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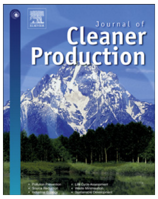

Enhancing sustainable production by the combined use of material flow analysis and mathematical programming

Hendrik Lambrecht*, Nikolaus Thißen

Institute for Industrial Ecology (INEC), Pforzheim University, Pforzheim, Germany

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ABSTRACT

Material and energy flow analysis (MEFA) is used by many companies for sustainability assessments of their production systems. MEFA generally leads to large and complex system models for which optimal operating conditions are hard to find manually. This article therefore presents an extension of MEFA towards mathematical programming that provides powerful methods for system optimization. A theoretic concept for this methodological integration is developed, illustrated by means of a simplified example and finally applied to a case study of an industrial waste treatment scenario. Technical feasibility is thus demonstrated. Moreover, the algebraic transformation of material flow models into mathematical programs reveals, on a conceptual level, the basic principles of an optimization-oriented MEFA.

1. Introduction

It is the credo of Industrial Ecology that concerns of the environment and sustainability should be tackled by regulating the material flows of society (Graedel and Allenby, 2010: 87). In particular, industrial production is deemed to play a key role in at least two senses: (i) industry is the portion of society that produces most goods and services and therefore controls an important part of all material flows within the technosphere. (ii) Firms possess the technological expertise needed for an environmentally benign design of products and processes (Lifset and Graedel, 2002: 3).

The most important method used by industrial ecologists is material and energy flow analysis (MEFA),[1] where material flows and stocks within a given system are systematically assessed (Brunner and Rechberger, 2004: 3). MEFA is a versatile method that can be the starting-point to analyze industrial production from all perspectives of sustainability. It is particularly suited for the environmental and economic dimensions, which can be treated in a methodologically consistent framework: material and energy flows at the boundaries of a company can be assigned economic and ecologic "costs" (Section 3.2). In the context of this article sustainability optimization thus consists in modifying the design or operational state of a production system so as to reduce these costs.

1.1. *Material flow networks as a specific method for MEFA*

The representation of material and energy flow models varies from flow chart diagrams and frequently used spreadsheet models to mathematical equations. A specific method are material flow networks (MFN) (Möller, 1994). At first, MFN have mainly been used for inventory analyses in Life Cycle Assessment (LCA) (Schmidt and Schorb, 1995). Their flexible approach to mapping industrial supply chains, as well as the fact that they have been implemented in the commercial material flow analysis software Umberto® (Schmidt and Häuslein, 1997), have led to their use by many companies, consultants and research institutes. MFN proved to be particularly useful for analyzing complex industrial production systems in the chemical industry (Bode et al., 2012; Thiβen, 2010; Viere et al., 2010).

MFN can be employed in a purely descriptive way to visualize material flows and metabolic rates within production systems thus

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* Corresponding author. Tiefenbronner Str. 65, D-75175 Pforzheim, Germany. Tel.: +49 7231286424; fax: +49 7231287424.
E-mail address: hendrik.lambrecht@hs-pforzheim.de (H. Lambrecht).

[1] List of abbreviations used in this article: Global Warming Potential (GWP), Life Cycle Assessment (LCA), Life Cycle Inventory (LCI), Life Cycle Inventory Analysis (LCIA), Linear Program (LP), Material and Energy Flow Analysis (MEFA), Material Flow Based Optimization [Problem] (MFBO),Material Flow Network (MFN), Mixed Integer Linear Program (MILP), Mixed Integer Non-Linear Program (MINLP), Mathematical Program (MP), Non-Linear Program (NLP), Non-Methane Volatile Organic Compounds (NMVOC), Process Flow Diagram (PFD), Rotor Concentrator (RC), Return On Investment (ROI), Thermal Oxidation (TO).

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revealing improvement potentials from a systemic perspective. But it is also possible to build detailed explanatory models that can be used for scenario analyses or to investigate the impact of individual improvement measures. In this context Bode et al. (2012: 1513) point out that MEFA with MFN.

- "is an excellent basis for communication in interdisciplinary teams,
- can be used at virtually any level of detail […],
- supports an understanding of complex systems […],
- has the potential in process engineering to reduce the time it takes to find the best solution"

Another important argument for using MFN in the context of sustainable production is the availability of interfaces to environmental impact assessment methods from LCA as well as cost accounting methods that support the evaluation of both environmental and economic performance.

1.2. Complexity and system optimization

MEFA of production systems typically results in large and complex models (e.g. Viere et al., 2010), where it becomes difficult to identify optimal states manually. An extension of MEFA by methods for automatic model optimization has therefore been proposed (Bode et al., 2012: 1513). A first step in this direction is material flow based optimization (Lambrecht and Schmidt, 2010). It involves (i) completing the MFN to a material flow based optimization problem (MFBO) and (ii) solving the MFBO using direct search heuristics in a simulation-based optimization framework. A major drawback of this approach is that the MFN enters the optimization process as a black box only used for evaluating the objective function. Additional information on its mathematical structure that could help optimization algorithms to find better solutions with less computing time is not available.

In this work, an alternative approach to *solving* a MFBO is elaborated. Instead of embedding the unmodified MFN in a simulation-based optimization approach, the entire MFBO is transformed into a mathematical program (MP). As MPs are typically formulated with algebraic languages, this approach is called *algebraic transformation*. As a direct consequence the mathematical structure of a MFN is disclosed thus rendering the application of powerful and efficient state-of-the-art solvers of mathematical programming possible. A more subtle but important side-effect is that this approach reveals important aspects of how MEFA should be carried out in the context of system optimization.

2. Approaches to sustainability optimization of production systems

This chapter describes the methodological basis for the *algebraic transformation*: mathematical programming (2.1), material flow networks (2.2) and material flow based optimization (2.3).

2.1. System optimization with mathematical programming

The ultimate goal of optimization in Operations Research is helping decision makers to find the best solution to complex planning problems. In many applications such problems can be formulated as a *parameter optimization problem*:

$$\min f(x) \quad \text{subject to. } x \in F \tag{1}$$

where a vector of parameters x is sought that minimizes a given performance measure f. In the language of Operations Research f and x are respectively called *objective function* and *decision variables*. In constrained optimization only decision vectors lying within the *feasible region F* are valid solutions to problem (1).

The most important paradigm for the formulation and solution of parameter optimization problems in Operations Research is *mathematical programming* (MP), where the feasible region is defined by a set of inequality and equality constraints:

$$x \in F \Leftrightarrow \begin{cases} g_i(x) \le 0, i = 1 \ldots n \\ h_j(x) = 0, j = 1 \ldots m \end{cases} \tag{2}$$

where g_i and h_j are analytic mathematical functions. Mathematical programs can be formulated and solved with so-called *algebraic modeling languages* (Fragnière and Gondzio, 2002). Modern algebraic modeling environments such as GAMS, AMPL or LINGO[2] provide interfaces to numerous powerful solvers that solve problems with thousands of decision variables and restrictions, even if they have unfavorable properties such as nonlinear, discontinuous or nonconvex functions (Bussieck and Vigerske, 2010; Mittelmann, 2013).

Since its early beginnings mathematical programming has been applied to optimize large and complex production systems such as refineries. Recent examples from the chemical industry primarily concern economic objectives (Grossman, 2005; Kallrath, 2002). But there is no reason, why it should not be applied to other objectives in the context of sustainable production as well. The main obstacle using MP in process improvement is that the algebraic representation of planning problems is only comprehensible to optimization experts, while other stakeholders in the companies like process engineers or managers often require quite different problem representations (Jones, 1996).

2.2. Material flow networks

In contrast, MFN offer a graphical and intuitive approach to analyzing and mapping production systems. Modeling with MFNs involves different levels that are briefly reviewed here. Fig. 1 shows the MFN of a fictive and strongly simplified production plant that will be used throughout this and the following chapters 3 and 4 to illustrate methods and theory.

First, the system structure is represented as a graph with two different node types: (i) T*ransitions* (rectangular nodes) represent single production units where materials are processed or transformed into other materials; (ii) *Places* (circular nodes) basically connect processes. Places may represent material stocks, e.g. a warehouse or a store. In most cases they merely connect processes and represent branching-points of material flows within the modeled system. They are also used to assess the material balance at the system boundary (P1–P5 and P9–P13 in Fig. 1). For formal reasons, transitions and places strictly alternate within the network. They are linked by *arrows* that correspond to the material flows. Measured data can be entered directly in this graphical model which, in this case, is purely *descriptive*.

On a second level, functional relationships between process inputs (x) and outputs (y) may be specified for the transitions. Details are given in Section 3.1 where the algebraic transformation of the resulting process submodels is discussed. By explicitly modeling how materials and energy are transformed in single process units, the material flow model actually becomes an *explanatory model*, where unknown *dependent* model variables can be calculated based on given *explanatory* variables. An explanatory model not only offers the possibility two replace costly

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[2] cf. www.gams.com, www.ampl.com and www.lindo.com.