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Screening LCA for Large Numbers of Products:

Estimation Tools to Fill Data Gaps

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Abstract

CIBA's Textile Dyes and Chemicals divisions use screening LCAs for their 1700 sales products to improve portfolio management and ecological process development. Material flow, energy, and waste data for in-house manufacturing processes are extracted from our company databases into our LCA system ECOSYS. For meaningful comparisons of whole life cycles, we must include LCA estimates for over 4000 raw materials from other suppliers. Even crude estimates are preferable to the frequently practiced omission of unknown process steps since they allow worst-case or sensitivity analyses. Sources for mass flows are (decreasing order of reliability): process literature (SRI-PEP Yearbook, Ullmann, Kirk-Othmer, patents), yields of analogous processes, theoretical stoichiometry. Energy demands come from literature, or from a set of standard operation estimates developed by our process engineers. Wastes/emissions, if not published, are derived from yields and elemental balances, estimated emissions of energy carriers (BUWAL-132), and typical end-of-pipe measures in CIBA. These data sets are kept as "added-burden modules" (ABM) in our system, each with a set of "inherent burdens", which are transformed to step-specific burden estimates by a "propagation" program, before the overall burdens of the whole process tree are cumulated. This program checks every process for actually measured burdens, before applying the attached ABM estimates to fill the gaps. Centralization of estimates as ABM with inherent burdens facilitates maintenance and adaptation. At present, well over 250 important intermediates were estimated and used in our product trees; many more follow rapidly.

This article is an example of how industry is using LCA to address environmental issues.

Keywords: Life cycle assessment; screening LCA; estimation procedures; computer-aided estimates; chemical processes; standard operations; process yields; chemical intermediates; chemical data sources

1 Introduction

During the last decade, life cycle assessment (LCA) has gained widespread acceptance as a tool [1] for the ecological process improvement. Presently, many LCA studies compare a narrow range of similar products or services that fulfill identical purposes. LCAs in the specialty chemical manufacturing industry must be more complex since they cover a large number of chemicals from a variety of substance classes, produced for a wide range of purposes in multi-step syntheses [2]. Comprehensive LCAs have not been performed for such complex environments thus far, although considerable work has been done on a number of chemicals (e.g. surfactants [3, 4]), and LCAs were considered part of a general environmental management system in a consumer goods company with a similarly complex product range [5].

In 1990, CIBA's Textile Dyes and Chemicals divisions started a program to perform at least screening LCAs on the whole range of their products (textile dyestuffs, auxiliaries and textile finishing agents; fluorescent whitening agents; paper dyes, coating and pulping agents; leather dyes and tanning agents; cosmetic ingredients). The results will not only be used for process optimization and communication with customers and authorities; beyond that, LCA shall serve as a tool for ecologically sound product development and strategic portfolio decisions, with the target of sustainable growth [6].

This ambitious task will cover over 1700 sales products manufactured in 17 production plants in Switzerland and eight other countries. Swiss operations alone comprise some 1600 production processes, with about 300 identifiable solid/special wastes and 2100 analyzed waste-water types.

It is not realistic to collect and manually enter all our pertinent raw data into one of the many commercial LCA software tools (summaries in [7–10]) since these are usually designed for stand-alone operation, i.e. not geared to the systematic, computer-aided extraction of environmental information already available in a variety of company-internal and external databases. Such automated data transfer is the only promising way to cope with the huge body of necessary data [11]; it requires a specially designed software.

Our syntheses start with 4700 raw materials or intermediates from other suppliers. Their manufacturing is not directly surveyable for us, and very few published LCA data exist [10]. Even for screening LCAs, we cannot restrict the scope to our in-house syntheses, but have to perform cradle-to-grave investigations [1]. Therefore, appropriate estimation procedures have to be developed to render at least "order-of-magnitude" figures and to fill the gaps in the complex product trees.

2 Data Acquisition from Company-Internal Data Systems

The part of the product-life cycle performed in our own company is the only sector that we can influence directly to achieve ecological product improvement. Data for this part are directly accessible in company databases: Chemical composition and material safety/ecotox data are maintained in our material safety data sheet system (MSDS). Mass flows and energy requirements are tracked in our standard calculation (STK) computerized database. Every waste is registered in a waste management database, with disposal route and analytical data. Site-specific waste water data are recorded in our waste water treatment plants (2000 sets in Basel, many more world-wide). Air emission data are kept decentrally by our power plants, incinerators, and catalytic waste air purifications.

None of these company databases was specifically designed for life cycle assessment; the data are kept up-to-date for other important (economical or legal) purposes. Our LCA system ECOSYS is a secondary user: Individual extraction routines collect LCA-specific data from a multitude of databases (also commercial LCA systems) in form of ASCII files for easy exchange; a single battery of loading processes integrate the data into ECOSYS, ensuring system integrity by a set of cross-checking and unit conversion processes. The logical structure of this data acquisition process is shown in **Figure 1**, together with the routes for manual data entry. The result is a set of process modules with information on input and output flows, energy requirements, emissions, and wastes. At present, more than 1600 chemical processes are documented, together with some 2300 waste and waste water information linked to them. The calculation program in ECOSYS connects them to product trees, and calculates the ecological burdens (extractions from natural resources, ad emissions to nature).

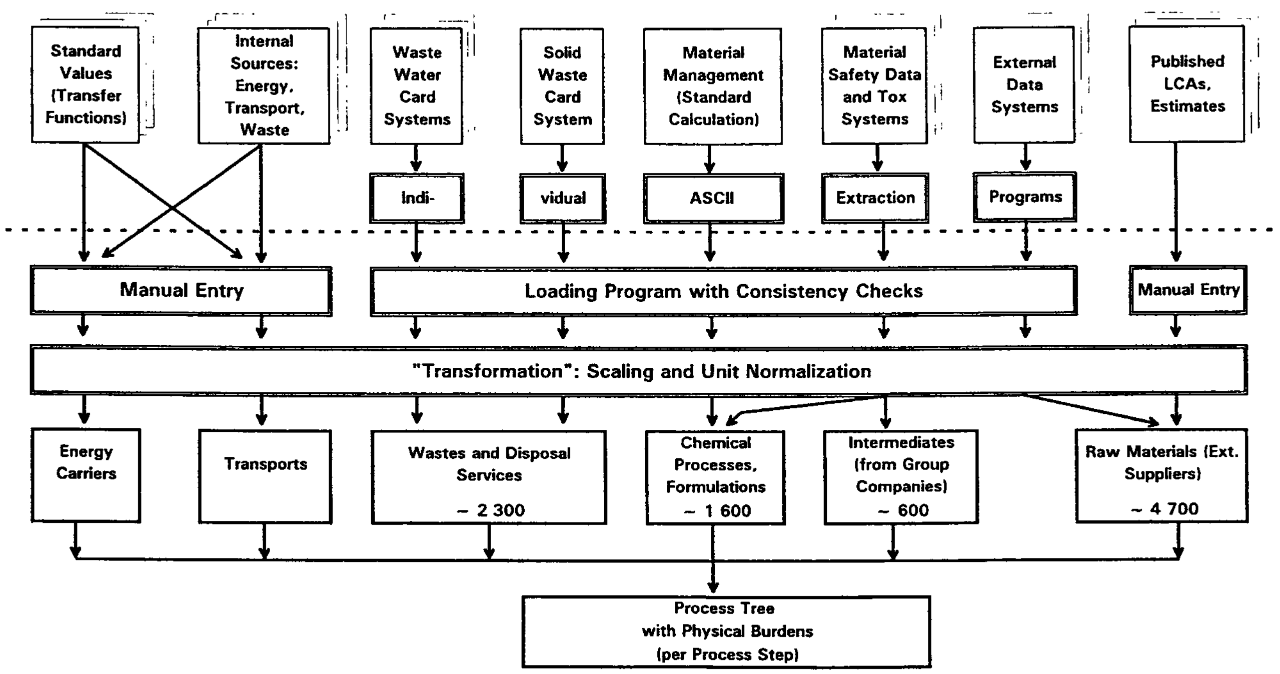

Fig. 1: LCA at CIBA: ECOSYS Data Acquisition.
Logical structure of data acquisition: From company-external and internal sources to ECOSYS modules in the process tree

3 Product Trees and Cradle-to-Grave Analysis

A simplified example of a product tree is shown in **Figure 2**. The product is made from two major intermediates (using auxiliary chemicals, solvents, etc.); process energy is partially generated in-house (steam and some electricity). Some waste treatment operations are directly performed by CIBA (water treatment, incineration), others by third parties. The two main intermediates are also synthesized by our company, but the process tree will eventually lead to third-party raw materials or intermediates. These are practically never directly extracted from the earth, so the cradle-to-grave product tree extends to the operations of third-party suppliers and a whole chain of raw materials processors, usually starting at crude oil extraction or other mining operations. As pointed out by BOUSTEAD [12], this outer part is not a simple, ramified tree, but a complex network, often with circular references.