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Combining environmental and economic performance for bioprocess optimization

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Keywords
Life cycle assessment, Techno-economic assessment, Biochemicals, Trade-offs, Single score

Abstract
Biochemical production faces economic and environmental challenges that need to be overcome to enable a viable and sustainable bioeconomy. We propose an assessment framework that consistently combines environmental and economic indicators to support optimized biochemical production at early development stages. We define internally consistent system boundaries and a comprehensive set of quantitative indicators from life cycle assessment and techno-economic assessment to combine environmental and economic performance in a single score. Our framework enables the evaluation of trade-offs across environmental and economic aspects over the entire biochemical life cycle. This approach provides input for optimizing future biochemicals in terms of overall sustainability, to overcome prevailing obstacles in the development of biochemical production processes.

Global demand for chemicals requires environmentally and economically sustainable alternatives
The doubling of biochemical production between 2011 and 2018 [1] is an important contributor to reducing dependency on fossil resources and related environmental impacts, and to supporting a circular economy [2]. This trend is predicted to continue based on growing demand for bio-based materials across sectors including packaging, automotive, building and consumer goods (12–42% growth by 2021 compared to 2011) [1]. Increased scale-up potential and know-how in manipulating cell factories and thermochemical technologies for selective and efficient production of target molecules has led to significant research and development (R&D, see Glossary) efforts to commercialize biochemicals [3,4].

Despite several reported environmental advantages of biochemicals, not all biochemicals are consistently more sustainable compared to functionally equivalent petrochemicals [5,6]. To optimize the sustainability performance of biochemicals, both environmentally and economically, it is important to understand where along a biochemical’s life cycle relevant
hotspots (i.e. environmental problems and major costs) occur, and how changes in life cycle inputs (resources used) and outputs (emissions) can reduce such hotspots [7–9].

Currently, biochemicals represent about 2% of the global commodity chemicals market, with projections exceeding 20% by 2025 [10]. Reaching this level of market contribution, however, requires addressing current economic sustainability challenges. For example, the lack of economic competitiveness of biochemicals renders their production vulnerable to fluctuations in supply and demand of fossil-based chemicals and bio-feedstocks [11]. Along with relatively complex supply chain dynamics, this currently hampers growth of the biochemicals market [8,12,13].

From an environmental perspective, there are additional challenges for biochemical production; biochemicals are not necessarily sustainable just because they are produced from renewable feedstocks [5,6]. For example, intensive use of synthetic fertilizers in crop-based bio-feedstocks contributes to increased eutrophication, rising demand for land leads to direct and indirect changes in land use, and the impact of water use increases with extended and intensified farming. Hence, claiming environmental sustainability of biochemicals based on reduced contribution to global warming (from reduced greenhouse gas emissions, which is often the main contributor to environmental impacts of fossil-based chemicals) can be misleading if other environmental impacts are neglected, which are mainly related to feedstock production and energy-intensive pretreatment and biorefinery processes [5,6]. To achieve an overall sustainable performance for biochemicals, both economic viability and environmental sustainability challenges need to be addressed [14–19].

Today, building block biochemicals are largely produced from agricultural crops (1st generation feedstock [20]), mostly with high technological readiness levels (TRLs) of 8 (first-of-a-kind commercial system) or 9 (full commercial application) [21] (see Table 1). Production capacities for building block biochemicals and derived polymers continue to grow approximately at the same rate as production capacity for building block petrochemicals, around 3-4% annually [22]. Biochemical production from lignocellulose or wood (second-generation feedstocks, [20]) has not yet reached high TRLs, due to relatively low fermentable sugar contents, high sugar conversion costs [23], and low technical process maturity [20]. The complexity of feedstock supply chains currently hampers economic viability of biochemicals from second-generation feedstocks [12]. Due to these challenges, new feedstock sources with low TRLs of 2-3 are being
explored; these include engineered crops, algae and urban residues like household waste (third- and fourth-generation feedstocks [19,6]. Among these emerging feedstocks, brown algae receive significant attention due to the absence of lignin in their biomass, thus avoiding the need for lignin removal [3,24]. Lignin removal is costly because of recalcitrance of lignocellulosic cellulose and toxic effects on microbial properties [25]. As promising feedstocks and associated pre-processing technologies emerge, it is critical to optimize these production systems in terms of both economic and environmental sustainability to achieve market competitiveness.

Table 1

<table>
<thead>
<tr>
<th>Bio-based building block chemicals [1]</th>
<th>Technological Readiness Level (estimated, if not found in literature)</th>
<th>Feedstock for bio-based products</th>
<th>Global Production Volumes/Capacities (kt/year) from different sources, from 2015 to 2019</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,4-Butanediol (1,4-BDO)</td>
<td>8-9 [21]</td>
<td>C5 and C6 Sugars [21]</td>
<td>~60 (estimated worldwide production capacity) [1] 3 [21]</td>
</tr>
<tr>
<td>1,5-Pentamethylenediamine (DN5), Cadaverine</td>
<td>8-9</td>
<td>Decarboxylation product of the amino acid lysine [26]</td>
<td>~50 (estimated worldwide production capacity) [1]</td>
</tr>
<tr>
<td>11-Aminoundecanoic acid (11-AA)</td>
<td>6-7</td>
<td>Castor oil [27]</td>
<td>~30 (estimated worldwide production capacity) [1]</td>
</tr>
<tr>
<td>2,5-Furandicarboxylic acid (2,5-FDCA)</td>
<td>5-6 [21]</td>
<td>Starch crops, 5-(Hydroxymethyl)furfural [21]</td>
<td>~30 (estimated worldwide production capacity) [1] 0.045 [21]</td>
</tr>
<tr>
<td>Adipic acid (AA)</td>
<td>4-5 [21]</td>
<td>Sugars [21]</td>
<td>~10 (estimated worldwide production capacity) [1] 0.001 [21]</td>
</tr>
<tr>
<td>Dodecanedioic acid (DDDA)</td>
<td>4-5 [21]</td>
<td>Plant oil feedstock [28]</td>
<td>~10 (estimated worldwide production capacity) [1]</td>
</tr>
</tbody>
</table>
In typical industrial biotechnology R&D paradigms, several decisions are made when designing a cell factory, which then often face enormous economic and environmental challenges upon scale-up to market level. For instance, during strain optimization, strains are mainly selected based on yield, titer and productivity. However, the presence of specific by-

<table>
<thead>
<tr>
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<th>Technological Readiness Level (estimated, if not found in literature)</th>
<th>Feedstock for bio-based products</th>
<th>Global Production Volumes/Capacities (kt/year) from different sources, from 2015 to 2019</th>
</tr>
</thead>
<tbody>
<tr>
<td>D-Lactic acid (D-LA)</td>
<td>8-9 [21]</td>
<td>Corn, cassava, sugar cane or beets, C5 and C6 sugars [21]</td>
<td>~20 (estimated worldwide production capacity) [1]</td>
</tr>
<tr>
<td>L-Lactic acid (L-LA)</td>
<td>8-9 [21]</td>
<td>Corn, cassava, sugar cane or beets, C5 and C6 sugars [21]</td>
<td>~700 (estimated worldwide production capacity) [1]</td>
</tr>
<tr>
<td>Lactide</td>
<td>8-9 [21]</td>
<td>Corn, cassava, sugar cane or beets [21]</td>
<td>~80 (estimated worldwide production capacity) [1]</td>
</tr>
<tr>
<td>Monoethylene glycol (MEG)</td>
<td>7-8</td>
<td>Sugarcane and second-generation sugars [21]</td>
<td>~310 (estimated worldwide production capacity) [1]</td>
</tr>
<tr>
<td>Monopropylene glycol (MPG)</td>
<td>7-8</td>
<td>Glycerol [22]</td>
<td>~130 (estimated worldwide production capacity) [1]</td>
</tr>
<tr>
<td>Sebacic acid</td>
<td>8-9</td>
<td>Castor oil [1]</td>
<td>~150 (estimated worldwide production capacity) [1]</td>
</tr>
</tbody>
</table>
products may lead to higher associated downstream processing costs. Similarly, for proper upstream conversion or downstream separation of impurities, extensive use of chemicals or utilities may result in increased environmental impacts. To consider such scale-up problems, the environmental and economic performance of biochemicals production should be evaluated early in the technology development process and ideally be combined to address possible trade-offs [29]. To evaluate both environmental and economic sustainability performance, different assessment methodologies and stakeholder perspectives must be included in an iterative approach. In response to this need, we propose the systematic combination of environmental life cycle impacts and techno-economic performance in a consistent decision support framework for optimizing biochemical production processes.

Performance assessment of biochemicals: Context and fundamentals

Assessing the economic viability of future technologies is an integral part of product development in biotechnology, mainly due to substantial development costs in turning ideas into commercialized products. To assess technical and economic feasibility, techno-economic assessment (TEA, see Box 1) is a widely used tool that helps companies to define internal optimization targets to reach market sustainability. To assess the environmental sustainability of biochemicals as emerging field, product life cycle assessment (LCA, see Box 1) is gaining more and more attention in support of the global sustainable development agenda and a viable bio-economy [6]. Technological improvements may at times lead to reduced environmental impacts, while in other cases, economic benefits may come at the expense of increased environmental burden. Only when combining both TEA and LCA in a consistent framework can related trade-offs be addressed to optimize biochemical production. In support of a combined framework, we discuss the strengths and limitations of applying TEA and LCA to biochemicals separately and in combination.

Box 1

Techno-Economic Assessment (TEA): TEA is a methodology built upon the information derived from thermodynamic and material data for process development and technical optimization. Data inputs are usually processed via process systems engineering (PSE) tools, such as Aspen© and SuperPro, which can estimate the economic viability of conceptual
biochemical production processes. TEA provides insights into the technological impacts and costs of various sections in the overall production process by assigning monetary values to all of the materials, energy and other consumables needed to run a production facility. Applying TEA has helped stakeholders to understand the long-term economic impacts of technologies at various commercialization levels [30–32].

**Life Cycle Assessment (LCA):** LCA is a standardized method that involves cradle-to-grave (for biochemicals from biomass extraction to product manufacturing, use stage, and end-of-life handling such as waste treatment) or cradle-to-gate (excluding use stage and waste handling) analyses of production systems. LCA provides comprehensive inventories (in the life cycle inventory, LCI, analysis phase) and related impact evaluations (in the life cycle impact assessment, LCIA, phase) of all upstream and downstream energy and other resource inputs and multiple environmental emission outputs [33,34]. LCA studies can be costly and time-consuming. However, the efficiency of conducting LCA can be increased by using TEA as a tool to generate the required process data on LCI inputs and outputs along the product life cycle [7].

**Assessing the economic sustainability of biochemicals**

To assess technical feasibility and economic sustainability of biochemicals, TEA is widely used, with numerous published studies [9]. Some examples are provided in Table 2. Existing TEA studies mostly focus on first- and second-generation feedstocks and specific process configurations in support of direct comparisons of different products and processes, while emerging feedstocks are rarely assessed to date. The National Renewable Energy Laboratory (NREL) has been one of the key contributors to this research field and has set the standard for high quality assessments [35].

**Assessing the environmental sustainability of biochemicals**

The environmental sustainability of biochemicals is becoming increasingly important in the development of biochemicals, with some studies applying LCA [5,6]. Examples are provided in Table 2. There are surprisingly few LCA studies available assessing commodity chemicals, such as lactic acid, succinic acid, and 1,3-propanediol. Moreover, many relevant life cycle stages, such as product application (use phase of the final product) and end-of-life handling (e.g. recycling, or waste disposal), are often not assessed. However, when life cycle stages are
neglected, environmental sustainability claims of biochemicals may quickly become questionable [6].

Parallel economic and environmental sustainability assessment

In addition to performing TEA and LCA separately for biochemicals, results from both tools can be combined to evaluate environmental and economic sustainability for optimizing individual processes [36] or to assess different process designs [37,38]. Some examples are given in Table 2. Combining TEA and LCA requires a broader perspective than process optimization. This includes covering the entire biochemical life cycle from feedstock selection to waste handling and considering the broad range of environmental impacts and economic indicators, including those related to process scale-up.

With growing demand for sustainable biochemicals, industrial biotechnology could immensely benefit from early-stage assessments that guide developing both economically and environmentally viable processes. This approach helps to identify trade-offs that a separate application of TEA and LCA would not be able to reveal, leading to unnecessary environmental or economic impacts that could be avoided from the earliest stages of process development.

However, a quantitative method that consistently combines a comprehensive set of indicators from both TEA and LCA and that translates these indicators into a combined score is currently missing. In response, we propose such a combined framework and discuss its application to the early stages of biochemical production process R&D.

Table 2

<table>
<thead>
<tr>
<th>TEA and/or LCA</th>
<th>Chemical or fuel type</th>
<th>Feedstock</th>
<th>Assessed environmental impact categories*</th>
<th>Application/Intention with study and Stage of development</th>
<th>Early stage</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>TEA</td>
<td>Biodiesel</td>
<td>Mixed wood and corn-stover</td>
<td>-</td>
<td>Process design</td>
<td>-</td>
<td>[40]</td>
</tr>
<tr>
<td></td>
<td>Biodiesel and co-production of succinic acid</td>
<td>Glycerine</td>
<td>-</td>
<td>Process design</td>
<td>-</td>
<td>[41]</td>
</tr>
<tr>
<td>Ethanol</td>
<td>Softwood</td>
<td>-</td>
<td>Process assessment</td>
<td>-</td>
<td>-</td>
<td>[42]</td>
</tr>
<tr>
<td>Drop-in</td>
<td>Jatropha</td>
<td>-</td>
<td>Process assessment</td>
<td>-</td>
<td>-</td>
<td>[43]</td>
</tr>
<tr>
<td>TEA and/or LCA</td>
<td>Chemical or fuel type</td>
<td>Feedstock</td>
<td>Assessed environmental impact categories*</td>
<td>Application/Intention with study and Stage of development</td>
<td>Early stage</td>
<td>Reference</td>
</tr>
<tr>
<td>----------------</td>
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<td>-------------------------------------------</td>
<td>----------------------------------------------------------</td>
<td>-------------</td>
<td>-----------</td>
</tr>
<tr>
<td>biofuels</td>
<td>Ethanol, PHB</td>
<td>Sugarcane</td>
<td>-</td>
<td>Process assessment</td>
<td>-</td>
<td>[44]</td>
</tr>
<tr>
<td></td>
<td>Ethanol, lactic acid, methanol</td>
<td>Lignocellulosic residues</td>
<td>-</td>
<td>Process assessment</td>
<td>-</td>
<td>[45]</td>
</tr>
<tr>
<td></td>
<td>Carboxylic acids</td>
<td>Sawdust</td>
<td>-</td>
<td>Process assessment</td>
<td>-</td>
<td>[46]</td>
</tr>
<tr>
<td>LCA</td>
<td>Succinic acid</td>
<td>Lignocellulosic residues</td>
<td>GHG, CED</td>
<td>Process assessment</td>
<td>-</td>
<td>[47]</td>
</tr>
<tr>
<td></td>
<td>Succinic acid</td>
<td>Corn</td>
<td>CC, EU, ET, HT, OD, MD, and many more</td>
<td>Process assessment</td>
<td>-</td>
<td>[48]</td>
</tr>
<tr>
<td></td>
<td>Lactic acid</td>
<td>Corn</td>
<td>GHG, CED</td>
<td>Process assessment</td>
<td>-</td>
<td>[49]</td>
</tr>
<tr>
<td></td>
<td>Lactic acid</td>
<td>Lignocellulosic residues</td>
<td>GHG, CED, PM, AC, ET, EU, HT, LU, OD</td>
<td>Process assessment</td>
<td>-</td>
<td>[50]</td>
</tr>
<tr>
<td></td>
<td>1,3-Propanediol</td>
<td>Corn</td>
<td>GHG, CED, EU, HT, ET, AC</td>
<td>Process assessment</td>
<td>-</td>
<td>[51]</td>
</tr>
<tr>
<td></td>
<td>1,4-Butanediol</td>
<td>Corn</td>
<td>GHG, CED</td>
<td>Process assessment</td>
<td>-</td>
<td>[52]</td>
</tr>
<tr>
<td></td>
<td>1,4-Butanediol</td>
<td>Corn, Lignocellulosic residues</td>
<td>GHG, CED</td>
<td>Process assessment</td>
<td>-</td>
<td>[47]</td>
</tr>
<tr>
<td>Combine TEA and LCA</td>
<td>Methane</td>
<td>Power-to-gas</td>
<td>GHG</td>
<td>Process design</td>
<td>-</td>
<td>[53]</td>
</tr>
<tr>
<td></td>
<td>Bioethanol</td>
<td>Rice straw</td>
<td>GHG</td>
<td>Process design</td>
<td>-</td>
<td>[54]</td>
</tr>
<tr>
<td></td>
<td>Biodiesel</td>
<td>Microalgae</td>
<td>GHG, NER</td>
<td>Process design</td>
<td>-</td>
<td>[55]</td>
</tr>
<tr>
<td></td>
<td>Bioethanol</td>
<td>Lignocellulosic residues</td>
<td>GHG, CED</td>
<td>Process design</td>
<td>-</td>
<td>[56]</td>
</tr>
<tr>
<td></td>
<td>Biodiesel</td>
<td>Microalgae</td>
<td>GHG, EcotA, POP, EUAC, LD50</td>
<td>Process design</td>
<td>-</td>
<td>[57]</td>
</tr>
<tr>
<td></td>
<td>Blendstocks</td>
<td>Lignocellulosic residues</td>
<td>GHG</td>
<td>Product enhancement</td>
<td>yes</td>
<td>[58]</td>
</tr>
<tr>
<td></td>
<td>Biodiesel</td>
<td>Microalgae</td>
<td>GHG</td>
<td>Process optimization</td>
<td>yes</td>
<td>[36]</td>
</tr>
<tr>
<td></td>
<td>3-HPA, 1,3-PDO, SA</td>
<td>Bio-feedstock</td>
<td>GHG</td>
<td>Process design</td>
<td>yes</td>
<td>[59]</td>
</tr>
<tr>
<td></td>
<td>Butanol,</td>
<td>Corn-stover</td>
<td>GHG</td>
<td>Process design</td>
<td>yes</td>
<td>[37]</td>
</tr>
<tr>
<td>TEA and/or LCA</td>
<td>Chemical or fuel type</td>
<td>Feedstock</td>
<td>Assessed environmental impact categories*</td>
<td>Application/Intention with study and Stage of development</td>
<td>Early stage</td>
<td>Reference</td>
</tr>
<tr>
<td>---------------</td>
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<td>---------------------------------------------</td>
<td>----------------------------------------------------------</td>
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<td>-----------</td>
</tr>
<tr>
<td>ethanol</td>
<td>Biodiesel, Glycerol</td>
<td>Macroalgae</td>
<td>GHG</td>
<td>Process design</td>
<td></td>
<td>[60]</td>
</tr>
<tr>
<td>Butanol</td>
<td>Lignocellulosic residues</td>
<td>GHG</td>
<td>Process design</td>
<td>yes</td>
<td></td>
<td>[38]</td>
</tr>
<tr>
<td>Phthalic anhydride</td>
<td>Lignocellulosic residues</td>
<td>GHG, WD, FD</td>
<td>Process design</td>
<td>-</td>
<td></td>
<td>[61]</td>
</tr>
<tr>
<td>Phenol Formaldehyde resins</td>
<td>Lignocellulosic residues</td>
<td>GHG, NER</td>
<td>Process design</td>
<td>yes</td>
<td></td>
<td>[62]</td>
</tr>
<tr>
<td>Higher alcohols</td>
<td>Ethanol</td>
<td>GHG</td>
<td>Process design</td>
<td>-</td>
<td></td>
<td>[63]</td>
</tr>
<tr>
<td>1,3-Butadiene</td>
<td>Bioethanol and naphtha</td>
<td>GHG, CED</td>
<td>Process design</td>
<td>-</td>
<td></td>
<td>[64]</td>
</tr>
<tr>
<td>Energy and biofuels</td>
<td>Lignocellulosic residues</td>
<td>GHG, AC, EU, OD</td>
<td>Product selection</td>
<td>-</td>
<td></td>
<td>[39]</td>
</tr>
<tr>
<td>Biodiesel</td>
<td>Microalgae</td>
<td>GHG</td>
<td>Process design</td>
<td>yes</td>
<td></td>
<td>[65]</td>
</tr>
<tr>
<td>Biogas</td>
<td>Manure</td>
<td>GHG</td>
<td>Process design</td>
<td>-</td>
<td></td>
<td>[66]</td>
</tr>
<tr>
<td>Cellulosic isobutanol, cellulosic ethanol, n-butanol</td>
<td>Lignocellulosic residues</td>
<td>GHG, EROI, CED</td>
<td>Product comparison</td>
<td>-</td>
<td></td>
<td>[67]</td>
</tr>
<tr>
<td>Succinie acid and biofuels</td>
<td>Lignocellulosic residues</td>
<td>GHG,LU</td>
<td>Process design</td>
<td>-</td>
<td></td>
<td>[68]</td>
</tr>
<tr>
<td>Biogas and biofuels</td>
<td>Lignocellulosic residues</td>
<td>GHG, CED</td>
<td>Process design</td>
<td>yes</td>
<td></td>
<td>[69]</td>
</tr>
</tbody>
</table>

*GHG = Greenhouse Gas Emissions, CC = Climate Change, CED = Cumulative Energy Demand, AC = Acidification, EU = Eutrophication, OD = Ozone Depletion, LU = Land Use, ET = Eco-Toxicity, HT = Human Toxicity, MD = Mineral Depletion, PM = Particulate Matter, NER = Net Energy Ratio, POP = Photochemical oxidation potential, GWP = Global Warming Potential, EcotA = Aquatic ecotoxicity, EUAC = Carcinogenic emissions to urban air, LD50 = Median lethal dose, WD = Water depletion, FD = fossil depletion, EROI = Energy Return On Investment.
**Consistent combination of economic and environmental indicators**

*Outlining a combined assessment framework*

The starting point for consistently combining TEA and LCA for assessing biochemicals at early development stages is to define a common **functional unit** (e.g., 1 kg of a target biochemical produced for a specific plastic product application), and derive common assessment boundaries for the technological system (e.g., aligning the assessed system by including incineration of unfermented bio-solids from the fermentation for energy production [7]). Chemical process modelling in the TEA component creates the required inventory data for the LCA, which aligns TEA and LCA in terms of data compatibility assessed processes. To finally align TEA cost outputs with environmental impact results, LCA impact indicators (e.g. climate change, eutrophication, land use [6]) are translated into monetarized damages using monetary valuation. This facilitates a consistent combination with TEA results into a single score reflecting total costs per functional unit. All proposed alignment aspects are illustrated in **Figure 1**.

![Figure 1](image-url)
While the monetized results for each TEA and LCA indicator help to identify the predominantly contributing processes (hotspots), combining all results into a single score helps to identify trade-offs across environmental and economic indicators. Both require considering a comprehensive set of TEA and LCA indicators, including for example impacts from indirect land-use change relevant for different feedstocks [7,70]. Our overall set of proposed indicators is presented in Figure 2.

Figure 2
Impact monetization has been used before in LCA studies [71–73], but has not yet been applied to arrive at a single score to combine TEA and LCA results for biochemicals. Results for resources-related LCA indicators (e.g. mineral- and fossil resource scarcity) and for all TEA indicators are already expressed in monetary values. Human health damages in LCA are commonly expressed as disability-adjusted life years (DALY), which can be translated into cost equivalents using, for example, a monetary value of 100,000 USD/DALY [74]. In analogy, ecosystem quality damages in LCA are expressed as lost species-years, which can be translated into cost equivalents using, for example, a value of 65,000 USD per lost species-year [72]. However, there are also challenges related to accurately and objectively monetizing human health and ecosystem damages. As demonstrated e.g. for damages from greenhouse gas emissions, there are substantial differences in monetary values for human health damages mainly due to differences in considered macro- and microeconomic factors, such as decreased working capacity and malnutrition [74]. Additional challenges are related to subjective value choices in the monetization [75], which involve moral questions that affect any framework adopting monetized values for human or environmental health. Uncertainty of monetary values is therefore high, which needs to be reflected when interpreting monetized damage results along with reporting the basis for the monetization, such as willingness to pay [72] or air quality impacts [76]. Hence, refined monetary values should be applied as soon as they become available for a given decision context and always be transparently reported. This can easily be accommodated, since our framework is modular, which would also allow for identifying those values that would render a proposed technology economically competitive in a specific decision context.

Application of the combined assessment framework

We applied our combined TEA and LCA assessment framework in an illustrative case study to evaluate trade-offs between different feedstocks and production systems for the “production and use of 1 kg of lactic acid, with 99.9% purity, for polylactic acid (PLA) household packaging application in the United States” as functional unit. LCA system boundaries were defined from cradle-to-grave, and TEA system boundaries were defined from cradle-to-gate (polymerization included) [7]. Waste handling at the end-of-life of biochemicals was excluded from the TEA in our simplified example as it is highly dependent on country- or
region-specific waste handling technologies, whereas waste treatment impacts during acid production is included in our cradle-to-gate assessment [7].

Figure 3 summarizes our combined TEA and LCA case study results for four scenarios. The scenarios cover three different bio-feedstock generations: corn, corn stover and macroalgae, and for macroalgae, we analyzed separately scenarios with and without biomass drying. The environmental sustainability costs (based on LCA results) of corn stover are 46.8% higher than for corn, driven by higher energy demand in feedstock processing. This is mainly due to increased energy consumption for the separation of fiber-rich corn stover biomass (assumed to be done via steam explosion), which is not needed to pre-treat corn biomass. We modeled this higher energy demand to be derived 88% from fossil resources matching the current US energy mix [7], which mostly affects damages on human health and natural resources.

![Figure 3](image)

Comparing the TEA results for lactic acid produced from corn (first-generation) and corn stover (second-generation) shows that economic costs of the second-generation feedstock are
25% lower. Despite lower overall yield, feedstock costs for corn stover are significantly less compared to corn. This is influenced by the monetary value assigned to a corn stover unit [35], which will increase significantly with plant size due to transportation and the low fraction of fermentable sugars present in corn stover [12]. Furthermore, the lower level of optimization and TRL of the corn stover process, along with its more fiber-rich biomass composition, requires a more intense separation process, which demands higher chemical concentrations and energy use. Therefore, the energy usage of second-generation process is one order of magnitude higher than that of the first-generation process. However, this only adds 0.5 USD per kg produced lactic acid in the TEA results as utility costs are only a minor contributor to overall TEA results. We emphasize that this example trade-off between lower economic costs but higher environmental costs of corn stover compared to corn can only be assessed in a combined TEA-LCA assessment.

When analyzing the results in further detail, we observe that for corn and corn stover, environmental impacts are highest for human health. For corn, these are driven by indirect land-use change, increasing the effect on global warming due to the increased demand for arable land [77]. In contrast, for corn stover, these impacts are driven by global warming related to the high energy demand of the biorefinery stage, due to intensive energy use during biomass pretreatment.

Feedstock costs for lactic acid produced from macroalgae (a third-generation feedstock) account for almost 50% of the total economic costs (based on TEA results) (see Figure 3). Energy utilities comprise about 20% of these costs, with drying as the main contributing process. Excluding drying results in a decrease in steam use of more than 100 MJ per kg lactic acid, but this has only a low effect on total costs per functional unit due to the low price of steam. On the other hand, analyzing the reduction in steam use in the LCA results shows that the related environmental impacts per functional unit are reduced by more than 40%. By comparing the total cost results for macroalgae-based lactic acid production, we can pinpoint the trade-offs between drying and not drying biomass, which a separate application of TEA and LCA would not have revealed.

**Concluding remarks**

We have described how a consistent combination of TEA and LCA into a single score can support decisions in early R&D stages of biochemical production processes. In addition to
combining LCA and TEA, there are other approaches focusing on multi-objective process optimization, for example pareto-based process optimization, usually called non-dominated or non-inferior [78], as well as data envelopment analysis focused on evaluating relative efficiency [79]. However, while such approaches might provide more objective results than a single score, they are often hard to interpret for decision makers.

With growing needs for chemicals that are aligned with global sustainable development goals and circular economy targets [80], industrial biotechnology can benefit from early-stage assessments that guide developing biochemicals that are both economically and environmentally sustainable. In this context, Figure 3 demonstrates that it is important to develop microbial fermentation strains that can feed on non-dried macroalgae without lowering biomass yield. Results from this assessment framework, with different scenarios, can furthermore help identify to what extent conversion yields to lactic acid or fermentation productivity are relevant when considering both economic and environmental sustainability. These combined results from the proposed assessment framework could serve as a yardstick by research organizations and companies to rank biochemical development projects based on their combined TEA and LCA performance. Furthermore, our framework could be applied iteratively to optimize entire production schemes with respect to a viable biochemical production idea from both an economic and environmental sustainability perspective.

Identifying combined economic and environmental hotspots provides insights into costs that could be mitigated by adopting certain strategies early in the biochemical development process. Energy-associated costs appear as a hotspot in TEA and LCA across our case study scenarios. For example, for macroalgae feedstock, drying the biomass has the biggest effect on energy use (accounting for more than 50% of the energy utilities). Removing macroalgae drying affects the TEA results only by 7%, but indirect LCA-related costs from energy use are reduced by 61% in countries relying on fossil fuels as a source for energy [7].

Overall, we have highlighted that it is crucial to account for both economic and environmental sustainability aspects for optimizing overall performance of biochemical production, thereby providing the foundation for increased market competitiveness. This can be accomplished by considering aligned systems (i.e. same process unit operations and energy and materials balances), using a comprehensive set of indicators to cover all product life cycle stages, and expressing TEA and LCA results in comparable units. While many research questions

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remain to be addressed for developing biochemicals (see Outstanding Questions), we hope that our proposed assessment framework can help the bioeconomy to become economically viable and environmentally sustainable in line with global sustainability targets and market goals.

**Disclaimer Statement**

The authors have no conflict of interest to disclose.

**Captions:**

Table 1. List of 17 building block chemicals, their technological readiness levels (TRLs), used feedstocks and current global production volumes.

Box 2. Techno-economic assessment (TEA) and life cycle assessments (LCA) for optimizing biochemical production.

Table 2. Techno-economic assessment (TEA) and life cycle assessment (LCA) studies applied individually or in combination to evaluate one or more processes in the production of biochemicals.

Figure 4. Early stage assessment framework for combined techno-economic assessment (TEA) and environmental life cycle assessment (LCA) as a decision support tool in biotechnology. The framework starts with acquiring the relevant raw data, followed by various alignment steps of both assessment methods, then impact aggregation and monetarization, finally aggregated into a single score for decision support.

Figure 5. Proposed approach for consistently combining indicators for environmental sustainability impacts using life cycle assessment (LCA), aggregated into areas of protection (AoP) and translated into monetized damage costs, with indicators for economic sustainability impacts using techno-economic assessment (TEA) into a monetary single score, expressed in total sustainability costs per given functional unit. *Environmental impacts include also impacts from indirect land-use change (iLUC).
Figure 6. Contribution of monetarized environmental impacts and economic impact costs to a total costs per functional unit of 1 kg of polylactic acid (PLA) from three different bio-feedstock generations and different process systems for macroalgae [7].
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Glossary

**Bio-feedstock:** an organic substrate that can be converted into biochemical products. Bio-feedstocks are divided into generations depending on the state of development of methods to use the biomass for biochemical production. Agricultural crops are defined as first-generation bio-feedstock, lignocellulose or wood as second-generation, and engineered crops, algae and organic (municipal and/or agricultural) wastes as either third- or fourth-generation bio-feedstocks (a general definition of third- and fourth-generation bio-feedstocks is currently not available).

**Building block biochemicals:** molecules that build the foundation of various secondary chemicals and intermediates derived for different applications and uses.

**Functional unit:** a quantitative description of the function or service of any given product system for which an assessment is performed. An example of a functional unit is “The utilization of 1 kg of lactic acid, with 99.9% purity, for household product packaging application in the United States”.

**Hotspots:** in assessment results, impacts that stand out compared to other results. Identifying hotspots in techno-economic and/or life cycle assessments shows where to focus future process optimization with respect to the chosen indicators for the given product.

**Life cycle:** here, the different stages a biochemical goes through during its lifetime. A full life cycle of biochemical production (e.g., derived via microbial fermentation) includes the following stages: 1) cultivation and harvesting, 2) biomass pretreatment, 3) fermentation and purification, 4) product making (application dependent, e.g. forming, molding), 5) use stage, and 6) waste handling.

**R&D:** research and development, referring to activities initiated to develop new products, services or product systems, or to further improve already available products, services or product systems.

**Trade-offs:** the increase in performance of one indicator and simultaneous decrease in performance in another indicator. Trade-offs occur, for example, when economic performance is improved due to a change in product composition or production system, which negatively affects environmental performance results, or vice versa. This is also referred to as ‘burden shifting’ from one aspect (that improves) to another (that gets worse).

**TRL:** technological readiness level, a tool developed by the National Aeronautics and Space Administration (NASA) to consistently and uniformly estimate the maturity of technologies.
scale ranges from TRL 1, which defines the lowest level of technological readiness, to TRL 9, which is the highest level of technological readiness, the technology in its final form.