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Eco-efficient process improvement at early development stage: identifying environmental and economic process hotspots for synergetic improvement potential

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Abstract

We present here a new eco-efficiency process improvement method to highlight combined environmental and costs hotspots of the production process of new material at a very early development stage. Production specific and scaled-up results for life cycle assessment (LCA) and production costs are combined in a new analysis to identify synergetic improvement potentials and trade-offs, setting goals for the eco-design of new processes. The identified hotspots and bottlenecks will help users to focus on the relevant steps for improvements from an eco-efficiency perspective and potentially reduce their associated environmental impacts and production costs. Our method is illustrated with a case study of nanocellulose. The results indicate that the production route should start with carrot pomace, use heat and solvent recovery and deactivate the enzymes with bleach instead of heat. To further improve the process, the results show that focus should be laid on the carrier polymer, sodium alginate, and the production of the *GripX* coating. Overall, the method shows that the underlying LCA scale-up framework is valuable for purposes beyond conventional LCA studies and is applicable at a very early stage to provide researchers with a better understanding of their production process.

Keywords

scale-up, sustainable chemistry, sustainable innovation, eco-design, eco-efficiency, process improvement

Introduction

Life cycle assessment (LCA) has been established as an internationally accepted tool to measure the environmental impact of processes, products and services. As such, it is helpful in assessing and informing the development of new materials and processes that aim to achieve a more sustainable profile. During the early development stages of R&D, the degree of flexibility is still high and changes can be implemented at relatively low costs.[1] Throughout the various phases from laboratory research to possibly mini- and then pilot-plant before finally building a large-scale production plant, the incurring costs for altering the process increase drastically.[2] As a consequence, it seems recommendable to define and find the right procedures as early in the development process as possible.

The problems with early stage assessments are threefold: a) the lack of data;[3] b) particularly for chemical processes, final large-scale production plants (machineries, reactors, pipes, etc.) are not at all comparable to their respective early stage lab-scale processes. This makes it impractical to use extrapolation factors from the laboratory results to predict environmental impacts; and c) the lab-scale process has not yet been optimized and lacks the economies of scales of a production plant. An LCA of a new product under development does not therefore sufficiently reflect its potential environmental impact.

In the literature, several studies and methods can be found that aim at integrating environmental impacts into process design. Sugyiama and co-workers presented a stage-gate decision framework for chemical process design.[4] They rely on the assumption that energy loss (during reaction and separation) is an indicator of potential environmental impacts and financial costs and is composed of five weighted values, namely the presence of water, product concentration, min. boiling point difference, inherent waste amount and reaction energy.[5] Specifically for the laboratory stage, a quick preliminary assessment of chemical processes was presented based on the aforementioned stage-gate decision framework.[6] In this method, five weighted economic and environmental parameters contribute to the final score. Other approaches proposed to model lifecycle inventory data and certain LCA impact categories of chemicals by only looking at the molecular structure of the target molecule.[7,8] In a review of early stage environmental assessment of bio-based chemicals, 33 methods were examined and categorized into two groups; full assessments and early stage methods.[9] The latter was thereby further broken-down into single- and multi-indicator methods. The authors concluded that the full assessments have a broad coverage of the environmental assessment issues. However, since those assessments are data intensive, it is difficult to apply them during R&D, especially at an early stage. On the other hand, early stage methods offer a limited coverage but can be more easily applied. It is stressed that the primary goal should be to identify critical issues as early as possible and steer the R&D in the right direction.

None of the cited articles assessed potential environmental impacts through the modeling of a scaled-up cradle-to-gate production plant of the specific lab process. Azapagic and co-workers describe in their methodology how to include sustainability consideration into process design during the various design stages.[10] Only in the detailed design stage is a cradle-to-gate LCA of the process included. However, this takes place at a more advanced stage and no indication on how the laboratory process can be translated into large-scale production is given. Having such a detailed LCA study already in the preliminary stage of the process design, would therefore help in improving the process design.

Studies to determine scaling laws for LCA with empirical data of different energy equipment have already been published.[11,12] The comparison of empirical data with theoretical engineering-based values helped to distinguish between learning and scaling effects.[13] For cases where a pilot plant has been installed and an LCA study of it has been performed, a scale-up method for chemical processes has been presented.[14,15] However, this requires an existing pilot plant which is only built in an advanced developmental stage. In order to fill this gap and include a scale-up during what would be the preliminary design stage, we developed an LCA scale-up framework.[16] The framework provides an indication in the form of mathematical formulas, estimates and generic data on how a chemical laboratory process can be scaled-up for lifecycle assessment studies of a large-scale production plant.

For a product to be successful on the market, the economic side is of decisive importance.. Hence, when assessing the sustainability of a material or product, the economic aspects should never be neglected. To predict the costs of a product at a commercial scale while it is still in the laboratory stage, similar difficulties occur as with the assessment of potential environmental impact. In order to obtain a comprehensive cost estimate, a lot of detailed knowledge about the production process is needed that is usually only available at an advanced stage. The literature offers a wide range of methods to estimate product costs. Niazi and co-workers classify these into four techniques, namely the intuitive and analogical as well as the parametric and analytical technique.[17] The first two are qualitative whereas the last two are quantitative techniques. They propose a decision support model to decide which technique should be chosen based on data quality and design stage. The qualitative techniques are used in the early design stages and mostly based on past data of similar processes. For case-based reasoning approaches – an intuitive technique that uses information on design, cost and time of previous products – neural networks have been used to estimate the cost of new product development.[18] In a recent publication, a model to simulate life cycle costs has been presented that uses an algorithm that relies on similar products.[19] Other quantitative methods include mathematical models for regression analysis.[20,21] The qualitative techniques on the other side, are more suitable for more advanced stages as detailed information is needed. Such techniques include methods such as operation- or activity-based approaches where a product is decomposed into components.[22,23] Galli and co-workers performed an economic assessment of a new lab-scale chemical production process to better understand the cost behavior with differing operating conditions.[24]

Eco-efficiency analysis is an attempt to combine environmental and economic aspects and was first introduced by Schaltegger and Sturm.[2525] The goal of this approach is to optimize a process or product in both aspects, meaning that profits are maximized while the environmental impact minimized. Eco-efficiency analyses can be applied to technologies at the micro-level or at the macro-level to explore its possible implications on wider society.[26] BASF has been developing and using such an eco-efficiency approach on numerous projects by combining LCA with life cycle costing (LCC).[27,28] In this approach, BASF applied a normalization of the LCA and LCC, which is then mostly used to inform alternative selection. For example, to choose the best indigo dye production and dyeing process or to assess alternative curing and water packaging systems.[29] Eco-efficiency analyses have also proven to be useful for procurement portfolio optimization.[3030] Most of these examples, however, include the assessment of already existing processes. A more recent study applied a methodology to combine the environmental and economic assessment of a new lab-scale process for eco-design purposes.[31] It helped to find the optimal operative conditions while optimizing both, costs and the environmental impact. Their results show the importance of performing the two assessments combined as they conclude that applying the evaluations independently would result in different operative conditions.

To include a similar assessment at a very early laboratory development stage for the purpose of highlighting eco-efficiency hotspots and bottlenecks for process design, the above-described eco-efficiency analyses are limited. To assess potential environmental impacts at the industrial production of a new material or process that is still in the laboratory research stage, a framework to scale-up chemical processes for LCA studies has been developed by these authors.[16] The results showed that the impact per output unit can be reduced considerably after scale-up.[32] Even more importantly, it demonstrated that the contributions of the single production steps can change drastically between laboratory and industrial scale. This leads to different hotspots in the two LCAs. An LCA based on the lab results only could therefore lead to inefficient or even wrong prioritization for process improvement. The same can be said about the costs and thus the eco-efficiency analysis. This means that to improve a production process from an eco-efficiency perspective at a very early stage, it is of pivotal importance to include scale-up calculations.

In this manuscript, we present a specific method to improve the projected eco-efficiency of the industrial production of a given production process even though it only exists at the laboratory scale. Our scale-up framework developed for LCA purposes is expanded to include variable production costs. This new method actually consists of combining eco-efficiency analysis and this expanded scale-up framework. Instead of focusing on alternative comparison and selection, our new method mainly targets and recognizes synergetic improvement potentials of a given process and helps therefore to set design goals by highlighting hotspots and bottlenecks at a very early research stage. A case study of nanocellulose illustrates the method.

Method for estimation of scaled-up production costs and eco-efficiency analysis

A comprehensive cost estimation of a production plant includes all involved costs, which are separated into capital and operating expenditures. Capital expenditure (or investment) comprises all costs that are incurred before production plus those incurred through maintaining the production operable, while operating expenditure comprises all costs incurred through the running of a production operation. Operating expenditures can further be separated into fixed and variable costs, which are characterized by their independency from or ligation to the production output, respectively. Variable costs thus comprise costs of the resources used for the production, such as raw material, energy and electricity inputs. Labor can, depending on the case, be part of the fixed or variable costs or even both.

Estimation of capital expenditure and fixed costs is difficult at such an early stage of development. The information obtained from the scale-up is insufficient and these expenses are highly case and site specific, i.e. they depend on the specific plant design, which normally takes place after the process has been established at a more advanced developmental stage.

The same is true of the estimation of labor, which is why it is excluded from the variable cost assessment in this paper. Including prices of capital expenditures (e.g. reactors) would also mean that the longevity and production output of the plant over its entire lifespan would require inclusion, information that is difficult to obtain or estimate at such an early state and that would go beyond the scope of the presented eco-efficiency analysis specifically designed for early stage process design.

However, an estimation of the variable costs (without labor) is possible with the available information from the scale-up. Analogously to the case of the environmental impact, hotspots can be identified and recommendations for improvements are possible.

By applying the LCA scale-up framework,[16] a lot of useful information about the process is obtained beyond the fundamental purpose of LCA. Hence, the results offer the possibility to include economic calculations by estimating the costs related to production. This is due to the fact that the scale-up provides detailed quantitative data about each process step. With a simple conversion of the quantitative input and output data into their respective prices, a first estimation of the variable production costs is obtained. So far, the scale-up framework does not include detailed estimation of the impact of all reactors and equipment but uses a consolidated average value for the entire infrastructure. In addition to the above-mentioned reasons and in order to be congruent with the environmental impact values and keep efforts of this eco-efficiency simple, the capital expenditures are not added on the economic portion. If one chooses to add such data, established methods can be used to estimate capital costs, such as those that have been applied in other studies.[24]

The LCA results and such cost estimations for the production phase can then be combined to an eco-efficiency analysis. We developed such an analysis that is used in combination with the LCA scale-up framework and applied for process improvement at a very early laboratory stage. By applying this new method at an early development stage, it helps to highlight and identify hotspots for synergetic improvement potential and trade-offs and thus will influence the eco-design of a new material, being the main goal of this analysis. The application of this method offers a competitive advantage to yield a more sustainable product.

The relative contribution (in %) of a component (e.g. an entire process step or a specific input) towards the overall results of the environmental impact (i.e. LCA results) is plotted against its contribution (in %) to the costs. Such a plot graphically illustrates the environmental-to-costs-behavior of every single component. Such a component has one of three states: it behaves proportionally (1), over-proportionally (2) or under-proportionally (3) in relation to environmental impact towards financial costs. That behavior describes components with equal, higher or lower relative LCA results compared to relative costs, respectively. The second group has a higher potential to reduce the environmental impact while the third group is more likely suitable for cost reduction. The closer a value is to group 1, the higher is the potential for a synergetic effect, reducing both at the same time. Therefore, components within (or close to) group 1 seem to be the most interesting for improvement opportunities, as they are attractive from an economic as well as an environmental perspective.

Focusing on proportionality alone, does not give any information about the relevance of a component. Hence, a certain minimal contribution (e.g. 20 %) has to be defined for each case. The minimal contribution is defined as the sum of the two contributions (i.e. LCA and costs). If it exceeds that minimal contribution, it is regarded as relevant for consideration to improve the process. The further a data point is located away from this relevance barrier, the higher it should be prioritized for a more detailed analysis. This procedure automatically gives an equal weighting factor to the potential environmental impact and financial costs. Since the aim is to evaluate and improve a production process relative to its momentary state, we suggest that this equal weighting for the process improvement should be used, allowing for an equal relative improvement of both impacts.

The minimal contribution has to be defined in each case according to the goals of the analysis. As a default mode, we suggest to calculate it as 200 % (potential environmental impact and financial costs each 100 %) divided by the number of steps/data points that are evaluated. This procedure easily highlights which data points are above average.

The weighting of the relevance barrier can also be changed based on the preference of the assessor who has to define the priorities. This is important to consider as there is no normalization with an external reference value. A higher weighting of the environmental impact would flatten the slope of the relevance barrier while a higher weighting of the costs would steepen it. As a result, also the proportionality barrier would change as it is always perpendicular to the relevance barrier. This also means that the distance to the proportionality barrier should be considered relative to the weighting.

The results are best illustrated graphically (Figure 1). The proportionality barrier divides the three groups, while the relevance barrier (here 20 %), running orthogonally to it, defines the case specific minimal amount at which a component becomes relevant for improvement considerations. Every component that lies on or above the relevance barrier is treated as relevant whereas those that are below are regarded as not relevant in relation to the entire process. The relevance barrier is therefore used to choose the components (e.g. process steps) that should be prioritized when addressing improvement efforts since they bear a higher potential (due to the larger contribution). Therefore, for process design aimed at improving environmental and financial costs impacts simultaneously, the components towards the upper right corner (close to proportionality barrier and far above the relevance barrier) allow for the greatest potential.

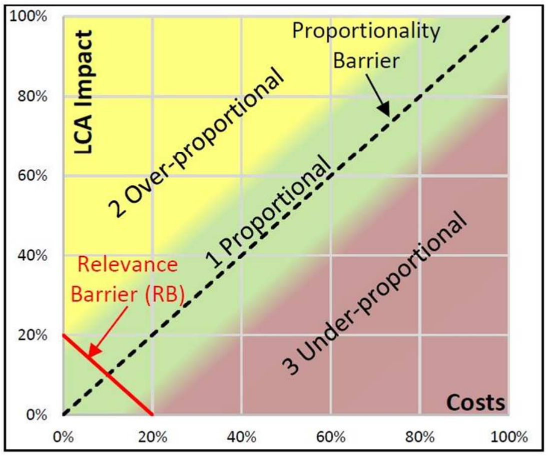

Figure 1. *Developed* e*co-efficiency analysis based on the scale-up results.*

Once a component has been identified, measures should be applied to improve it. As a result, the entire process should become more favorable from an eco-efficiency perspective. However, this has to be performed and monitored systematically to ensure that the targeted improvement measures do indeed lead to a more eco-efficient process. Figure 2 shows an example of the position of a process step that has been identified as a hotspot. After improvement measures have been undertaken, the point will most likely shift in this graph. This can include six different scenarios. In the ideal case, both impacts have been lowered, meaning that a clear improvement (++) has been achieved and the measures were successful. The opposite scenario would yield higher values for both impacts and thus a worsened process (--). In between these extreme scenarios, there is the possibility that one impact (e.g. LCA) has been lowered while the other (e.g. costs) increased. In such a case, it is not as clear whether an overall improvement has been achieved, as it requires the comparison of two factors that are not comparable *per se*. To be comparable, a monetary value must be given to the potential environmental impact (or vice versa), which is subject to a separate field of research. This evaluation is therefore in many cases subjective depending on the importance that an assessor gives to each potential impact. Our suggestion is to use the relevance barrier, which already includes a weighting. Based on this weighting, the indifference line which runs parallel to the relevance barrier and through the identified step should be used as threshold. Everything that lies below this line (+) is therefore considered as an overall improvement of the examined step while the contrary is the case above the line (-).

While the previous point holds true in most cases, an improved eco-efficiency of an identified step does not guarantee that the process has been improved overall. Changes to that step might affect (positively or negatively) other steps in the process. However, as the step has been identified as a hotspot with large contribution, it is unlikely that the production process as a whole is affected negatively. To assure that this case is excluded, an alternative assessment of the entire process is performed as a last step. The difference with an alternative assessment is that two different processes are compared on an absolute scale (i.e. points and Euros (EUR)). Here, a relevance barrier does not seem useful. Therefore, it is only distinguished between a clear process improvement (++) or impairment (--). No conclusive recommendation is given for the areas in between, leaving it in the competence of the assessor.

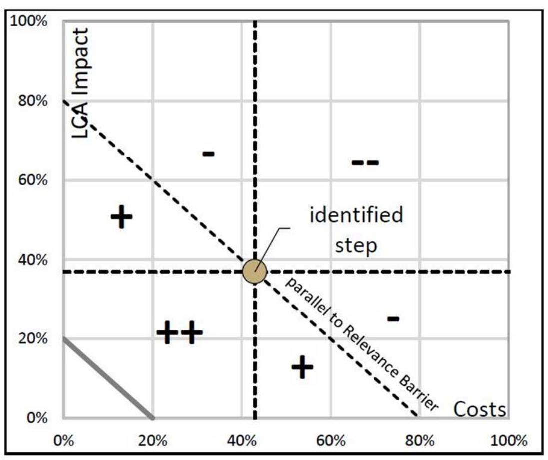

Figure 2. *Graphical illustration of areas of improvement as well as impairment.*

Case study

The case study considers a specific nanocellulose production process that uses food waste as a starting material and is still in the laboratory development stage. The process has already been scaled up by the authors, using the LCA scale-up framework to perform a cradle-to-gate LCA study.[32] Those data are, on the one hand, used for the assessment of potential environmental impact through the here-described eco-efficiency analysis and, on the other side, serve as the basis to calculate the production costs.

Only two production routes are compared from an eco-efficiency perspective to choose the more promising in the first step. Then, this selected alternative is used to illustrate the application of the eco-efficiency method. As a result, targeted recommendations are given to improve the production process. After implementation of the improvements, the results are recalculated for comparison and validation of the measures.

Eco-efficiency analysis and improvement potential. All data about the scale-up and the LCA impact using the ReCiPe endpoint indicator[33] are obtained from our LCA scale-up study.[32] As a background database, the *ecoinvent* v3.1 with the cut-off system model was used[34] and the live cycle impact assessment was calculated with the *OpenLCA* v1.4.1 software. As a cradle-to-gate study, the functional unit is 1 kg of produced nanocellulose yarn starting from the carrot waste source. The system boundaries for the LCA include all the steps including the solvent recycling and waste treatment steps whereas the obtained by-products from the enzamatic step are cut-off. A flow chart with the system boundaries can be found in the supporting information. In order to estimate the costs, we used the life cycle inventory (LCI) of the scaled-up nanocellucose production process. Every input was translated into its purchase price using average prices. However, the outputs, such as waste, were excluded. Details about prices and sources for chemicals, electricity and other inputs, are specified in the supporting information. Two alternatives are compared that only differ in the starting materials used as cellulosic sources, i.e. whole carrot waste and carrot pomace. The used LCA impact data excludes the infrastructure to be in line with the costs. Furthermore, besides the exclusion of the waste treatment, the costs have the system boundaries as the environmental impact for the functional unit of 1 kg of produced nanocellulose yarn.

According to the above-described method, we first choose the more eco-efficient of the two alternatives. Hereby, the eco-efficiency analysis clearly shows that the pomace is the preferable material given that it has a lower impact from both perspectives, environmental and costs (Figure 3). Hence, the pomace case is chosen as the more eco-efficient alternative and will be used in the following steps to improve the process itself.

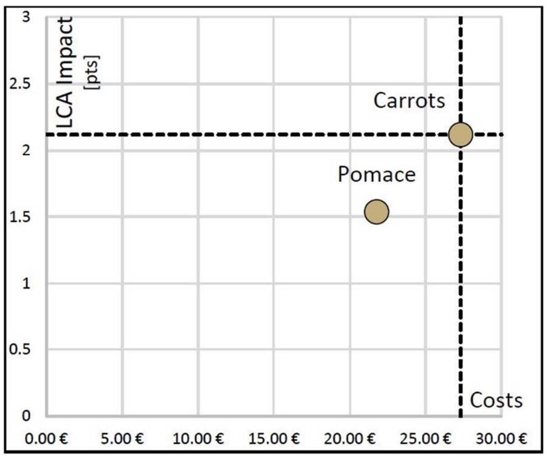

Figure 3. *Eco-efficiency per kg of produced nanocellulose yarn comparison of alternative starting materials.*

Figure 4 displays environmental-cost-behavior of the pomace case, divided into process steps. The relevance barrier was defined at 20 % with an equal weighting.

The analysis of the process steps reveals that only two steps are located above the relevance barrier, the *GripX* production – a coating copolymer that is synthesized separately and used to functionalize the cellulose – and the sodium alginate – the carrier polymer for the cellulose yarn spinning. Of these, the former can be found much further from the relevance barrier and, at the same time, displays an almost perfect proportionality. This makes it an ideal candidate for synergetic process improvement. Sodium alginate, on the other hand, is characterized by an under-proportional behavior. Therefore, the highest improvement potential can be obtained through focusing on the *GripX* (5) first and then the sodium alginate (6) which is why, for the next step, we focus on the improvement of the *GripX* step.

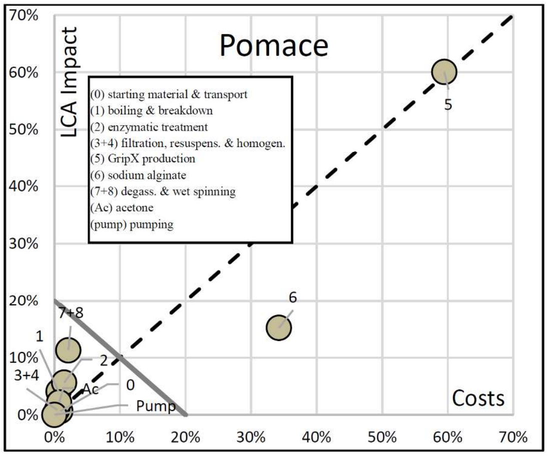

Figure 4. *Eco-efficiency analysis of the NanoCelluComp technology divided into process step.*

In order to improve the *GripX* production step, an eco-efficiency analysis of this step split into inputs sources is performed (Figure 5). Here the picture is clear that the materials used in the process contribute almost exclusively to the entire impact of both. When looking more closely into the production process this becomes more evident as vast amounts of solvents, especially ethanol with 1000 l/batch and dimethyl sulfoxide (DMSO) with 500 l/batch, are processed and disposed of afterwards. As a logical improvement step, the amount of these materials must be reduced. As these solvents are not part of the product but only used as processing materials, the implementation of measures to regain and reuse them appears to be feasible. Therefore, a distillation of the solvent waste seems to be a good option, although this will require additional heating energy.

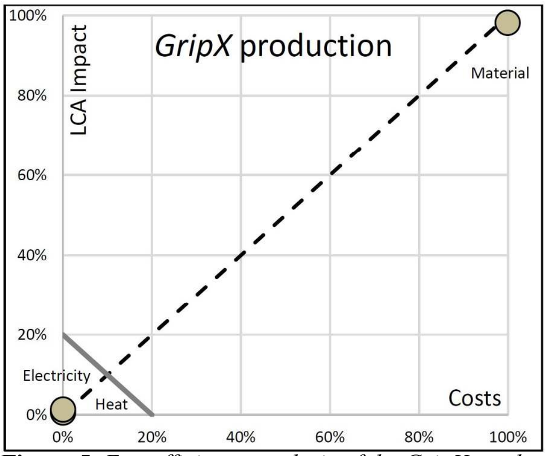

Figure 5. *Eco-efficiency analysis of the GripX production (5) step divided into input sources.*

The distillation has been included and the results recalculated (see supporting information for further specifications). Figure 6 shows the shift of step 5 after the improvement measure. The values are left relative to the overall impacts of the process without distillation for comparability reasons. Including the distillation has the effect that the *GripX* production comes closer to the barrier and switches from a proportional to clearly over-proportional behavior. It is also visible that, based on the assumptions, all the other steps are not influenced by this measure. Sodium alginate is now the component with the largest distance to the relevance barrier. This distance is mainly due to the large cost contribution, which is evidenced by the high degree of under-proportionality. Since step 5 is clearly improved from both perspectives and none of the other steps are affected, it is obvious that the overall impact of the entire process has been improved from an eco-efficiency perspective. This would make the last step, the alternative comparison before and after the measure, unnecessary. However, for the sake of completeness and illustration purposes, an alternative comparison is performed here to verify whether an eco-efficiency improvement has occurred. As anticipated, Figure 7 shows that after the inclusion of the distillation the eco-efficiency of the entire process has been improved.

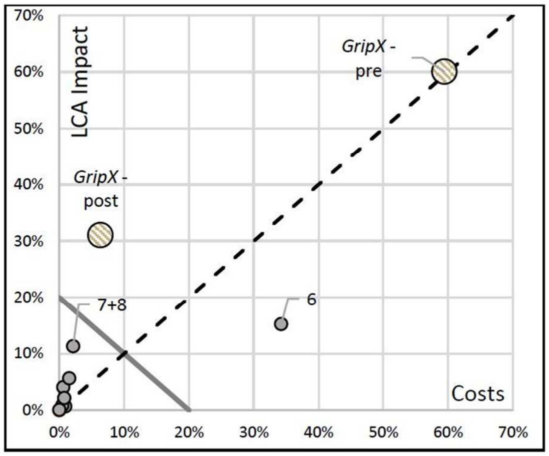

Figure 6. *Eco-efficiency shift of the GripX production step after (post) inclusion of distillation.*

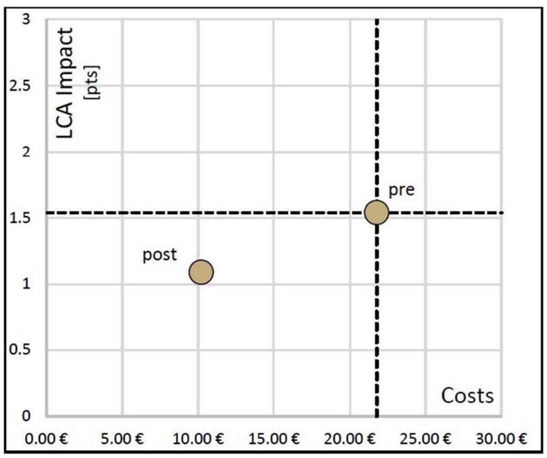

Figure 7. *Eco-efficiency per kg of produced nanocellulose yarn comparison before (pre) and after (post) inclusion of distillation.*

The presented procedure could now potentially be applied again for further process improvement with the sodium alginate (6) and the *GripX* (5) steps being the most likely to be addressed.

With solvent recovery, sodium alginate becomes a main cost factor in the yarn production. Given that the costs for the microfibrillated cellulose (MFC) production (steps 1-5) are significantly lower, spinning a yarn with a higher MFC/alginate ratio would result in lower costs. However, this is restricted by the technical feasibility of altering that ratio. Also, a higher ratio would mean a larger amount of *GripX* needed, as its quantity is coupled to the MFC, ultimately resulting in a greater potential environmental impact.

While the above-described case was used as an illustrative example using two of the calculated scenarios (i.e. 1P and 3P), the scaled-up nanocellulose production process has already been simulated and investigated from an LCA perspective using various additional production route scenarios.[32] Therefore, we applied the eco-efficiency analysis to compare all the scenarios and select the most promising one, of which, briefly, recommendations about the improvement potential are given. Details about the translation into costs of the different scenarios (Table 1) can be found in the supporting information.

Table 1. *Explanation of the different nanocellulose production systems. Adapted from Piccinno, F.; Hischier, R.; Seeger, S.; Som, C. Predicting the environmental impact of a future nanocellulose production at industrial scale: Application of the life cycle assessment scale-up framework. Journal of Cleaner Production 2018, 174, 283–295).[32] Copyright 2018 Elsevier.*

Name	Starting Material	Enzyme Deactivation	Distillation*	Heat recov. from steps	Acetone scenario
1 C	Waste of whole carrots	heat	-	-	Emission to air
2 C	Waste of whole carrots	ClO_2	-	-	Emission to air
3 C	Waste of whole carrots	heat	68/95 %	-	Emission to air
4 C	Waste of whole carrots	heat	68/95 %	1 & 2	Emission to air
5 C	Waste of whole carrots	ClO_2	68/95 %	1	Emission to air
1 P	Carrot pomace waste	heat	-	-	Emission to air
2 P	Carrot pomace waste	ClO_2	-	-	Emission to air
3 P	Carrot pomace waste	heat	68/95 %	-	Emission to air
4 P	Carrot pomace waste	heat	68/95 %	1 & 2	Emission to air
5 P	Carrot pomace waste	ClO_2	68/95 %	1	Emission to air
6 P	Carrot pomace waste	ClO_2	68/95 %	1	No acetone used
7 P	Carrot pomace waste	ClO_2	68/95 %	1	Combustion of acetone vapor

*recycling rates of solvents: H_2O and AcOH 68 %; DMSO and EtOH 95 %

A comparison of the various scenarios shows that the pomace cases with the solvent recovery (3P–7P) are clearly favorable (Figure 8) from an eco-efficiency perspective as both impacts are clearly improved. The inclusion of heat recovery (4P–7P) and deactivation of the enzymes with ClO_2 (5P–7P) instead of heat further improves the process. The difference between the three most promising scenarios (5P–7P) lies only in the handling of the acetone for solvent exchange while spinning the yarn. However, although it is the least favorable of those three, the system where the acetone vapor is burned (7P) seems to be the most realistic for implementation. Also the heat recovery from the acetone burning step is not considered, which would improve the results slightly. Therefore, the eco-efficiency analysis for the process improvement recommendations is performed with system 7P.

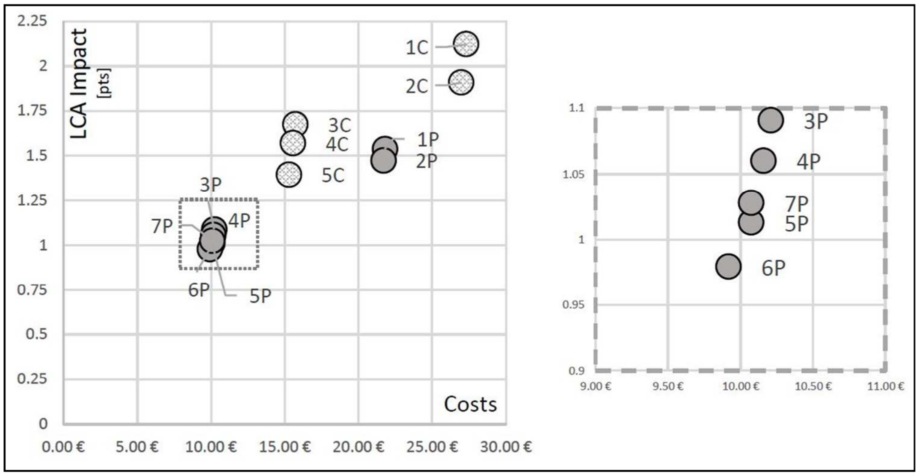

Figure 8. *Eco-efficiency alternative comparison of nanocellulose production process routes per kg nanocellulose yarn.*

The separation by source clearly shows that the material accounts for the greatest contribution (Figure 9). It displays an under-proportional behavior, hence its contribution to the potential environmental impact is lower in comparison to financial costs. Reducing the material consumption through various measures (e.g. recycling, higher yield, etc.) could have a large effect from a cost perspective, while still having a meaningful reduction of the potential environmental impact. However, if cost reduction should be targeted through the exchange of a material with an alternative of a cheaper unit price, this might cause a higher potential environmental impact (depending on the material), changing the results of this eco-efficiency analysis. This is the reason why a before-after comparison is always recommendable. Heat and electricity are the other two impact sources regarded as relevant. Both behave over-proportionally, especially in the case of heat. The use of less heating energy would thus mainly result in a relevant reduction of the potential environmental impact. The impact of the electricity consumption only surpasses the relevant state by a small amount.

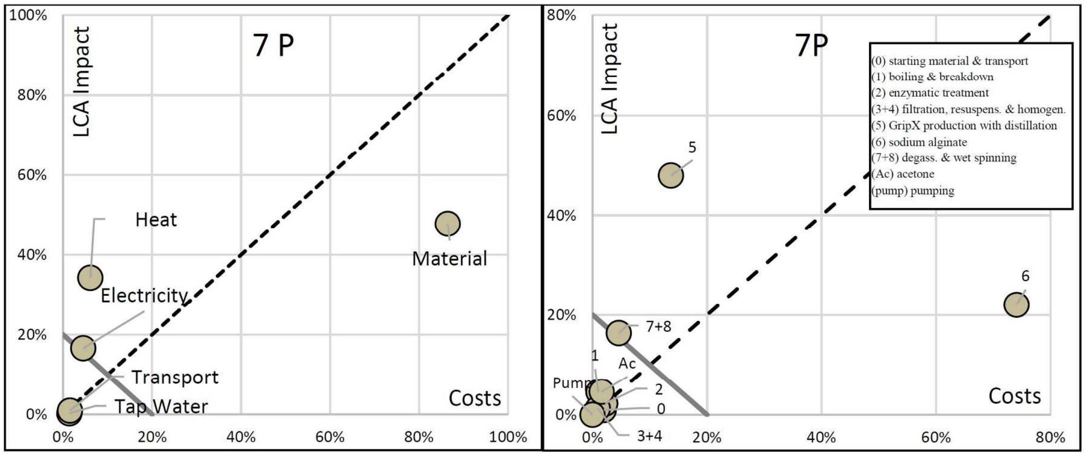

Figure 9. *Eco-efficiency analysis of the NanoCelluComp technology divided into source (left) and process steps (right).*

The analysis of the process steps reveals that sodium alginate (6), as well as the *GripX* production (5), are the two components with the highest relevance. However, the respective proportionalities are not ideal, which limits the synergetic optimization potential of the single process steps. The combination of both steps results in a very high synergetic potential given that one behaves clearly under-proportional, while for the other the opposite is the case. The alginate's distance to the relevance barrier is mainly due to the large cost contribution deriving from its high purchase price, evidenced by the high degree of under-proportionality. The opposite is the case for the over-proportional *GripX* where the cost contribution has been lowered considerably thanks to the distillation. However, its contribution to the potential environmental impact stays relatively high due to the heating involved. The third relevant process step, that just surpasses the relevance barrier, is the spinning and degassing step (7+8). The over-proportional behavior is explained by the high electricity use within this step.

Overall, the highest improvement potential of system 7P based on the analysis can therefore be obtained through first focusing on sodium alginate (6) and *GripX* (5) together and to a lesser extent, the degassing and spinning step (7+8).

Possible measures that should be investigated to improve the impact of the alginate include replacing it with a different carrier polymer, improving the yield, buying in larger amounts to reduce the purchase price and, as mentioned above, spinning at higher MFC/alginate ratio.

The impact of the *GripX* production might be reduced by replacing the solvents with other more environmentally-benign alternatives, regaining the heat from the distillation (not yet included in the calculations) and improving the yield. In contrast to the sodium alginate measure, a lower MFC/alginate spinning ratio would improve the impact caused by the *GripX* itself. Therefore, if technically feasible, the state after the improvement has to be compared as a whole to see whether changing the ratio in any direction makes sense at all.

Lastly, the spinning and degassing step might be improved through higher yields and replacement of the wet spinning with a different spinning technique.

Discussion

The case study demonstrates that the here presented new method for eco-efficiency analysis at very early development stages can provide highly valuable information to inform the prioritization of possible approaches for process improvement. The scale-up framework behind it is crucial in predicting the potential environmental impact and financial costs of the production process at a large scale. One of its advantages lies in the fact that new hotspots might be identified that would otherwise, by only looking at the lab-scale process, been missed. However, the scale-up framework for a theoretically scaled-up and predicted production plant has an influence on the quality of the data and leads to some degree of uncertainty. Hence, the results of this method should rather be regarded as indicators than as exact values, meaning that if two data points lie close to one another then they should be regarded as equal for the here described procedure.

While the method does include certain aspects of BASF's method, such as the two-dimensional plotting of costs versus LCA impact, by graphically illustrating the results, it is clear how our analysis differs. Our method focuses on the improvement of the production process, i.e. from cradle to gate only, meaning that no use phase or end-of-life consideration is included for the assessment of potential environmental impact or financial costs. This differs from other methods as they used life cycle costs or purchase prices as well as the full LCA where possible.[29] Furthermore, our method includes a procedure on how to obtain the required environmental and costs data but does not contain a normalization factor for these results.

The eco-efficiency analysis is specifically designed to be used with the scale-up data at an early development stage. Although it could also be applied without a scale-up on an existing process, we do not see its advantage over other eco-efficiency analyses in this regard. Hence, we strongly suggest to use it with the scale-up as that is where it differentiates itself from other eco-efficiency analyses and can provide additional insights. The application of the presented eco-efficiency method without performing the scale-up procedure, i.e. using the lab values, could lead to inefficient improvement recommendations. This has already been shown with the data in the LCA scale-up study of the same case where the relative contributions of the single steps have shifted considerably.[32] The same is true for the scaled-up variable costs and ultimately the eco-efficiency analysis. For that reason, the same limitations that apply to the scale-up framework are also limiting factors for this eco-efficiency method. Those include the limitation to only certain types of processes as well as the uncertainty of predicting future processes.

One key advantage over many other methods is that our method provides data with a higher degree of detail at such an early stage. Although it can be applied at a very early stage, i.e. the preliminary design stage according to Azapagic and co-workers,[10] the results in terms of degree of detail can be positioned between the early stage and full assessment methods.[9] Also, the costs are obtained without using a separate method to the LCA assessment, meaning that the scale-up is useful for both, resulting in a more straightforward procedure. However, the cost calculation is very simple and limited to considering only variable costs. Expansion of the costs modeling through inclusion of fixed costs and capital expenditures – possibly through combination with existing and established methods – could be a goal for further improvement. However, one needs to bear in mind that this would result in greater complexity as well.

The described analysis provides additional insights and information when compared to a study focusing on the LCA results or costs only. This is not as evident in the here presented case study as the results for improvement recommendations are similar to the LCA scale-up study. However, even in this study, the advantage can be seen. When comparing the LCA impact of sodium alginate (6) with the degassing and spinning (7+8) step for the 7P scenario, the values are close to each other making it difficult to identify a clear favorite (especially when uncertainty of the results is considered). However, as soon as the eco-efficiency is assessed the relevance of the sodium alginate becomes much greater and should therefore be prioritized.

We deliberately chose not to include any normalization calculations linked to external data (e.g. environmental impact of a geographical area) as this constitutes a different field of research and compromises the results. In our opinion, at this stage the relevance of the impacts is best judged by the assessor him or herself. As it would be reasonable to include a normalization step for the alternative selection to put the impacts into relation, this is not necessarily true for the process improvement analysis, which constitutes the core part of this method. As a new process or material – making it difficult to find a normalization reference (especially for the costs) –, we mainly see the contribution of the single steps towards the entire process to be the most relevant part. The advantage hereby is that an optimization from the point of the as-is state is achieved.

A broader range of real-case applications of the method will hopefully help to further refine it in future by pointing out its limitation.

The presented process improvement eco-efficiency analysis method for process improvement should be applied whenever an LCA scale-up study is performed. Only the addition of the economic perspective allows to obtain a more holistic picture and understanding of the production process and helps in setting design goals towards more eco-efficiency and, thus, sustainability. Given that all this can be achieved with minor efforts once a scale-up study has been performed, our method is a valuable additional step for process eco-design at a very early stage already.

Supporting Information

Background data for the various production systems and the cost calculations can be found in the Supporting Information document.

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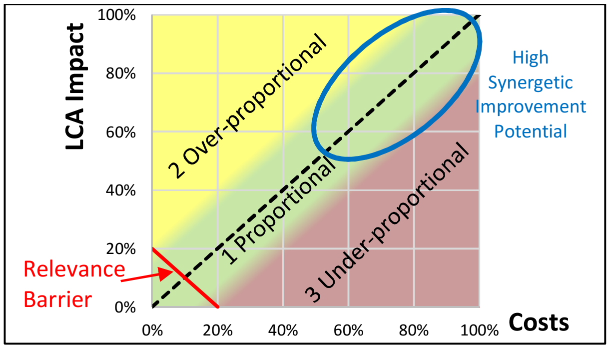

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