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Use of the life-cycle assessment (LCA) toolbox for an environmental evaluation of production processes*

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Abstract: Green chemistry not only emphasizes the central production process of the "green" chemical, but it ultimately requires a life-cycle conceptual approach for each chemical product. A life-cycle conceptual approach comprises the consideration of all stages along the life cycle of a chemical (i.e., raw material extraction, pre-production, production, use, recycling, and disposal) as well as the consideration of environmental impacts caused by by-products and auxiliaries (such as solvents and additives, but also technical facilities which have to be provided to produce the green chemical). A significant improvement in the evaluation of green chemical products can be approached by the complementary use of the methodologies of life-cycle assessment (LCA) and risk assessment. The use and combination of both methodologies can be performed by a separate use of the instruments (depending on the scope, definition, and application of LCA), an iterative use of LCA and risk assessment, or a complete integration of both instruments. Pros and cons of these approaches are discussed.

INTRODUCTION

Recently, a definition of green chemistry was given by the OECD (OECD Workshop on Green Chemistry, 15–17 October 1998, Venice):

> "The broad framework of Sustainable Development strives to maximise resource through activities such as energy and non-renewable resource conservation, pollution prevention, risk minimization, low levels of waste at all stages, durability, reuse and recycling. Sustainable Chemistry strives to accomplish these ends through design, manufacture and use of efficient and effective, more environmentally benign products and processes".

Such a definition clearly not only emphasizes the central production process of the "green" chemical, but it ultimately requires a life-cycle conceptual approach for each chemical product. A life-cycle conceptual approach comprises the consideration of all stages along the life cycle of a chemical (i.e., raw material extraction, pre-production, production, use, recycling, and disposal) as well as the consideration of environmental impacts caused by by-products and auxiliaries (such as solvents and additives, but also technical facilities which have to be provided to produce the green chemical). A life-cycle conceptual approach also addresses and compares different environmental problems such as global warming, ozone depletion, acidification, and ecotoxicity. Current discussions on green chemistry mainly focus on the selected stage of the production process, and thus the basis for decision making and risk management might be erroneous and misleading. A significant improvement in the evaluation of green chemical products can be approached by the complementary use of the methodologies of life-cycle assessment (LCA) and risk assessment.

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TECHNICAL DESCRIPTION OF THE LCA METHODOLOGY

General applications of the LCA methodology are the development and improvement of chemicals, technical products, and processes as well as services, the strategic planning in companies (as the instrument allows for the identification of the most critical life stage or the most critical emission of the functional unit) public policy making (as many LCAs are comparative assertions disclosed to the public) and last, but not least, marketing.

The LCA procedure itself has been laid down in ISO 14040 ff. as a normative reference. It is a stepwise procedure with mandatory and optional elements.

1. In the first step, the ultimate goal and the application of the results have to be defined. It has to be laid down as to whether a comparative assertion disclosed to the public will be performed since such a scope triggers several sub-steps and the final results presentation. Additionally, system boundaries have to be laid down as they, to a great extent, will finally influence the LCA results.
2. The second step comprises the input and output analysis. Any material and energy flow within the system boundaries and also entering and leaving the system is documented. “Material”, in this context, can either be complex products or chemical emissions along the life cycle.
3. The third step is the impact assessment being divided into several sub-steps. First, the inventorized material and energy flows are assigned to environmental problems operationalized as impact categories (classification). The second sub-step, the characterization, tries to assess the contribution of the assigned input/output data to the respective impact category to result finally in an impact profile. This can be achieved by using models, which combine the input/output data from the inventory and a so-called indicator expressing the environmental effects or damages. In general, the indicators allow, in terms of being “units”, for an aggregation of all emission-based contributions within each impact category. If appropriate, characterization factors are used to quantify the contribution of each single emission to the respective category. The models range from quantitative and internationally accepted ones to expert- or even value-based individual models.
4. The last step of an LCA is the interpretation phase. Value choices for the impact categories with their subsequent weighting can, for example, be made in order to focus on a single aspect that has been documented in the goal definition.

Figure 1 shows a typical result of a LCA obtained upon impact assessment. The material and energy flow as given by the inventory have been assigned to the impact categories and subsequently characterized. On one of the axes, the commonly considered impact categories are listed. On the other axis, the numerical indicator results expressed as mass units—such as ozone depletion potential, gobal warming potential, etc. of the assessed functional unit—are given to result in the impact profile. When comparing two chemical products of the same functional unit, the number of the global warming potential of product A can directly be compared with the respective number obtained for product B. In case no comparative assertion is to be performed, the results obtained after characterization have to be normalized. The normalization refers the product-based emissions to those of a reference, i.e., a political or economic unit such as a country or the OECD.

DISADVANTAGES OF LCA METHODOLOGY IN RESPECT TO THE APPLICABILITY FOR COMPARATIVE ASSERTIONS IN GREEN CHEMISTRY

Though the approach of LCA excellently integrates many aspects of environmental protection and is in fact a helpful innovative tool in green chemistry, it also has some major shortcomings. As already mentioned, the results of the impact assessment are expressed as numerical indicator results with the underlying information usually not being related to space and time. However, detailed information also on temporal and spatial aspects is needed in most cases for decision making by the engineer, manager, or stakeholder. Furthermore, the scientific knowledge and state-of-the-art concerning the detailed

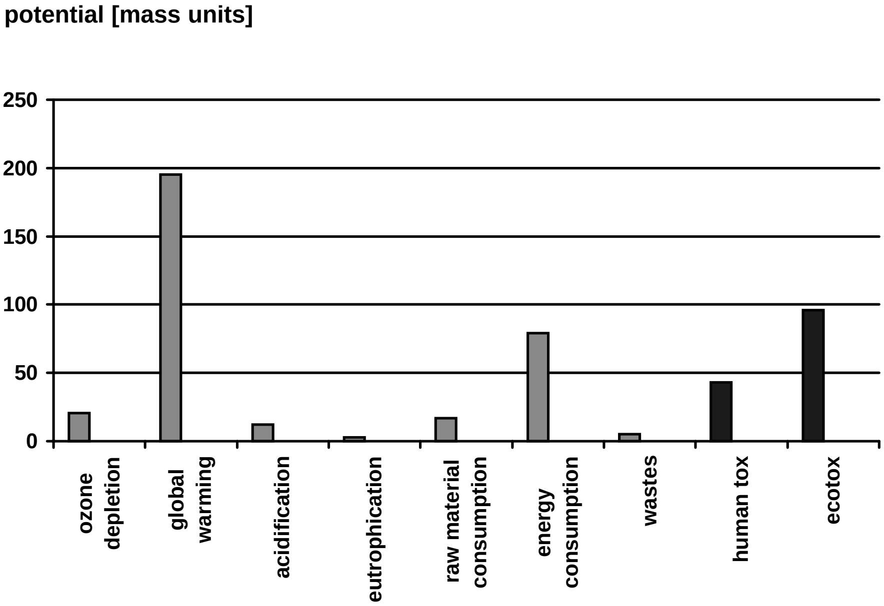

Fig. 1 Impact profile of a chemical product.

chemical's assessment is not implemented sufficiently, even though it is possible to do so.

SOLUTION: COMBINED USE OF LCA AND RISK ASSESSMENT FOR STRATEGIC PLANNING AND ECO-DESIGN IN GREEN CHEMISTRY

A possibility to cope with the mentioned disadvantages of LCA is not the alternative but complementary use of the instrument of human and environmental risk assessment. On a local, regional, or even continental scale and by scenario-based approaches the risk assessment tries to describe and predict as precisely as possible the probability of environmental damage caused by emitted chemical substances. In order to be consistent with respect to the used terminology, the different definitions of "risk assessment" are shortly introduced:

- "the estimation of the probability of clearly defined environmental effects occuring as a result of the exposure to a chemical
- estimation of the probability or likelihood of undesirable events such as injury, death or the decrease in the mass or productivity of fish, wildlife. Risk is a function of hazard and exposure; ecological risk is a function of (eco)toxicological hazard and environmental exposure
- Comparing the concentration in the environmental compartments (PEC) with the concentration below which unacceptable effects on organisms will most likely not occur (PNEC)" [1].

As a consequence, from a reduced data availability, routinely, the "predicted effect concentrations" (PEC) and the "predicted, no effect concentrations" (PNEC) approach is followed. Such an approach is, for example, laid down in detail in the Technical Guidance Documents in support of the risk assessment of New and Existing Chemicals in the European Union. The PEC can either be a deterministic value assessed by using scenarios or a predefined percentile of a concentration distribution function. The PNEC can either be extrapolated by using extrapolation factors or by assuming an organism's sensitivity distribution and, again, on the selection of a certain percentile of the curve.

At least three possibilities exist to combine the LCA and the risk assessment approaches in order to obtain as much output as possible:

1. separate use of instruments depending on the scope definition and application of LCA

2. iterative use of LCA and risk assessment
3. complete integration of both instruments

1. Separate use of instruments depending on the scope definition and application of LCA in green chemistry

The first approach is basically the introduction of a life-cycle conceptual approach in conventional standard methodologies for the protection of humankind and the environment. For each stage along the life-cycle of a chemical product, an adopted tool is selected, and assists in solving the occurring problems. The selection of the most appropriate tool is based on the producer's experience with the chemical product under consideration; however, it also might be based on existing regulations.

Appropriate tools could be, among others:

Tool	Life-cycle stage
the analysis of material and energy fluxes	for the stage of raw material extraction and the pre-production phase
the handling of hazardous substances	for the production phase with main emphasis on worker protection
a hazard ranking for emitted compounds	to optimize an environmentally critical production sub-process
a detailed risk assessment	for the production site
a scenario-based risk assessment approach	for final consumer protection

As for any approach, advantages and disadvantages exist. One of the advantages is the fact that the selected instruments are exactly adjusted to the occurring problem. This is not necessarily the case when exclusively using the LCA tool. Recently, after the initial enthusiasm for using the LCA tool as a universally applicable instrument, a shift towards problem-oriented solutions is observable. Thus, for most cases, the selected tools are not overloaded and the obtained results are not misinterpreted. Additionally, the combination of voluntary measures and regulations might eventually result in de-regulations, though this is still discussed quite controversially. One of the major disadvantages is the fact that the selection of an appropriate tool depends to a great extent on experience. Experience, on the other hand, might be misleading, and thus the application of the LCA tool could lead to false decisions.

2. Iterative use of LCA and risk assessment

A second approach which more consequently introduces risk assessment in life-cycle thinking is the possibility to iteratively combine both methodologies:

1. The basis for such an iteration is the application of the LCA screening method. This screening method identifies hazardous emissions by the use of a classification system, which is defined by substance-inherent properties and thus, in fact, reflects the hazard of the emitted compounds. Elements of such a procedure can for example be taken from the EU-Directive on Classification and Labeling, which also aims at an appropriate description of substance inherent properties without the need for information on concentrations in the environment [1].
2. By referring to the information obtained by the inventory, the sources of the screened hazardous emissions can be identified in most cases. In principle, two situations can occur: either a high number of sources with low emissions or a low number of sources with intensive emissions lead to the impact assessment results.

3. By focusing on the latter, an appropriate risk assessment can be performed that refers to the specific local and temporal situation of the emission sources but that also still refers to the functional unit as defined by the goal definition.
4. As a further option, a refined LCA could be performed using the detailed information obtained by the risk assessment. Such a refined LCA is an option only, since it does not give additional output, but presents valid information for one single assessment tool.

Again, advantages and disadvantages for the described approach exist. First, of course, it can be stated that such an iterative approach is highly flexible and can strictly be oriented at the goal definition. However, on the other side, the use of the approach should not be overstressed, and the approach should not be applied unflexibly. This could lead to trivial results. And this again could result in some lack of credibility of the whole instrument of LCA.

3. Complete integration of both instruments

The last, and most elegant, way to combine the LCA and risk assessment tool is the integration of both methods. This can be done by deriving characterization factors—hereinafter called impact scores—on the basis of hazard or risk assessment. An example is given by the following equations:

$$\text{Impact score (ecotoxicity, water)} = I_{\text{exposure}}\,(\text{water}) * [\text{accumulation factor} + I_{\text{effect}}\,(\text{water})]$$

with:

$$I_{\text{exposure}}\,(\text{water}) = \log E$$

and:

$$E = \text{emission [kg]} \times \text{distribution factor} \times \text{degradation factor}$$

and:

$$I_{\text{effect}}(\text{water,soil}) = \frac{\log(\text{PNEC}_{\text{i}} / \text{PNEC}_{\text{max}})}{\log(\text{PNEC}_{\text{min}} / \text{PNEC}_{\text{max}})} 7$$

The suggested hazard assessment methodology is a typical scoring system [2]:

1. Various exposure and effects of related criteria are defined. This example is for the exposure part:
   - the percentage of the emitted compound distributed into the compartment under consideration. This is calculated by using, e.g., the MACKAY level I model [3,4]
   - the degradability of the compound expressed by degradation factor

   For the effects part, the criteria are the direct effects (expressed as PNEC) and the indirect effects (expressed as the accumulation potential).
2. In a second step the criteria are weighted according to their relevance for the environment. The weight is expressed as a numerical score. In our case the effects and exposure parts are weighted equal and given the number of 10 each.
3. In a third step the scores are scaled. This can be done either continuously by defining an upper and lower limit or discontinuously by defining property classes for the criteria. For the criteria "degradability" and "accumulation", discontinuous scales are defined by property classes. Factors are assigned to the classified properties. Depending on the inherent properties of the considered emitted substance, the compound is allocated to one of the classes and factors.

   For calculating the direct effects score a continously scaled score is needed. The effects are expressed as PNEC. The score is scaled by defining an upper limit, the PNEC_{min}, and a lower limit, the PNEC_{max}. The PNEC_{min} is an extremely low PNEC (and thus represents high toxicity) selected by convention to form the upper part of the scale. The PNEC_{max} is a very high PNEC (and thus it represents extremely low toxicity) and is selected by convention to form the lower part of the scale.

The results of such a procedure are, for each of the emitted compounds, impact scores for the aquatic (and also the terrestrial) compartment. The impact scores are numerical figures and demonstrate the “relative risk” of the compounds. The numerical figures are meaningless as such. Therefore, they are referred to a reference substance, in our case 1, 4-dichlorobenzene (see also refs. 5 and 6). This is in accordance with the procedure for other impact categories. For example, for the impact category of global warming, all compounds are referred to the potential of CO_2 which is set equal to one [7]. After such a normalization the scores are added for all emitted compounds of the functional unit or of a selected stage along the life cycle to result finally in the aquatic and terrestrial ecotoxicological impact potential.

Advantages of such an integrated approach are obvious: The knowledge and experience from the chemicals assessment is used as far as possible. As a basic requirement, the dialog between LCA appliers and experts in the field of chemicals assessment needs to be intensified, and this has, so far, not sufficently been the case. Several attempts exist to do so, for example, using scientific workshops and conferences as a platform.

One of the major shortcomings of the integrative approach is the fact that an immense data input is needed. Since information is not always available, the use of defaults is inevitable. As a consequence thereof, results seem to be precise, but in fact, the level of precision varies from one LCA to another without having a highly transparent way of presentation. As long as LCA appliers are aware of this problem, misleading final discussions and decisions can be avoided.

CONCLUSIONS

Concluding from the given overview it can be stated that approaches exist to combine various tools for an integration of a life-cycle conceptual approach in the assessment and evaluation of green chemicals. None of the approaches has advantages or disadvantages only, but the appropriate method should be selected in dependence on the application. The applier has to be aware of the limitations and result variations and must responsibly take care of a transparent presentation of results. The presented approaches and further concepts to combine different tools in environmental management and decision making might further diverge in future. The level of sophistication will increase, and this will make the results even less comparable.

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