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Review

Integration of LCA, TEA, Process Simulation and Optimization: A systematic review of current practices and scope to propose a framework for pulse processing pathways

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ABSTRACT

It is now common practice to conduct either a life cycle assessment (LCA) or techno-economic analysis (TEA) to assess the feasibility and sustainability profiles of specific technologies or product supply chains. Although numerous studies have proposed integrated frameworks for combining LCA and TEA for specific sectors, such a framework has not been proposed for the pulse protein processing sector to date. The goal of the current analysis was to propose such a framework including, in addition, integration of process simulation and optimization capabilities, that can enable assessing and improving the sustainability of existing and emerging pulse protein extraction pathways (i.e., dry fractionation, wet fractionation, hybrid) based on a combination of technical, economic, and environmental performance criteria. A systematic review of published articles was used to identify the key characteristics of sector-specific integrated frameworks and to subsequently propose a comparable framework for pulse processing pathways, taking into consideration relevant attributes of LCA and TEA studies of agri-food processing systems. Different system boundaries and functional units are commonly utilized for LCA (cradle to gate) and TEA/process simulation (gate to gate), but the proposed framework proposes using the same functional units (both mass and functionality based) based on output material. In addition to adhering to the ISO 14044 standard for LCA and established TEA methodologies, the proposed framework recommends integrating process simulation, genetic algorithm-based multi-objective optimization, GIS models for spatially explicit raw material production scenarios, and use of analytical hierarchy process to facilitate multi-criteria decision making.

1. Introduction

Technology improvement based on technical, economic, and environmental indicators is critical to addressing future market demands in a sustainable manner (Mahmud et al., 2021; Wiedmann et al., 2020; Söderholm, 2020). Life cycle assessment (LCA) and techno-economic analysis (TEA) are widely used tools to evaluate the sustainability of process technologies based on environmental, technical, and economic criteria (Mahmud et al., 2021; Rajendran and Murthy, 2019).

LCA is used to quantify inputs and outputs along product supply chains in terms of resources and emissions, respectively, and to identify environmental impacts caused by a product/system throughout its life cycle. This method plays a vital role in support of sustainability measurement and management efforts for a wide variety of technologies and services. Key applications include identifying supply chain "hotspots" for improvement, assessing the environmental performance of specific technologies, facilitating policy formulation and decision-making, and comparing different interventions in terms of a variety of sustainability outcomes (Takacs and Borrion, 2020). TEA is a tool to evaluate a process or product system based on technical and economic performance criteria (Zimmermann et al., 2020b). It is most commonly used to study single supply chains but, like life cycle costing (LCC) and LCA, it can also include upstream and downstream phases. TEA can also support process optimization as well as R&D and investment decision-making (Zimmermann et al., 2020a).

To date, several review articles have summarized the findings of LCA and TEA studies to evaluate the feasibility of different technologies considering both environmental and economic outcomes. Most of them

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focused on alternative fuels, biofuels, or renewable energy generation technologies to reduce GHGs emissions (Davidson et al., 2021; Ince et al., 2021; Kargbo et al., 2021; Tibesigwa et al., 2021). Microalgae or algal and yeast-based biorefinery technologies have also been addressed in numerous LCA and TEA studies (Cruce et al., 2021; Kannah et al., 2021; Karpagam et al., 2021; Liyanaarachchi et al., 2021). Rahman et al. (2020) and Veilleux et al. (2020) summarized the findings of studies focusing on electrification and power grids. Some other areas of study are the electrochemical reduction of CO_2 (Somoza-Tornos et al., 2021); plant fiber processing (Ramesh et al., 2020); extraction of seed oils (Lavenburg et al., 2021); conversion of agro-food residues to natural dyes (Phan et al., 2021); and removal and recovery of ammonia nitrogen (Chen et al., 2021b), etc.

It is currently common practice to employ LCA or TEA individually to assess a process or product system. However, a more systematic integration of LCA and TEA could enable a better understanding of the synergies and trade-offs between environmental and economic performance and facilitate decision-making in a more consistent, transparent, and systematic manner (Awasthi et al., 2021; Mahmud et al., 2021; Wunderlich et al., 2021). On this basis, a number of recent studies have proposed frameworks for integrated LCA and TEA in order to identify the best-suited pathways in specific sectors. These include, for example, frameworks for assessing biorefineries (Shi and Guest, 2020), the development of chemical technologies (Wunderlich et al., 2021), and biomass conversion technologies (Kim et al., 2022). Mahmud et al. (2021) reviewed 25 papers that employed LCA and TEA simultaneously but limited their scope to mostly renewable energy and wastewater treatment technologies. They summarized the methodological challenges for integrating LCA and TEA and recommended developing an integrated LCA-TEA tool that also incorporates optimization capabilities (Mahmud et al., 2021).

In complement to LCA and TEA, technology process simulation and optimization can also be used to obtain more benefits/outcomes with minimum/optimal inputs and less environmental impacts (Laitinen et al., 2021; Zhu et al., 2022). In process simulation, the product system is represented as a mathematical model outlined with numeric solutions under different conditions and constraints. The mathematical model may include mass balance, energy balance, and/or momentum balance with different fundamental equations. In recent times, the use of process simulation has been seen in different research fields either for conceptualizing designs or as a decision-making tool (Mangili et al., 2019; Sitter et al., 2019; Tula et al., 2020). For simulating the real-world process/system in the virtual world to design efficient and effective processes (Asprion and Bortz, 2018), researchers use a wide range of software – Aspen Plus (Nezammahalleh et al., 2018), SuperPro Designer (Cheng and Rosentrater, 2017), UniSim (Foo, 2023), ProSim Plus (Morales-Mendoza et al., 2018), EMSO (Elias et al., 2021), ChemCAD (Pérez Sánchez et al., 2022), gPROMS (Näf, 1994), PRO/II (Frutiger et al., 2018), etc.

Optimization, especially multi-objective optimization considering environmental, economic, and technical objective functions, can enable a comprehensive sustainability assessment. Though Azapagic and Clift (1998) first proposed the integration of LCA with optimization, this type of integrated assessment has since attracted the interest of researchers from diverse industrial sectors, including manufacturing (Dabbaghi et al., 2021; Faridmehr et al., 2021); power generation (Bahlawan et al., 2021a; b); agriculture (Cobo et al., 2020; Khanali et al., 2021); construction (Galimshina et al., 2021; Trinh et al., 2021; Zhang et al., 2021); etc. There are two principal approaches to optimization – deterministic and stochastic methods - and numerous algorithms are now available including a genetic algorithm (Hafyan et al., 2020a, 2020b; Karar et al., 2021; Khadem et al., 2022), artificial neural network (Khadem et al., 2022; Nagapurkar and Smith, 2019b), fuzzy analytical hierarchy process (Tang and You, 2018b), Brute Force Monte Carlo simulation (Karar et al., 2021), simulated annealing method (Karar et al., 2021), etc.

Process simulation and optimization have been used in combination in a variety of studies - for example, to evaluate bio-ethanol production processes (Kadhum et al., 2018; Kristianto and Zhu, 2017); algal biofuel industries and bio-refineries (García-Casas et al., 2022; Gong and You, 2017; Kern et al., 2017); CO_2 capture and utilization (Do et al., 2022); acid production from fruit bunches (Hafyan et al., 2020b); micro-grid/conventional grid integration (Nagapurkar and Smith, 2019a, 2019b); lipid extraction from microalgae (Nezammahalleh et al., 2018); biochemical production (Hafyan et al., 2020a); adiabatic compressed air energy storage (Li et al., 2021a); furfural production (Thompson et al., 2021); recycling plastic waste (Zhao and You, 2021); aluminum hot stamping processes (Xiao et al., 2022), and multiple gas feed sweetening processes (Zhu et al., 2022), etc. Integrating process simulation and optimization with LCA and TEA is thus an emerging research area requiring further development to address the sustainability challenges of clean technologies. This is particularly the case with alternative protein production processes.

The market for plant-based protein is predicted to grow to USD 140 billion by 2029 (Richter, 2019; Saget et al., 2021a; Tziva et al., 2020) - especially for proteins from pulses, which contain 18–36% protein, important nutrients, minerals, and vitamins (FAO, 2016; Peoples et al., 2019). This growth in demand for plant-based proteins to substitute animal proteins, especially in western countries, is driven in part by sustainability concerns (Aschemann-Witzel et al., 2021; Forbes, 2019; Potter and Röös, 2021; Vinnari and Vinnari, 2014). There has hence been significant growth in the pulse processing industries to meet the demand for different pulse-based products such as pulse flour, pulse protein, pulse starch, and pulse fiber (Pulse Canada, 2021).

It has been suggested that the development of improved pulse-processing technologies should be prioritized to further enhance the acceptability and sustainability of pulse-based foods (Varela-Ortega et al., 2021). Dry fractionation and wet fractionation are the two most common processing technologies to extract pulse protein from dried pulses. Both are energy-intensive processes that make large contributions to the overall sustainability impacts of processed pulse products (Vogelsang-O'Dwyer et al., 2020).

Methods to improve the quality of the extracted protein and make the processing systems more sustainable with respect to yields and energy efficiency continue to evolve, but it is unclear which among them result in the best sustainability outcomes, and more information regarding priority intervention points is required to support continued evolution in the sector. While several researchers have considered various aspects of pulse processing pathways, (Alonso-Miravalles et al., 2019; Heusala et al., 2020a; Lie-Piang et al., 2021; Saldanha do Carmo et al., 2020; Vogelsang-O'Dwyer et al., 2020; Zhu et al., 2021), no systematic review of LCA and TEA studies of pulse processing pathways has been reported to date, nor have any proposals for an integrated framework for combining process simulation and optimization with LCA and TEA in order to improve the technical efficacy, economic feasibility, and environmental sustainability of pulse processing pathways been advanced.

In order to address this gap, the current review, therefore, aims at answering the following specific questions.

1. What are the required methodological choices for integrating LCA and TEA?
   a) What is the current state of the art in sector-specific integrated frameworks?
   b) What are the specific characteristic components/key features of an integrated LCA/TEA framework?
   c) Are the functional unit and system boundaries the same for TEA and LCA? If not, how do they differ?
   d) Are uncertainties quantified and reported for both TEA and LCA? If so, how? Are the methods similar, different, or integrated?
   e) What are the current practices for employing process simulation, optimization, and other modelling approaches in the integrated LCA/TEA frameworks?

2. What is the current state of the art of LCA and TEA studies of agri-food processing pathways/technologies?
   a) Are the functional units mass-based or functionality-based?
   b) What are the common data sources used in these studies?
   c) What are the most commonly used impact categories for studying agri-food processing pathways? Is there any recommendation about specific impact categories for food processing pathways?
   d) What is the current practice to include process simulation and optimization in TEA studies of agri-food processing pathways/technologies?
   e) What are the common economic analyses carried out in TEA studies of agri-food processing pathways/technologies?
   f) What are the common allocation methods for agri-food processing pathways?
3. On the basis of information derived from questions 1 and 2
   a) What are the gaps/limitations of existing integrated LCA/TEA approaches? Is it necessary to develop sector-specific frameworks?
   b) If yes, what framework can be proposed for integrating LCA, TEA, process simulation, and optimization for pulse processing pathways?

This review consists of the following sections – i) Methods section explaining the search strategy and how the review questions will be answered; ii) Results and Discussions section summarizing the findings after reviewing selected pieces of literature followed by a proposed framework and a brief discussion about how the proposed framework can facilitate eco-design; and iii) Conclusions covering main findings, limitations, and recommendations.

2. Methods

For this study, published articles were selected following the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) systematic review method (Moher et al., 2009). The PRISMA method consists of three stages – search strategy, screening criteria, and extraction and synthesis of data. The following sections explain the PRISMA method in detail for review questions 1 and 2. The systematic review method for selecting and screening published articles is presented in Fig. 1.

2.1. Search strategy

2.1.1. Review question 1 (R1)

The Web of Science search engine and keyword combinations with logical operators "AND", "OR" and "NOT" were used to identify relevant peer-reviewed literature. The combination of search keywords and logical operators for review question 1 were – ALL ("LCA" OR "life cycle assessment" OR "life cycle analysis" OR "life cycle") AND ALL ("TEA" OR "Techno-economic Analysis" OR "techno economic" OR "techno-economic" OR "techno-economic assessment") AND ALL ("Integration" OR "integrated" OR "comprehensive" OR "combination" OR "combined" OR "framework" OR "template" OR "new approach" OR "systematic guideline" OR "process simulation" OR "optimisation" OR "optimization" OR "simulation" OR "process modelling").

2.1.2. Review question 2 (R2)

For identifying published primary research articles on LCA and/or TEA of agri-food processing pathways to answer review question 2, the combination of search terms and logical operators were – ALL ("LCA" OR "life cycle assessment" OR "life cycle analysis" OR "life cycle" OR "TEA" OR "Techno-economic Analysis" OR "techno economic" OR "techno-economic" OR "techno-economic assessment") AND ALL ("processing" OR "extraction" OR "fractionation") AND ALL ("agri-food" OR "pulse" OR "legume" OR "Flour" OR "pea" OR "lentil*" OR "chickpea" OR "wheat" OR "grain*" OR "seed" OR "corn" OR "faba" OR "Soybean" OR "bean" OR "plant protein" OR "protein crop" OR "lupine" OR "peanut" OR "oat" OR "quinoa") NOT ALL ("biorefin*" OR "biomass" OR "waste*"). As the main aim of this study is to propose an integrated framework for pulse processing pathways, studies using different agri-foods or their wastes for biorefinery or any biomass-based products were excluded using the NOT logical operator, considering that the processing pathways of those studies are different from the targeted ones.

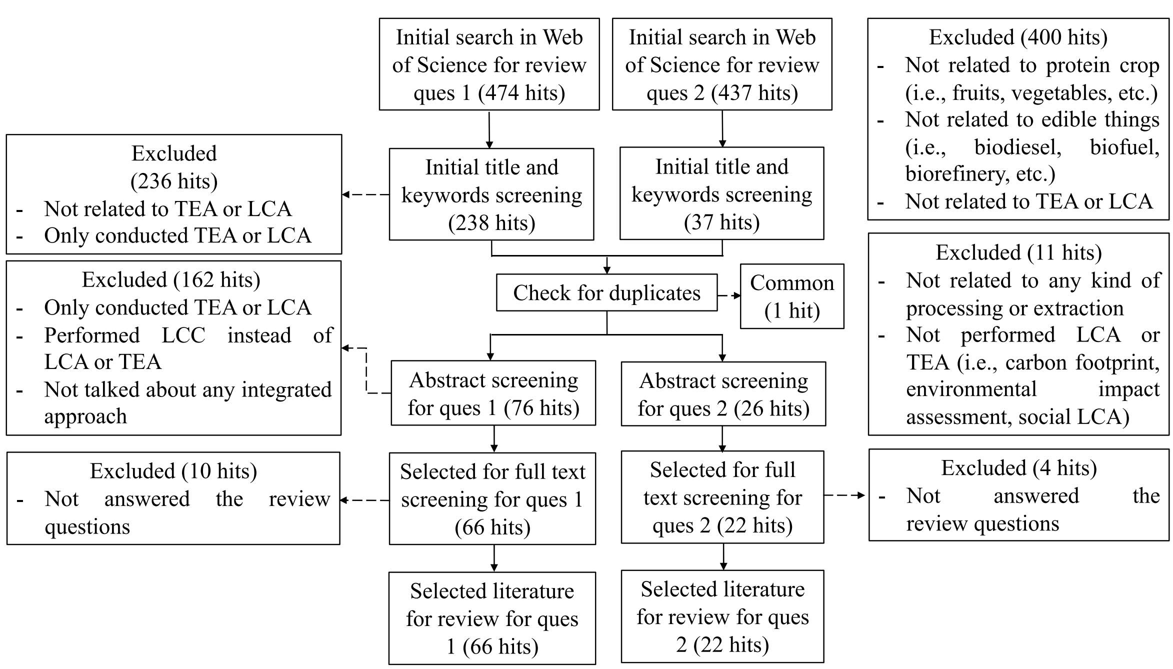

Fig. 1. PRISMA systematic review method for selecting literature for review

2.2. Screening criteria

2.2.1. Review question 1 (R1)

The initial search on the Web of Science resulted in 474 research articles. The temporal scope was from 2017 to 2021, as an initial search without temporal boundary revealed that most of the articles were published within this period. A second-tier screening was carried out by analyzing the titles and keywords for relevance, which excluded 236 hits. These articles were excluded if they were not related to LCA and TEA, or if they did not report a combined LCA/TEA. The abstracts of the selected articles were then consulted to identify those that performed LCA, and TEA simultaneously and described integrated approaches or frameworks. Articles performing LCC instead of LCA or TEA were excluded as LCC will only cover the economic feasibility aspects, excluding the technical and environmental perspectives. Screening of the abstracts excluded 162 hits; hence 76 hits were selected for full-text review in support of answering review question 1. Another 10 papers were excluded during the full-text screening, resulting in a final count of 66 articles consulted.

2.2.2. Review question 2 (R2)

The initial search resulted in 437 research articles for the temporal scope of 2017–2021. After the initial screening of the titles and keywords, only 37 papers were identified for the full review. Articles that were not related to any type of protein crop (i.e., vegetables, fruits) and/or edible outputs (i.e., biodiesel, biofuel), or that were not related to LCA or TEA, were excluded based on their titles and keywords. Full abstract screening excluded another 11 hits that were not related to any processing or extraction process or did not conduct LCA or TEA (i.e., carbon footprint, social LCA). 26 hits were selected for full-text screening, which resulted in the exclusion of 4 more hits. On this basis, a total of 22 articles comprised the final sample of literature consulted to answer review question 2.

2.3. Extraction and synthesis of data

2.3.1. Review question 1 (R1)

R1 aimed at identifying the required methodological choices for integrating LCA and TEA for a sector-specific framework. An Excel-based synthesis table was used to collate information from the articles (Table S1) regarding - a) the product/system studied; b) characteristic elements of the framework (functional unit, system boundary, economic analysis, uncertainty and sensitivity analyses, allocation method); c) current practices with respect to process simulation and optimization; and d) integration of other modelling approaches in the framework.

2.3.2. Review question 2 (R2)

The current state of the art for LCA and TEA studies of agri-food processing (in particular, protein-crop processing) pathways was determined by reviewing articles specific to processing that were employing either LCA, TEA or both. An Excel-based synthesis table was used to collate information regarding a) characteristic elements of the LCA studies (system boundary, functional unit, data sources, allocation method, LCIA methods and impact categories, uncertainty and sensitivity analyses, and statistical analysis) (Table 1a); and b) characteristic elements of the TEA studies (system boundary, functional unit, data sources, integration of process simulation and optimization, economic analysis, and sensitivity analysis) (Table 1b).

2.3.3. Review question 3 (R3)

One of the main objectives was to develop an integrated framework for LCA, TEA, process simulation, and optimization for pulse processing pathways. From the information obtained from R1, key features and gaps in the integrated frameworks were identified and the need for sector-specific frameworks was highlighted. Based on the information obtained from R2, where the main characteristic elements of LCA and TEA along with process simulation and optimization for agri-food processing/extraction pathways were summarized, a new integrated approach was proposed specifically for pulse-processing pathways (i.e., dry fractionation, wet fractionation). The new proposed framework aims to incorporate all the relevant features of the previously considered integrated frameworks in order to support integrating LCA, TEA, process simulation, and optimization for assessing the sustainability of pulse processing pathways from environmental, technical, and economic perspectives.

3. Results and Discussions

3.1. Existing integrated frameworks for LCA and TEA

3.1.1. Sector-specific integrated frameworks

Among the 66 reviewed articles, almost half (30 articles) developed integrated frameworks to assess the technical, economic, and environmental feasibility of technology pathways related to renewable fuel production (i.e., biofuel, solar, electro fuel), biorefineries and/or biomass-based industries. An additional 12 focused on the production and distribution of heat, power, gas and/or electricity, microgrid systems and power plants, 8 developed integrated frameworks for energy storage systems, and 6 targeted different waste management systems (i.e., plastic, solid waste, wastewater, sewage sludge). Some of the frameworks proposed methodologies specifically for agricultural and biochemical production techniques. Combined LCA and TEA methodologies to assess techno-economic-environmental sustainability were proposed for agricultural systems (Lan and Yao, 2019); biochemical production from fruits/vegetables (Hafyan et al., 2020a, 2020b; Thompson et al., 2021); guar gum production (Summers et al., 2021); ketone ammoximation production (Wang et al., 2020); and lithium recovery from geothermal brine (Huang et al., 2021), etc. (Table S1). An integrated framework specifically for the fractionation of protein crops, however, was not observed in the literature considered.

3.1.2. Characteristic elements of the integrated frameworks

i. System Boundary and Functional Unit

When integrating LCA and TEA, it is evident from the reviewed literature that it is not mandatory to consider the same system boundary and functional unit. Most of the reviewed articles considered only the processing stages (industry gate-to-gate) for TEA, process simulation, and optimization, but the system boundary of the LCA was often different (i.e., cradle-to-grave or cradle-to-gate). The aims of TEA, process simulation and optimization are mainly to improve processing techniques at the industry level. That is one of the main reasons for disregarding other background systems and downstream processes.

The functional units were explicitly defined for all LCAs, but most did not define a FU for the TEA. Instead, the studies either referred to the input materials rather than the outputs, or processing capacity (amount/time) or did not mention any specific unit of analysis. Ideally, however, such analyses should have the same functional unit when combining LCA and TEA, as the methods are being employed in an integrated manner. For optimizing or getting efficient output/result from the process, an output-based functional unit is recommended. Moreover, while comparing two or more product systems, there should be a common ground of comparison, which is why output-based functional units are preferable. Pérez-López et al. (2018) explicitly stated that the FUs of the LCA (1 kg diesel) and TEA (1 gal diesel) were different due to the nature of the available data, which were both output and mass-based. Noteworthy is that defined FUs for the LCAs were always mass-based. However, depending on the studied product system, functionality-based functional units may sometimes be more suitable.

ii. Economic Analysis

Table 1a
Summary of reviewed articles to identify the current state of the art for LCA studies for agri-food processing pathways

ID	References	Product/System	Functional Unit	System Boundary	Data sources	Allocation Method	LCIA Method	Impact categories	Methods of uncertainty analysis	Statistical Analysis	Sensitivity/ Scenario Analysis
1	Cancino-Espinoza et al. (2018)	Production and distribution of organic quinoa	Mass based	Cradle to packaging	Primary, Ecoinvent, EMEP/EEA emission inventory guidebook 2013	–	IPCC 2013, IPCC 2006, ReCipe 2008	13 midpoint categories	Monte Carlo Simulation, geometric standard deviation using Pedigree Matrix	Mann-Whitney-Wilcoxon test	Based on different FUs and emission factors
2	Câmara-Salim et al. (2020)	Comparing different types of agricultural systems for cultivating Galician wheat	Mass based	Cradle to farm	Ecoinvent, primary, literature	Economic and mass allocation	Recipe 1.12 hierarchist	5 midpoint categories	–	–	–
3	Miguel and Ruiz (2021)	Comparison between industrially produced bean and pork stew	Mass based	Cradle to grave	Primary, Ecoinvent, Agri-footprint, Industry Data LCA Library 2.0, Quantis World food LCA database	Avoided and/or economic allocation and/ or system	EF 3.0 (adapted) v1.0 as PEF guidelines	16 midpoint categories	–	–	–
4	Bai et al. (2021)	Production of edible vegetable oils, comparison among soybean, rapeseed, and peanut oils	Mass based	Cradle to industry gate	National statistical yearbooks, factories, CPLCID	–	ReCipe 2016	18 midpoint and 3 endpoint categories	Monte Carlo Simulation	–	For validating LCIA method
5	Khatri et al. (2017)	Production of edible mustard oil	Mass based	Cradle to gate	Primary Data, literature and published models	System expansion, mass, and economic allocation	ReCipe 2008 hierarchist	9 midpoint and 3 endpoint categories	Pedigree matrix for data quality assessment	Hypothesis testing - ANOVA, post hoc test, Tukey's Honestly Significant Difference test	–
6	Ferreira et al. (2019)	Wine and olive oil production with and without Pulsed Electric Field treatment	Mass based	Cradle to gate	Industrial trials, European Reference Life Cycle Database (ELCD), Ecoinvent	–	ReCipe	5 midpoint categories	–	–	–
7	Heusala et al. (2020b)	Production of oat protein concentrate (OPC) and faba bean protein concentrate (FBC) and comparing these with other protein sources	Mass based	Cradle to gate	Literature, processing factories, VTT Technical Research Centre of Finland LTD.,	Economic allocation	IPCC 2013	2 midpoint categories	–	–	Based on various economic prices in allocation method, and different emission factors
8	Heusala et al. (2020a)	Different food products containing oat protein concentrate	Mass based and functionality based	Cradle to processing	Literature and other published models	Economic allocation	IPCC 2013	2 midpoint categories	–	–	Sensitivity analysis with various input values and economic parameters
9	Lie-Piang et al. (2021)	Effect of reducing the degree of refining in four different extraction process to	Mass based and functionality based	Cradle to processing gate	Literature, experimental data, Agri-footprint 5.0, patent	Mass (dry matter) allocation	ReCipe 2016 v1.03 method	–	–	–	–

(continued on next page)

Table 1a (*continued*)

ID	References	Product/System	Functional Unit	System Boundary	Data sources	Allocation Method	LCIA Method	Impact categories	Methods of uncertainty analysis	Statistical Analysis	Sensitivity/ Scenario Analysis
		get plant-based proteins									
10	Saerens et al. (2021)	Comparing plant-based burger patties to meat burger patties	Mass based	Cradle to gate	Models of LCA Food DK database, Ecoinvent, pilot scale production facility of DIL of Germany, primary data	Economic and mass-based allocation	ReCipe v1.08	16 midpoint and 2 endpoint categories	Monte Carlo Simulation and Pedigree matrix	–	Sensitivity and scenario analyses based on assumptions, calculations and/ or uncertainties
11	Tidåker et al. (2021)	Comparing cultivation of five Swedish pulses grown in both conventional and organic production systems with some imported pulses	Mass based	Cradle to consumer	GaBi database, Swedish Board of Agriculture, literature, Swedish National Inventory Report	Allocation based on mass and protein content	IPCC 2013	Midpoint categories	–	–	–
12	Saget et al. (2021b)	Comparing plant and beef-based patties	Mass based and functionality based	Cradle to fork	Literature, manufacturing companies, Agri-footprint, Ecoinvent	Economic and biophysical allocation based on energy flows and other causal relationships	–	16 midpoint categories	Monte Carlo Simulation	–	Sensitivity analysis with additional cattle systems from different regions
13	Svanes et al. (2020)	Comparing environmental impacts of production of rapeseed and turnip rapeseed, rape oil and press cake, and some common animal protein sources	Mass based	Cradle to gate	Primary data, Ecoinvent, Agri-footprint	Economic allocation	ILCD 2011 Midpoint + v1.11/EC-JRC Global, equal weighting, EDIP 2003v1.07, ReCipe 2016 Endpoint v1.04/ World (2010) H/A, Ecological Scarcity 2013 v1.06/Ecological Scarcity 2013, IMPACT 2002+ v2.15/IMPACT 2002+	13 midpoint categories	–	–	Sensitivity analysis was conducted to determine the importance of allocation based on varying prices.
14	Saget et al. (2021c)	Comparing mayonnaise made with aquafaba as the emulsifying agent and traditional mayonnaise made with egg yolk	Mass based	Cradle to factory gate	Agri-footprint, Ecoinvent, primary data	–	–	16 midpoint categories	Monte Carlo Simulation	Modified null hypothesis significance test (NHST)	Sensitivity analysis for different regional electricity mixes

Table 1b
Summary of reviewed articles to identify the current state of the art of TEA studies for agri-food processing pathways

ID	References	Product/System	Process simulation/ Optimization	Economic Parameters and analysis	Functional Unit	System Boundary	Data sources	Sensitivity Analysis
1	Aktas-Akyildiz et al. (2018)	Small industrial scale extraction of β-glucan (BG) from oat and barley fractions, comparison among scenarios with varying raw materials, other cases with modifications in any unit processes	Process simulation based on mass and energy balance	Price of different inputs, fixed and variable operating costs	Functionality based	Processing and extraction	Experimental research results and literature	Based on various key cost parameters
2	Cheng and Rosentrater (2017)	Soybean oil production by hexane extraction process	Process simulation based on mass balance	Capital investment, operating cost, revenues, and profits, gross profit, gross margin, net profit, return on investment	Mass based	Processing and extraction	Literature, SuperPro Designer database, the inventory record of the Iowa State University Center for Crops Utilization Research (CCUR) pilot plant	Contribution analysis with fluctuating economic conditions
3	Somavat et al. (2018)	Yellow, blue, and purple corn processing for anthocyanin extraction and ethanol production using modified dry grind process	Process simulation based on material and energy balance	Capital investment, operating cost, profitability analysis based on internal rate of return	Mass based	Processing and extraction	USDA Model, previous dry grind models, cost models of SuperPro Designer	Based on various extraction method, and various percentage increase in the price of colored corn
4	Kayathi et al. (2021)	Extraction of Ƴ-Oryzanol from defatted rice bran using supercritical carbon dioxide (SC–CO_2)	The response surface methodology was applied to optimize the handling parameters such as temperature, pressure, and CO_2 flow rate.	CAPEX and OPEX, gross operating margin, net present value, payback period	Mass based	Processing and extraction	Aspen Plus, National Center for Biotechnology Information databank, Aspen Process Utility databank	Based on various temperature, pressure, and CO_2 flow rate
5	Archacka et al. (2020)	Production of probiotic preparations using optimized corn flour medium and spray-drying protective blends	Process model simulation at industrial scale and optimization	Factory gate prices excluding transport or delivery charges, gross profit, gross margin, net profit, return on investment, net present value	Mass based	Processing and extraction	SuperPro Designer Database, quotations from local and global suppliers	Sensitivity of unit production cost and the number of batches per year was estimated in the simulation.
6	Cheng and Rosentrater (2019)	Extruding expelling of soybeans to produce oil and meal	Process simulation based on mass balance	Fixed capital investment and operating costs, return on investment, payback time, gross margin, internal rate of return, net present value	Mass based	Processing and extraction	SuperPro Designer Database, operational records of the Center for Crops Utilization, Iowa State University, literature	Based on various operating costs to examine the factors having significant effects on the net profit of the process
7	Kurambhatti et al. (2019)	Impact of fractionation process of corn dry grind ethanol process	Process simulation models	Fixed capital investment and operating costs, revenues, profitability analysis based on internal rate of return	Mass based	Processing and extraction	SuperPro Designer Database	Based on various operating costs to examine the factors having significant effects on the net profit of the process

Discounted cash flow analysis was the most commonly listed (72.7%) economic analysis in the reviewed articles. On the other hand, 24.2% did not explicitly mention specific types of economic analysis. Net present value (NPV) (64.6%) and internal rate of return (IRR) (37.5%) were used as a means of profitability measure under discounted cash flow analysis. Some of the reviewed articles mentioned conducting discounted cash flow rate of return (DCFROR) analysis by combining NPV and IRR (DeRose et al., 2019a, b; Manouchehrinejad et al., 2020; Pérez-López et al., 2018; Rodgers et al., 2021; Sahoo and Mani, 2019; Somers and Quinn, 2019; Vega et al., 2020; Zapata-Boada et al., 2021). Different studies used different terms for the cost parameters (i.e., fixed cost, operating cost), and 31.8% of reviewed articles mentioned the terms CAPEX/OPEX (Capital Expenditure/Operating Expenditure) for calculating the cost associated with studied systems. Levelized Cost of Energy (LCOE) was another economic metric for some studies (Abdon et al., 2017; Falter et al., 2020; Li et al., 2021c; Nagapurkar and Smith, 2019a, 2019b; Parra et al., 2017; Singlitico et al., 2020; Tang and You, 2018a). Other mentioned economic criteria were payback period (Chen et al., 2021a; Nickel et al., 2020; Resurreccion et al., 2021; Salazar et al., 2021; Wang et al., 2019), present value ratio (Chen et al., 2021a; Resurreccion et al., 2021), benefit-cost ratio (Chen et al., 2021a), capital recovery factor (Shemfe et al., 2018), investment cost model (Li et al., 2021a), commodity price modelling and real options analysis (Kern et al., 2017), and return on investment (Wang et al., 2019). Economic analysis methods and parameters are mostly dependent on the availability of data and it is highly likely to use secondary data sources such as software databases for assembling the data for economic parameters.

iii. Allocation Methods

Less than half of the studies (27 articles) described the allocation methods used to handle the multi-functionality of the systems. Of those that did, different allocation methods were reported for different unit processes. Economic allocation was the most commonly utilized allocation method (33.3%), despite this occupying the "last resort" tier in the ISO 14044 multifunctionality hierarchy. Some studies avoided allocation via substitution (Levasseur et al., 2017; Rodgers et al., 2021) or system expansion for some unit processes (Basuhi et al., 2021; Gong and You, 2017; Kadhum et al., 2018; Pérez-López et al., 2018; Singlitico et al., 2020; Vega et al., 2020; Zhao and You, 2021). Allocation based on mass (Hafyan et al., 2020a; Resurreccion et al., 2021; Summers et al., 2021), energy content (Bressanin et al., 2020; DeRose et al., 2019b; Elias et al., 2021; Falter et al., 2020; Rodgers et al., 2021; Shi and Guest, 2020; Somers and Quinn, 2019), and exergy (Manouchehrinejad et al., 2020) were also reported in some studies.

iv. Uncertainty and Sensitivity Analyses

Some studies mentioned considering the uncertainties of input parameters but did not clearly state the measurement method (Kristianto and Zhu, 2017). Most (15 articles) used Monte Carlo Simulation for uncertainty measurement, especially for economic parameters/economic risk analysis. Lan and Yao (2019) proposed an integrated measurement method based on a stochastic approach. Thomassen et al. (2018) used Oracle Crystal Ball software for uncertainty management. The use of the Latin Hypercube Sampling method (Bressanin et al., 2020; Li et al., 2021b) and composite probability distribution method (Usack et al., 2019) were also reported. Model and parameter uncertainties are very common for LCA and TEA studies, hence it is important to address and report these uncertainties.

Sensitivity analysis was performed in most of the reviewed articles. 47 performed sensitivity/scenario analysis considering various input/model parameters, especially economic parameters, to identify the influence of these input parameters on the results. Some also conducted sensitivity/scenario analyses by varying yield percentage (Larnaudie et al., 2020), carbon tax (Nagapurkar and Smith, 2019b), production locations (Falter et al., 2020), transportation distance (Somers and Quinn, 2019), and weights used in the Analytic Hierarchy Process (AHP) method (Wang et al., 2019). Elias et al. (2021) and Shi and Guest (2020) employed global sensitivity analysis. Elias et al. (2021) also used the Standardized Elementary Effects (SEE) method and the optimized Morris Sampling Strategy for sensitivity analysis. Finally, some articles used Spearman's Rank Correlation Coefficient (Li et al., 2021b; Shi and Guest, 2020), finite difference method (Nickel et al., 2020), or parametric applicability analysis (Ifaei and Yoo, 2019) in sensitivity/scenario analysis (Table S1).

3.1.3. Integration of process simulation, optimization, and other methods with LCA and TEA

Integration of LCA and TEA with process simulation and optimization models were very common among these frameworks. 42.4% of reviewed articles combined process simulation based on mass and energy balances with the LCA and TEA methodologies. Most used Aspen Plus software for process simulation and the Aspen Plus database was one of the key data sources. However, Nagapurkar and Smith (2019a) used Matlab and Elias et al. (2021) used EMSO – an equation-oriented simulator for the process simulation component. Few publications provided a description of how process simulation was used to optimize technical performance, which was then used to improve economic and environmental performances. Process simulation could be used to improve sustainability using these 5 steps – i) define system boundary, ii) perform process simulation, iii) obtain mass and energy balance, iv) build LCI and OPEX/CAPEX data inventory, and v) estimate environmental and economic impacts (Fig. 2). The last four steps could also be used to optimize technical, economic, and environmental performances.

Among the 66 articles, 17 employed different optimization models with one or multi-objective functions. The genetic algorithm was the most widely applied optimization method (Hafyan et al., 2020a, 2020b; Li et al., 2021a; Nagapurkar and Smith, 2019a, 2019b). Genetic algorithm is based on principles of biological evolution or natural selection – survival of the fittest - to find solutions for both constrained and unconstrained optimization problems. Some studies mentioned employing different optimization methods like VIKOR, and mixed integer linear and nonlinear programs (Table S1). For every optimization model, there are at least one or, in some cases, two or three objective functions. Most of the studies set the objective function to minimize either the Levelized Cost of Energy (LCOE) or investment capital cost or production cost or maximize either the profit or net present value. Some of them also included minimizing environmental impacts as an objective function to combine the outputs of LCA and TEA for optimizing any techniques (Hafyan et al., 2020a, 2020b; Li et al., 2021a; Singlitico et al., 2020; Zhao and You, 2021). Hafyan et al. (2020b) set the objective to minimize Hazard Identification and Ranking Index (HIRA), and Kristianto and Zhu (2017) targeted maximizing production in their optimization models. Pinch analysis in a heat exchanger was carried out to maximize heat integration and recovery by DeRose et al. (2019a) and Nickel et al. (2020), while Thompson et al. (2021) included Pareto Analysis in their framework for facilitating decision-making (Table S1).

Integrating attributional LCA with TEA, process simulation, and optimization methods is a common practice. However, a small subset of researchers also proposed integrated frameworks based on consequential LCA methodology (Gong and You, 2017; Zhao and You, 2021). Though process simulation based on mass and energy balances was employed in most of these studies, a dedicated open-source platform for biorefinery simulation, BioSTEAM simulation, was also employed by Li et al. (2021b) and Shi and Guest (2020).

Integrating social LCA or social impact assessment methodology with environmental LCA and TEA to cover all the pillars of sustainability – social, economic, and environmental - was reported by several researchers (Table S1). Vega et al. (2020) included territorial metabolism LCA in their integrated framework. In addition, using GIS-based models or geospatial analysis techniques was reported for spatially explicit frameworks (Resurreccion et al., 2021; Singlitico et al., 2020). Combining GIS models is a key element of regionalized analyses. Some studies combined other modelling frameworks with LCA, TEA, process simulation and optimization (Table S1). For instance, Nagapurkar and Smith (2019b) combined Artificial Neural Networks, and Lan and Yao (2019) integrated Agent-based modelling where each farm was an agent deciding the crop type to produce. Analytic Hierarchy Process (AHP) and fuzzy modelling approaches were reported in some studies (Hafyan et al., 2020a; Tang and You, 2018a; Wang et al., 2019). Other than AHP, the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) approach was also included in some of the multi-criteria decision-making frameworks (Chen et al., 2021a; Hafyan et al., 2020a; Tang and You, 2018a, 2018b). Both TOPSIS and AHP are used to rank among different options, but AHP enables including multiple stakeholders' opinions. Considering the nature of the studied system, some researchers combined Hazard Identification and Ranking (HIRA), Fire and Explosion Damage Index (FEDI), and Toxicity Damage Index (TDI) with LCA, TEA, process simulation, and optimization (Hafyan et al.,

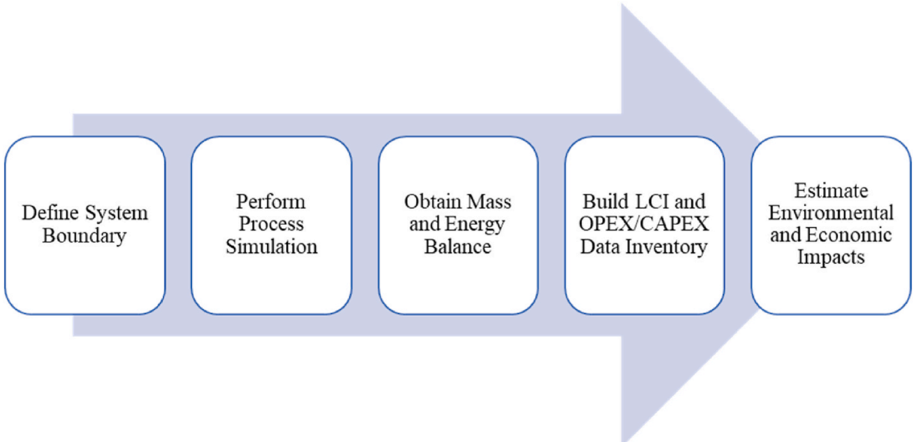

Fig. 2. Integration of process simulation with LCA and TEA

2020a, 2020b).

3.2. Current state of the art for LCA and TEA studies of agri-food processing pathways

3.2.1. Characteristic elements of LCA studies

i. System Boundary and Functional Unit

Among the 22 articles reviewed, 14 carried out LCA and 7 conducted TEA. Only 1 article performed both (Potrich et al., 2020). All the LCA studies claimed to follow the ISO 14040/14044 framework for attributional LCA for either characterizing the associated environmental impacts or identifying the hotspots in the systems. Cradle-to-gate was the most common system boundary and all utilized mass-based functional units. However, some studies also included functionality-based functional units to compare the results based on protein content (Heusala et al., 2020a; Lie-Piang et al., 2021), which seemed effective for studying protein crops and their products and comparing them with other protein sources. Saget et al. (2021b) considered Nutrient Density Unit (NDU) as the functional unit. Considering multiple functional units, including functionality-based, affords more scope to compare the studied systems with other systems (for example, to compare protein crops with animal-based protein sources). Functionality-based units (i.e., 1 kg of protein from beans/peas) also enable comparing different systems which have different levels of output. For instance, dry and wet fractionation have different levels of protein content in the final product (protein concentrate/isolate). For comparing these two fractionation pathways, a functionality-based unit will be more suitable.

Some studies mentioned excluding certain unit processes from their system boundary. For instance, activities such as manure production (Cancino-Espinoza et al., 2018), transport of straw from the field to other locations (Câmara-Salim et al., 2020), environmental burdens of equipment and infrastructure and their installation, maintenance, and cleaning (Lie-Piang et al., 2021; Miguel and Ruiz, 2021), production of pesticides (Heusala et al., 2020b), transport to home from the grocery store (Tidåker et al., 2021), etc. were explicitly excluded in some studies. Cancino-Espinoza et al. (2018) excluded the impacts of manure production on the basis that it was considered a residue from the previous production process, but they considered transport and on-field emissions after spreading the manure. They also suggested excluding questionable responses/outliers (i.e., farms with extremely high production or fertilizer used) (Cancino-Espinoza et al., 2018). Excluding some unit processes to make the system boundaries comparable among different product systems is also recommended. For example, Câmara-Salim et al. (2020) did not include field emissions of pesticides and heavy metals when comparing bread production using wheat from Galician wheat farming systems. They also disregarded the transport of straw from field to other locations (Câmara-Salim et al., 2020). If it has previously been shown in other studies that some unit processes have negligible impacts, this may also provide grounds for excluding them. For example, Heusala et al. (2020b) excluded pesticide production and Tidåker et al. (2021) excluded emissions or sequestration due to soil carbon change, on the basis that they had previously been shown to contribute negligibly to the footprint of Danish and Swedish production systems, respectively. Moreover, it is very common to ignore the impacts associated with infrastructure where it can be reasonably assumed that they make a minor contribution to impacts based on lifetime (Heusala et al., 2020b; Lie-Piang et al., 2021; Miguel and Ruiz, 2021).

ii. Data Sources

Primary data was collected directly from the associated farms and industries/manufacturing companies in some studies (Câmara-Salim et al., 2020; Cancino-Espinoza et al., 2018; Khatri et al., 2017; Svanes et al., 2020). It appears to be common practice to collect primary data for at least the foreground systems to ensure data quality and accuracy. Primary data for the production stage of different protein crops were collected for some studies. For example, Cancino-Espinoza et al. (2018) collected primary data from 13 farms regarding the production of organic quinoa. Similarly, 107 farmers were surveyed to collect primary data for rapeseed production in Svanes et al. (2020). For background systems and where primary data were missing, studies commonly used literature data or previously published models. Ecoinvent and Agri-footprint life cycle inventory databases were used for background data in most of the studies. Some studies also used other regionalized datasets to ensure geographically and temporally representative inventories (Table 1a).

iii. Allocation Methods

Most of the studied systems produced co-products, like wheat straw (Câmara-Salim et al., 2020), mustard straw and cake (Khatri et al., 2017), oat straw, oil, and starch (Heusala et al., 2020a, 2020b), or starch and fiber-rich fractions while processing protein concentrates (Heusala et al., 2020b; Lie-Piang et al., 2021). Economic allocation was the most common approach (57.1%) in these studies despite this occupying the lowest tier in the ISO 14044 allocation hierarchy (Table 1a). Mass-based allocation was used in some studies for some unit processes (Table 1a). Câmara-Salim et al. (2020) mentioned using economic allocation instead of mass allocation depending on the nature of co-products (i.e., straw and wheat, flour and bran) and the disparity in their values but used mass allocation for lower quality seeds in the seed production phase because they had no economic value. Miguel and Ruiz (2021) avoided allocation as specific inventory data were available to enable subdivision. System expansions both in the processing and consumption phases of beef and pork stew were carried out by Miguel and Ruiz (2021) for the recycling of fat residues and packaging materials, respectively. Comparing the results based on different allocation methods, Khatri et al. (2017) reported that the results of economic allocation were almost twice the results of mass allocation and significantly higher than system expansion for an edible mustard oil production study. Khatri et al. (2017) recommended not using mass-based allocation for edible oil systems because it would result in allocating more to the co-products (straw and oil meal) rather than the oil – which seems to be a less than compelling rationale. Tidåker et al. (2021) and Saget et al. (2021b) allocated based on protein content and metabolic energy requirements for tissue growth in livestock, respectively. Choosing a justifiable allocation procedure is one of the most important steps in LCA as the LCA results are very sensitive to allocation methods (Heusala et al., 2020b; Saget et al., 2021a, 2021b).

iv. LCIA Methods and Impact Categories

ReCipe method and midpoint categories were most commonly used in the reviewed articles. IPCC 2013 and IPCC 2006 were used in some of the studies to account for GHGs emissions. Midpoint impact categories are seemingly preferred due to the uncertainty associated with endpoint impact categories. Along with midpoint impact categories (most common), some studies also considered endpoint impact categories to identify impacts on human health and ecosystem services (Table 1a). Most of the studies used all the midpoint impact categories available in the chosen methods suites. However, some focused on specific impact categories without any clear justification. The choice of specific impact categories should always be well-justified and consistent with the goal and scope of the study. Climate change or carbon footprint was included as an impact category in every study considered. Agricultural and/or urban land use was prioritized in some studies, mostly related to crop production (Heusala et al., 2020a, 2020b; Saerens et al., 2021). Freshwater and marine eutrophication, freshwater and marine ecotoxicity, terrestrial acidification, human toxicity, and fossil depletion were among the other most commonly utilized impact categories (Câmara-Salim et al., 2020; Ferreira et al., 2019; Khatri et al., 2017; Saerens et al., 2021).

v. Uncertainty and Sensitivity Analyses

Only 6 articles (27.3%) reported uncertainty analysis. Monte Carlo Simulation and Pedigree matrix were the primary methods used for uncertainty measurement (Table 1a). 8 articles performed sensitivity/scenario analysis with respect to the choice of functional unit, emission factors, input parameters and economic prices for allocation, different cattle systems, and different regional electricity mixes (Table 1a). Bai et al. (2021) performed a sensitivity analysis to validate using the ReCipe method for LCIA.

vi. Statistical Analyses of Primary Data Quality

Some studies carried out statistical tests to validate the accuracy of the primary data. Cancino-Espinoza et al. (2018) performed a Mann-Whitney-Wilcoxon test. Hypothesis testing using ANOVA, Post Hoc test, and Tukey's Honestly Significant Difference (HSD) was carried out by Khatri et al. (2017). Saget et al. (2021c) mentioned performing a modified null hypothesis significance (NHST) test (Table 1a). Statistical analyses are useful when the study uses primary data from different stakeholders, and it is necessary to validate their consistency, accuracy, and representativeness.

vii. Other Features

Unique indicators were also identified for some of the reviewed articles, which were very specific to the studied product systems. For example, Cancino-Espinoza et al. (2018) computed a dimensionless indicator to calculate the cumulative energy demand for edible protein – edible protein energy return on investment (ep-EROI). Miguel and Ruiz (2021) calculated an aggregated impact score using a "circular footprint formula" (CFF) from the EC product environmental footprint (PEF) methodology. Carbon opportunity cost (Saget et al., 2021b), the effect of soil carbon change (Svanes et al., 2020), and the use of Dumas analysis for calculating protein content (Lie-Piang et al., 2021) were also reported.

3.2.2. *Characteristic elements of TEA studies*

i. System Boundary and Functional Unit

All of the TEA studies reviewed had the same system boundary (processing facility gate to gate) as they only considered the processing and extraction stages. None applied cut-off criteria. Most studies used a mass-based functional unit, except for Aktas-Akyildiz et al. (2018) who used a functionality-based functional unit (1 g of soluble β-glucan in the product). Interestingly, many studies considered the input material amount (Cheng and Rosentrater, 2017, 2019; Kayathi et al., 2021) or the processing capacity (Kurambhatti et al., 2019; Somavat et al., 2018) as functional units instead of outputs (Table 1b). In general, however, it is advisable that the functional unit refers to the output material because increasing the sustainability of the output should be the main priority and it will also enable comparing different systems producing the same outputs.

ii. Data Sources

Most studies either used Aspen Plus or SuperPro Designer software for process simulation and used the databases associated with the software. Moreover, some also used experimental results from laboratories for process simulation (Aktas-Akyildiz et al., 2018; Archacka et al., 2020). Other sources were databases of different organizations or research centers (i.e., Center for Crops Utilization, Iowa State University), a USDA model, and quotations from local and global suppliers (Table 1b). Somavat et al. (2018) mentioned using Lang Factor for calculating data, which is one of the most common approaches in biofuel and bioprocessing-related TEA studies. Most of these TEA studies utilized either secondary data or estimated or assumed data for their economic analysis (Table 1b).

iii. Process Simulation and Optimization

All studies performed process simulations based on mass and/or energy balances in Aspen Plus or SuperPro Designer software. Only 2 studies carried out optimization (Archacka et al., 2020; Kayathi et al., 2021). Kayathi et al. (2021) applied response surface methodology for optimizing different handling parameters (i.e., temperature, pressure, CO_2 flow rate). Archacka et al. (2020) utilized the simplex-centroid design method to optimize the composition of protective blends for spray drying in probiotics preparation from corn flour (Table 1b). Preferred optimization methods will depend on the studied product system and the considered objective functions.

iv. Economic Analysis

Economic analyses were carried out mainly based on fixed capital investment (CAPEX), fixed/variable operating costs (OPEX), and revenue. The capital investment cost, operating cost, and revenues for the studied facilities/systems were calculated or estimated. Feasibility and/

or profitability analysis was carried out based on the capital and operating costs. Feasibility analyses were conducted by calculating gross profit, gross margin, net profit, net present value, return on investment, and payback period. Profitability analysis was carried out based on the internal rate of return (Table 1b).

v. Sensitivity Analysis

Most studies performed sensitivity/scenario analysis based on various cost/economic parameters to find out which parameter affected the profit the most (Table 1b). Moreover, Somavat et al. (2018) carried out a sensitivity analysis with varying temperatures, pressures, and CO_2 flow rates in the process model.

3.2.3. Characteristic elements of combined LCA and TEA studies

There are some common elements between LCA and TEA. However, there are also numerous differences. Process simulation is often performed in TEA, which is not the case for LCA. LCA also relies on more

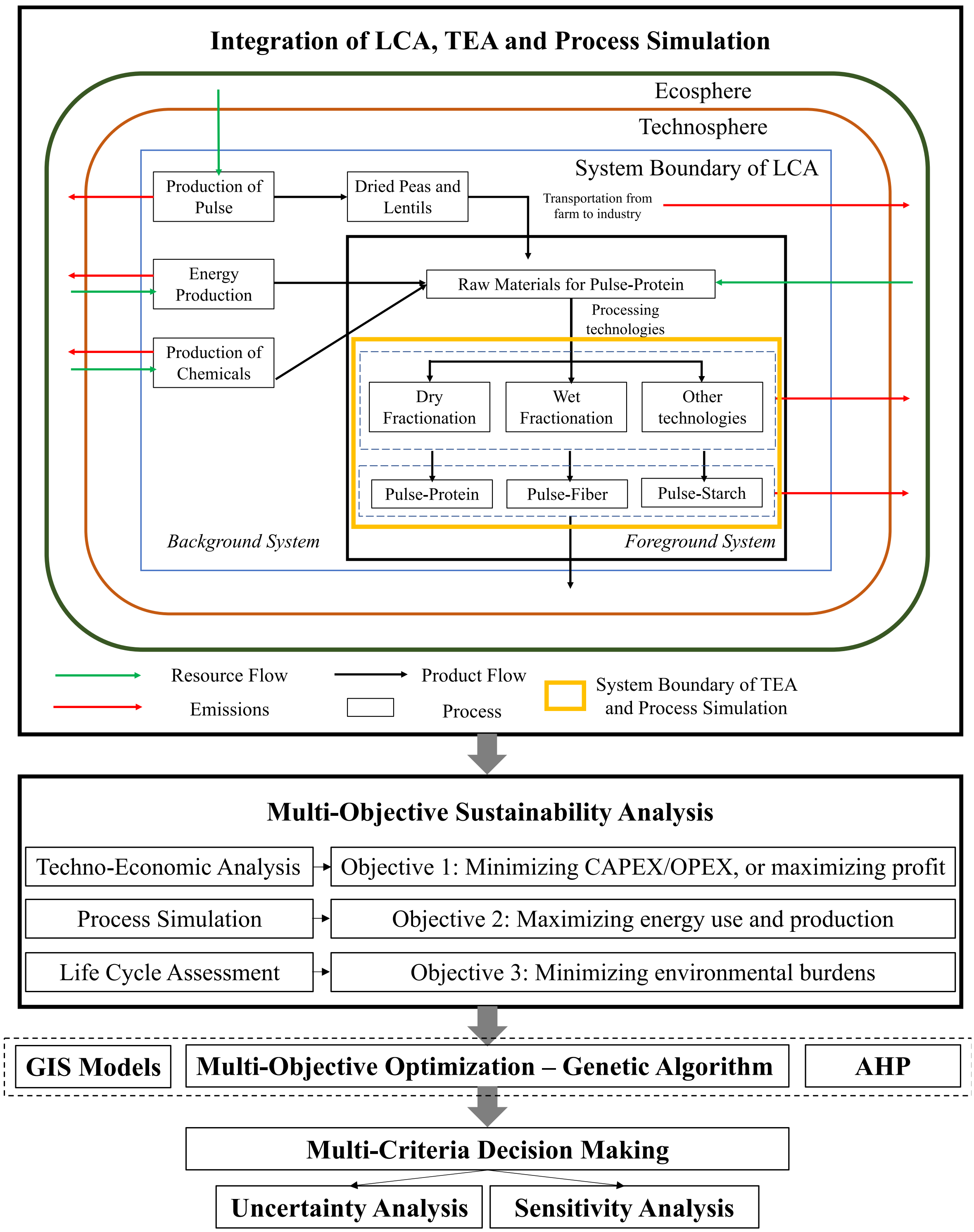

Fig. 3. Proposed integrated framework for multi-criteria decision-making combining LCA, TEA, process simulation and optimization

granular data inventory than is commonly used for TEA. Only 1 study performed both LCA and TEA to compare four different solvent recovery methods in soybean oil extraction (Potrich et al., 2020). In this study, a cradle-to-gate attributional LCA considering a mass-based input (1 metric ton of soybean) as the functional unit was performed, but the system boundary for the TEA was gate-to-gate and the functional unit was mass-based processing capacity (125 tons input per hour). Process simulation and optimization employed the EMSO platform. This process simulation and the Aspen database were their main data sources. For the LCA component, they only considered global warming potential using IPCC 2006 and Invensys as LCIA methods. Allocation was based on energy content. A sensitivity analysis was carried out to evaluate the impact of the price of bagasse and electric energy sales on the net present value (Potrich et al., 2020).

3.3. *Proposed integrated sustainability framework for pulse processing pathways*

Based on the literature considered, it is apparent that an integrated assessment framework for agri-food processing pathways, especially for pulse processing pathways (Table S1; Section 3.1), has not been developed to date. Considering the growing demand for plant-based protein, it is important to evaluate the feasibility of existing and emerging technologies/pathways for pulse fractionation through an integrated sustainability lens, where sustainability profiles based on environmental, technical, and economic criteria can be developed, and optimized solutions can be identified. Based on common practices identified from the literature, but with some notable departures to ensure compliance with the ISO 14044 standard for LCA and employment of suitable methods for TEA, process simulation, and optimization, such a framework is proposed to address this gap. Fig. 3 represents the schematic diagram of the proposed integrated framework, which includes LCA, TEA (with process simulation) and multi-objective optimization for multi-criteria sustainability decision-making in the pulse processing sector. Any process simulation software (i.e., ProSim Plus, Aspen Plus, SuperPro Designer) can be utilized in this integrated framework for technical analysis along with the available LCA software (i.e., OpenLCA, SimaPro). The following sections describe and justify the framework while making connections with current practices as observed in the reviewed articles.

3.3.1. *System boundaries and functional units*

Based on the reviewed articles in R1, it is very common to consider different system boundaries for LCA (cradle to gate) and TEA/process simulation (gate to gate), hence this is a core feature of the proposed framework. The schematic diagram of the framework represents the system boundaries of LCA and TEA (with process simulation) containing a generic process flow diagram for protein crop fractionation/processing techniques (Fig. 3), which can be adjusted based on the studied product system. For instance, if the dry fractionation of peas or beans is the targeted product system, the system boundary of the TEA (with process simulation) will include only the unit processes for obtaining protein concentrates from dried peas or beans. Environmental impacts associated with the background systems (i.e., raw materials production, energy production) should, however, be included in the LCA, despite that optimization of foreground systems may be prioritized.

Despite that different functional units have been used for LCA and TEA in many studies, when integrating these two methodologies, the functional units should ideally be the same. They may include both mass (e.g., 1 kg of pulse protein) and functionality (e.g., 1 kg of protein in the final product) based functional units, defined in terms of the output material. Consideration of functionality-based FUs will enable comparing different pathways producing different levels of protein content in the final product (i.e., protein concentrate from dry fractionation and protein isolate from wet fractionation). Moreover, it will also enable the practitioner to compare processing techniques of plant-based and animal-based proteins. Although many TEA studies consider input material or processing capacity as the functional units (findings from R2), it is here proposed that the focus should be on optimizing output material and/or enhancing the sustainability of the output, which is particularly important for supporting product comparisons and for sustainability communication and marketing.

3.3.2. *Data sources*

Data for foreground systems should be directly collected from pulse processors, with data from published models, patents, technical/industrial reports, and databases such as Ecoinvent and Agri-footprint used for background systems. Data gaps in the processing stage may be filled using process simulation results. For economic analysis, market research reports may be useful along with the databases of a simulation software like Aspen Plus, SuperPro Designer, and/or ProSim Plus.

3.3.3. *Life cycle impact assessment*

In order to be consistent with ISO 14044, all relevant midpoint impact categories associated with protein crop production and processing supply chains should be included (findings from R2). Midpoint impact categories that are most relevant for evaluating agri-food processing techniques are i) climate change, ii) stratospheric ozone depletion, iii) terrestrial acidification, iv) freshwater and marine eutrophication, v) terrestrial, freshwater and marine ecotoxicity, vi) photochemical oxidant formation, vii) human toxicity, viii) particulate matter formation, ix) land use (land occupation and biodiversity), x) water depletion, and xi) fossil and mineral depletion. This is a notable departure from comparable frameworks, most of which only consider global warming potential. Indeed, for compliance with the ISO 14044 standard, all relevant impact categories should be included. However, for the optimization phase, it may be justifiable to include only the most significant ones when seeking to minimize environmental burdens. Endpoint impact categories can also be considered, but with attention to the additional uncertainty this contributes to model results.

3.3.4. *Allocation methods*

Considering the multi-functionality of the studied system (pulse protein extraction), allocation choices should also be ISO 14044 compliant, but sensitivity analyses employing alternative allocation keys including mass, gross chemical energy content, and economic values can be considered. In LCA, mass and gross chemical energy content-based allocation should be prioritized. However, for economic analysis (TEA), allocation based on economic values can be an option. Sensitivity analysis for different allocation methods is always advisable.

3.3.5. *Economic analysis*

The most suitable approach for the economic analysis appears to be by calculating or estimating CAPEX/OPEX for the functional unit. Data can be collected from primary sources or secondary sources like reports and software databases. Rather than just mentioning capital expenditures and operating expenditures, some economic analysis should be reported too. Discounted cash flow analysis was the most commonly used method in the reviewed articles (findings from R1 and R2). Feasibility analysis can be conducted based on gross margin, gross profit, net profit, return on investment, payback period, and net present value. Profitability analysis based on the internal rate of return can also be carried out (Table 1b).

3.3.6. *Multi-objective sustainability analysis and optimization*

The proposed framework for sustainability analysis and optimization (Fig. 3) takes into account three performance criteria – technical, economic, and environmental - to formulate the objective functions. The three primary objective functions for multi-objective optimization should be: i) minimizing CAPEX/OPEX or maximizing profit/net present value (related to the economic analysis), ii) maximizing energy use efficiency and productive output (related to process simulation and technical analysis), and iii) minimizing environmental burdens for significant impact categories (related to the LCA). This multi-objective optimization problem can be most efficiently solved by using a genetic algorithm method, which will give a Pareto-Optimal solution with optimal capacities, production, biomass allocation, etc. while also revealing the potential trade-offs among the objective functions (Hafyan et al., 2020a, 2020b; Han et al., 2021). For designing the optimization framework, decision variables (i.e., biomass availability, production/yield of different outputs, operating conditions – temperature, pressure, flow rate, conversion rate, etc.) and constraints (i.e., mass and energy balances, market demand, equipment fabrication, operating conditions) must be defined. Decision variables will be varied within their lower and upper bounds to create optimal solutions with regard to the defined constraints. Sometimes, to avoid numerous iterations for genetic algorithms, the simulation model can be simplified via regression models (Hafyan et al., 2020b).

3.3.7. Integration of GIS models and AHP

To make the assessment framework more robust for context-specific decision support, GIS-based spatially explicit models and Analytic Hierarchy Process (AHP) can also be applied. For instance, geographically explicit background models for pulse production can enable regionalized LCIA results based on the source of raw materials. In addition, since multi-objective optimization will result in multiple optimal solutions (Pareto solutions), the integration of AHP will facilitate finding the best solution by incorporating different stakeholders' perspectives. Different weights can be assigned for the objective functions based on the preferences of, pulse producers, processors, plant-protein consumers, etc.

3.3.8. Uncertainty and sensitivity analyses

Although the existing frameworks did not explicitly mention uncertainty analysis, the proposed framework includes uncertainty analysis for the input and model parameters. Monte Carlo Simulation and the Pedigree Matrix approach are commonly used for uncertainty measurement (Table S1, 1a and 1b). Sensitivity/scenario analyses should consider varying input and economic parameters to assess the influence of these parameters on the process outputs and results. Sensitivity analyses should also be carried out with varying functional units, allocation methods, and weights for AHP, and to validate the use of the selected LCIA methods (i.e., ReCipe, IMPACT WORLD+) and their specific characterization and/or emission factors (Tables 1a and 1b). This proposed framework will enable multi-criteria decision-making to identify the most suitable pulse processing pathways based on a multi-criteria sustainability lens.

3.3.9. Facilitating eco-design

Eco-design aims to integrate consideration of environmental impact indicators into product design, taking into account each stage of a product's life cycle (Bhamra and Lofthouse, 2016). Eco-design may inform materials substitution, optimization of machinery, controlling the use phase, or goals related to transitioning towards a circular economy (Spreafico and Landi, 2022). Integrating the environmental aspects into product design and development is an emerging research area. This proposed framework can enable stakeholders to utilize eco-design in the plant-protein sector in order to support appropriate design decisions and solutions, including the conceptualization and development of sustainable products (Spreafico and Landi, 2022). Spreafico and Landi (2022) underscored some misperceptions that designers have about eco-knowledge and eco-design. For instance, if there is no quantitative assessment framework, designers may be strongly influenced by perceptions triggered by emotional and aesthetic aspects (Maccioni and Borgianni, 2020). That's why a systematic quantitative assessment framework such as that proposed herein can facilitate eco-design in the plant-protein sector by directing stakeholders/designers toward optimizing the structure of the product system, reducing energy and/or material consumption, substituting raw materials, and reducing production cost and environmental burdens.

4. Conclusions

Existing integrated frameworks for LCA and TEA have a small number of sector-specific characteristics. Integrated system boundaries, functional units, and application of uncertainty measurement techniques are uncommon. Most of the frameworks did not explicitly define all the characteristic elements of LCA and TEA methodologies.

Both LCA and TEA are widely used to evaluate the environmental, technical, and economic feasibilities of existing and/or emerging pathways/technologies. Integrating process simulation and optimization into such frameworks is an emerging area, with few published examples to date. Different researchers have combined these methods in different ways, depending on the studied systems. It is hence important to develop a dedicated framework for pulse processing pathways. The framework herein constitutes a multi-criteria decision-making tool based on multi-objective sustainability assessment and optimization, which can be used for assessing and optimizing the sustainability of pulse processing pathways. It can also be adaptable for any other agri-food processing techniques.

One of the main limitations of this framework is, however, the absence of the social pillar of sustainability. Another is its exclusive focus on the processing stages (the most energy-intensive aspect of the supply chain of plant proteins). It does not currently support the optimization of downstream and/or upstream processes, although the addition of this capability merits further consideration/research. In addition, as LCA heavily depends on data (Junqueira et al., 2018), in the absence of quality data, other assessment matrices like the eco-efficiency index (Mangili et al., 2019) may be used. Although the proposed framework suggests integrating MCDM methods like AHP to include stakeholders' preferences for different criteria (i.e., economic, technical, environmental), there are still scopes to develop other integrated frameworks for weighted sustainability assessment for agri-food processing systems. For example, there are already weighted performance metrics that have been developed for designing chemical processes (Gonzalez-Garay and Guillen-Gonsalbez, 2018; Mangili et al., 2019), manufacturing (Shi et al., 2022); dairy processing (Benoit et al., 2019); waste management (Young et al., 2000); chemical production (Radzuan et al., 2019); etc.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2023.136804.

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