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

André Weidenhaupt* and **Konrad Hungerbühler**

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

André Weidenhaupt* and **Konrad Hungerbühler**

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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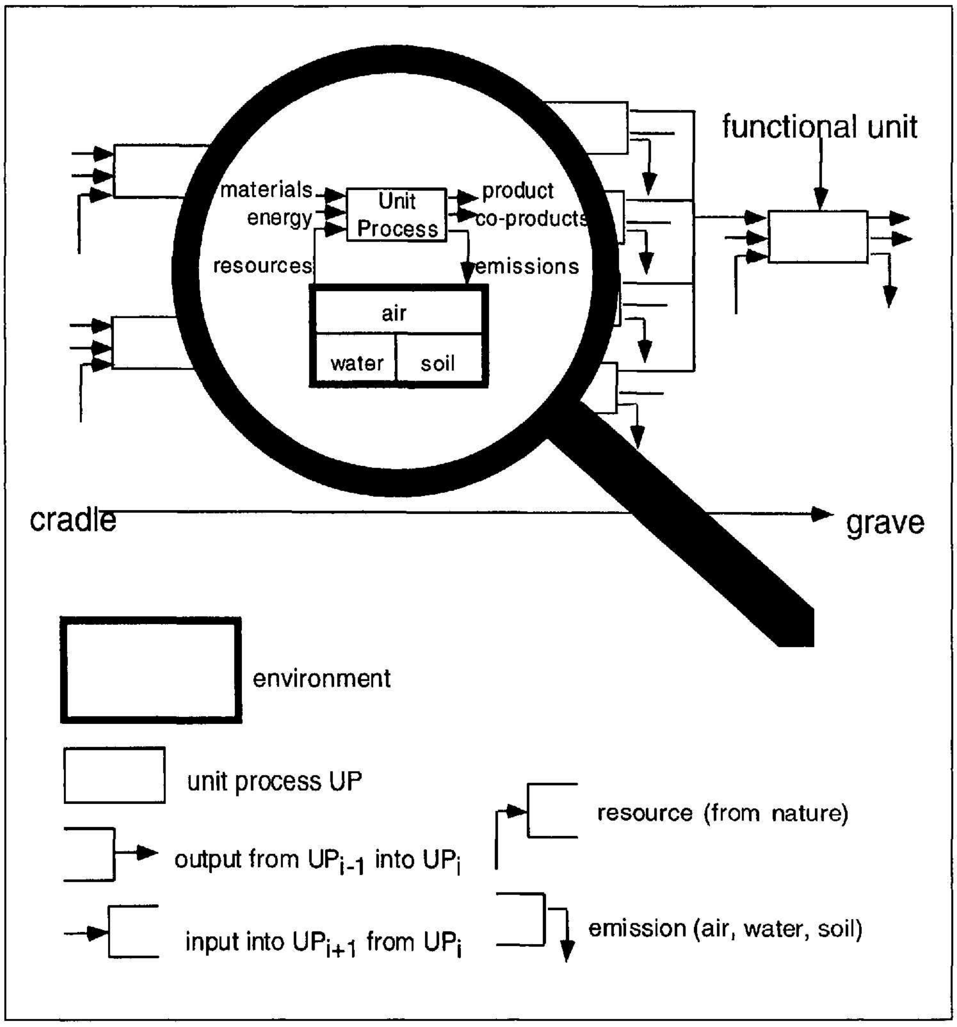

Fig. 1. *System boundaries of a product or service* (*i.e.*, the functional unit) *from cradle to grave* (life-cycle thinking). Note that the life cycle is an assembly of single unit processes with inputs (energy, materials, and resources) and outputs ((co-)products, waste and emissions to air, water, and soil).

Table. *List of Available Life-Cycle Impact Assessment Methods* (not comprehensive)

Critical Volumes [4] BUWAL 132	One-step quantitative method, emissions are weighted and aggregated according to their immission limits within each single environmental compartment (air, water, soil)
EPS [5] (the Swedish enviro-accounting method)	One-step quantitative environmental evaluation according to safeguard subjects with a willingness to pay valuation
Ecological Scarcities [6] (CH-Eco-points method) BUWAL 133	One-step quantitative valuation method which expresses valuation in Ecopoints based on the relation between the actual flow and a flow considered as critical for each single emission
CML [7] Impact Oriented Classification	Three-step (classification, characterization, normalization) quantitative valuation method leading to 14 environmental impact classes (*e.g.* global warming potential, ozone depletion potential, ...)
CML + MET [7]	CML characterization combined with a distance-to-target approach for the valuation step based on the Dutch National Environmental Plan
Eco-indicator 95 [8]	Four-step (classification, characterization, normalization, valuation) method using a similar set of environmental impact classes than the CML method with an additional distance-to-target approach for valuation

2. Life-Cycle Assessment and Life-Cycle Design

Life-cycle assessment (LCA), according to the guidelines of the Society of Environmental Toxicology and Chemistry (SETAC) [3] and the ISO 14040 series of draft standards, is a method capable of dealing with a product's (service's) potential environmental impact in a so-called cradle-to-grave approach. This consists of four distinctive phases:

1) the goal and scope definition (GSD), the phase dealing with system boundaries and setting the functional unit,

2) life-cycle inventory (LCI) consisting of energy and material balances, as well as emission inventories as shown in *Fig. 1*,

3) life-cycle impact assessment (LCIA) that
  - classifies (*e.g.* global warming potential (GWP), ozone depletion potential (ODP)),
  - characterizes (*e.g.* GWP in CO_2 equivalents, ODP in CFC-11 equivalents),
  - normalizes (gives a relation between the specific emission listed in the inventory and the pollutant's total annual emission) and
  - evaluates (the different classes are weighted to yield an overall aggregated value) the emissions and resource use of the LCI (a list of different life-cycle impact assessment methods is given in in the *Table*) and

4) an interpretation step that is necessary to assure an adequate discussion at each single stage of the LCA.

However, there is a considerable controversy both in academia and in industry about the above-listed impact assessment methods, as all of these include a valuation step and tend to aggregate all emissions and resource consumption to one single value. Valuation is considered by decision makers as being rather subjective and case-and/or context-dependent. For instance, chemical industry, insurance companies, consumers, *etc.* are influenced by different values within their decision-making processes. For this reason, there is a series of comprehensive reviews that compare and analyse LCIA methods with respect to their adequacy for giving a macro view of potentially harmful environmental impacts [9–13].

Furthermore, time horizons and costs to perform a detailed LCA study most often exceed the time frame for product development in industry and are thus not attractive for decision makers. For this reason, there is an obvious need for simplifying the LCA procedure as it has been proposed in the report of the SETAC-Europe LCA Working Group on Screening and Streamlining [14]. According to the SETAC-Europe group, a simplified or 'streamlined' LCA is a three-step procedure covering

1) a comprehensive screening assessment of the whole life cycle,
2) the simplified LCA focusing on the most important environmental impacts and/or life-cycle stages,
3) a thorough assessment of the reliability of the overall results.

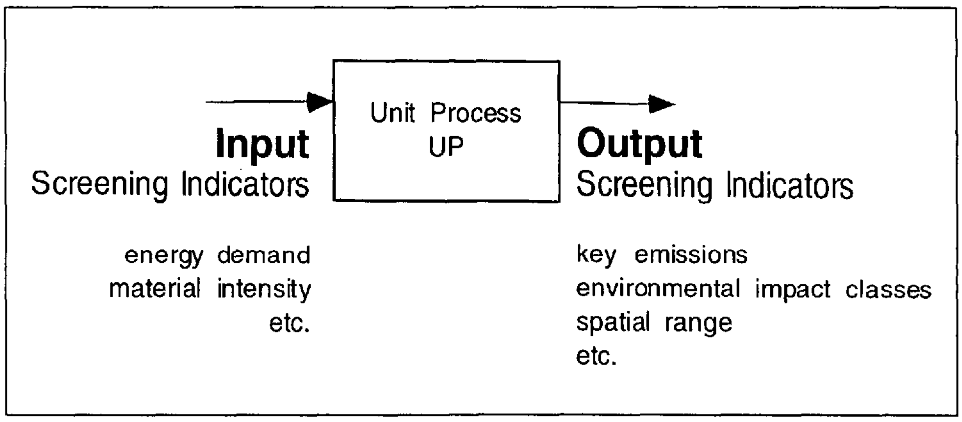

Fig. 2. *Input- and Output-Screening indicators in a life-cycle unit process perspective*

3. Screening Indicators for Product Development

For integrating life-cycle thinking into product design it is far better to consider LCA as a set of flexible approaches/tools rather than a rigid instrument. This alternate approach has already been proposed by several product designers and applied for certain industrial applications [15–17]. Thus, for product design purposes, the first step of the above-described simplified LCA procedure, the screening step, seems most adequate: screening is a process that sifts through the full life cycle and all relevant environmental aspects of a product system to identify the most important areas for further investigation and/or improvement. The concept of screening implies the use of screening indicators and should be performed according to specified one-step or iterative procedures, including panels of experts, checklists, qualitative valuation matrices [2], or benchmarking. With respect to chemical product design, the approach of *Dow-Europe S.A.* is to choose six screening indicators (energy demand, material intensity, resource intensity, waste intensity, health environment & safety (HES), and service intensity) in a six-dimension radar plot [17]. This is a step towards the overall goal of integrated product design.

However, care needs to be exerted when screening indicators are used, because there is no guarantee that all environmentally important aspects of a life cycle will be covered by the chosen set of screening indicators. This is the case, if either *input-screening indicators* or *output-screening indicators* are exclusively used in the screening step. Examples of single *input-screening indicators* are, *e.g.* energy demand, MIPS (material intensity per service unit), key input materials/resources. *Output-screening indicators* include, *e.g.* key emissions, individual environmental impact classes (*e.g.* global warming potential, ozone depletion potential). In this context, a comprehensive combination of screening indicators (looking at inputs and outputs) will increase the reliability of screening (*Fig. 2*). Furthermore, screening indicators which do not include the life-cycle thinking, *i.e.*, that cannot be applied to all stages of the life cycle, should not exclusively be applied for screening purposes. Among such screening indicators are, *e.g.* percent of recycled material, recyclability or degradability which focus at life-cycle stages after consumption of products.

3.1. *Input-Screening Indicators*

The life-cycle inventory has its origins in basic chemical engineering mass balances and/or economic tools which assess the overall efficient use of materials/resources and energy [18]. As this concept is familiar to any chemical engineer, the following input-screening indicators should be included in the overall concept of life-cycle design of chemical products:

Energy demand: In this case, the life-cycle inventory is limited to energy consumption data and energy balances [19] and, additionally, may distinguish the type of the energy generation process, *i.e.*, energy from fossil fuels, renewable energy sources, and/or electricity from nuclear power plants. The idea being, that several environmentally important emissions are strongly linked to (fossil) energy demand and that depletion of fuel resources is important.

MIPS (material intensity per service unit) [20]: The *MIPS* concept consists of a life-cycle inventory method in which only system inputs (resources) are taken into account. All inputs are added up, based on their mass, *i.e.*, no difference is made between the type of material (*e.g.* 1 kg of mercury + 1 kg of granite = 2 kg of used material). The sum of masses is related to the functional unit, which yields the MI. The idea of MIPS is that important impacts on the environment are related to resource consumption and transport of material. It is based on the assumption that a 'dematerialized' system, *i.e.*, a system using less materials, is a 'better' system. Another similar approach is the *FIPS* method, *i.e.*, the area intensity per service unit.

When *key substances* are used as screening indicators, the life-cycle inventory is limited to data of a single substance or a group of substances, *e.g.* heavy metals, all nitrogen compounds, organic chlorine compounds, greenhouse gases. This concept is not limited to input-screening indicators and is commonly referred to as *substance flow analysis* (SFA) [21].

3.2. *Output-Screening Indicators*

In order that screening indicators give a realistic picture of the interface between technosphere and ecosphere of a product life cycle, it is crucial to have an appropriate set of objectively defined output-screening indicators based on a natural science approach. Such screening indicators enable a more accurate description of the environmental effects of a chemical substance in all environmental compartments (air, soil, water, and biota).

As stated above, the choice of one or several *key substances* screens both the input and output side of a product's life cycle. The choice of the key substances depends on the branch of industry to be investigated and on the goal of the study. An impact assessment will thus be reduced to the impacts of the investigated substances. With respect to completeness, we should consider the use of *summary parameters* (*e.g.* total organic carbon (TOC), volatile organic carbon (VOC), chemical oxygen demand (COD)) as possible screening indicators, as these are very often subject to monitoring and thus readily available, even though it is almost impossible to evaluate potential harms of such a heterogeneous mix of chemical substances. Furthermore, there are tendencies, at least in the United States, to restrict the choice of key substances to those toxic substances listed in the US-Environmental Protection Agency (US-EPA) Toxic Release Inventories (TRIs) [22].

The use of *environmental impact classes (EIC)* (e.g. global warming potential (GWP), ozone depletion potential (ODP, nutrification potential (NP)) according to the center of environmental sciences (CML) of Leiden University (NL) [7] is a promising alternative. EIC-based screening indicators are designed to take potential effects of the product's life cycle into account. Yet, care needs to be exerted when choosing the EIC, because several EIC strongly correlate with certain input-screening indicators. A combination of both energy demand and GWP, for instance, will give information about the use of fossil fuels exclusively.

If life-cycle design should meet the need to identify associations between emissions and potential hazards, it is crucial that the *environmental fate* of the chemicals listed in the emission inventory are taken into consideration when designing screening indicators. Although some of the above-mentioned EIC consider environmental fate implicitly (*e.g.* GWP, ODP), other classes tend to ignore this crucial issue. This renders it hard to achieve an overall consistency, when trying to integrate environmental fate into LCIA, as has already been proposed by *Wegener Sleeswijk* and *Heijungs* [23]. Furthermore, *Guinée et al.* [24] introduced a fate model for the environmental impact class *toxicity* by applying the software USES 1.0 [25], based on a Mackay Level III unit-world model [26]. Although this concept follows the principles of environmental product risk assessment [27] by comparing environmental exposure with potential toxic effect concentrations, its overall complexity as well as its limited transparency reduces its adequacy for screening purposes.

We think however, that screening indicators should reflect environmental fate. Thus, an adaptation of multimedia models is a promising approach to achieve this overall goal. In this context, the definition of the purely exposure-based screening indicators *spatial range* and *persistence* as has been proposed by *Scheringer* [28], is a promising concept that should be included in our list of screening indicators for life-cycle design. In a circular model based on a set of single Mackay-type level III multimedia worlds, *Scheringer* tends to define two proxies for an exposure-based assessment of organic chemicals. In our context, *persistence* or temporal range (in time units) is a screening indicator which considers the duration of any exposure caused by inventory emissions, whereas *spatial range* (in space units) describes the potential of any emission for global pollution, classifying the inventory in long/short term and local/global pollutants. These two indicators can be used even in an early stage of product development, as there are several methods that allow an early evaluation of substance properties according to their environmental fate in the field of environmental chemistry [29].

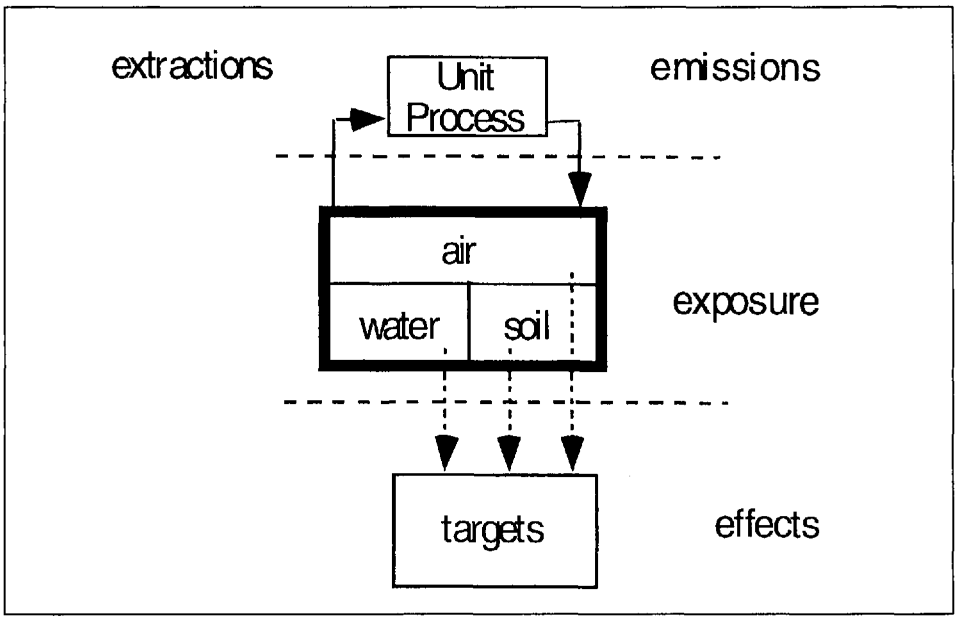

Fig. 3. *Extractions and emissions as interactions of the unit process with the environment leading to an exposure with potential effects on diverse targets* (*e.g.* biota, stratospheric ozone layer)

4. Case Studies

We have investigated the concept of life-cycle design with screening indicators or, as we call it prospective LCA, within a couple of case studies. Among others, we might cite the use of perchloroethylene in textile dry cleaning [30] and the comparison of several reactive red cotton dyestuffs [31]. In both cases, we first performed a detailed LCA study to evaluate the adequacy of possible screening indicators. *Energy demand* proved to be a good screening indicator on the input side. Furthermore, we found that we could use both perchloroethylene in the textile dry-cleaning study and the respective textile dyestuffs together with naphthalenesulfonic acids as their precursors in the dyeing works study as *key substances* for screening purposes. More generally, we think that with respect to highly emissive applications, it is wise to include the main substances in the set of screening indicators. Yet, as this selection does not cover the whole life cycle, we also recommend, additionally, the inclusion of *summary parameters* which represent the most emissive life-cycle stages adequately (*e.g.* TOC in case of textile dyestuffs and VOC in case of textile dry cleaning, respectively) in the first screening step. A further refinement will be achieved in subsequent iterative screening steps.

5. Outlook

Although there seems to be a large amount of available screening indicators, there is only little knowledge in how far a specific set of proxies [32] is suitable to describe potential harmful effects on both man and the environment. Even though completeness might never be achieved, we have the strong feeling that a systematic natural science approach will lead to screening indicators that integrate both environmental fate and potential effects in industrial design and decision-making processes. The adaptation of fate models for polar and/or (de-)protonable substances on the one hand, and a systematic prediction concept for potential toxic effects (*Fig. 3*) on the other hand are two steps which both lead in this direction and will be pursued in our group with respect to further develop the concept of prospective LCA.

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