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Life-Cycle Assessment of Chemical Production Processes: A Tool for Ecological Optimization

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Abstract. Life-cycle assessment (LCA) has gained in recent years widespread acceptance as an environmental management tool to assess and valuate the environmental impacts (resource consumption and emissions to nature) of products and processes, covering the whole life cycle from cradle (extraction of raw material) to grave (final disposal). Applied to chemical manufacturing, LCA allows to compare the ecological performance of synthesis processes, guide process developers to weak points and improvement options, and avoid suboptimizations. In our Consumer Care Chemicals Division, we apply LCA routinely to sales products as well as manufacturing-process chains, and we developed a specialized LCA computer system ECOSYS for that purpose. Material flow, energy, and waste data for all in-house manufacturing processes are extracted from our company data bases into ECOSYS. For meaningful comparisons of whole life cycles, we must include LCA results for the raw materials bought from other suppliers, and since such data are rarely available, appropriate estimation procedures were developed. The multitude of ecological burdens calculated over the life cycle can be judged and compared by a variety of valuation schemes, *e.g.* according to the Swiss BUWAL or the modern Eco-indicator 95 method. ECOSYS is not restricted to existing, operational processes, but allows the process developer to test his hypothetical designs (*e.g.* derived from a simulation tool) at a very early stage. If process alternatives use different raw materials, a narrow judgement on data for the process step alone may lead to suboptimization, whereas LCA results that consider all preceding syntheses of intermediates allow a more objective comparison. As an example, two synthesis paths for DNS (4,4'-dinitro-2,2'-stilbenedisulfonic acid disodium salt) were compared: The older, established route uses NaOCl in aqueous media as an oxidant, whereas the method more recently introduced in one of our production plants is based on air oxidation in liquid ammonia. The latter produces considerably less waste and is favorable with respect to many ecological parameters, including energy consumption, over the whole life cycle.

1. Introduction: What is LCA?

Life-cycle assessment (LCA) is an environmental management tool that examines the ecological consequences of making and using products or providing services [1], covering the whole life cycle from cradle to grave (*Fig. 1*). The process is structured and has several phases (*Fig. 2*, *cf.* [2]). The first step, goal and scope definition, defines the questions to be answered and sets the boundaries of the investigation; the cutoff rules applied here are often decisive for the outcome and the comparability of the study. The subsequent phase, life-cycle inventory analysis (LCI), quantifies the consumption of resources (including energy carriers), the wastes generated, and the emissions to the environment associated with the whole life cycle of a product or process, from the extraction of the raw materials (cradle) to the final disposal (grave). This part is the best-understood section of LCA, well documented [3][4], and presently standardized by ISO [5]. In many ways, LCI resembles a classical product cost calculation; in place of the manufacturing costs (in various currencies), environmental interventions (the various extractions and emissions) are cumulated over the whole life cycle.

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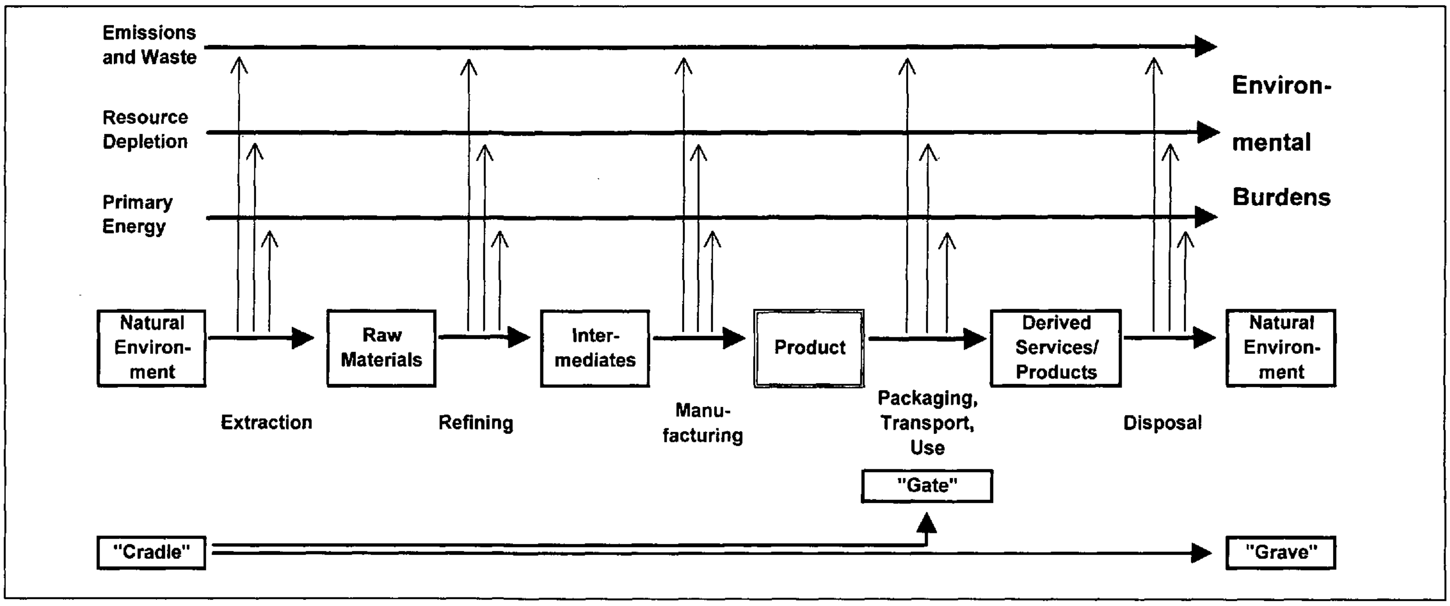

Fig. 1. *Life-cycle assessments/envorinmental burdens of a product*

Unfortunately, unlike cost calculation, LCA cannot (yet) rely on internationally accepted exchange rates for the various 'currencies' (emissions and impacts). The third phase, impact assessment (LCIA) attempts to cope with this problem, trying to answer questions, such as 'how many kg of CO_2 (greenhouse gas) are equivalent to 1 g of FCKW (stratospheric ozone depleting agent)?', and reducing the multitude of extractions and emissions to a small set of ecological key figures, possibly even a single indicator. Several older methods based their comparisons on legal immission limits [6][7] or national emission target values [8]. More modern approaches [9][10] group the various interventions into environmental impact classes (biotic/abiotic resource depletion, global warming, ozone depletion, acidification, nutrification, photooxidant formation, *etc.*), then characterize their weight *inside* their class, and finally valuate the relative importance of the various impact classes themselves. Classification and characterization are derived from scientific results (*e.g.* atmosphere physics), whereas the valuation is based on societal value/priority systems, political target values (considering the 'distance to target' of the actual environmental situation), and sometimes even monetary considerations [11]. The various impact assessment strategies may all have their individual merits, and standardization has not been achieved, though ISO adopted the matter [12].

The final step, interpretation (formerly called improvement assessment [1]) draws the conclusions (not only from the valuation results, but also directly from important individual findings in the inventory) according to the goal and scope of the study and derives recommendations to decision. The decisions themselves and the subsequent actions lie outside the scope of the LCA, since they must include performance, economic, and social aspects.

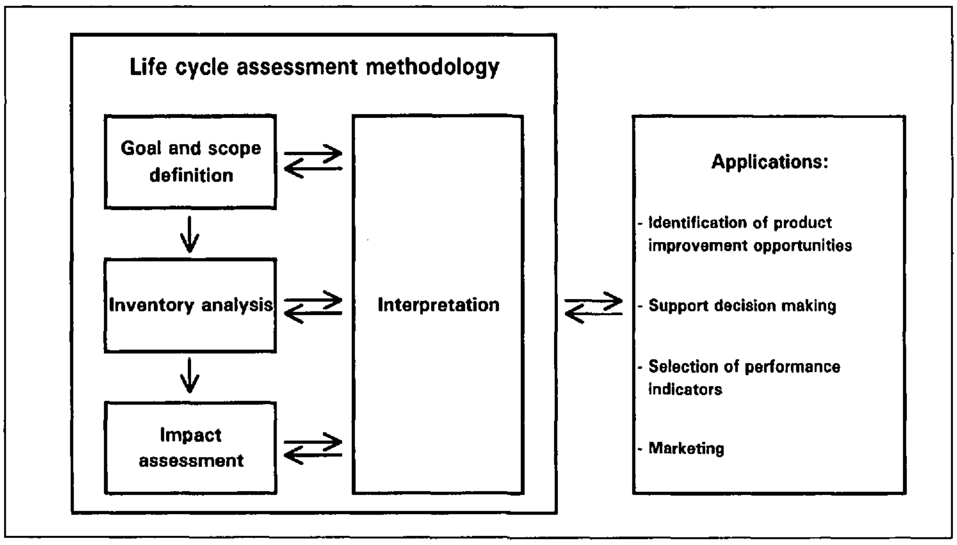

Fig. 2. *ISO Draft International Standard 14040, phases of an LCA*

2. LCA of Chemical Production Processes

In recent years, life-cycle inventories were compiled for a wide range of chemicals, such as commodity thermoplastics and their monomers [13], or detergent ingredients [14] and their precursors [15]. Mostly, these studies were focused on a rather narrow class of chemicals, and they responded to some public concern about their ecological impact.

In 1990, *Ciba Specialty Chemicals* embarked on an ambitious program to perform LCAs on the whole range of products manufactured by the Textile Dyes Division and the Consumer Care Chemicals Division (textile finishing agents; fluorescent whitening agents; paper dyes, coating and pulping agents; cosmetics ingredients). This project was not triggered by any external pressure, but resulted from our corporate 'Vision 2000' to strike a fair balance between our economic, social, and environmental responsibilities. Its results will be used for the traditional, 'internal' applications (process optimization) and the well-known 'external' purposes, such as communication with our customers, support for eco-labelling, and dialogue with authorities. Beyond that, LCA shall serve as a tool for the ecologically sound development of new products and

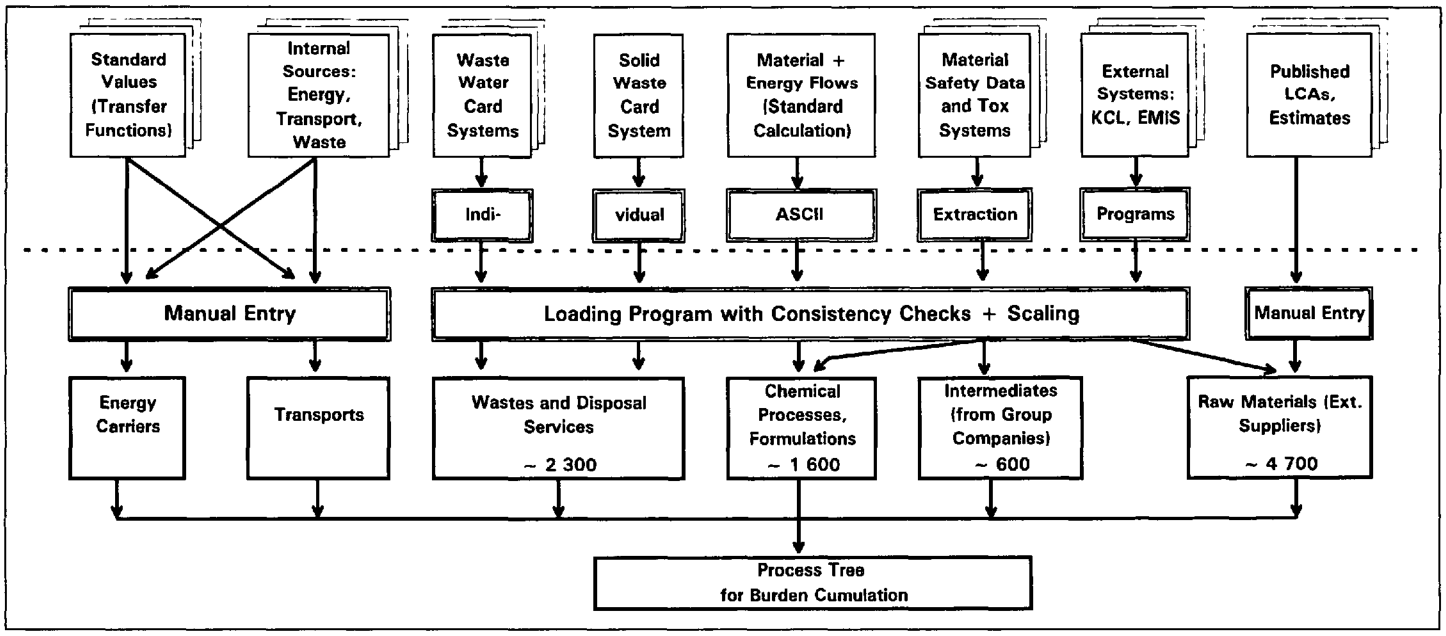

Fig.3. *LCA at* Ciba Specialty Chemicals, *ECOSYS data acquisition from international and external data sources* (data bases)

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finally give our management the necessary ecological information for strategic portfolio decisions, with the target of sustainable growth [16].

The details of this systematic LCA project were given in [17][18]. It covers over 1 700 sales products manufactured in some 1600 production or formulation processes, with some 300 identifiable solid/special wastes and 2100 distinguishable (analyzed) wastewater types. In-house syntheses start with 4700 raw materials/ intermediates from other suppliers. Since most manufacturers of such chemicals do not publish (and rarely perform) LCAs, estimation methods were developed for frequently used intermediates [18] to close data gaps and cover the whole process tree, cradle to grave. It is quite obvious that the omission of the raw-material contributions to the LCA distorts the results, favoring single-step syntheses from advanced intermediates and unjustifiably 'punishing' backward-integrated multistep manufacturing sequences [19].

LCA calculations of the required complexity can neither be done manually, nor is a manual collection and entry of all the pertinent raw data conceivable. Rather, we have to draw on the multitude of data systems maintained in our company for purposes other than LCA, such as the standard calculation system STK (material and energy flows of our manufacturiung processes), solid waste and wastewater data bases, and material safety-data sheet collections; automatized data transfer is the only promising way to cope with the huge body of data necessary [17]. Commercial LCA software packages are normally not geared to such systematic, computer-aided extraction of environmental information already available in company-internal data systems and also in external data bases such as EMIS [20] (containing the data of [21] and [22]) or KCL ECODATA [23]. Therefore, we developed our own, specialized LCA software tool ECOSYS [17][18] and the necessary interfaces to ensure the free flow of information from our company data bases (*Fig. 3*). Data are kept in process modules which are linked to form process trees of any degree of complexity. A calculation routine follows these trees, cumulating the environmental burdens of all involved steps over the whole life cycle, another routine performs impact assessments according to any desired method [6–10]. Other programs analyze the trees and show the total use of any commodity (electricity, fuel oil, common solvents, *etc.*) over the full cycle, or the major contributors of any requested burden ('which processes contribute 90% of the total SO_2 liberated in the whole life cycle?'), thus pointing out improvement options.

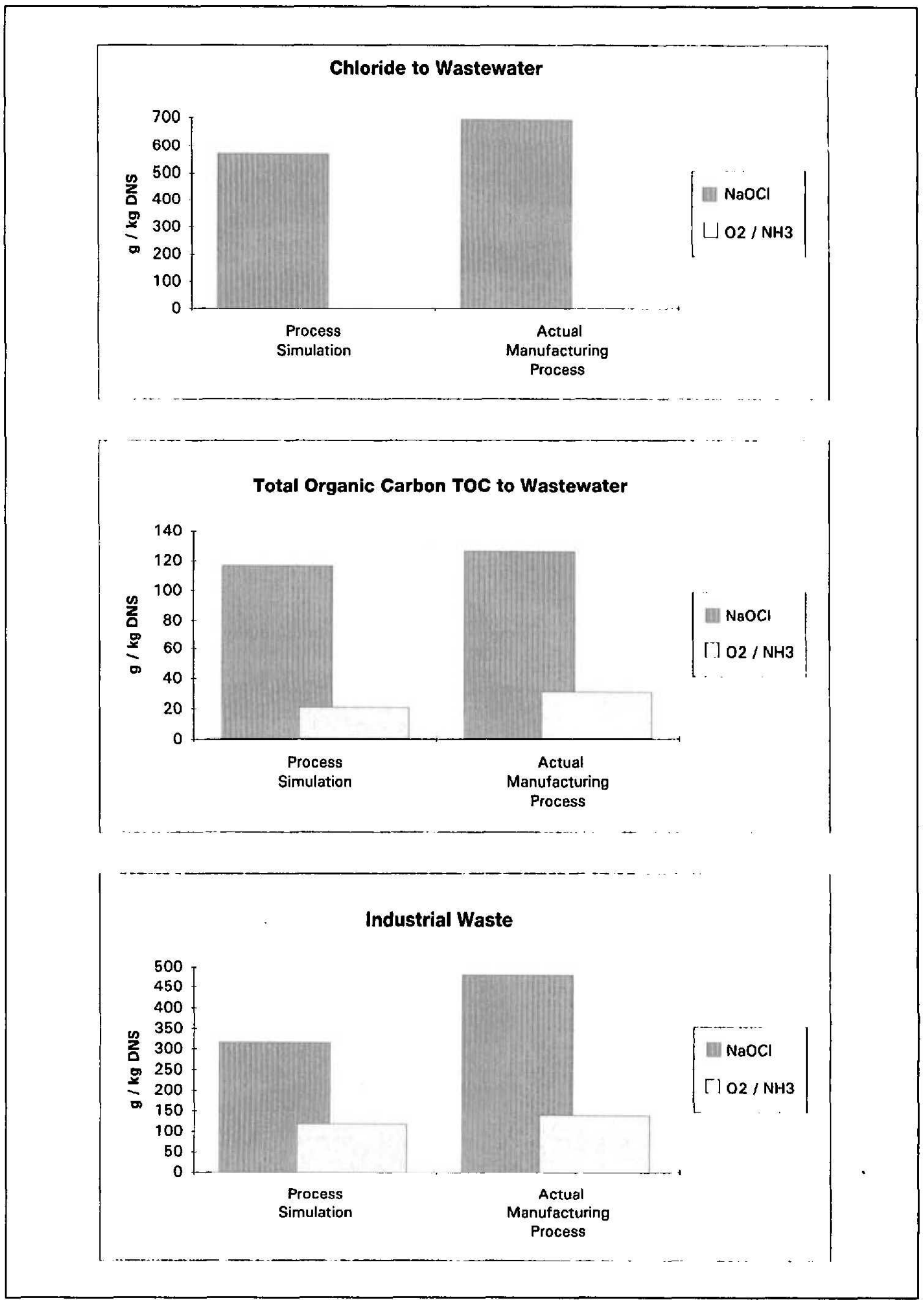

Fig. 4. *DNS synthesis process alternatives, judged by individual emissions, before and after implementation*

3. Ecological Process Optimization with ECOSYS

ECOSYS is equally efficient to calculate LCAs for established manufacturing processes (documented in our STK) and to provide life-cycle estimates for new processes under development, even before production has started. An example is the manufacturing of DNS (4,4'-dinitro-2,2'-stilbenedisulfonic acid disodium salt), which serves as an intermediate for several of our sales products, mostly optical brighteners. The traditional method synthesizes one molecule of DNS from two units of *para*-nitrotoluenesulfonic acid (PNTS) by oxidation with sodium hypochlorite (NaOCl) in aqueous solution. For a new production site, we investigated a more modern, technically sophisticated route using air oxidation of PNTS in liquid ammonia (O_2/NH_3). Judged on process mass flow data alone, the new method promised a considerable waste reduction [24]; however, since different raw materials were required, a life-cycle approach was chosen to determine whether the overall balance would also be favorable for the modern synthesis.

Since the process was not yet operational, a simulation tool (ASPEN®) was

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used to estimate mass flow data and energy requirements. These figures (which are routinely derived for process development in any case) were entered into ECOSYS as a chain of hypothetical process steps and compared with older process simulation data for the traditional synthesis. Since DNS is used as an intermediate for further syntheses and not released into the environment, a reduced 'cradle-to-gate' LCA (*Fig. 1*) was sufficient for our purpose.

Fig. 4 (left-hand side) shows how some critical emissions can be improved by the choice of the new process: Chloride in the effluent is reduced to negligible amounts (since no hypochlorite is used), and the higher specificity and yield of the new process eliminates 80% of the total organic carbon discharge to wastewater and 60% of the solid waste. Better yields also lead to a lower demand for the precursor PNTS, and consequently, most other emissions are reduced and less resources used. The overall energy consumption is reduced by 14%. Of course, the whole new process chain has to be considered, especially the synthesis of the solvent NH_3, but also the avoided burdens from NaOCl electrolysis. The overall balance (*Fig. 5*) shows that the new process is ecologically more favorable, judged by the Swiss BUWAL method [8] (–50% of the impact) as well as by the Eco-indicator valuation [10] (–35%).

When the O_2/NH_3 synthesis route became operational in the new plant, realistic (standard calculation) data could be gathered, reflecting the scaleup from process simulation to manufacturing practice (*Figs. 4* and *5*, right-hand side). Our process simulation tended to underestimate some burdens, so the absolute values of all indicators are higher for the real-life processes. However, the trend in favor of the modern process is even more clear, although it leads to somewhat higher methane, ammonia, and N_2O emissions. The reduction in most other parameters is so pronounced that the BUWAL points are lowered by 65% and the Eco-indicator by 54%.

These findings indicate that our LCA system can serve as a useful complement to more traditional process-modelling software systems, and that it allows a meaningful ecological judgement at a rather early stage of process development, taking into consideration the influences of changing raw materials and yields as well as the ecological impacts of the new process itself.

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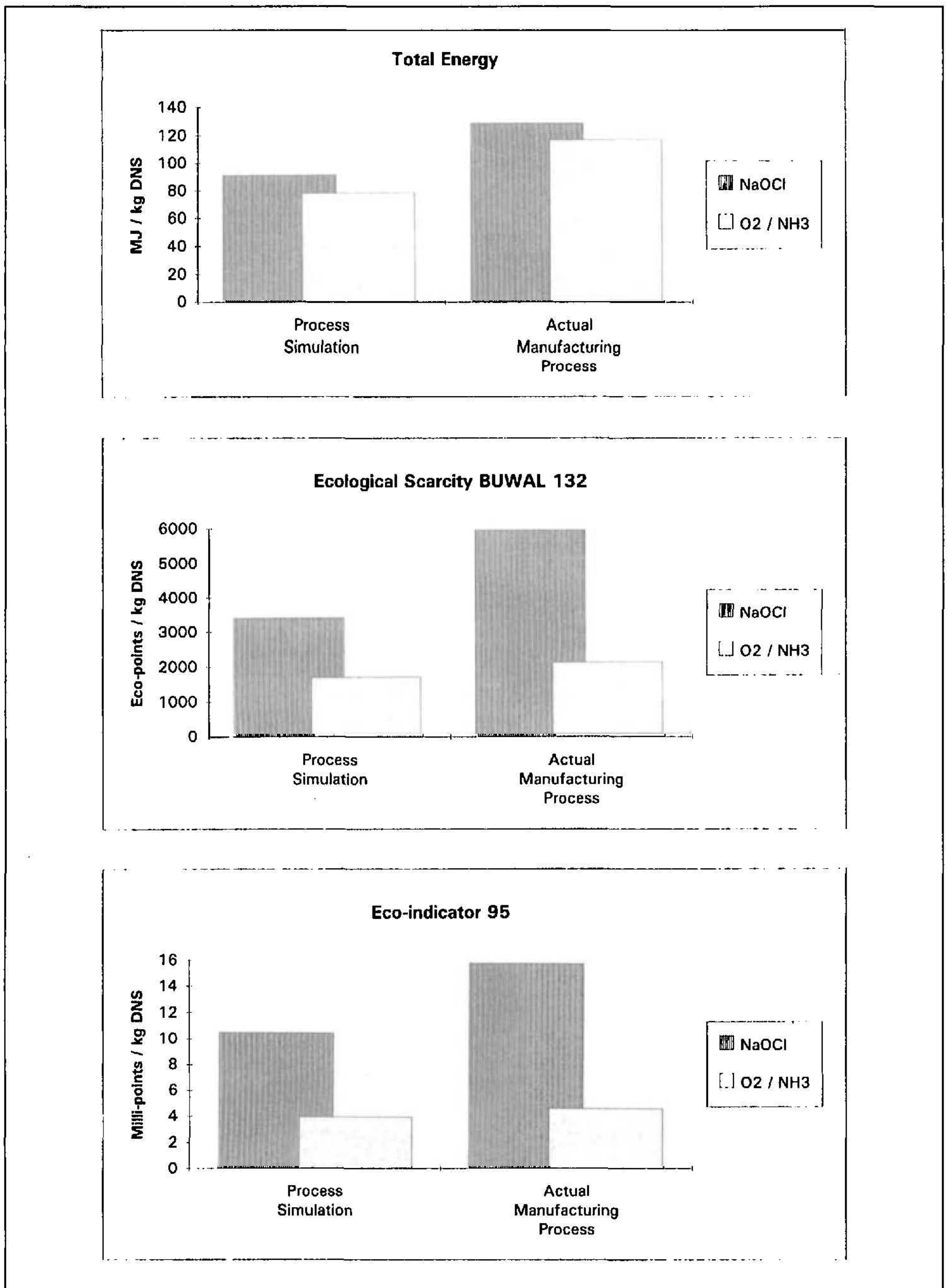

Fig. 5. *DNS synthesis process alternatives, judged by environmental burden numbers* (valuation), *before and after implementation*

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Integrated Product Design in Chemical Industry. A Plea for Adequate Life-Cycle Screening Indicators

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Abstract. The ever expanding growth of energy and material fluxes and the associated environmental impact challenge the chemical industry to integrate ecological issues into the design of new chemical substances and products (integrated product design). To achieve this goal, product developers as well as marketing and application specialists need appropriate tools for incorporating ecological issues at every stage of product development. Life-Cycle Design, an approach based on the screening indicators of the streamlined Life-Cycle Assessment (LCA) method, is an appropriate concept that can be used even at early development stages. Still today, however, many product designers regard screening indicators, *e.g.* energy and/or material intensity, summary emission indicators (DOC, TOC, VOC, *etc.*) as rather subjective judgements, even if they are based on experts' knowledge, panel discussions, *etc.* Thus, there is a strong need for defining an appropriate set of objective screening indicators based on a natural science approach. These enable an accurate description of environmental effects of a chemical substance in all environmental compartments (air, soil, water, and biota). In this work, we present a conceptual framework for screening indicators that take into account both process inputs and outputs at every single life-cycle stage. Finally, first results based on several case studies (solvents, dyestuffs, ...) are shown.

1. Introduction

Society's ever expanding growth of energy and material fluxes is paralleled by an increasing pollution of water, soil, air, and biota by anthropogenic compounds. Simultaneously, a decrease of nonrenewable resources leads us to a situation where the basic necessities of human life are becoming more and more endangered. Thus, the chemical industry is now challenged to integrate ecological and societal issues into its design of new chemical substances and products, in order to keep providing the solutions that fulfill society's needs (integrated product design) [1][2]. This new challenge calls for better tools, allowing product developers as well as marketing and application specialists to effectively evaluate products and processes with respect to their potential environmental impacts. Also, these tools must take into account legal compliance and consumer needs, as well as marketing aspects, in early stages of product/process development.

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