... 1
1.1.2 Motivation ..... 2
1.2 Elements of LCA ..... 4
1.3 Background of the book ..... 7
1.4 Structure of the book ..... 8
1.4.1 Outline ..... 8
1.4.2 Notation ..... 9
2 The basic model for inventory analysis ..... 11
2.1 Representation of processes and flows ..... 11
2.2 The inventory problem and its solution ..... 16
2.3 General formulation of the basic model for inventory analysis ..... 20
2.4 Some notes on the basic model ..... 23
2.5 Geometric interpretation of inventory analysis* ..... 24
2.6 An interpretation of the scaling factors* ..... 27
2.7 An interpretation of the intensity matrix* ..... 28
3 The refined model for inventory analysis ..... 33
3.1 Cut-off ..... 33
3.1.1 Formulation of the problem ..... 34
3.1.2 Adding hollow processes to the technology matrix* ..... 35
3.1.3 Replacing non-zero numbers for flows that are cut-off by zeros* ..... 36
3.1.4 Removing cut-off flows from the technology matrix ..... 36
3.1.5 Brief discussion ..... 38
3.2 Multifunctionality and allocation ..... 39
3.2.1 Formulation of the problem ..... 40
3.2.2 The substitution method ..... 41
3.2.3 The partitioning method ..... 46
3.2.4 The surplus method* ..... 49
3.2.5 Other methods* ..... 51
3.2.6 Brief discussion ..... 56
3.3 System boundaries ..... 56
3.3.1 Economic and environmental flows ..... 57
3.3.2 Cut-off ..... 58
3.3.3 Other product systems ..... 59
3.3.4 Goods and wastes ..... 60
3.4 Choice of suppliers ..... 62
3.4.1 Formulation of the problem ..... 62
3.4.2 Comparison of alternative systems ..... 63
3.4.3 Representing a mixing process ..... 64
3.4.4 Brief discussion ..... 66
3.5 Closed-loop recycling ..... 67
3.5.1 Formulation of the problem ..... 68
3.5.2 Solution with the pseudoinverse ..... 69
3.5.3 Comparison with the partitioning method* ..... 70
3.5.4 Comparison with the substitution method* ..... 71
3.5.5 Brief discussion ..... 72
3.6 Inclusion of aggregated systems* ..... 73
3.7 Some special unit processes and flows ..... 76
3.7.1 Consumption processes ..... 77
3.7.2 The reference flow ..... 77
3.7.3 Transport processes ..... 79
3.7.4 Storage processes ..... 80
3.7.5 Waste treatment processes ..... 81
3.7.6 Waste flows ..... 81
3.7.7 Environmental flows ..... 83
3.8 More than one reference flow ..... 83
3.8.1 The comparison of product alternatives ..... 84
3.8.2 A database of inventory tables ..... 85
3.8.3 Structural universality and sleeping processes ..... 86
3.9 Types of final demand ..... 88
3.9.1 Cradle-to-grave analysis ..... 88
3.9.2 Cradle-to-gate analysis ..... 88
3.9.3 Gate-to-grave analysis ..... 89
3.9.4 More general analyses ..... 89
3.10 General formulation of the refined model for inventory analysis ..... 90
3.11 An extended example ..... 92
4 Advanced topics in inventory analysis* ..... 99
4.1 Alternative ways of formulating and solving the inventory problem ..... 99
4.1.1 The sequential method ..... 100
4.1.2 Petri nets ..... 101
4.1.3 Linear programming ..... 102
4.1.4 Cramer's rule ..... 102
4.2 Expansion of the inverse as a power series ..... 103
4.3 Feedback loops in the technology matrix ..... 105
4.3.1 Solution with matrix inversion ..... 106
4.3.2 The network as an infinite sequence ..... 107
4.3.3 Algebraic manipulation of systems of equations ..... 108
4.3.4 The use of a power series expansion ..... 108
4.4 Singularity of the technology matrix ..... 110
4.5 Allocation in economic models ..... 112
4.5.1 The supply/use framework ..... 112
4.5.2 Negative scaling factors: the Hawkins-Simon condition1 ..... 114
4.5.3 The technology assumptions ..... 115
5 Relation with input-output analysis* ..... 117
5.1 Basics of input-output analysis and its environmental extension ..... 117
5.2 Comparison of LCA and IOA ..... 121
5.3 IOA instead of LCA ..... 123
5.4 Hybrid analysis ..... 124
5.4.1 Tiered hybrid analysis ..... 125
5.4.2 Internally solved hybrid analysis ..... 128
6 Perturbation theory ..... 131
6.1 Some general results ..... 132
6.1.1 Perturbation of the technology matrix ..... 133
6.1.2 Perturbation of the intervention matrix ..... 136
6.1.3 Perturbation of the final demand vector ..... 136
6.1.4 Some examples ..... 138
6.2 Uncertainties and their propagation ..... 140
6.2.1 Uncertainties in data ..... 140
6.2.2 Uncertainties in results ..... 143
6.3 Discrete choices ..... 145
6.4 Monte Carlo simulations ..... 146
6.5 Change of technology ..... 147
6.6 Numerical stability ..... 148
6.6.1 Round-off ..... 148
6.6.2 Rescaling ..... 149
7 Structural theory ..... 151
7.1 Some definitions ..... 151
7.2 Summary measures ..... 152
7.2.1 The condition number ..... 153
7.2.2 Other characteristics ..... 153
7.2.3 Correlation analysis ..... 154
7.2.4 Multivariate methods ..... 154
7.3 Visual tools ..... 157
7.3.1 Spy plots ..... 158
7.3.2 Other graphics ..... 158
8 Beyond the inventory analysis ..... 161
8.1 Impact assessment ..... 161
8.1.1 Impact categories and characterisation models ..... 162
8.1.2 Derivation of characterisation factors* ..... 163
8.1.3 Classification ..... 165
8.1.4 Characterisation ..... 168
8.1.5 Normalisation ..... 169
8.1.6 Grouping* ..... 170
8.1.7 Weighting ..... 170
8.2 Interpretation ..... 172
8.2.1 Contribution analysis ..... 172
8.2.2 Structural analysis ..... 177
8.2.3 Perturbation analysis ..... 178
8.2.4 Uncertainty analysis ..... 182
8.2.5 Key issue analysis ..... 183
8.2.6 Comparative analysis ..... 184
8.2.7 Discernibility analysis ..... 185
9 Further extensions* ..... 189
9.1 Non-linear models ..... 189
9.2 Spatially differentiated models ..... 192
9.3 Dynamic models ..... 194
10 Issues of implementation* ..... 195
10.1 Sparse matrices and location matrices ..... 195
10.2 Matrix inversion ..... 198
10.2.1 The inverse ..... 198
10.2.2 The pseudoinverse ..... 199
10.3 Statistics of very long series ..... 200
10.4 Design of software for LCA ..... 201
A Matrix algebra ..... 205
A. 1 General concepts ..... 205
A. 2 Special matrices ..... 206
A. 3 Basic operations ..... 207
A. 4 Basic properties ..... 209
A. 5 Partitioned matrices ..... 212
A. 6 Systems of linear equations ..... 213
B Main terms and symbols ..... 217
C Matlab code for most important algorithms ..... 219
References ..... 223
Index ..... 235

## Chapter 1

## Introduction

This chapter introduces the aim of this book and motivates the importance of its topic. It does so in relation to a brief introduction of life cycle assessment (LCA), in which the various types of activities are outlined as well. Finally, the structure of the book is presented, along with a reading guide.

### 1.1 Purpose of the book

### 1.1.1 Aim

This book presents and discusses the computational structure of life cycle assessment. Under the computational structure, we will capture the arithmetical rules that are involved in carrying out an LCA study. However, this book is not a book with computational recipes only. Two other aspects receive a large emphasis as well. These are the background of the computational recipes, including argumentations and proofs, even though sometimes heuristically, references to related mathematical rules, and aspects that relate to the numerical implementation of the computational recipes. For this latter, the book will not provide computer source codes, but it will concentrate on the algorithmic aspects, even though some example pieces of Matlab code are given in Appendix C. Thus the computational structure is understood here to cover the mathematical structure as well as the algorithmic structure.

The computational structure will be formulated in terms of explicit mathematical equations. It will become apparent that use of matrix algebra provides an elegant, concise and powerful formalism. One should note that
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 $5 \times 5$ 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

$$
\begin{equation*}
\mathbf{s}=\mathbf{A}^{-1} \mathbf{f} \tag{1.1}
\end{equation*}
$$

in which $\mathbf{f}$ is the final demand vector, $\mathbf{A}$ is the technology matrix (and $\mathbf{A}^{-1}$ its inverse), and $\mathbf{s}$ 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
multiplied with the corresponding factor by which the process participates in the system." In this, he is one of the few authors that explicitly introduce the concept of scaling factors, but he does not provide a method to obtain them in a concrete situation. The report of SETAC's Working Group on Inventory Enhancement (Clift et al. (1998)) ignores the topic entirely. Another famous SETAC-publication (Fava et al. (1991, p.15)) is more explicit: "The calculation procedure is relatively straightforward ... The calculations can usually be performed by common spreadsheet software on a personal computer." This is, however, no longer true. As we will see in subsequent chapters, the theory involves concepts such as linear spaces, singular value decomposition, the pseudoinverse of a matrix, and the condition number of a matrix. Of course, there are a few texts in which the topic is addressed. For an overview, see Section 1.3.

It is the authors' experience that a good knowledge of the computational structure of LCA is important for several reasons:

- it is a prerequisite in the construction of a method that really can claim to have scientific validity;
- it is useful to gain an understanding of the logic of LCA in a university course;
- it guides the design and implementation of reliable LCA software (so proves the aforementioned failure of most commercial programs to deal with system with feedback loops);
- it may shed lead new light on established topics, such as co-product allocation;
- it enables a further exploration of advanced topics, such as uncertainty analysis.

In conclusion, the aim of this book is to provide a comprehensive description of the present state of scientific knowledge of the computational structure of LCA.

### 1.2 Elements of LCA

The general ISO 14040 standard (ISO, 1997, p.2) defines LCA as the "compilation and evaluation of the inputs, outputs and the environmental impacts of a product system throughout its life cycle." The LCA technique is
structured along a framework with a number of steps or activities in each of these steps. There are four phases:

- goal and scope definition;
- inventory analysis;
- impact assessment;
- interpretation.

A short summary of these phases follows.
Goal and scope definition deals with the clear and unambiguous formulation of the research question and the intended application of the answer that the LCA study is supposed to provide. Important elements of the goal and scope definition are the choice of the functional unit, the selection of product alternatives to be analysed, and the definition of the reference flows for each of the alternative systems.

The inventory analysis is concerned with the construction of these product systems. These systems are composed of unit processes, like industrial production, household consumption, waste treatment, transportation and so on. System boundaries and flow charts of linked unit processes are drawn for each alternative product system, and quantitative data as well as qualitative data for representativeness, etc. are collected during this phase. For those unit processes that are multifunctional, i.e. that provide more than one function, an allocation step is made. A final step of the inventory analysis is the aggregation of the emissions of chemicals and the extractions of natural resources over the entire product system, in such a way that a quantitative match with the system's reference flow is achieved. The final table of these aggregated emissions and extracted is referred to as the inventory table.

The result of the inventory analysis is often a long list with disparate entries, such as carbon dioxide, nitrogen oxides, chloromethane and mercury. The impact assessment aims to convert and aggregate these into environmentally relevant items. In particular, we mention here the step of characterisation, in which the inventory results are transformed into a number of contributions to environmental impact categories, such as global warming, acidification, and ecotoxicity. We also mention the optional normalisation in which the characterisation results are related to a reference value, such as the annual global extent of these impacts. We finally mention the weighting, in which priority weights are assigned to the characterisation
or normalisation results, and which may result into one final score for each alternative product system.

During the course of the LCA, many choices and assumptions must be made. Moreover, uncertainty may be introduced with every data item. The interpretation phase deals with the meaning and robustness of the information obtained and processed in the previous phases. The interpretation may include comparisons with previously published LCA studies on similar products, uncertainty and sensitivity analyses, data checks, external comments, and much more. It is also the place in which a final judgement and decision is outspoken.

In using the LCA technique for carrying out an LCA study, one may distinguish several types of activities.

- There are activities, related to the design of the system, the collection of data, the making of assumptions and choices, and so on. This, for instance, includes steps like the drawing of system boundaries, the collection of process data, the choice of allocation method, and the choice of an impact assessment method.
- There are computational activities, related to transforming or combining data items into a certain result. For instance, emission data are related to the functional unit, aggregated over all unit processes in the system, multiplied with appropriate characterisation factors, and so on.
- There are activities that relate to the procedural embedding of an LCA project. Depending on the topic of study and the intended application, different stakeholders may be involved in certain ways. For certain applications, critical review by an independent expert is essential.
- There are activities, related to the planning of the LCA. For instance, one can start with a small-size LCA, to explore the potentials and bottlenecks, and then to reiterate the steps in a more complete way. Uncertainty analyses can give rise to further reiterations.
- There are activities, related to the reporting of an LCA. All types of requirements on what to report and how to report can be imposed to obtain transparent and reproducible reports.

The ISO-standards for LCA do not clearly separate these different types of activities. However, emphasis is, apart from the presentation of framework and the definition of terms, mainly on procedural embedding and
reporting. Most importantly for this book, the ISO-standards for LCA do not cover the computational structure. One can easily confirm this by observing the absence of mathematical equations. This leaves a large degree of freedom for the present book. Many new technical terms will be introduced; examples are technology matrix and final demand vector. In fact, besides a presentation of the computational structure, this book aims to propose a standard nomenclature for a number of concepts; see Appendix B. Notation is also free, as there are no reserved symbols in the LCAcommunity (except perhaps one older proposal by Heijungs \& Hofstetter (1995)). Throughout this book a consistent notation will be used. It is summarised in Appendix B as well. A number of new non-mathematical terms are introduced; we mention in particular hollow processes (Section 3.1), brands of economic flows (Section 3.4) and sleeping processes (Section 3.8). Finally, for a few terms that do occur in the ISO-standards, we have found reason to introduce a different meaning; here we mention reference flows (Section 3.7.2) and grouping (Section 8.1.6).

As already indicated, this book discusses the computational structure of LCA, without reference to the procedural embedding and without reference to the planning aspects. This means, for instance, that this book may well describe the mathematics of comparing product alternatives on the basis of a weighting procedure, while the ISO-standards state that such an activity is not appropriate. The point is that ISO's reluctance derives from procedural grounds, while the mathematics is in itself without problems. The mathematics remains valid even when someone decides to operate outside the ISO-framework, or when the ISO-standards are changed in this respect.

### 1.3 Background of the book

Most method-oriented texts on LCA focus on formulating guidelines (cf. Guinée et al. (2002)). In addition to that, there are many articles and reports in which specific topics are discussed, such as models for assessing impacts of acidification or data quality. There are only few texts in which the computational structure is discussed. To the extent that they are relevant for the present book, their material has been included. Important references in this respect include Projektgemeinschaft Lebenswegbilanzen (1991), Heijungs et al. (1992), Möller (1992), Frischknecht et al. (1993), Heijungs (1994), Schmidt \& Schorb (1995), Heijungs (1996), Heijungs (1997), Heijungs \& Frischknecht (1998), Huele \& van den Berg (1998) and Heijungs \& Kleijn (2001).

In addition to that, other references that are relevant throughout the text are on linear algebra. Many texts, at various levels of sophistication and rigour, are available. Apostol (1969), Stewart (1973), Gentle (1997) and Harville (1997) provide good and accessible reviews. Albert (1972), Jennings \& McKeown (1977) and Golub \& Van Loan (1996) provide more specialised texts at an advanced level.

Finally, the topic of numerical analysis and computer algorithms is treated in many books, some emphasising the theoretical aspect and others providing easy-to-use computer codes. We have made use of the books by Jennings \& McKeown (1977), Hamming (1986), Thisted (1988), Press et al. (1992) and Cheney \& Kincaid (1999).

### 1.4 Structure of the book

### 1.4.1 Outline

This book discusses the computational structure of LCA. Much of the discussion will be directed to the computational aspects of inventory analysis. While many books on LCA would be structured along four core chapters, each of them dealing with one single phase of the LCA framework, this book presents the material in a different way. There is no chapter on goal and scope definition (although the reference flow is introduced in Section 2.1), and impact assessment and interpretation are treated in one single chapter (8).

Chapter 2 presents the basic computational model for inventory analysis. It introduces the representation of unit processes, economic flows and environmental flows, and it presents and solves the inventory problem: how to obtain the environmental flows associated with a functional unit.

Chapter 3 further develops the inventory analysis. We will see that the basic model falls short in many practical cases. This failure has to do with various complications that distort the ideal required for the basic model. These complications are, most importantly, cut-off and multifunctionality, the second type of complication giving rise to the allocation problem. This chapter also explores how the basic model works for a number of difficult situations.

Chapter 4 discusses advanced topics of the inventory analysis and is mainly intended for discussing very specific points. This chapter may be omitted without affecting the readability of the subsequent chapters. The same applies to Chapter 5 which ties the discussion to input-output analysis, a tool that is familiar in economics for more than sixty years and that
shares certain features with LCA.
In Chapter 6, we abandon the idea of point estimates of data, and develop how the computational rules can be used to statistically deal with uncertainty. Both an analytical and a numerical treatment are included.

Chapter 7 discusses analytical explorations of the data on the basis of theoretical considerations. This leads to summary measures of the structure of the data and their dependencies.

All computational aspects beyond the inventory analysis are discussed in Chapter 8: impact assessment and interpretation.

Chapter 9 briefly explores a more general theory for LCA, in which the usual simplifying assumptions of linearity and steady state are abandoned.

A final chapter (10) is devoted to more information-technical topics: algorithms for the inversion of a matrix under special conditions, memory requirements, and so on.

Some sections contain special topics that can be omitted without distorting the readability of subsequent text. These sections are indicated with an asterisk $\left({ }^{*}\right)$.

The book assumes that the reader has a basic knowledge of matrix notation and manipulation. A concise review of matrix algebra is provided as an appendix (A). The first few chapters require a smaller background in mathematics than the chapters later on do. Especially Chapter 2, which discusses the basics, has been written in a more accessible way, to make sure that the basics can be understood by a wide audience. Chapter 3 is already more involved, and especially Chapter 6 requires quite some background.

### 1.4.2 Notation

In this book, a consistent notation will be employed throughout. Appendix B gives an overview of the most important symbols and the name of the concepts they represent. Furthermore, we have adhered to the convention that italic letters (like $x$ ) indicate scalars, that roman bold lowercase letters (like $\mathbf{x}$ ) indicate vectors and that roman bold uppercase letters (like $\mathbf{X}$ ) indicate matrices. A superscript T indicates the transpose of a vector or matrix, a superscript -1 the inverse of a matrix, a superscript + the pseudoinverse of a matrix; see Appendix A for the definitions of these concepts. Other symbols that are placed after or on top of a symbol, like primes $\left(x^{\prime}\right)$, hats $(\hat{x})$, dots $(\dot{x})$ and tildes ( $\left.\tilde{x}\right)$, are used to refer to another variable, and their meaning differs per occurrence. Sometimes, we will write a row vector for a column vector to save space, e.g. writing

$$
\mathbf{x}=\left(\begin{array}{lll}
1 & 2 & 3
\end{array}\right)^{\mathrm{T}} \text { instead of } \mathbf{x}=\left(\begin{array}{l}
1 \\
2 \\
3
\end{array}\right)
$$

## 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

$$
\left(\begin{array}{c}
\text { litre of fuel }  \tag{2.1}\\
\mathrm{kWh} \text { of electricity } \\
\mathrm{kg} \text { of carbon dioxide } \\
\mathrm{kg} \text { of sulphur dioxide }
\end{array}\right)
$$

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

$$
\mathbf{p}=\left(\begin{array}{c}
-2  \tag{2.2}\\
10 \\
1 \\
0.1
\end{array}\right)
$$

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 $x$-coordinate indicates by convention a point at the left of the origin. Here, the negative co-ordinate indicates an input, while the other three positive coordinates 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 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

$$
\left(\begin{array}{c}
\text { litre of fuel }  \tag{2.3}\\
\mathrm{kWh} \text { of electricity } \\
\mathrm{kg} \text { of carbon dioxide } \\
\mathrm{kg} \text { of sulphur dioxide } \\
\text { litre of crude oil }
\end{array}\right)
$$

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

$$
\mathbf{p}_{1}=\left(\begin{array}{c}
-2  \tag{2.4}\\
10 \\
1 \\
0.1 \\
0
\end{array}\right)
$$

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

$$
\mathbf{p}_{2}=\left(\begin{array}{c}
100  \tag{2.5}\\
0 \\
10 \\
2 \\
-50
\end{array}\right)
$$

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

$$
\mathbf{P}=\left(\mathbf{p}_{1} \mid \mathbf{p}_{2}\right)=\left(\begin{array}{cc}
-2 & 100  \tag{2.6}\\
10 & 0 \\
1 & 10 \\
0.1 & 2 \\
0 & -50
\end{array}\right)
$$

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 $\mathbf{p}_{1}, \mathbf{p}_{2}$ or $\mathbf{p}_{j}$ in general. An individual element of a process matrix can be referred to as $(\mathbf{P})_{i j}$ where $i$ denotes the index of the row and $j$ the index of the column. Observe that $(\mathbf{P})_{i j}=\left(\mathbf{p}_{j}\right)_{i}=p_{i j}$. 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 $5 \times 2$.

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

$$
\mathbf{P}=\left(\frac{\mathbf{A}}{\mathbf{B}}\right)=\left(\begin{array}{cc}
-2 & 100  \tag{2.7}\\
10 & 0 \\
\hline 1 & 10 \\
0.1 & 2 \\
0 & -50
\end{array}\right)
$$

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 $\mathbf{A}$ that represents the flows within the economic systems will be referred to as the technology matrix. Matrix $\mathbf{B}$ 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 $\mathbf{A}$ and $\mathbf{B}$ is equal, and it is also equal to that of the unpartitioned process matrix $\mathbf{P}$.

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 $\phi$ 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

$$
\begin{equation*}
\mathbf{f}=\binom{0}{1000} \tag{2.8}
\end{equation*}
$$

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:

$$
f_{i}= \begin{cases}\phi & \text { if } i=r  \tag{2.9}\\ 0 & \text { otherwise }\end{cases}
$$

Vector $\mathbf{f}$ 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 $\mathbf{f}$, we need to reserve vector elements for each of these flows. We will proceed to define

$$
\mathbf{g}=\left(\begin{array}{l}
g_{1}  \tag{2.10}\\
g_{2} \\
g_{3}
\end{array}\right)
$$

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

$$
\mathbf{q}=\left(\frac{\mathbf{f}}{\mathbf{g}}\right)=\left(\begin{array}{c}
0  \tag{2.11}\\
1000 \\
\hline g_{1} \\
g_{2} \\
g_{3}
\end{array}\right)
$$

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 $s$ and write in the example case

$$
\begin{equation*}
\mathbf{s}=\binom{s_{1}}{s_{2}} \tag{2.12}
\end{equation*}
$$

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

$$
\begin{equation*}
a_{11} \times s_{1}+a_{12} \times s_{2}=f_{1} \tag{2.13}
\end{equation*}
$$

In the concrete case, this amounts to

$$
\begin{equation*}
-2 \times s_{1}+100 \times s_{2}=0 \tag{2.14}
\end{equation*}
$$

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:

$$
\begin{equation*}
a_{21} \times s_{1}+a_{22} \times s_{2}=f_{2} \tag{2.15}
\end{equation*}
$$

or with the coefficients inserted,

$$
\begin{equation*}
10 \times s_{1}+0 \times s_{2}=1000 \tag{2.16}
\end{equation*}
$$

Simultaneous solution of these two equations yields

$$
\begin{equation*}
\mathbf{s}=\binom{s_{1}}{s_{2}}=\binom{100}{2} \tag{2.17}
\end{equation*}
$$

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

$$
\left\{\begin{array}{l}
a_{11} \times s_{1}+a_{12} \times s_{2}=f_{1}  \tag{2.18}\\
a_{21} \times s_{1}+a_{22} \times s_{2}=f_{2}
\end{array}\right.
$$

can be written as

$$
\left(\begin{array}{ll}
a_{11} & a_{12}  \tag{2.19}\\
a_{21} & a_{22}
\end{array}\right)\binom{s_{1}}{s_{2}}=\binom{f_{1}}{f_{2}}
$$

or even more concisely as

$$
\begin{equation*}
\mathbf{A s}=\mathbf{f} \tag{2.20}
\end{equation*}
$$

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 s:

$$
\begin{equation*}
\mathbf{s}=\mathbf{A}^{-1} \mathbf{f} \tag{2.21}
\end{equation*}
$$

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

$$
\mathbf{A}=\left(\begin{array}{cc}
-2 & 100  \tag{2.22}\\
10 & 0
\end{array}\right)
$$

and

$$
\mathbf{A}^{-1}=\left(\begin{array}{cc}
0 & 0.1  \tag{2.23}\\
0.01 & 0.002
\end{array}\right)
$$

Straightforward multiplication yields

$$
\mathbf{s}=\mathbf{A}^{-1} \mathbf{f}=\left(\begin{array}{cc}
0 & 0.1  \tag{2.24}\\
0.01 & 0.002
\end{array}\right)\binom{0}{1000}=\binom{100}{2}
$$

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 predetermined 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

$$
\begin{equation*}
g_{1}=b_{11} \times s_{1}+b_{12} \times s_{2} \tag{2.25}
\end{equation*}
$$

In the concrete case, this amounts to

$$
\begin{equation*}
g_{1}=1 \times s_{1}+10 \times s_{2} \tag{2.26}
\end{equation*}
$$

Inserting the values for $s_{1}$ and $s_{2}$, we find for $g_{1}$

$$
\begin{equation*}
g_{1}=1 \times 100+10 \times 2=120 \tag{2.27}
\end{equation*}
$$

More generally, we have

$$
\left\{\begin{array}{l}
g_{1}=b_{11} \times s_{1}+b_{12} \times s_{2}  \tag{2.28}\\
g_{2}=b_{21} \times s_{1}+b_{22} \times s_{2} \\
g_{3}=b_{31} \times s_{1}+b_{32} \times s_{2}
\end{array}\right.
$$

or in matrix notation

$$
\begin{equation*}
\mathbf{g}=\mathbf{B} \mathbf{s} \tag{2.29}
\end{equation*}
$$

In the example case, we have

$$
\mathbf{B}=\left(\begin{array}{cc}
1 & 10  \tag{2.30}\\
0.1 & 2 \\
0 & -50
\end{array}\right)
$$

Matrix multiplication gives

$$
\mathbf{g}=\mathbf{B} \mathbf{s}=\left(\begin{array}{cc}
1 & 10  \tag{2.31}\\
0.1 & 2 \\
0 & -50
\end{array}\right)\binom{100}{2}=\left(\begin{array}{c}
120 \\
14 \\
-100
\end{array}\right)
$$

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 $(\mathbf{g}=\mathbf{B s})$ 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:

$$
\begin{equation*}
\forall i: \sum_{j} a_{i j} s_{j}=f_{i} \tag{2.32}
\end{equation*}
$$

for the balance equation, and

$$
\begin{equation*}
\forall k: g_{k}=\sum_{j} b_{k j} s_{j} \tag{2.33}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathbf{g}=\mathbf{B A}^{-1} \mathbf{f} \tag{2.34}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathbf{g}=\left(\mathbf{B A}^{-1}\right) \mathbf{f} \tag{2.35}
\end{equation*}
$$

which we will write as

$$
\begin{equation*}
\mathrm{g}=\boldsymbol{\Lambda} \mathbf{f} \tag{2.36}
\end{equation*}
$$

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

$$
\begin{equation*}
\boldsymbol{\Lambda}=\mathbf{B A}^{-1} \tag{2.37}
\end{equation*}
$$

This notation makes clear that the matrix $\boldsymbol{\Lambda}$ 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

$$
\boldsymbol{\Lambda}=\left(\begin{array}{cc}
0.1 & 0.12  \tag{2.38}\\
0.02 & 0.014 \\
-0.5 & -0.1
\end{array}\right)
$$

This matrix can, for instance, be applied to

$$
\begin{gather*}
\mathbf{f}=\binom{0}{1000} ; \mathbf{f}=\binom{0}{1} ; \mathbf{f}=\binom{10}{0} \\
\mathbf{f}=\binom{10}{1000} ; \mathbf{f}=\binom{-10}{0} ; \text { etc. } \tag{2.39}
\end{gather*}
$$

The meaning of these different types of final demand vectors will be discussed in Section 3.9. Using the matrix $\boldsymbol{\Lambda}$ 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 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 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

$$
\begin{equation*}
\mathbf{A s}=\mathbf{f} \tag{2.40}
\end{equation*}
$$

is met.
Proof Applying a scaling vector 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,

$$
\begin{equation*}
\tilde{f}_{i}=a_{i 1} \times s_{1}+a_{i 2} \times s_{2}+\cdots \tag{2.41}
\end{equation*}
$$

As this applies for all economic flows, it follows that

$$
\begin{equation*}
\tilde{\mathbf{f}}=\mathbf{A} \mathbf{s} \tag{2.42}
\end{equation*}
$$

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

$$
\begin{equation*}
\tilde{\mathbf{f}}=\mathbf{f} \tag{2.43}
\end{equation*}
$$

or equivalently

$$
\begin{equation*}
\mathbf{f}=\mathbf{A} \mathbf{s} \tag{2.44}
\end{equation*}
$$

Q.E.D.

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

$$
\begin{equation*}
\mathbf{s}=\mathbf{A}^{-1} \mathbf{f} \tag{2.45}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathbf{A} \mathbf{s}=\mathbf{A}\left(\mathbf{A}^{-1} \mathbf{f}\right)=\left(\mathbf{A} \mathbf{A}^{-1}\right) \mathbf{f}=\mathbf{f} \tag{2.46}
\end{equation*}
$$

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 nonsingular. 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

$$
\begin{equation*}
\mathbf{g}=\mathbf{B s} \tag{2.47}
\end{equation*}
$$

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

$$
\begin{equation*}
g_{k}=b_{k 1} \times s_{1}+b_{k 2} \times s_{2}+\cdots \tag{2.48}
\end{equation*}
$$

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
as the effective neglect of temporal and spatial patterns are subjects for discussion in Chapter 9.

### 2.5 Geometric interpretation of inventory analysis*

Using the concepts of linear spaces suggests a link with Cartesian space, for which a geometric interpretation is readily available. Let us start with the economic flows. The basis for this subspace is

$$
\begin{equation*}
\binom{\text { litre of fuel }}{\mathrm{kWh} \text { of electricity }} \tag{2.49}
\end{equation*}
$$

We can easily visualise the basis in a rectangular graph in which the first basis vector is $\hat{\mathbf{p}}_{1}=\left(\begin{array}{ll}1 & 0\end{array}\right)^{\mathrm{T}}$, represents 1 litre of fuel, and is shown as a vector to the right. The second basis vector $\hat{\mathbf{p}}_{1}=\left(\begin{array}{ll}0 & 1\end{array}\right)^{\mathrm{T}}$ represents 1 kWh of electricity and is shown as an upward vector.

Then, the unit process production of electricity, $\mathbf{p}_{1}$, can be represented as a vector, starting from the origin $\left(\begin{array}{ll}0 & 0\end{array}\right)^{\mathrm{T}}$ and ending in $\left(\begin{array}{cc}-2 & 10\end{array}\right)^{\mathrm{T}}$. The unit process production of fuel, $\mathbf{p}_{2}$, also starts at the origin; it ends in $\left(\begin{array}{cc}100 & 0\end{array}\right)^{\mathrm{T}}$. The notion of a linear space implies that vectors can be added with the parallelogram rule, and that vectors may be multiplied with a scalar number. See Figure 2.1 for an illustration of the two unit processes $\mathbf{p}_{1}$ and $\mathbf{p}_{2}$ and their sumvector $\mathbf{p}_{1}+\mathbf{p}_{2}$.


Figure 2.1: Geometric interpretation of two unit processes and their sum in a two-dimensional linear space representing two economic flows.

In the example case, we had two unit processes. There was one additional item: the final demand vector $f$. It can be drawn in the graph as a vector starting from the origin and ending in $\left(\begin{array}{ll}0 & 1000\end{array}\right)^{\mathrm{T}}$. The inventory problem now consists of the question of finding the appropriate linear combination of unit process vectors, such that the resulting vector exactly coincides with the final demand vector. See Figure 2.2.


Figure 2.2: Geometric interpretation of how a linear combination of two unit processes $\mathbf{p}_{1}$ and $\mathbf{p}_{2}$ add up to the final demand vector $\mathbf{f}$.

A final step in the geometric interpretation is the addition of the environmental dimensions. However, the full example would require a graph in five dimensions. Therefore, we will restrict the illustration to only one environmental flow: kg of carbon dioxide. We extend the graph with a projected axis to represent depth. The basis of the new space is thus

$$
\left(\begin{array}{c}
\text { litre of fuel }  \tag{2.50}\\
\mathrm{kWh} \text { of electricity } \\
\mathrm{kg} \text { of carbon dioxide }
\end{array}\right)
$$

The basis vector is $\hat{\mathbf{p}}_{3}=\left(\left.\begin{array}{ll}0 & 0\end{array} \right\rvert\, 1\right)^{\mathrm{T}}$ represents 1 kg of carbon dioxide. The first unit process, production of electricity, ends in the point with co-ordinates $\left(\begin{array}{cc}-2 & 10 \mid 1\end{array}\right)^{\mathrm{T}}$, the second one in $\left(\begin{array}{cc|c}100 & 0 \mid 10\end{array}\right)^{\mathrm{T}}$. Now the system-wide aggregation. For the economic flows, this is the exogenously determined final demand vector. For the environmental flows, this
is the inventory vector, which is not yet known. We could write these together as $\left(\begin{array}{ll}0 & 1000 \mid ?\end{array}\right)^{\mathrm{T}}$, where the question mark indicates that this co-ordinate is unknown. This three-dimensional aggregated vector has thus fixed values for the co-ordinates in the first and second dimension, but can temporarily assume any value for the co-ordinate in the third dimension. This corresponds with a straight line that passes through $\left(\begin{array}{ll}0 & 1000 \mid 1\end{array}\right)^{\mathrm{T}}$, $\left(\begin{array}{ll}0 & 1000 \mid 0\end{array}\right)^{\mathrm{T}},\left(\begin{array}{ll}0 & 1000 \mid-1\end{array}\right)^{\mathrm{T}}$, etc. See Figure 2.3. Now, we can interpret the inventory problem as finding a linear combination of the unit process vectors, such that the resulting vector falls on the line that is defined by the final demand vector.


Figure 2.3: Geometric interpretation of the inventory problem as the problem of locating the point on an axis parallel to the axis that defines the environmental flow ( kg of carbon dioxide) and passing through the point that is defined by the final demand vector $\mathbf{f}$.

Recall that we have left out the environmental flows kg of sulphur dioxide and litre of crude oil for simplicity. If we add the fourth dimension, kg of sulphur dioxide, the final demand vector defines not a line in three dimensions, but a plane in four dimensions. And adding another dimension for litre of crude oil means that the final demand vector defines a three-dimensional object (a hyperplane) in five dimensions.

The final geometric interpretation of the inventory problem is thus to
find a linear combination of the unit process vectors, such that the resulting vector falls on the hyperplane that is defined by the final demand vector, and to locate the exact co-ordinates of this resulting vector.

### 2.6 An interpretation of the scaling factors*

In Section 2.2 the notion of a scaling factor was introduced, as a factor which can serve to scale a unit process up or down. The idea is that a unit process is modeled as an activity that can be described with constant technical coefficients, i.e. representing a linear technology (cf. Axiom 1). The inventory problem was formulated as a geometrical problem in a linear space: find coefficients $s_{1}, s_{2}, \ldots$, such that a linear combination of the vectors that represent the economic part of the unit processes exactly matches with the final demand vector:

$$
\begin{equation*}
s_{1} \mathbf{p}_{1}+s_{2} \mathbf{p}_{2}+\cdots=\mathbf{f} \tag{2.51}
\end{equation*}
$$

This is only a valid interpretation if the vectors that represent the economic part of the unit processes and the final demand vector are indeed to be represented in the same linear space, and that the meaning of the coordinates, is therefore the same for unit processes and final demand. The scaling factors are then pure, i.e. dimensionless, numbers. There is, however, an arbitrary element involved in the way a unit process is represented. If a unit process is given as $\mathbf{p}_{j}$, an arbitrary multiple $c \times \mathbf{p}_{j}$ could serve as an equally good representation. For instance, one can represent the unit process of electricity production per 10 kWh of electricity, per 100 kWh of electricity, per 1.23 kWh of electricity, and so on. And if this unit process in the original representation receives a scaling factor $s_{1}$, it would receive a scaling factor $s_{1} / c$ in the revised representation. There is no preferred representation, and the scaling factors have no absolute meaning.

It is, however, possible to revise the scheme a bit (Heijungs, 1998). This starts with the acknowledgement that the descriptive data of a unit process are almost never recorded per 10 kWh , per 100 kWh , per 1.23 kWh , etc. A convenient way of measuring and straightforward recording of such data is per unit of time. The inputs and outputs of a unit process can be measured during an hour, a day, or a year. The descriptive data of a unit process then assume a form like $3.15 \times 10^{10} \mathrm{kWh} /$ year or $10 \mathrm{kWh} /$ second. Then the step of rescaling the data of a unit process to a convenient size, such as 10 kWh , is no longer needed. The final demand vector, however, remains unaffected by such a redefinition of the basis of the linear space
that defines the co-ordinates of the unit processes. It may still be 1000 kWh of electricity. This then leads to a readjustment of the meaning of the scaling factors. In the previous representation, a scaling factor of 100 meant that the arbitrarily rescaled unit process needed to be multiplied with an equally meaningless factor of 100 . In the revised representation, the scaling factor bears a dimension: it is 100 second. Moreover, it can be interpreted as that the reference flow defined in the final demand vector requires that the unit process of electricity production is involved for 100 seconds. The electricity generator is thus allocated, so to speak, for 100 seconds to the function investigated.

The advantage of the new representation is three-fold:

- the step of scaling all unit process data to some convenient round number of output is not needed;
- the scaling factors receive a clear meaning;
- the process data can be entered in their actual extent, which may be convenient for the construction of databases that serve more purposes than LCA alone.

A disadvantage is that the basis that defines the co-ordinate system is not any longer universally applicable to both unit processes and final demand vector. This then also implies that the geometrical interpretation of Section 2.5 does not apply for this setup.

### 2.7 An interpretation of the intensity matrix*

In Section 2.2 we have introduced the matrix $\boldsymbol{\Lambda}$ as

$$
\begin{equation*}
\boldsymbol{\Lambda}=\mathbf{B A}^{-1} \tag{2.52}
\end{equation*}
$$

and given it the name intensity matrix. Some comments are in order: what does the matrix mean, and whence the name intensity matrix?

Let us first study the case of a technology matrix that consists of one number only. Let

$$
\begin{equation*}
\mathbf{A}=(10) \tag{2.53}
\end{equation*}
$$

denote that the system contains one process which produces 10 kWh of electricity. Let us assume that the intervention matrix is

$$
\mathbf{B}=\left(\begin{array}{c}
1  \tag{2.54}\\
0.1 \\
0
\end{array}\right)
$$

which keeps to mean emission of 1 kg of carbon dioxide and of 0.1 kg of sulphur dioxide, and no in- or outflow of crude oil. Then

$$
\boldsymbol{\Lambda}=\left(\begin{array}{c}
1  \tag{2.55}\\
0.1 \\
0
\end{array}\right)(10)^{-1}=\left(\begin{array}{c}
0.1 \\
0.01 \\
0
\end{array}\right)
$$

Applying this to a (degenerate) final demand vector

$$
\begin{equation*}
\mathbf{f}=(1) \tag{2.56}
\end{equation*}
$$

representing 1 kWh of electricity, we find

$$
\mathbf{g}=\left(\begin{array}{c}
0.1  \tag{2.57}\\
0.01 \\
0
\end{array}\right)
$$

We thus see that the meaning of the coefficient 0.1 for $\boldsymbol{\Lambda}_{11}$ is that it represents the carbon dioxide intensity of electricity (in kg per kWh ). Similarly, the coefficient 0.01 for $\boldsymbol{\Lambda}_{21}$ represents the sulphur dioxide intensity of electricity.

This suggest to assign to $\boldsymbol{\Lambda}$ the interpretation of a matrix of environmental intensity coefficients per unit of economic flow. However, this is too rapid a conclusion. Let us expand the technology matrix to the case of two processes and two flows:

$$
\mathbf{A}=\left(\begin{array}{cc}
-2 & 100  \tag{2.58}\\
10 & 0
\end{array}\right)
$$

Retrieving the intervention matrix

$$
\mathbf{B}=\left(\begin{array}{cc}
1 & 10  \tag{2.59}\\
0.1 & 2 \\
0 & -50
\end{array}\right)
$$

one finds

$$
\boldsymbol{\Lambda}=\left(\begin{array}{cc}
1 & 10  \tag{2.60}\\
0.1 & 2 \\
0 & -50
\end{array}\right)\left(\begin{array}{cc}
-2 & 100 \\
10 & 0
\end{array}\right)^{-1}=\left(\begin{array}{cc}
0.1 & 0.12 \\
0.02 & 0.014 \\
-0.5 & -0.1
\end{array}\right)
$$

When applied to a final demand vector

$$
\begin{equation*}
\mathbf{f}=\binom{0}{1} \tag{2.61}
\end{equation*}
$$

again representing 1 kWh of electricity, we find

$$
\mathbf{g}=\left(\begin{array}{c}
0.12  \tag{2.62}\\
0.014 \\
-0.1
\end{array}\right)
$$

This is different from the $\mathbf{g}$ obtained for the case of one process and one flow, in spite of the fact that the specification of the process of electricity production is almost similar. The difference can be interpreted as an increase of environmental interventions: 0.02 kg extra emission of carbon dioxide, 0.004 kg extra emission of sulphur dioxide, and 0.1 litre extra extraction of crude oil (mind the removal of the minus sign for crude oil). The only difference in process specification is that the process of electricity production is assumed to consume fuel: 0.2 litre per 1 kWh electricity. We may also observe that the final demand vector that represents 1 litre of fuel,

$$
\begin{equation*}
\mathbf{f}=\binom{1}{0} \tag{2.63}
\end{equation*}
$$

yields

$$
\mathbf{g}=\left(\begin{array}{c}
0.1  \tag{2.64}\\
0.02 \\
-0.5
\end{array}\right)
$$

as inventory vector. Rescaled with a factor of 0.2 , we find 0.02 kg of carbon dioxide, 0.004 kg of sulphur dioxide, and -0.1 litre of crude oil, which exactly accounts for the extra interventions of the delivery 1 kWh electricity. Thus, we arrive at an interpretation that the vector

$$
\boldsymbol{\Lambda}_{2}=\left(\begin{array}{c}
0.12  \tag{2.65}\\
0.014 \\
-0.1
\end{array}\right)
$$

represents the system-wide (or cradle-to-grave) interventions of supplying 1 kWh of electricity, i.e. one unit of economic flow number 2. Similarly,

$$
\boldsymbol{\Lambda}_{1}=\left(\begin{array}{c}
0.1  \tag{2.66}\\
0.002 \\
-0.5
\end{array}\right)
$$

represents the system-wide (or cradle-to-grave) interventions of supplying 1 litre of fuel, i.e. one unit of economic flow number 1.

Hence, one may interpret a column of the intensity matrix as the systemwide interventions for supplying one unit of the good or service that is referred to by that column. Altogether, it seems reasonable to assign to $\boldsymbol{\Lambda}$ the interpretation of a matrix of system-wide environmental intensity coefficients per unit of economic flow. We refer to Section 3.8.2 for a longer discussion.

