



Combining Environmental and Economic Performance for Bioprocess Optimization

Ögmundarson, Ólafur; Sukumara, Sumesh; Herrgård, Markus J.; Fantke, Peter

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2

3 **Combining environmental and economic performance for**

4 **bioprocess optimization**

5 Ólafur Ögmundarson^{a,b,1,*}, Sumesh Sukumara^b, Markus J. Herrgård^{b,2}, Peter Fantke^{a*}

6

7 ^a Quantitative Sustainability Assessment, Department of Technology, Management and
8 Economics, Technical University of Denmark, Produktionstorvet 424, 2800 Kgs. Lyngby,
9 Denmark

10 ^b The Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark,
11 Kemitorget 220, 2800 Kgs. Lyngby, Denmark

12

13 *Corresponding authors:

14 Ólafur Ögmundarson: Tel.: +354 7885528, e-mail: olafuro@hi.is

15 Peter Fantke: Tel.: +45 45254452, e-mail: pefan@dtu.dk

16

17 ¹Current affiliation: Faculty of Food Science and Nutrition, University of Iceland, Reykjavík, Iceland

18 ²Current affiliation: BioInnovation Institute, Ole Maaløes Vej 3, 2200 Copenhagen N, Denmark

19

20

21 ORCID:

22 Ólafur Ögmundarson: <https://orcid.org/0000-0003-3171-2388>

23 Sumesh Sukumara: <https://orcid.org/0000-0002-7924-458X>

24 Markus J. Herrgård: <http://orcid.org/0000-0003-2377-9929>

25 Peter Fantke: <http://orcid.org/0000-0001-7148-6982>

26

27 Twitter:

28 ^a https://twitter.com/QSA_DTU

29 ^b <https://twitter.com/DTUBiosustain>

30 ¹ https://twitter.com/mat_naer_hi

31

32 Facebook:

33 ^b <https://www.facebook.com/biosustain/>

34 ¹ <https://www.facebook.com/pg/hi.foodsciencenutrition/community/>

35 ^c <https://www.facebook.com/BioInnovationInstitute/>

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36 **Keywords**

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

38

39 **Abstract**

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

50

51 **Global demand for chemicals requires environmentally and economically** 52 **sustainable alternatives**

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

61 Despite several reported environmental advantages of biochemicals, not all biochemicals
62 are consistently more sustainable compared to functionally equivalent petrochemicals [5,6]. To
63 optimize the sustainability performance of biochemicals, both environmentally and
64 economically, it is important to understand where along a biochemical's **life cycle** relevant

65 **hotspots** (i.e. environmental problems and major costs) occur, and how changes in life cycle
66 inputs (resources used) and outputs (emissions) can reduce such hotspots [7–9].

67 Currently, biochemicals represent about 2% of the global commodity chemicals market,
68 with projections exceeding 20% by 2025 [10]. Reaching this level of market contribution,
69 however, requires addressing current economic sustainability challenges. For example, the lack
70 of economic competitiveness of biochemicals renders their production vulnerable to fluctuations
71 in supply and demand of fossil-based chemicals and **bio-feedstocks** [11]. Along with relatively
72 complex supply chain dynamics, this currently hampers growth of the biochemicals market.
73 [8,12,13].

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

86 Today, **building block biochemicals** are largely produced from agricultural crops (1st
87 generation feedstock [20]), mostly with high technological readiness levels (**TRLs**) of 8 (first-of-
88 a-kind commercial system) or 9 (full commercial application) [21] (see **Table 1**). Production
89 capacities for building block biochemicals and derived polymers continue to grow approximately
90 at the same rate as production capacity for building block petrochemicals, around 3-4% annually
91 [22]. Biochemical production from lignocellulose or wood (second-generation feedstocks, [20])
92 has not yet reached high TRLs, due to relatively low fermentable sugar contents, high sugar
93 conversion costs [23], and low technical process maturity [20]. The complexity of feedstock
94 supply chains currently hampers economic viability of biochemicals from second-generation
95 feedstocks [12]. Due to these challenges, new feedstock sources with low TRLs of 2-3 are being

96 explored; these include engineered crops, algae and urban residues like household waste (third-
 97 and fourth-generation feedstocks [19,6]. Among these emerging feedstocks, brown algae receive
 98 significant attention due to the absence of lignin in their biomass, thus avoiding the need for
 99 lignin removal [3,24]. Lignin removal is costly because of recalcitrance of lignocellulosic
 100 cellulose and toxic effects on microbial properties [25]. As promising feedstocks and associated
 101 pre-processing technologies emerge, it is critical to optimize these production systems in terms
 102 of both economic and environmental sustainability to achieve market competitiveness.

103

104 **Table 1**

Bio-based building block chemicals [1]	Technological Readiness Level (estimated, if not found in literature)	Feedstock for bio-based products	Global Production Volumes/Capacities (kt/year) from different sources, from 2015 to 2019
1,3-Propanediol (1,3-PDO)	8-9 [21]	Corn glucose, sugars and glycerol [21]	~130 (estimated worldwide production capacity) [1] 128 [21]
1,4-Butanediol (1,4-BDO)	8-9 [21]	C5 and C6 Sugars [21]	~60 (estimated worldwide production capacity) [1] 3 [21]
1,5-Pentamethylenediamine (DN5), Cadaverine	8-9	Decarboxylation product of the amino acid lysine [26]	~50 (estimated worldwide production capacity) [1]
11-Aminoundecanoic acid (11-AA)	6-7	Castor oil [27]	~30 (estimated worldwide production capacity) [1]
2,5-Furandicarboxylic acid (2,5-FDCA)	5-6 [21]	Starch crops, 5-(Hydroxymethyl)furfural [21]	~30 (estimated worldwide production capacity) [1] 0.045 [21]
Adipic acid (AA)	4-5 [21]	Sugars [21]	~10 (estimated worldwide production capacity) [1] 0.001 [21]
Dodecanedioic acid (DDDA)	4-5 [21]	Plant oil feedstock [28]	~10 (estimated worldwide production capacity) [1]

Bio-based building block chemicals [1]	Technological Readiness Level (estimated, if not found in literature)	Feedstock for bio-based products	Global Production Volumes/Capacities (kt/year) from different sources, from 2015 to 2019
D-Lactic acid (D-LA)	8-9 [21]	Corn, cassava, sugar cane or beets, C5 and C6 sugars [21]	~20 (estimated worldwide production capacity) [1]
L-Lactic acid (L-LA)	8-9 [21]	Corn, cassava, sugar cane or beets, C5 and C6 sugars [21]	~700 (estimated worldwide production capacity) [1]
Lactide	8-9 [21]	Corn, cassava, sugar cane or beets [21]	~80 (estimated worldwide production capacity) [1]
Epichlorohydrin (ECH)	8-9 [21]	Glycerol [22]	~490 (estimated worldwide production capacity) [1]
Ethylene	8-9 [21]	Glucose [1], sugar cane, sweet sorghum, corn [21]	~200 (estimated worldwide production capacity) [1] 200 [21]
Isosorbide	7-8 [21]	Glucose [1]	~20 (estimated worldwide production capacity) [1]
Monoethylene glycol (MEG)	7-8	Sugarcane and second-generation sugars [21]	~310 (estimated worldwide production capacity) [1]
Monopropylene glycol (MPG)	7-8	Glycerol [22]	~130 (estimated worldwide production capacity) [1]
Sebacic acid	8-9	Castor oil [1]	~150 (estimated worldwide production capacity) [1]
Succinic acid (SA)	8-9 [21]	C5 and C6 sugars [21]	~70 (estimated worldwide production capacity) [1] 38 [21]

105

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107

108

109

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-

110 products may lead to higher associated downstream processing costs. Similarly, for proper
111 upstream conversion or downstream separation of impurities, extensive use of chemicals or
112 utilities may result in increased environmental impacts. To consider such scale-up problems, the
113 environmental and economic performance of biochemicals production should be evaluated early
114 in the technology development process and ideally be combined to address possible **trade-offs**
115 [29]. To evaluate both environmental and economic sustainability performance, different
116 assessment methodologies and stakeholder perspectives must be included in an iterative
117 approach. In response to this need, we propose the systematic combination of environmental life
118 cycle impacts and techno-economic performance in a consistent decision support framework for
119 optimizing biochemical production processes.

120

121 **Performance assessment of biochemicals: Context and fundamentals**

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

135

136 **Box 1**

137 **Techno-Economic Assessment (TEA):** TEA is a methodology built upon the information
138 derived from thermodynamic and material data for process development and technical
139 optimization. Data inputs are usually processed via process systems engineering (PSE) tools,
140 such as Aspen[®] and SuperPro, which can estimate the economic viability of conceptual

141 biochemical production processes. TEA provides insights into the technological impacts and
142 costs of various sections in the overall production process by assigning monetary values to all of
143 the materials, energy and other consumables needed to run a production facility. Applying TEA
144 has helped stakeholders to understand the long-term economic impacts of technologies at various
145 commercialization levels [30–32].

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

155
156 *Assessing the economic sustainability of biochemicals*

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

164
165 *Assessing the environmental sustainability of biochemicals*

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

172 neglected, environmental sustainability claims of biochemicals may quickly become
173 questionable [6].

174

175 *Parallel economic and environmental sustainability assessment*

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

183 With growing demand for sustainable biochemicals, industrial biotechnology could
184 immensely benefit from early-stage assessments that guide developing both economically and
185 environmentally viable processes. This approach helps to identify trade-offs that a separate
186 application of TEA and LCA would not be able to reveal, leading to unnecessary environmental
187 or economic impacts that could be avoided from the earliest stages of process development.
188 However, a quantitative method that consistently combines a comprehensive set of indicators
189 from both TEA and LCA and that translates these indicators into a combined score is currently
190 missing. In response, we propose such a combined framework and discuss its application to the
191 early stages of biochemical production process R&D.

192

193 **Table 2**

TEA and/or LCA	Chemical or fuel type	Feedstock	Assessed environmental impact categories*	Application/Intention with study and Stage of development	Early stage	Reference
TEA	Biodiesel	Mixed wood and corn-stover	-	Process design	-	[40]
	Biodiesel and co-production of succinic acid	Glycerine	-	Process design	-	[41]
	Ethanol	Softwood	-	Process assessment	-	[42]
	Drop-in	Jatropha	-	Process assessment	-	[43]

TEA and/or LCA	Chemical or fuel type	Feedstock	Assessed environmental impact categories*	Application/Intention with study and Stage of development	Early stage	Reference
	biofuels					
	Ethanol, PHB	Sugarcane	-	Process assessment	-	[44]
	Ethanol, lactic acid, methanol	Lignocellulosic residues	-	Process assessment	-	[45]
	Carboxylic acids	Sawdust	-	Process assessment	-	[46]
LCA	Succinic acid	Lignocellulosic residues	GHG, CED	Process assessment	-	[47]
	Succinic acid	Corn	CC,EU,ET,HT,OD, MD, and many more	Process assessment	-	[48]
	Lactic acid	Corn	GHG, CED	Process assessment	-	[49]
	Lactic acid	Lignocellulosic residues	GHG,CED,PM,AC,ET, EU,HT,LU,OD	Process assessment	-	[50]
	1,3-Propanediol	Corn	GHG,CED,EU,HT,ET, AC	Process assessment	-	[51]
	1,4-Butanediol	Corn	GHG,CED	Process assessment	-	[52]
	1,4-Butanediol	Corn, Lignocellulosic residues	GHG,CED	Process assessment	-	[47]
Combine d TEA and LCA	Methane	Power-to-gas	GHG	Process design	-	[53]
	Bioethanol	Rice straw	GHG	Process design	-	[54]
	Biodiesel	Microalgae	GHG, NER	Process design	-	[55]
	Bioethanol	Lignocellulosic residues	GHG, CED	Process design	-	[56]
	Biodiesel	Microalgae	GHG, EcotA, POP, EUAC, LD50	Process design	-	[57]
	Blendstocks	Lignocellulosic residues	GHG	Product enhancement	yes	[58]
	Biodiesel	Microalgae	GHG	Process optimization	yes	[36]
	3-HPA, 1,3-PDO, SA	Bio-feedstock	GHG	Process design	yes	[59]
	Butanol,	Corn-stover	GHG	Process design	yes	[37]

TEA and/or LCA	Chemical or fuel type	Feedstock	Assessed environmental impact categories*	Application/Intention with study and Stage of development	Early stage	Reference
	ethanol					
	Biodiesel, Glycerol	Macroalgae	GHG	Process design	-	[60]
	Butanol	Lignocellulosic residues	GHG	Process design	yes	[38]
	Phthalic anhydride	Lignocellulosic residues	GHG, WD, FD	Process design	-	[61]
	Phenol Formaldehyd de resins	Lignocellulosic residues	GHG, NER	Process design	yes	[62]
	Higher alcohols	Ethanol	GHG	Process design	-	[63]
	1,3-Butandiene	Bioethanol and naphtha	GHG, CED	Process design	-	[64]
	Energy and biofuels	Lignocellulosic residues	GHG,AC,EU,OD	Product selection	-	[39]
	Biodiesel	Microalgae	GHG	Process design	yes	[65]
	Biogas	Manure	GHG	Process design	-	[66]
	Cellulosic isobutanol, cellulosic ethanol, n-butanol	Lignocellulosic residues	GHG,EROI, CED	Product comparison	-	[67]
	Succinic acid and biofuels	Lignocellulosic residues	GHG,LU	Process design	-	[68]
	Biogas and biofuels	Lignocellulosic residues	GHG,CED	Process design	yes	[69]

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

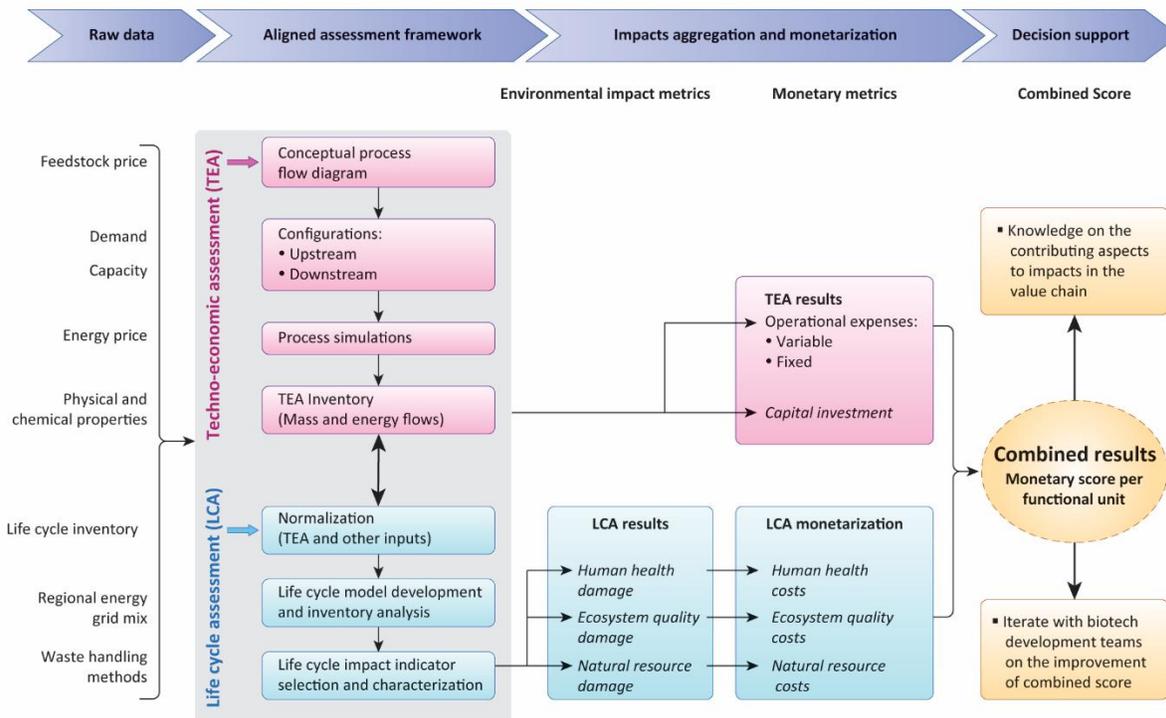
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201 **Consistent combination of economic and environmental indicators**

202 *Outlining a combined assessment framework*

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

214

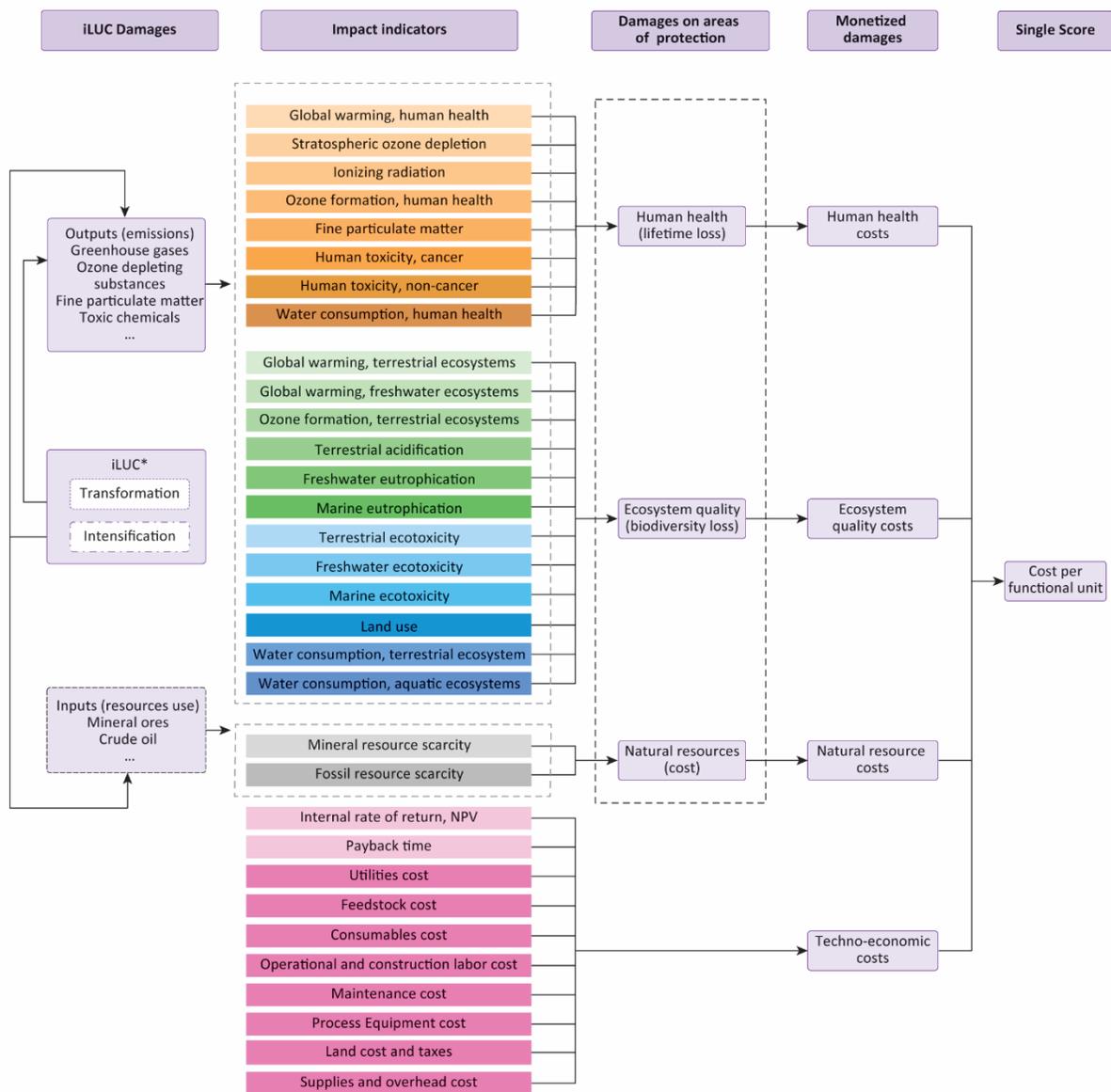


215

216 **Figure 1**

217

218 While the monetized results for each TEA and LCA indicator help to identify the
 219 predominantly contributing processes (hotspots), combining all results into a single score helps
 220 to identify trade-offs across environmental and economic indicators. Both require considering a
 221 comprehensive set of TEA and LCA indicators, including for example impacts from indirect
 222 land-use change relevant for different feedstocks [7,70]. Our overall set of proposed indicators is
 223 presented in **Figure 2**.
 224



225
 226 **Figure 2**
 227

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

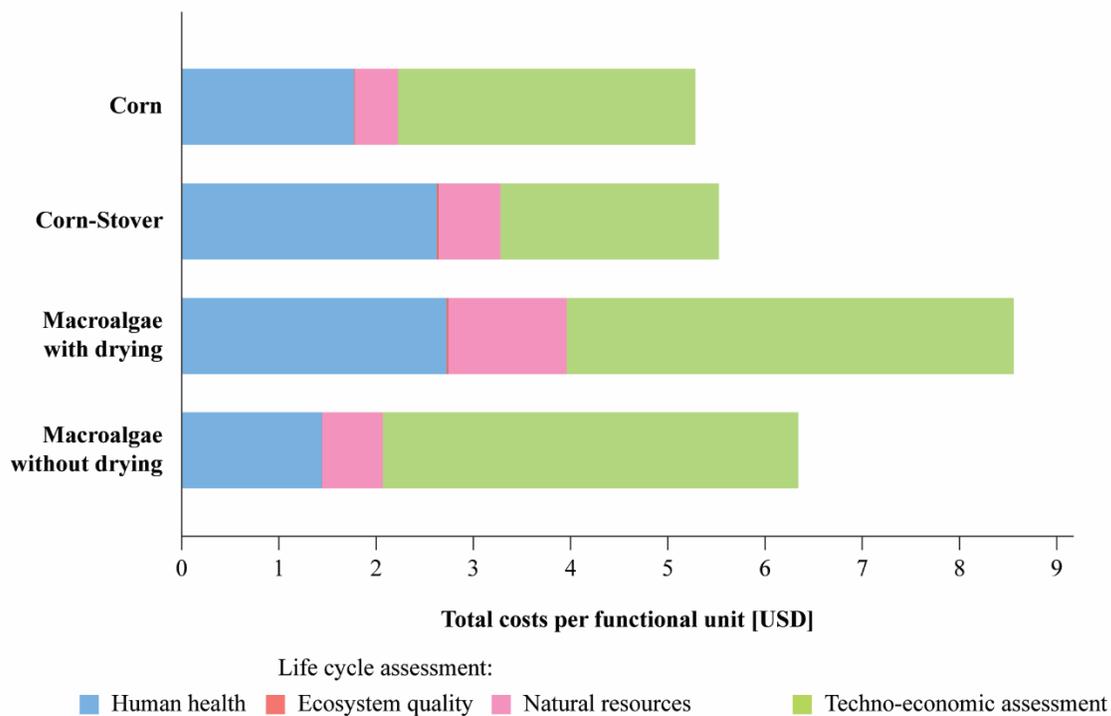
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251 *Application of the combined assessment framework*

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

259 region-specific waste handling technologies, whereas waste treatment impacts during acid
260 production is included in our cradle-to-gate assessment [7].

261 **Figure 3** summarizes our combined TEA and LCA case study results for four scenarios.
262 The scenarios cover three different bio-feedstock generations: corn, corn stover and macroalgae,
263 and for macroalgae, we analyzed separately scenarios with and without biomass drying. The
264 environmental sustainability costs (based on LCA results) of corn stover are 46.8% higher than
265 for corn, driven by higher energy demand in feedstock processing. This is mainly due to
266 increased energy consumption for the separation of fiber-rich corn stover biomass (assumed to
267 be done via steam explosion), which is not needed to pre-treat corn biomass. We modeled this
268 higher energy demand to be derived 88% from fossil resources matching the current US energy
269 mix [7], which mostly affects damages on human health and natural resources.
270



271
272 **Figure 3**

273
274 Comparing the TEA results for lactic acid produced from corn (first-generation) and corn
275 stover (second-generation) shows that economic costs of the second-generation feedstock are

276 25% lower. Despite lower overall yield, feedstock costs for corn stover are significantly less
277 compared to corn. This is influenced by the monetary value assigned to a corn stover unit [35],
278 which will increase significantly with plant size due to transportation and the low fraction of
279 fermentable sugars present in corn stover [12]. Furthermore, the lower level of optimization and
280 TRL of the corn stover process, along with its more fiber-rich biomass composition, requires a
281 more intense separation process, which demands higher chemical concentrations and energy use.
282 Therefore, the energy usage of second-generation process is one order of magnitude higher than
283 that of the first-generation process. However, this only adds 0.5 USD per kg produced lactic acid
284 in the TEA results as utility costs are only a minor contributor to overall TEA results. We
285 emphasize that this example trade-off between lower economic costs but higher environmental
286 costs of corn stover compared to corn can only be assessed in a combined TEA-LCA assessment.

287 When analyzing the results in further detail, we observe that for corn and corn stover,
288 environmental impacts are highest for human health. For corn, these are driven by indirect land-
289 use change, increasing the effect on global warming due to the increased demand for arable land
290 [77]. In contrast, for corn stover, these impacts are driven by global warming related to the high
291 energy demand of the biorefinery stage, due to intensive energy use during biomass
292 pretreatment.

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

303

304 **Concluding remarks**

305 We have described how a consistent combination of TEA and LCA into a single score
306 can support decisions in early R&D stages of biochemical production processes. In addition to

307 combining LCA and TEA, there are other approaches focusing on multi-objective process
308 optimization, for example pareto-based process optimization, usually called non-dominated or
309 non-inferior [78], as well as data envelopment analysis focused on evaluating relative efficiency
310 [79]. However, while such approaches might provide more objective results than a single score,
311 they are often hard to interpret for decision makers.

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

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

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

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

341

342 **Disclaimer Statement**

343 The authors have no conflict of interest to disclose.

344

345 Captions:

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

348

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

351

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

355

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

361

362 **Figure 5.** Proposed approach for consistently combining indicators for environmental
363 sustainability impacts using life cycle assessment (LCA), aggregated into areas of protection
364 (AoP) and translated into monetized damage costs, with indicators for economic sustainability
365 impacts using techno-economic assessment (TEA) into a monetary single score, expressed in
366 total sustainability costs per given functional unit. *Environmental impacts include also impacts
367 from indirect land-use change (iLUC).

368

369 **Figure 6.** Contribution of monetarized environmental impacts and economic impact costs to a
370 total costs per functional unit of 1 kg of polylactic acid (PLA) from three different bio-feedstock
371 generations and different process systems for macroalgae [7].

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566 **Glossary**

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

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

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

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

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

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

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

595 **TRL:** technological readiness level, a tool developed by the National Aeronautics and Space
596 Administration (NASA) to consistently and uniformly estimate the maturity of technologies. The

597 scale ranges from TRL 1, which defines the lowest level of technological readiness, to TRL 9,
598 which is the highest level of technological readiness, the technology in its final form.

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