Guiding innovation with integrated life-cycle assessment (LCA) and techno-economic assessment (TEA) - the case of CO_2-containing polyurethane elastomers

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Why an integrated assessment?

As societies face global challenges such as climate change, population increase with limited resources or health issues they become aware of and raise questions about ecological and societal impacts of chemical innovations. As a consequence, the goals of research, development and deployment (RD&D) of such technologies become more complex and diverse. For example, companies experience increasing pressure from stakeholders such as governments or the general public who force them into rethinking their strategies which can often no longer be based on monetary gains alone.

Innovations are guided by the interplay of technical improvement and assessment: A technology is being researched, developed and deployed with a specific goal. The chances of realizing this goal are continuously checked alongside the RD&D and feedback is given in order to guide the innovation to the set goal. However, this mechanism, presents multiple challenges which lead to chemical innovation projects experiencing low success rates and long cycle times. Challenges emerge from a variety of risks and a lack of reliable guidance posed by complex decision-making[1,2]. This raises the necessity for an improved assessment methodology, leading to more comprehensive and accurate assessment results which provide a sound basis for subsequent decisions.

Improved technical performance is in the core of most chemical innovations. Techno-economic assessment (TEA) has long been regarded as obligatory and remains a decisive part of every assessment as deployment of chemical technologies is only possible in environments that are first and foremost driven by economic prospects. In addition, life-cycle assessment (LCA) was introduced to include an ecological perspective. Thus, assessments of chemical innovations are typically carried out at the three-sided interface of technical performance with economic viability and with ecological sustainability. In this context, technical performance parameters on the one hand present the limiting frame in which both with ecological and economic impacts can occur; and on the other hand suggest options which benefit the set goal.

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How to integrate life-cycle assessment (LCA) and techno-economic assessment (TEA)

Definitions

"Assessment means assigning a positive or negative value to a certain criterion."[3] Criteria are aspects of assessments that are judged individually and whose values cannot directly be transferred into each other. Criteria are conventionally assigned to different assessment fields such as life-cycle, techno-economic or social impact assessment. In LCA, all impact categories can be seen as criteria. The single most important criterion for TEA is profitability. Efforts have been made to identify other economic criteria[4] but remain inconclusive. Technical aspects such as energy efficiency of a process or product properties are not suitable criteria in the established understanding of 'assessment' as only the effects of technical performance can be assessed[3]. Indicators answer to an associated criterion by taking on measurable values[3]. Figure 1 illustrates the hierarchy of assessment fields, criteria and indicators for examples in LCA and TEA.

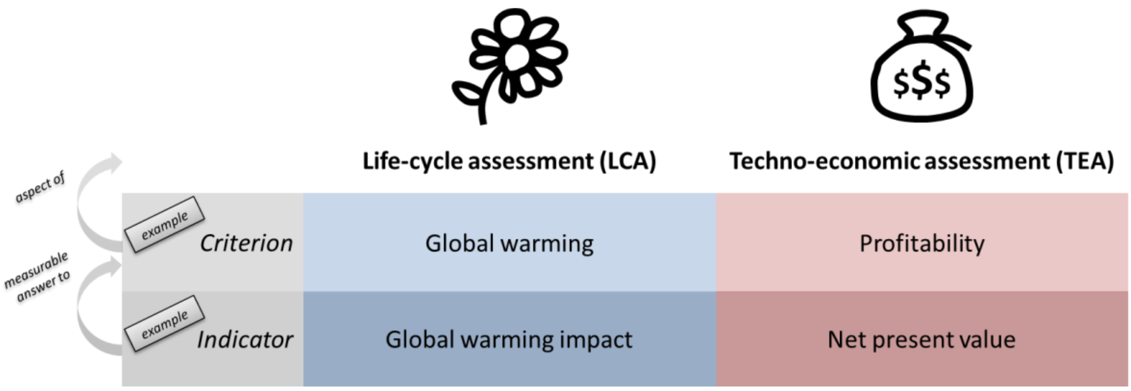

Figure 1: Life-cycle assessment and techno-economic assessment with example criteria and example indicators

Assessment structures

Every assessment can be described broken down into the four phases that the ISO standards 14040 and 14044 present for LCA[5,6]: goal and scope definition (I), [life-cycle] inventory analysis (II), [life-cycle] impact assessment (III), interpretation phase (IV). However, the specific contents need to be detailed for different assessment types. While exhaustive descriptions of LCA phase contents are available[5–7], only recently, detailed descriptions of TEA phase contents (for the chemical industry) have been published[3,4].

Approaches on integrated assessment

Both TEA and LCA provide interpreted indicators to a subsequent decision making step. In order to ensure that TEA and LCA can be weighted in a single decision, both assessments need to have the same basis, especially refer to the same goal. An approach for aligning TEA and LCA was suggested in a report on TEA & LCA Guidelines[4] written by a consortium of researchers from TU Berlin, IASS Potsdam, RWTH University and the University of Sheffield. This approach and is briefly outlined below. Indicators calculated on the same basis can be fed into a Multi-Criteria Decision Analysis (MCDA) which allows for a single decision based on multiple separated criteria and identification or balancing of trade-offs. A shared scope and calculation basis is especially important when calculating composite assessment indicators such as CO_2 abatement cost. For the depth of alignment or integration of assessments, three types of studies are distinguished[4]:

1 'Qualitative Integration': Mostly for early TRLs, two separate studies on the same product system, allowing for only qualitative comparison of hot-spots

2 ‘Alignment and Combined Indicators’: Two separate studies with aligned scopes and inventories, combined indicators are presented in addition to solely economic or ecological indicators
3 ‘Fully Integrated’: One combined study comprising indicators from different assessment fields

Type 2 studies can vary in their degree of alignment. Aligned scopes help to provide the same depth of analysis. Issues that need to be addressed in the goal and scope phase (I) are: the elements of the technology, *i.e.* system boundaries, and the scenario in which the technology is deployed, *i.e.* especially the time and geographical situation. Assessment methodology depends heavily on the available data about the technology in focus[3,8]. The availability of data is strongly linked to technology maturation which itself can be described with technology readiness levels (TRL). Following the analysis of data availability by TRL rating, a joint collecting of inventory (phase II) data can be carried out. Substantial overlaps of LCA and TEA can primarily be found in their inventories: Commonly, at least mass and energy balances are required for both assessments. Joint data collection helps to exploit synergies and reduce overall assessment effort. In the following phase (III), data are “tagged” with potentials such as cost (TEA) or global warming potential (LCA) in order to yield the respective impacts. An example for aligned studies is given in the following.

A case study – the CroCO_2PETs project

I - Goal and Scope

The case study is provided by the CroCO_2PETs project, a project funded by the European Commission’s Climate-KIC as part of the ‘enCO_2re’ flagship program within the Horizon 2020 framework. Focus of this project is the development of various types of elastomers from polyols that contain double bond moieties and carbon dioxide as building blocks. For this report, the focus is on densely cross-linked elastomers that are produced in a two-step process: First, the production of the novel polyols and second, an elastomer formation. The polyol production was invented and is currently carried out by Covestro Deutschland AG. The elastomer formation can be described as similar to a network curing step with simultaneous urethanization with polyisocyanates and further cross-linking with double bond linking agents. As the resulting elastomer can be a drop-in or near drop-in solution for conventional cast polyurethane elastomers, the system boundaries for both assessments enclose only the elastomer system, *i.e.* the polyol formation and all components in the elastomer recipe (*e.g.* polyisocyanates). The technical performance is examined at end product level as this is where the novel polyol structure comes into effect.

In addition, LCA and TEA studies in this project agreed on essential indicators in preparation of a multi-criteria optimization which reaches beyond the type 2 study descriptions. The project consortium found that the simultaneous analysis of the effects of altered polyol composition on Shore hardness, glass transition temperature and gelation time (technical performance parameters) and also global warming impact (GWI, of LCA) and cost of goods manufactured[*] (COGM, of TEA) allow for a sound feedback and recommendations for future development. For this optimization, the functional unit was defined as 1 kg of elastomer system. In case of the LCA, the avoided burden approach for the CO_2-supply from the ammonia plant was chosen. This approach is equivalent to the system expansion approach used in the LCA report.[9] In contrast to the LCA report, environmental impacts of the end-of-life treatment were not assessed in the optimization.

* For this optimization problem only, the scope of the TEA is restricted to the ‘cost side’ (*cf.* [3]), *i.e.* the cost estimation (COGS), for the following reasons: 1) The final property picture is incomplete, only a few (core) properties are examined, the ‘market side’ depends on the applicability of the material for special situations and cannot be generalized. 2) The form of the end product remains unknown; and is usually broadly diversified. Production cost estimation for a whole product groups is not possible. / The Scope of COGS is further restricted to COGM due to general expenses being very company-specific and mostly dependent on non process-related activities.

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Data availability was evaluated to be at mid TRL. LCA and TEA methodologies were chosen accordingly. As for the time and geographical situation, location US gulf coast, plant building date 2017, project time span 10 years and nominal plant capacity 100 kt/a were fixed. At this stage, the LCA is independent thereof. Further economic assumptions were based on typical textbook values[10–12] and practitioners experience.

II - Inventory

As main overlap between both the LCA and the TEA, the material and energy balances were identified. Collection of common data was carried out jointly and common assumptions were discussed: Environmental impacts of the side product occurring in the polyol production were allocated according to a mass allocation. The mass balance for the polyol production step was taken from pilot trials and presents the most important basis for both assessments. The demand of energy and utilities was limited to the polyol production in accordance with the system boundaries; amounts were taken from pilot trials. For the optimization, the energy balance was assumed to be independent of the mass balance.

The TEA inventory was complemented with capital investment, indirect operational expenditures and respective market data. Data for global warming impacts and costs were separately collected and evaluated for the LCA and TEA studies. Data could be obtained from relevant data bases, calculated with appropriate methods and assumed according to best practices in chemical engineering and financing. Data quality and consistency were judged by the practitioners.

III - Impact & indicator calculation

Calculation of indicators was carried out independently in the LCA and TEA study, each following best practices in their fields and using adequate software. In accordance with the goal and scope of the studies, the LCA study calculated various impact categories (*e.g.* global warming, fossil resource depletion), the TEA study calculated various indicators for the criterion profitability (*e.g.* amortization time, ROI).

In preparation of the multi-criteria optimization, the TEA calculations were altered to yield the results related to the functional unit: Absolute annual figures were divided by the effective plant capacity, returning per-kg cost increments; capital investment was allocated to the project life span similar to static capital budgeting.

IV - Interpretation

The single studies' results were discussed within the project consortium and cannot be disclosed in this report. In comparison to the benchmark system, positive impacts on both cost and GWI could be reported for the novel elastomer systems. For both studies, the material inputs show the predominant influence on both GWI and cost; the material GWI and costs, in total, exceed the contributions of the process itself.

The optimization problem is an extension of the aligned base LCA and TEA studies. It is defined in both assessments' goal and scope parts as it is a common goal of the project. The optimization was prepared in the subsequent phases of inventory collection and calculation of impacts or indicators in addition to the regular base studies' calculations. The optimization problem itself can be seen as part of the interpretation as it discusses the combination of base calculation results. For the optimization, a common model was programmed in MATLAB comprising a variable notation of the material balance, fixed GWI and cost increments for additional items and quantified structure-property relationships of the produced elastomers.

The combined assessment reveals that most chemicals in this system influence the result in the same direction for both assessments, *i.e.* an increase of the weight content of chemicals leading to a higher overall GWI also leads to higher overall cost and *vice versa*. It is suspected that this effect can be attributed to the general rule-of-thumb that for materials which incorporate more steps in the previous value-chain, the burden of both cost and GWI is increased as a result of the energy consumption added with each step. Moreover, it could be shown that for this kind of elastomers, the Shore hardness can for example be affected in the following ways:

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- Substantial increase with increasing urethane cross-linking density – entailing higher GWI and COGM
- Moderate increase with increasing CO_2 content – entailing lower GWI and COGM

As the Shore hardness is a decisive parameter of technical performance, it is assumed that higher sales prices can be achieved – an exact price-performance-correlation remains unknown. Similar correlations could be shown for other key technical performance parameters. It is suggested to expand this study to a simultaneous analysis of a full set of relevant technical parameters.

Consequences for decision making

The abovementioned chemistry and process establish a product group that is examined separately in the CroCO_2PETs project. The studies are continuously carried out and feedback is given to the project management allowing for iterative product development. The combined study is expected to play a major role in tailoring solutions for customers in need of a certain set of technical performance properties. In this way, it can facilitate the market entry and boost the product's success.

Conclusion and …what's next?

Judging an innovation's value becomes more and more difficult by reason of an increasing number of criteria across different fields of assessment. In order to come to a single decision about the continuation or alteration of a research, development and deployment pathway, it becomes necessary to align or integrate different assessments. Today, the most prevalent assessments are techno-economic and life-cycle assessment.

This report applies the recommendations introduced in a recent report on TEA & LCA Guidelines[4] for the integration of aforementioned assessments. A type 2 alignment was chosen. As a consequence two different studies were carried out but aligned to face a common goal and scope and joint collection of inventory data – leading to results that can be weighed by decision makers. In addition, proper alignment made it possible to set up a common model for simultaneous optimization of GWI and cost given desired technical performance parameters. The separated but aligned base assessments and the common model showing interrelations of LCA, TEA and technical performance help to guide the development of the novel CO_2-containing elastomers and thus prove to be a valuable tool for project management.

This concept is open for extensions to a multitude of criteria and indicators which will lead to a holistic assessment. Model descriptions showing the interrelations of a complete set of technical performance parameters to ecological and economic impacts (on the market) are encouraged. Challenges arising for full integration of different LCA and TEA such as combined indicators, system boundaries, burden allocation or cutoff criteria need to be tackled in upcoming research. The inclusion of social or risk perspectives remains another challenge for future research.

Detailed descriptions of methodology as applied for this case study as well as quantitative results will be shown in future publications by the same authors.

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