



## Research Paper

# Pathway development for brewer's spent grain valorization using multi-objective optimization

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## ARTICLE INFO

## Keywords:

Superstructure Optimization  
Early-Stage Biorefinery Design  
Minimum Selling Price  
Carbon Footprint Analysis  
OUTDOOR

## ABSTRACT

Brewer's spent grain (BSG) is a major biowaste stream in the European beer industry used for animal feed, biogas and landfilling. Its composition offers potential for producing a variety of value-added products, making it crucial to benchmark valorization technologies for better management. In response to this sectorial need, the study applies a methodological framework previously developed open-source OUTDOOR software to the brewing industry context. A multi-objective optimization was performed for a superstructure that includes all possible BSG valorization pathways, guiding decision-making in biorefinery design, and assessing the economic and environmental sustainability of the process.

Beyond traditional valorization options, a comprehensive review of potential products and conversion pathways—including biological, thermochemical and extraction routes—was conducted based on biomass characterization. A Pareto efficiency analysis was applied to integrate the two optimization objectives, using earnings before interest and taxes (EBIT) and minimum selling price (MSP) to evaluate economic performance, and the carbon footprint analysis compliant with ISO 14067 to assess environmental impact.

Results indicate animal feed as the most profitable route, with an EBIT approximately 10 % higher than the best second alternative (compost). Environmentally, compost exhibits the smallest carbon footprint, around 91 % lower than the next best option (biogas). Ethanol and hydrochar stood out for their environmental value and proximity to market competitiveness, based on MSP. An evaluation of cascade conversion strategies suggested that the combination of multiple valorization routes is only viable through synergies between pathways, i.e. if obtaining one product facilitates the remaining routes through increased yields or resource efficiencies.

## 1. Introduction

The global beer industry generates substantial quantities of biowaste, particularly in the form of brewers' spent grain, with around 20 kg/hL of beer produced (Liu et al., 2025). In the European context, beer production reached 166.73 million hL in 2022, with Germany at the forefront, followed by Spain and Poland, resulting in an estimated 3.67 million tons of BSG generated annually across the region (Naibaho et al., 2024). Currently, about 70 % of this residue is repurposed as animal feed, while 10 % is utilized for biogas production via anaerobic digestion (AD), and the remaining 20 % is disposed of in landfills (Aradwad et al.,

2025), giving space for more efficient and, a priori, more sustainable applications following the waste hierarchy (European Parliament and Council, 2008).

The composition of spent grains plays a crucial role in determining their potential for valorization as they are rich in fibers, proteins, and bioactive compounds that make them ideal candidates for innovative applications in food, biofuels or cosmetics (Xiros and Christakopoulos, 2012). For example, the Danish company *Agrain* has implemented a sustainable and profitable route to upcycle BSG into spent grain flour, yielding 200 kg/ton and saving both 44–88 kg of CO<sub>2</sub> and 400 m<sup>2</sup> of agricultural land, compared to producing the same amount of wheat

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<https://doi.org/10.1016/j.wasman.2026.115558>

Received 3 October 2025; Received in revised form 1 March 2026; Accepted 21 April 2026

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flour (Agrain, 2025). However, the properties can vary depending on the brewing method, type of beer brewed, the addition of adjuncts, pre-processing of the grains, or the separation process, complicating the design of biorefinery processes for their optimal recovery (Xiros and Christakopoulos, 2012).

Since BSG is a promising raw material for obtaining high-value-added compounds, numerous valorization strategies have been investigated in recent years. Its high dry carbon content makes it particularly suitable to produce bioalcohols (ethanol and butanol) or biogas, thermochemical methods have also been studied to exploit its energy content in hydrochar production, antioxidant phenolic compounds and high-value proteins can be extracted, and also a considerable proportion of fibers that can be used to produce dietary supplements (arabinoxylan) or prebiotics (xylitol) (Puligundla and Mok, 2021).

For a given type of BSG, identifying the most effective valorization strategies requires a simultaneous analysis of all available technological pathways and their possible combinations. Therefore, superstructure optimization (more information on the approach in Section 2 of Supplementary Material) emerges as a suitable tool by capturing all feasible flowsheets in a set of processes. Its effectiveness has been demonstrated by Van der Hauwaert et al., (2025a) with a framework for the sustainable design of a biorefinery for potato waste considering the uncertainty of the solutions, or in a later study for the tomato pulp with an environmental-economic optimization (Van der Hauwaert et al., 2025b). Arango-Manrique et al., (2024) extended similar methodologies to citrus waste by systematically comparing different valorization routes for orange peel waste through conceptual design. Elyasi et al., (2021) formulated an integer superstructure model to determine sustainable platforms for the conversion of household waste into bioenergy, microbial protein and biochemicals. Additionally, Guerras et al., (2021) employed a multilayer superstructure approach for the product portfolio optimization for olive industry residues.

A key factor for biorefinery systems is their environmental sustainability, as their development is driven by the role they are expected to play in the transformation toward a future bioeconomy. A clear environmental benefit must be demonstrated from the initial stages of process design, while maintaining economic viability to ensure market competitiveness and minimize investment risks. This requires a multi-objective optimization approach in the superstructure to balance environmental and economic perspectives. Consequently, the objective of this study is to identify the optimal valorization route for BSG that both maximizes EBIT and minimizes carbon footprint analysis (CFA), and steams from the specific needs of the brewing industry. Given the wide range of options of routes and products available for valorizing BSG—many of them at early stages of development—and the intrinsic variability of this biomass stream, a superstructure-based multi-objective optimization approach is employed to systematically benchmark alternative pathways according to the objectives of interest. The methodological framework is here adapted to the agro-industrial context, enabling the assessment of standalone and cascading configurations within a unified environment. It serves as a practical decision-support tool for residue valorization systems like BSG, and illustrates how optimization-based approaches can be effectively applied to prioritize the processing strategies under sector-specific constraints.

Section 3, Results, begins with raw material characterization and a systematic review of potential products, selecting the best technological route to obtain each one through a pre-multi-objective economic optimization based solely on EBIT. Next, the MSP of the products is used as a complementary decision-making aid for stakeholders, and multi-product valorization cascade schemes are explored to maximize resource use. Finally, Section 4, Conclusions, summarizes the main findings and potential future improvements in the results.

## 2. Material and methods

### 2.1. Data acquisition

The data used in the construction of each unit operation of the superstructure was obtained from bibliographic sources, specified in greater detail in Section 5 of the Supplementary Material. Specifically, the parameters for calculating the cost of each equipment using the factorial method were extracted from process engineering design manuals (Woods, 2007), while the operating expenses for utilities (electricity and head demand) were estimated using scaling-up methods (Piccinno et al., 2016).

On other hand, the operating conditions (temperature and pressure), reaction yields (material balances), and separation efficiencies for each route were extracted from the references specified in Table 1. For its elaboration, the literature search combined terms related to the feedstock (e.g., “brewer’s spent grain”, “BSG”, “spent grain”) with terms associated with valorization routes and process performance (e.g., “valorization”, “utilization”, “biorefinery”, “extraction”, “fermentation”, “anaerobic digestion”, “hydrothermal carbonization”, “yield”, “recovery”, “efficiency”, and “operating conditions”). Also, the search was guided by two research questions: (i) which BSG valorization routes or technologies have been experimentally evaluated, and (ii) which studies report quantitative operating conditions and experimental performance data suitable for consistent integration within the superstructure model. For the study screening strategy, only peer-reviewed studies written in English and published after 2005 were considered, excluding conference papers and contributions containing only abstracts. Articles with original quantitative data obtained by the authors were selected and the precision of the experimental campaign was verified through statistical analysis. Furthermore, an uncertainty analysis was not applied to the compiled values to avoid misinterpretations, as the studies were conducted under heterogeneous brewing conditions.

Regarding the stage of establishing connections between processing routes to create cascades, it was guided by a physicochemical characterization following the methodology of Rovira-Cal et al., (2025). This characterization considers the composition of BSG, including hemicellulose, cellulose, proteins, lignin, lipids and starch, as further described in Section 3.1 of this document. According to the aforementioned approach, recovering using extraction methods for secondary metabolites (proteins, lipids or polyphenols) present in lower concentrations but with high market value were prioritized, to avoid their degradation into other and less valuable intermediate products. Bioconversion techniques for substrates with high sugar content were incorporated in a second stage. Finally, end-of-cycle alternatives comprise those that do not require detailed prior characterization of the residue (only dry matter and elemental composition), as they are suitable for wide variety of residues (anaerobic digestion). Also, to select several technologies at the same level, a descending order was established based on market value.

In the environmental CFA, background data for electricity consumption and waste treatment processes were retrieved from the regional data sets (RERs) of the consequent version of the Ecoinvent database v3.9.1 when available (Weidema, 2003), choosing European conditions given the limits of the study.

### 2.2. Superstructure model

The superstructure optimization problem aims to determine the optimal flow diagram between a set of potential processes and their interconnections, which varies according to the objective function. It is represented by a mathematical model of equations (Eqs. (1)–(5)) that describes the optimization criterion (Eq. (1)), the constraints on unit operations (Eqs. (2)–(4)), and the logical rules that determine the selection of the route in the network (Eq. (5)) (Van der Hauwaert et al., 2024).

$$\min F(x, y) = (f_{econ}(x, y), f_{env}(x, y)) \quad (1)$$

$$g(x, y) \geq 0 \quad (2)$$

$$h(x, y) = 0 \quad (3)$$

$$x^{LO} \leq x \leq x^{UP} \quad (4)$$

$$x \in X, y \in \{0; 1\}^n \quad (5)$$

where  $F$  is a vector of the objective functions  $f_{econ}(x, y)$  and  $f_{env}(x, y)$ , corresponding to economic and environmental criteria, respectively. Vector  $x$  represents the continuous variables of the model, which describe operating parameters (mass flow, equipment sizing, etc.) with lower and upper bounds  $x^{LO}$  and  $x^{UP}$ , in a continuous feasible region  $X$ . Vector  $y$  denotes the binary variables responsible for selecting or not a specific unit process. Vectors  $g$  and  $h$  are inequality and equality constraints, used in a set of generic equations (Eqs. (2)–(3)) that represent the series of possible operations that a unit process can carry out. Nonlinear equations (e.g., for capital cost equations) were piecewise linearized resulting in a mixed integer linear problem (MILP).

The economic criterion in the multi-objective problem (Eq. (1)) was defined as the maximization of the EBIT (Eq. (6)).

$$\max \text{EBIT} = (\text{PROFITS} - (\text{CAPEX} + \text{OPEX})) / \text{cap}^{LOAD} \quad (6)$$

EBIT (in €/ton of BSG) is determined based on total annualized capital costs (CAPEX) over a plant lifetime of 20 years using an interest rate of 5 %, total annual operating costs (OPEX) and annual profit (PROFITS), normalized by the annual load of incoming BSG ( $\text{cap}^{LOAD}$ ).

Regarding the environmental criterion in the multi-objective function (Eq. (1)), minimization of the carbon footprint was considered in accordance with ISO 14067 (Eq. (7)).

$$IS_{u,CFA} = \sum_{a \in A} F_a \cdot EF_{a,CFA} \quad (7)$$

where  $IS_{u,CFA}$  is the impact score or environmental burden of unit  $u$ , measured in  $\text{CO}_2$ -equivalents per kg of BSG as functional unit.  $F_a$  denotes the activity data for activity  $a$  (energy consumption, raw material flow entering the unit, or waste flow sent for treatment).  $EF_{a,CFA}$  is the factor that translates the load into carbon footprint, combining both the conversion of flows into emissions using Ecoinvent v3.9.1, and their characterization into GWP100 with ReCiPe 2016 (H) following the Intergovernmental Panel on Climate Change (2021) guidelines.

In the CFA performed it was assumed that the products would be introduced as new to the market, not replacing existing alternatives for the same use. A gate-to-gate approach was also adopted to avoid the uncertainties associated with the use and end-of-life stages of the resultant products, as some of them are not yet commercially validated and therefore data on the mechanical and chemical properties as well as on the targeted markets are not available.

On the other hand, since many of the alternatives studied are emerging and still in the development phase, they lack established value chains and market prices constitute one of the main sources of uncertainty in the analysis. In this context, the MSP was calculated as a tool to evaluate the economic viability of the routes, providing the price at which EBIT falls to zero (Eq. (8)), ensuring coverage of all capital and operating costs normalized by the annual capacity of each product ( $\text{cap}^{PROD}$ ).

$$\text{MSP} = (\text{CAPEX} + \text{OPEX}) / \text{cap}^{PROD} \quad (8)$$

### 2.3. Computational and optimization framework

The optimization problem was formulated using the open-source tool OUTDOOR (Kenkel et al., 2021), and the graphical user interface developed by Van der Hauwaert et al., (2025b). In the software, the set

of generic constraint equations (Eqs. (2)–(3)) are used to describe: (1) mass balances of input and output streams; (2) utility operating expenses (electricity, heating and cooling); (3) equipment capital expenditure; (4) basic environmental impacts ( $\text{CO}_2$ ); and (5) heat exchange network cost using pinch analysis. Regarding the environmental modelling, the open-source package Brightway2 (Mutel, 2017) for life cycle assessment (LCA) was used, and biogenic  $\text{CO}_2$  emissions were considered neutral (0) so that they do not contribute to the net increase in greenhouse gases (GHG), as they come from the carbon absorbed from the atmosphere by biomass. To view the complete mathematical model behind OUTDOOR we refer to the Supplementary Material of Van der Hauwaert et al., (2025b).

For multi-objective optimization of the superstructure, each of the possible valorization pathways for the BSG was evaluated using a Pareto efficiency analysis. This approach identifies the non-dominated alternatives (optimal) for the economic and environmental objectives, which form the so-called Pareto front. These calculations were performed on a laptop with an Intel® Core™ Ultra 7 155U processor, 1.70 GHz, 12 cores, 14 logical processors, and 16 GB of RAM.

## 3. Results and discussion

### 3.1. Biomass characterization

The BSG primarily consists of barley grain husks, but endosperm fragments can also be present. As revised by Lisci et al. (2022), the chemical profile is mainly based on hemicellulose (arabinoxylans), cellulose and a considerable amount of proteins and lignin, while lipids and residual endosperm starch are also a part and contribute to their dry weight. Besides, wet BSG typically contains a high moisture content, up to 80 % wet matter, which must often be significantly reduced for further processing (Russ et al., 2005). An overview of the biomass characterization and the variability reported in the literature is provided in Section 3 of Supplementary Material.

### 3.2. Superstructure formulation

The process of constructing the superstructure involved developing a conceptual map that represents all possible valorization pathways for BSG. A structured approach was followed, organizing the design of each product route into several process intervals. Each interval represents a specific step in the biorefinery and includes all possible unit operations that can be employed. Specifically, four intervals were evaluated: (1) pretreatment; (2) extraction processes; (3) reactions; and (4) downstream and purification.

Table 1 provides a literature review of the technological basis for unit operations, operating conditions, and yields included in the optimization model. Target products include conventional applications for direct use such as animal feed or composting, and the potential emerging routes identified in Section 1 of this document based on waste composition. The level of development of the valorization methods is highly heterogeneous. Most extraction-based processes (antioxidants, proteins, arabinoxylan) remain at laboratory scale, often under tightly controlled conditions and with limited process integration. Thermochemical routes (hydrochar) show higher technological readiness but are still demonstrated mainly in batch-scale studies. Biological processes such as anaerobic digestion, ethanol, and butanol fermentation span from lab to pilot scale depending on the study, but typically involve intensive pretreatment steps that limit industrial maturity. Even if the reported yields can potentially improve as the methods become mature, the evaluation in this work is restricted to the values in Table 1.

To more easily manage all combinations and reduce computational complexity in the multi-objective system, a preliminary single-objective optimization step was performed to identify the economically favorable conversion path for each product, maximizing EBIT. The results obtained and the small superstructure employed for each scenario are

**Table 1**  
Examples of BSG valorization methods including various pretreatments and their product yield.

Product	ID	Unit operation	Process conditions	Yield	Reference
Animal feed	1	Extrusion	120 °C; 20 MPa; 5 min; S/L 1:1	59.9 g/100g <sub>BSG</sub>	(Kletscher et al., 2014)
Compost	2	Composting	55 °C; 60 % humidity; C/N 25:1; Continuous aeration	71.5 g/100g <sub>BSG</sub>	(Murphy and Power, 2006)
Biogas	3	Anaerobic Thermophilic Digestion	55 °C; 100 g <sub>BSG</sub> /L; Inoculum: mixed animal manure; Co-digestion: <i>Helianthus tuberosus</i> L. 10 g/L; pH 7; CH <sub>4</sub> yield 61 %; 10–16 days	8.6 L <sub>CH<sub>4</sub></sub> /100g <sub>BSG</sub>	(Robertson et al., 2010)
	4	Ultrasonic Pretreatment, and Anaerobic Mesophilic Digestion	Ultrasonic: Ultrasonic power 53 W; 179.45 g <sub>BSG</sub> + 1,43 L <sub>water</sub> ; 1 h; 0.29 MWh/1000kg <sub>BSG</sub> Anaerobic Digestion: 35 °C; 41.16 g <sub>BSG</sub> /L; Broth composition: 179.45 g <sub>BSG</sub> , 1,43 L <sub>water</sub> , 1.7 L <sub>inoculum</sub> ; pH 7–8; 50 days; Total volatile solids (TVS) of BSG 73.6 % Solvent: water; 30 °C; 121.9 min; L/S 10 mL/g; 1 atm	7.896 L <sub>CH<sub>4</sub></sub> /100g <sub>BSG</sub> ; 107.28 L <sub>CH<sub>4</sub></sub> /kg <sub>TVS</sub>	(Buller et al., 2022)
Anti-oxidant phenolics	5	Solid-Liquid Extraction	Solvent: 0.75 % NaOH in water; 100 °C; 15 min; L/S 20:1	542 mgGA <sub>eq</sub> /100g <sub>BSG</sub>	(Moreira et al., 2012)
	6	Microwave-Assisted Conventional Extraction	Solvent: 0.5 EtOH/water (v/v); 120 °C; Flow rate: 2 mL/min; 10.34 MPa	1.31 g <sub>ferulic acid</sub> /100g <sub>BSG</sub>	(González-García et al., 2021)
	7	Pressurized Liquid Extraction	Solvent: water; 120 °C; Flow rate: 4 mL/min; 10 MPa	19.3 % (wt.); 1471 ± 25 mgGA <sub>eq</sub> /100g <sub>BSG</sub> ; 6384 ± 444 mmol TE/100g <sub>BSG</sub>	(Herbst et al., 2021)
Arabin-oxylan	8	Pressurized Liquid Extraction	Solvent: CO <sub>2</sub> ; 40 MPa; 80 °C; S/F 706 g <sub>CO<sub>2</sub></sub> /g <sub>BSG</sub> ; 4 h	17.8 % (wt.); 2130 ± 1 mgGA <sub>eq</sub> /100g <sub>BSG</sub> ; 9944 ± 391 mmol TE/100g <sub>BSG</sub>	(Herbst et al., 2021)
	9	Supercritical Fluid Extraction	Extraction: S/L 1:2 (w/v); solvent: KOH or NaOH 0.1 M, 0.5 M and 4 M; room temp.; 24 h; 81–83 % (wt.) protein recovery from original 8.65 g <sub>protein</sub> /100g <sub>BSG</sub> ; pH 11–12; AX Precipitation: pH 3 (citric acid 2.3 M), then pH < 2 (HCl 12 M); 70 % (v/v) aqueous EtOH; yield from original AX content 79 % (wt.) Total AX 25.8 % (wt.); Thermal Pretreatment; S/L 10 % (w/v); 90 °C; 30 min; Enzymatic Hydrolysis; Laminex Super 3G: 1000 ppm; Attenuzyme Pro: 500 ppm; UltraFlo FABI: 100 ppm; Alcalase: 200 ppm; 35 °C; Fermentation; Lactiplantibacillus plantarum F10; inoculum volume 1 % (v/v); 220 rpm; pH 6.8, 6 h; yield from original AX content 21.3 % (wt.)	5.70 g <sub>extract</sub> /100g <sub>BSG</sub> ; 16.6 mgGA <sub>eq</sub> /g <sub>extract</sub> ; 94 mgGA <sub>eq</sub> /100g <sub>BSG</sub>	(Alonso-Riño et al., 2022)
Hydrochar	10	Sequential Alkali Acid Extraction	Extraction: S/L 1:12 (w/v); S: NaOH 1.5 M; room temp.; 400 W, 20 kHz; 15 min; initial pH unspecified; CaCl <sub>2</sub> 8 % (w/v); pH 4 (HCl 6 M); extract yield 13.60 % (wt.); total sugar content 85 % (wt.); AX fraction in extract 60.46 %; yield from original AX content 58.47 % (wt.)	17 g <sub>AX</sub> /100g <sub>BSG</sub>	(Vieira et al., 2014)
	11	Thermal Pretreatment, Simultaneous Enzymatic Hydrolysis and Fermentation	250 °C; 0 h; HHV 31.75 MJ/kg; Energy yield 55.92 %; C content: 71.14 %; O/C: 0.19, H/C: 1.18 (mol/mol)	4.6 g <sub>AX</sub> /100g <sub>BSG</sub>	(Lynch et al., 2021)
Ethanol	12	Ultrasound-Assisted Extraction	230 °C; 6 h; LHV 30.3 MJ/kg; Energy yield 60 %; Fixed C content: 33.7 % dry; O/C: 0.27, H/C: 1.4 (mol/mol)	8.2 g <sub>AX</sub> /100g <sub>BSG</sub>	(Liu et al., 2023)
	13	Microwave-Assisted Hydrothermal Carbonization	Phosphoric acid hydrolysis: 155 °C; 0 min; 2 % w/w Enzymatic hydrolysis: 24 h; pH 4.8; 50 °C; Cellic CTec2 15 FPU/g; β-glucosidase 15 IU/g Fermentation: Ethanogenic <i>E. coli</i> SL100; pH 6.5; 37 °C; 300 rpm; 100 h	43.69 g/100g <sub>BSG</sub>	(Lorente et al., 2020)
Ethanol	14	Hydrothermal Carbonization	Supercritical fluid extraction: 40 MPa; 100 °C; S/F 30 g <sub>CO<sub>2</sub></sub> /g <sub>BSG</sub> Acid hydrolysis: 0.37 M H <sub>2</sub> SO <sub>4</sub> ; L/S: 10 g <sub>liquid</sub> /g <sub>BSG</sub> ; glucose recovery 18.3 g/100g <sub>BSG</sub> Fermentation: <i>S. cerevisiae</i> ; pH 4.5; 25 °C; inoculum volume 12.25 % (v/v); 150 rpm; 9 h	42.0 g/100g <sub>BSG</sub>	(Ulbrich et al., 2017)
	15	Acid hydrolysis, enzymatic hydrolysis, and fermentation	Acid-alkali hydrolysis: 1.25 % (v/v) H <sub>2</sub> SO <sub>4</sub> , 1:8 w/w; 120 °C; 17 min; followed by 2 % (v/v) NaOH, 1:20 w/w; 120 °C; 90 min Enzymatic hydrolysis: 2.24 % (v/v) cellulase and 1 % (v/v) β-glucosidase (Novozymes), 8 % (w/v) substrate; 45 °C; 120 rpm 72 h; cellulose to glucose conversion efficiency 97 %	17.5 g/100g <sub>BSG</sub> ; 0.0222 L/100g <sub>BSG</sub>	(Rojas-Chamorro et al., 2020)
	16	Supercritical fluid extraction, acid hydrolysis, and fermentation		14.83 g/100g <sub>BSG</sub>	(Lisci et al., 2024)
	17	Acid-alkali hydrolysis, enzymatic hydrolysis, and fermentation		26 g/100g <sub>BSG</sub>	(Liguori et al., 2015)

(continued on next page)

Table 1 (continued)

Product	ID	Unit operation	Process conditions	Yield	Reference
Butanol	18	Autohydrolysis, enzymatic hydrolysis, and fermentation	Fermentation: S. cerevisiae NRRL YB 2293; 50 g <sub>glucose</sub> /L; pH 6.0; 30 °C; 120 rpm; 48 h	16.8 g/100g <sub>BSG</sub> (BLGII 1762); 16.0 g/100g <sub>BSG</sub> (PE-2)	(Pinheiro et al., 2019)
			Autohydrolysis: 160 °C; 5 min; solid loading 25 % (m <sub>BSG</sub> /v <sub>water</sub> ) Enzymatic hydrolysis: Cellic CTec2 enzyme (15 FPU/g <sub>BSG</sub> ); 50 °C; 200 rpm; 120 h		
	19	Microwave-Assisted Hydrothermal, Enzymatic Hydrolysis, and Fermentation	Fermentation: S. cerevisiae BLGII 1762 (brewing yeast) and PE-2 (industrial bioethanol yeast); 60 g <sub>glucose</sub> /L; pH 4.8; 30 °C; 150 rpm; 48 h Microwave: 1800 W; 192.7 °C; 5.4 min; S/L 10 % (w/v); S: water; 82 % sugar recovery; 43 g <sub>fermentable sugars</sub> /100 g BSG; Enzymatic Hydrolysis: enzyme: Cellic CTec2 enzyme complex; 50 °C; pH 4.8; 48 h; 15 FPU/g of solid enzyme loading; glucose recovery 69.5 %; Fermentation: Clostridium beijerinckii DSM 6422; Reinforced Clostridial Medium; 35 °C; 135 rpm; 48 h (inoculum); 120 h fermentation	4.6 g <sub>butanol</sub> /100g <sub>BSG</sub>	(López-Linares et al., 2019)
Protein	20	Acid Hydrolysis, Enzymatic Hydrolysis, and Fermentation	Acid Hydrolysis; BSG: 23.1 glucan, 15.5 xylan, arabinan 7.4 % (wt.) per 100 g <sub>BSG</sub> ; 10.4 % (wt.) sulfuric acid (96 %); pH 1; 121 °C; 30 min; Enzymatic hydrolysis; Celluclast 1.5 L (Cellulase): 15 FPU/g <sub>BSG</sub> and Novozyme 188 (β-Glucosidase): 15 IU/g <sub>BSG</sub> ; pH 5.3; 50 °C; Fermentation; Clostridium beijerinckii DSM 6422; pH 6.5; 96 h; 35 °C; glucose yield 97.6 ± 1.8 %	7.5 g <sub>butanol</sub> /100g <sub>BSG</sub>	(Plaza et al., 2017)
	21	Laccase Pretreatment, Enzymatic Hydrolysis, and Fermentation	Laccase: 10 U/g <sub>BSG</sub> laccase; 150 rpm, 28 °C; 24 h; incubation: 50 °C, 6 h; Enzymatic Hydrolysis; 15 mg <sub>protein</sub> /g <sub>glucan</sub> Cellic CTec 2 Xylanase; S/L 10 % (w/v); 250 rpm; 50 °C; 72 h; Fermentation; Clostridium acetobutylicum DSMZ 792; pH 6.5; inoculum 6.25 % (v/v); glucose yield 99 %; 40 g <sub>sugar</sub> /L; 25 g <sub>butanol</sub> /g <sub>sugar</sub> ; 37 °C	10 g <sub>butanol</sub> /100g <sub>BSG</sub>	(Giacobbe et al., 2019)
	22	Pressurized Liquid Extraction	S: 0.35 EtOH/water (v/v); 155 °C; Flow rate: 0.3 mL/min; 10 MPa	11.6 g <sub>protein</sub> /100g <sub>BSG</sub>	(Spinelli et al., 2016)
Xylitol	23	Ultrasonic Extraction	S/L 2 g <sub>BSG</sub> /100mL; solvent: sodium carbonate buffer; pH 10; 81.4 min; ultrasonic power 98.2 W/100 mL	9.64 g <sub>protein</sub> /100g <sub>BSG</sub>	(Tang et al., 2010)
	24	Sequential Alkali Acid Extraction	22.63 ± 2.24 g <sub>protein</sub> /100g <sub>BSG</sub> Alkaline: 110 mM NaOH, 1:20 (w/v), 50 °C, 2 h; pH > 12; protein in liquid phase 17.73 g <sub>protein</sub> /100g <sub>BSG</sub> ; yield 78 % Acid: 1 M H <sub>2</sub> SO <sub>4</sub> , 1:20 (w/v), 121 °C, 1 h; pH < 1; protein in liquid phase 3.86 g <sub>protein</sub> /100g <sub>BSG</sub> ; yield 79 %; Combined: yield 95 %	21.59 g <sub>protein</sub> /100g <sub>BSG</sub>	(Qin et al., 2018)
Xylitol	25	Acid Hydrolysis and Fermentation	L/S 8 (g/g); Acid hydrolysis; Solvent 100 mg/g <sub>BSG</sub> H <sub>2</sub> SO <sub>4</sub> ; 17 min; recovery of sugars 92.7 % (wt.); Fermentation: Candida guilliermondii; pH 6.5; 30 °C; 24 hr; 200 rpm	0.7 g <sub>xylitol</sub> /100g <sub>BSG</sub>	(Mussatto and Roberto, 2005)

provided in Section 4 of the Supplementary Material.

The most cost-effective processes for each product are specified below using the identificatory given in Table 1: (3) thermophilic AD for biogas production (Robertson et al., 2010); (5) production of phenolic antioxidants by conventional solid-liquid extraction with water as a green solvent (Moreira et al., 2012); (12) production of arabinoxylan using advanced ultrasonic extraction techniques (Liu et al., 2023); (13) development of hydrochar as a biomaterial by microwave-assisted hydrothermal carbonization (Lorente et al., 2020); (18) biological production of ethanol with auto- and enzymatic hydrolysis followed by fermentation (Pinheiro et al., 2019); (20) butanol synthesis through sequential acid-enzymatic hydrolysis and fermentation (Plaza et al., 2017); and (22) protein recovery for microbial processes using pressurized liquid extraction (Spinelli et al., 2016). These routes, together with the technologies that present a single option (animal feed, compost and xylitol), form the basis of the final multi-objective superstructure illustrated in Fig. 1.

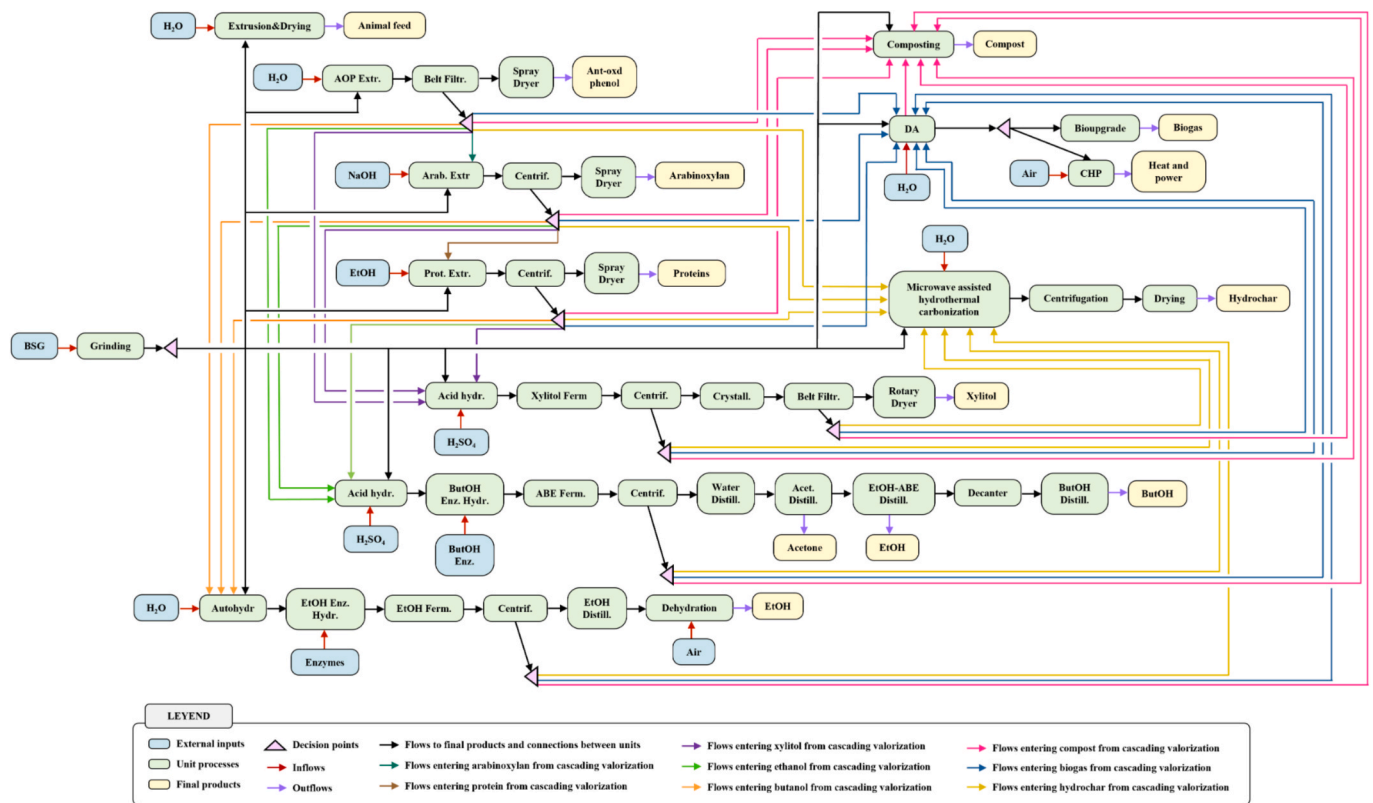
Additionally, the superstructure design incorporates potential synergies between processing routes, and a common upstream grinding unit

to reduce particle size and increase the efficiency of downstream extraction and conversion processes. Regarding the initial system design, an annual waste processing volume of 4.800 t/year was estimated for each subproblem, equivalent to the amount handled by the Danish company Agrain to produce brewing flour (Ingredients Network, 2023), with an input fee of 59 €/ton of BSG, corresponding to the cost of avoiding landfill waste management in Denmark (Bolwig et al., 2019). Finally, it should be noted that the construction of the facility was set for early 2020 to mitigate high uncertainty on equipment costs due to drastic change after COVID 19 pandemic.

### 3.3. Multi-objective optimization

To explore the trade-offs between the economic and environmental dimensions of the multi-objective problem, Table 2 evaluates the BSG valorization pathways, providing EBIT and CFA values, along with the production flows and total system mass throughput.

In view of the results obtained, two alternatives stand out as non-dominated, forming the Pareto frontier of the system. On the one



**Fig. 1.** Comprehensive superstructure of BSG valorization pathways, extracted from the graphical interface of OUTDOOR software. The blue boxes (■) indicate external inputs to the unit processes, the green boxes (■) are the unit processes, and the yellow boxes (■) are the final products. The pink triangles (◀) represent the decision points where the optimization problem must determine how the flows are divided. External inputs and outputs flows are highlighted with red (→) and lilac arrows (→). Black arrows (→) represent processes directly linked to the individual production of the 10 main products (animal feed, phenolic antioxidants, arabinoxylan, proteins, compost, biogas, hydrochar, xylitol, butanol and ethanol). All remaining-colored arrows indicate the transfer of secondary flows from the pathways to other processes for the establishment of cascades: dark green (→) to arabinoxylan, brown (→) to proteins; purple (→) to xylitol; light green (→) to ethanol; orange (→) to butanol; pink (→) to compost; dark blue (→) to biogas, and yellow (→) to hydrochar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

**Table 2**  
Key performance, impact and profitability indicators by product.

Product	EBIT (€/ton BSG)	Flow (t prod/h)	Yield (g/g)	CFA (kg CO <sub>2</sub> -eq/kg BSG)
Animal feed	63.24	600.00	–	1.18
Antioxidants	–265.02	2.40	0.01	0.12
Arabinoxylan	–1,344.47	390.00	0.65	1.24
Proteins	–3,919.03	99.80	0.17	2.27
EtOH	–437.83	190.00	0.32	0.57
Xylitol	–1,263.17	21.40	0.04	2.07
Compost	57.52	430.00	0.72	0.01
Hydrochar	–122.39	290.00	0.48	1.16
Butanol	–2,495.90	26.20	0.04	1.83
Biogas	–837.44	270.00	0.45	0.11

hand, animal feed represents the most profitable option, providing the highest EBIT, while compost is distinguished by its lower environmental impact. The remaining pathways present lower economic and CFA performance and are therefore considered dominated compared to these solutions. Starting from the same production volume and waste costs specified in Section 3.2, the process lines would be designed to process 3 tons/h of BSG at 80 % moisture content, producing 0.6 tons/h and 0.43 tons/h of feed and compost, respectively.

There are numerous articles on valorization options for BSG, but few include a CFA calculation for the development technologies, and comparison among the available literature is complicated due to the diversity of processes and methodologies employed. However, the results obtained in Table 2 are consistent with the gate-to-gate assessment by

Newman et al., (2025) for laboratory-scale hydrocarbon production (1.18 kg CO<sub>2</sub>-eq/kg BSG). Similarly, the estimated CFA for biogas coincides with that reported by Sancioleto et al., (2022) for the anaerobic digestion of generic food waste (0.11 kg CO<sub>2</sub>-eq/kg BSG). Composting shows very low system impacts (0.01 kg CO<sub>2</sub>-eq/kg BSG), in line with studies reporting minimal direct emissions under ideal operating conditions (Assandri et al., 2025). In contrast, routes such as ethanol (Jia et al., 2025) or proteins (da Fonseca et al., 2024) have a greater footprint in the literature by being expressed per unit of product, adopting cradle-to-grave boundaries, and analyzing substantially different production processes.

It should be mentioned that the result obtained is in line with the current valorization of the by-product in the European context. As examples, the Danish company Biograin collects wet BSG from breweries to transform it into cattle, pig, and mink feed (BioGrain, 2025). The Netherlands-based Duynie Group concentrates the fiber and protein fraction of the residue for use in pet food (Duynie, 2025). Finally, Terra Compostaje Regenerativo is a Spanish company that implements sustainable composting solutions that recover organic waste, including BSG (Terra Compostaje Regenerativo, 2025).

### 3.4. Minimum selling price

When dealing with new valorization products, some of them with an uncertain selling price, estimating profits may not reflect the potential of the market. As an alternative, the MSP was calculated for the different routes, defined as the one that leads to an EBIT of zero. This indicator allows the decision maker to assess how far a new valorization product is

to reach a break-even point and to become an interesting profitable alternative.

As animal feed was the best solution in terms of EBIT, the MSP was calculated only for those solutions with a lower CFA than the reference solution. The rationale is that these products would be environmentally beneficial and profits would be attained if the MSP could be reached. Thus, the relationship between the economic and environmental performance of the pathways shown in Fig. 2.A identifies the antioxidant phenolics, ethanol, biogas, and hydrochar production pathways in the quadrant of interest; while the representation in Fig. 2.B of the EBIT ranges according to the current maximum and minimum price values reported in the literature, highlights that none of the options are competitive according to the available information.

The results of MSP determined by Eq. (8) for the four routes

identified with the greatest environmental potential are shown in Table 3, as well as the maximum and minimum range of current sales prices reported in the literature.

In view of the results, ethanol and hydrochar are feasible alternatives to achieve a financially sustainable operation if production processes are optimized, economies of scale are generated, or specific markets with higher added value are accessed. In contrast, antioxidant phenolics exhibit much more price uncertainty, making their short-term commercial competitiveness difficult to assess, although they may find opportunities in specialized markets with willingness to pay for added-value molecules.

Additionally, the MSP can be contextualized against the literature, while noting that differences in process configuration, scale, and economic assumptions limit direct comparison. For ethanol, the MSP

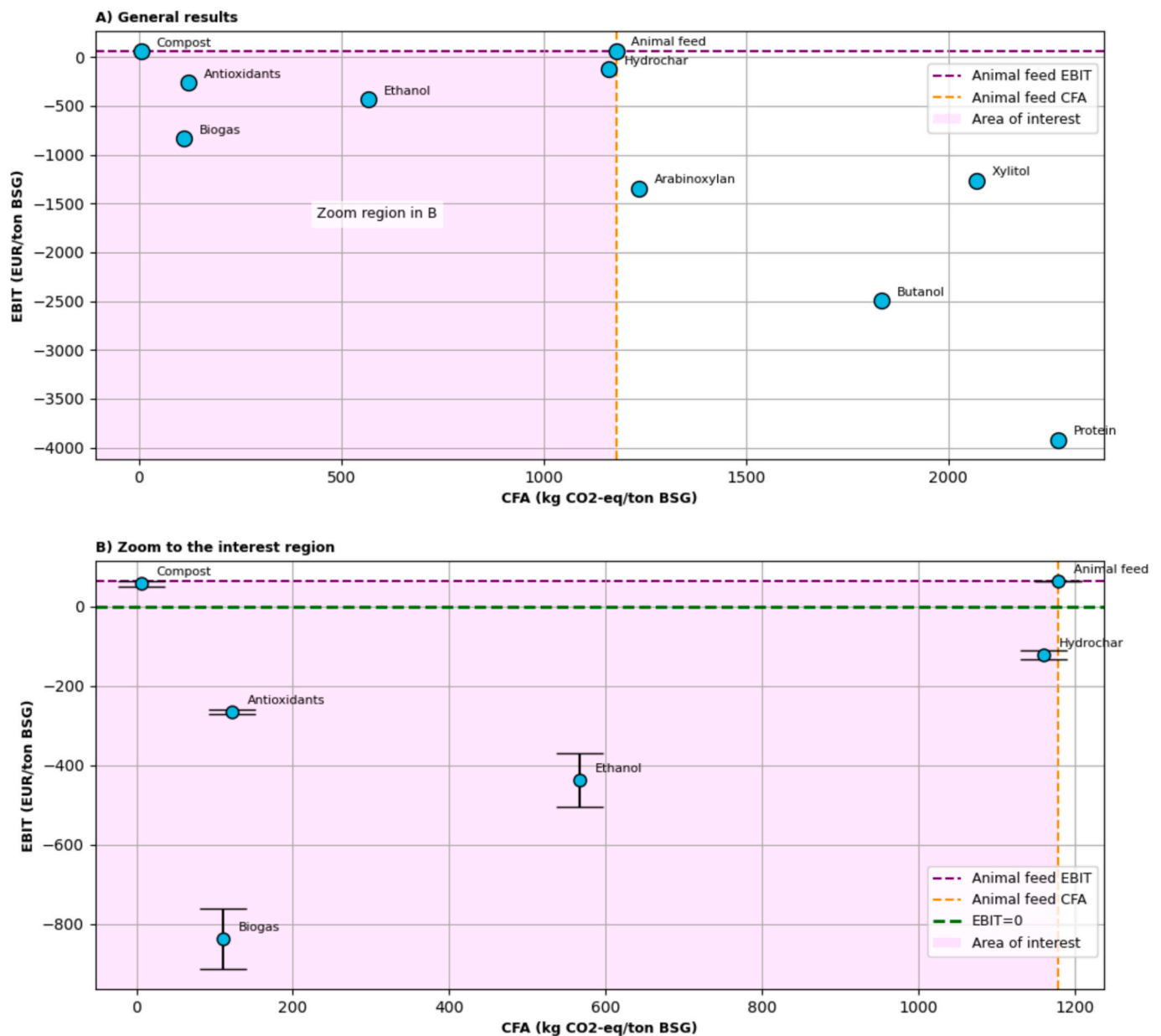


Fig. 2. (A) Relationship between economic performance (EBIT, €/ton BSG) and environmental impact (CFA, kg CO<sub>2</sub>-eq/ton BSG) for the studied valorization pathways of BSG. The cyan points (●) represent each product. Purple (---) and orange (---) dashed lines indicate the reference EBIT and CFA for the animal feed solution. The magenta shaded area (■) highlights the area of interest, corresponding to the zoom region in (B). (B) Zoom of the quadrant of interest, showing only products with lower CFA than animal feed. Green (---) dashed line marks the objective EBIT = 0 for the MSP calculation. Error bars on cyan points represent uncertainty in EBIT for the corresponding product, calculated from reported ranges in the literature. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

**Table 3**

Current prices with reported ranges, estimated MSP, and required increase factors to achieve zero EBIT for the most promising valorization pathways.

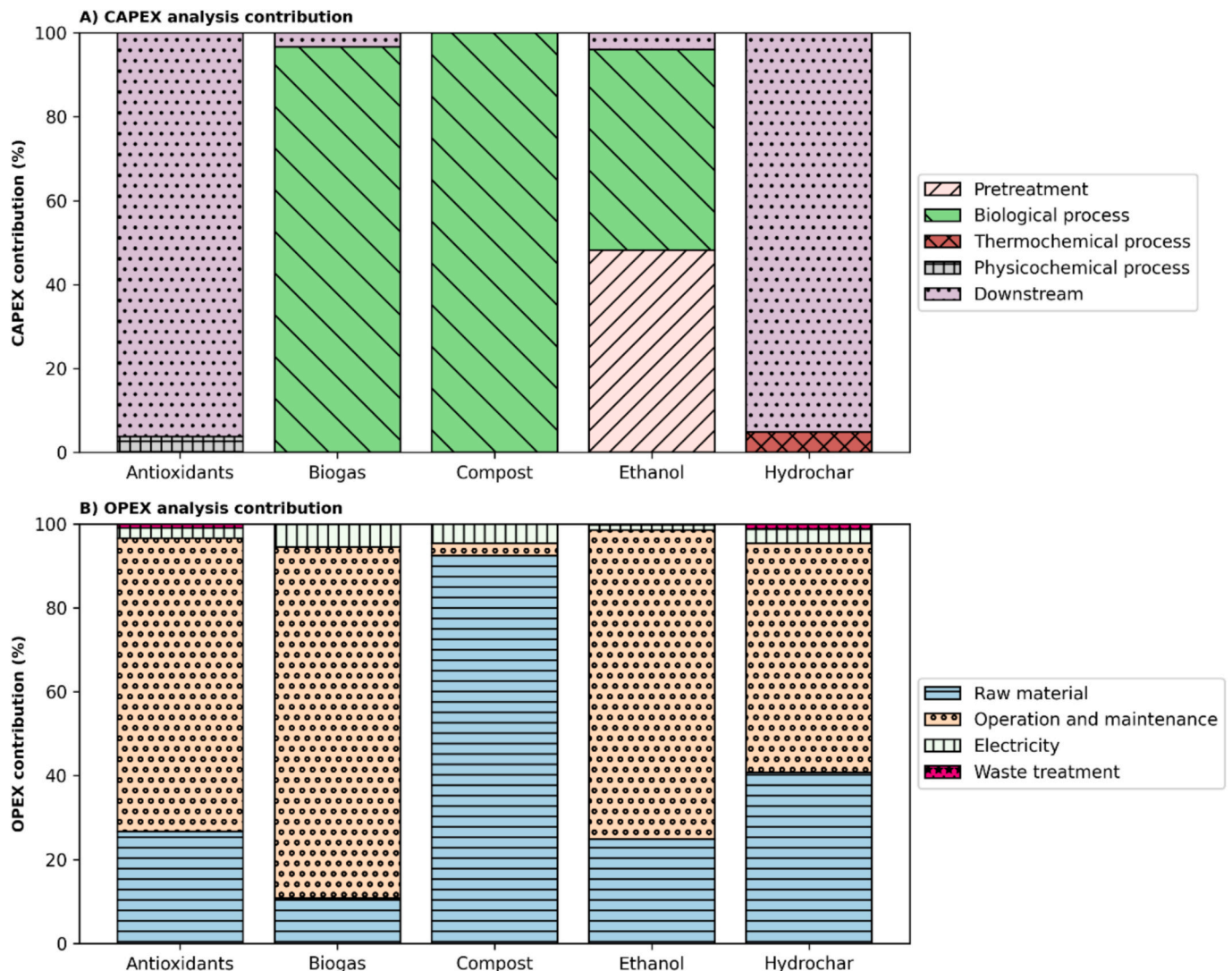
Interest product	Current price (€/ton)	Price range (€/ton)	MSP (€/ton)	Increase factor	Bibliographic reference
Antioxidants	5,500	4,000–6,500	71,755	13.05	(Shi et al., 2025)
EtOH	931	854–1,290	2,314	2.49	(Business Analytiq, 2025)
Hydrochar	180	150–200	433	2.41	(Fernández-Sanromán et al., 2021)
Biogas	555	388–555	2,416	4.35	(YCharts, 2025)

obtained is lower than the value reported by [Jia et al., \(2025\)](#) in a cradle-to-gate LCA and techno-economic assessment (3,900–8,600 \$/ton). The difference can be attributed to: (1) smaller production scale (4,800 t/year vs. 2,000 t/d); (2) different process configuration; and (3) the economic metric used (EBIT = 0 vs. NPV = 0). For hydrochar, the techno-economic evaluation of [Mugoronji et al., \(2022\)](#) suggested profitable production with a selling price of 200 \$/ton for a 70 % conversion yield from BSG. The MSP reported in the study is higher and the result is explained by the lower conversion yield and by the smaller production scale (4,800 t/year vs. 36,000 t/year), which increases the unit cost.

To guide the development of technologies toward scenarios of

greater economic viability, it is essential to identify the limiting factors that determine benefits. Therefore, [Fig. 3](#) shows the relative contribution of the capital investment and operating stages for each production system of interest.

The total investment required is determined based on direct and indirect cost factors and the acquisition cost of the facility's equipment. The downstream processing section constitutes the limiting stage for thermochemical or extraction processes due to the presence of expensive suspended solids handling units (filters, centrifuges, dryers) or thermodynamically unfavorable separations. In contrast, the results associated with biological processes indicate that research should focus on increasing conversion in fermentations, reducing residence time and



**Fig. 3.** (A) Percentual breakdown of the total CAPEX for each non-dominated product of interest per unit process. Each equipment has been grouped into 5 categories, including: Pretreatment: hydrolysis; Biological: fermentation, compost; Thermochemical: hydrothermal carbonization; Downstream: filtration, centrifugation, distillation, dehydration, drying. (B) Percentual breakdown of the total OPEX for each non-dominant product of interest by the expenditures items considered: Raw materials: feedstock, reagents, enzymes, solvents; Operation & maintenance: labor, equipment, maintenance; Electricity: unit operations; Waste treatment: solid, liquid, gaseous effluents.

energy consumption. Optimizing the specified bottlenecks would significantly contribute to increasing the facility's profitability, reducing not only the percentage of capital costs to be deposited, but also the operation and maintenance items in OPEX, determined as a percentage of CAPEX and predominant in all products analyzed except compost. Improving the management of material flows and auxiliary services would also contribute to a lesser extent to an improvement in EBIT, as they directly depend on operating conditions, the performance of key stages, energy efficiency, and the utilization of byproducts.

It is worth highlighting the low expected yields of biogas production from BSG compared to other valorization routes for the substrate composition, which contains a high proportion of lignocellulosic fractions that are not readily biodegradable under anaerobic conditions (Bochmann et al., 2015). Although AD is often considered a simple and robust technology, its profitability from BSG is hampered by both the limited methane yield, due to long retention times and low conversion efficiency, and the high management costs of the residual solids, which are largely composed of poorly biodegradable lignocellulosic fibers that remain after digestion (Atelge et al., 2020). A possible alternative to improve its performance would be to study co-digestion strategies with more biodegradable substrates, which could improve overall methane productivity and process stability (Edunjobi et al., 2024).

### 3.5. Cascading integration of production routes

The goal of biorefinery system design is to achieve improved environmental performance in industrial production, so it is essential not to limit oneself to the economic study of MSP of individual products in isolation, but rather to analyze the potential of integrating conversion routes to maximize waste utilization and generate synergies. The total number of possible combinations in the problem's superstructure increase exponentially with the number of considered products (combinatorial explosion), so it was decided to limit the calculation to the designs located within the quadrant of interest in Fig. 2.A, while maintaining a realistic view of the viable options. Specifically, the routes evaluated were: (1) phenolic antioxidants and compost; (2) phenolic antioxidants and ethanol; (3) phenolic antioxidants and biogas, obtaining compost as a by-product; (4) phenolic antioxidants and hydrochar; (5) ethanol and compost; (6) ethanol and biogas, obtaining compost as a by-product; (7) ethanol and hydrochar; (8) phenolic antioxidants, ethanol and compost; (9) phenolic antioxidants, ethanol and biogas, obtaining compost as a by-product; (10) phenolic antioxidants, ethanol and hydrochar.

When applying Eq. (8) for the product cascades, it was assumed that market prices for raw materials such as biogas, compost, and hydrochar would remain stable. Furthermore, ethanol price variation was allowed except when combined with antioxidants, where it was considered a stable product since the uncertainty of the cascade was concentrated in the other, higher-value compound.

Under these considerations, only the chains that included compost achieved a slight improvement in the MSP compared to the individual route, since as it represents the only suboptimal product with profitable production, its inclusion in any cascade tends to improve the overall economics of the process. In designs (1) and (8) according to the previous nomenclature, an MSP for phenolic antioxidants of 71,443 and 189,277 €/ton is obtained, with a reduction in this parameter of 0.44 % and 2.61 %, respectively. Similarly, for design (5), the MSP of ethanol decreases to 2,249 €/ton with the incorporation of compost, representing a 2.80 % improvement compared to the individual valorization.

### 3.6. Limitations and context

First, it was decided to select the process from Table 1 with the highest EBIT of each product when building the superstructure in Fig. 1, since profitability is often the first obstacle to industrial adoption. However, this introduces a bias toward economic performance that

exclude alternatives with better environmental performance. If the preliminary selection is based on reducing the CFA, there are differences in the prioritized set of processes. Starting from a solution space already conditioned by one dimension, the diversity of possible trade-offs between economic and environmental objectives in multi-objective optimization is reduced. This highlights the importance of testing the robustness of results against different preliminary assumptions. Future studies could therefore address the problem by constructing parallel superstructures based on environmental criteria or by incorporating sensitivity analyses to explicitly assess how initial decisions affect the equilibrium results in multi-objective optimization. EBIT and CFA could also be considered simultaneously in the preliminary selection stage, although this significantly increases the computational demand and data requirements.

Secondly, the scope of the environmental assessment was defined from the outset as a CFA, a common approach in biorefinery impact analyses (Broeren et al., 2017), due to its close relationship with energy inventories and its relevance to the decarbonization targets established in the EU Taxonomy. It is important to integrate environmental criteria from the early design stages, as this modifies decisions compared to purely economic optimization. In this case, the environmental criterion is based on a single midpoint impact indicator which is considered as objective, together with the economic criterion, in the multi-objective optimization. While this choice does not capture the full spectrum of environmental impacts, multi-objective life cycle optimization studies in biorefinery systems have shown that climate change impacts are often strongly correlated with other damage-oriented objectives such as human health and ecosystem quality (Kopton et al., 2023). This is mainly due to the dominant contribution of energy demand across several impact categories, and in such cases, Pareto-optimal solutions tend to coincide. However, impact categories related to resource depletion or specific toxicity pathways may display different behaviors and introduce additional trade-offs. By not representing the full environmental profile of each product, relevant impacts in other categories may be overlooked. An alternative could be the aggregation of multiple impact categories into a single environmental indicator through normalization, grouping and weighting as defined by ISO 14040. While such aggregation can facilitate decision-making, it inherently involves normative choices and value judgments that may reduce methodological robustness in early-stage process design. For this reason, weighted single-indicator approaches are better suited as complementary analyses or sensitivity checks rather than as primary optimization objectives. Having said that, this work should be then regarded as an ongoing study, and future developments will extend the multi-objective optimization framework by comparing Pareto fronts based on multiple midpoint impact categories within an LCA perspective.

Additionally, a single-objective optimization could be proposed by converting impacts to an economic value using environmental prices, which express the cost that society is willing to pay to avoid introducing one kilogram of pollutant into the environment. Although the analysis is simplified, the economic and environmental trade-offs are also flattened by not performing impact profiling, so that a process could have a positive EBIT but generate very negative environmental performance in a specific category. It is also worth mentioning that environmental prices are less suitable for studies that differ from the geographical and temporal conditions for which they were established, so their use must recognize the existence of a high degree of uncertainty in the results (the Bruyn et al., 2017).

It is also necessary to highlight the limitations of the conservative modeling approach applied to cascade analysis. By evaluating each chain as an independent pathway and redirecting only residual solids as feedstock for subsequent processes, the true synergies that could be achieved integrating extraction, bio- and thermoconversion stages (enabling gentler pretreatments or eliminating redundant units) are not captured. The implementation of this approach was not possible due to the lack of experimental data and literature that quantify yield

improvements or present a more detailed characterization of the composition of intermediate streams. Thus, there is a need for research into the integration of emerging pathways for BSG valorization, which is essential for assessing how cascading strategies could reduce costs and improve economic and environmental competitiveness within a circular bioeconomy framework. Rovira-Cal et al., (2025) similarly emphasize that many biorefinery optimization methodologies continue to evaluate valorization routes in isolation, without detailing opportunities for sequential integration to recover multiple compounds from the same stream. Their proposal—based on a three-level compositional characterization of biomass—highlights the importance of exploring all plausible combinations, which aligns with the superstructure logic applied in this study. Furthermore, it incorporates a multi-criteria framework (economic, environmental, and social) for route prioritization using an Analytic Hierarchy Process (AHP), reinforcing the importance of holistic assessments from the early design stages.

Finally, it is important to highlight the limitations related to industrial scalability. Despite the potential of biorefineries, their widespread adoption remains limited by economic and systemic barriers. As evidenced in the study, emerging biorefinery designs are not yet cost-competitive with fossil fuel-based alternatives, especially considering the variability of raw materials and underdeveloped supply chains (Javourez et al., 2024). Therefore, future work should address broader organizational and systemic scales, considering aspects of geographical feasibility (facility location) or the logistical optimization of a given design (Mota et al., 2015). Complementarily, industrial symbiosis is presented as a strategy to achieve circularity and identify material flow needs in a region, allowing for the efficient sharing of resources, energy, and waste among different stakeholders (Demartini et al., 2022). The integration of these strategies is essential for biorefineries to become established as solutions that are not only technically viable, but also economically sustainable and socially relevant within the framework of a circular bioeconomy.

#### 4. Conclusions

This study presents a multi-objective optimization framework for evaluating conventional and emerging biorefinery configurations for BSG valorization, showing that animal feed production remains the most economically competitive option—yielding approximately 10 % higher profitability than the second-best alternative (compost), while compost stands out as the nondominated alternative with the lowest carbon footprint, exhibiting impacts about 91 % lower than the next optimal option (biogas). The combined analysis of trade-offs and MSP was used as a decision-making tool, and ethanol and hydrochar represented the most promising alternatives for further Research and Development (R&D) investment due to their proximity to the benchmark EBIT, while phenolic antioxidants would require significant improvements in process performance or market conditions to achieve the desired economic competitiveness.

A thorough assessment of CAPEX and OPEX contributions revealed that the performance of biological processes and downstream solid-liquid separation operations were bottleneck parameters whose improvement would bring suboptimal designs closer to greater economic profitability and market competitiveness. Moreover, the study of cascade conversion routes to maximize the utilization of BSG waste demonstrated limited improvements compared to isolated production processes when incorporating compost synthesis, but the lack of experimental data on performance synergies or equipment highlighted the need for further research into integrated designs.

Finally, the implementation of the framework in OUTDOOR, an open-source platform that integrates superstructure optimization with environmental and economic assessment should be noticed. Together with its intuitive graphical interface, it proved to be a powerful decision-support tool. By enabling systematic exploration of alternatives and simplifying the mapping of complex superstructures, this integrated

environment contributed to the identification of optimal and balanced solutions, reinforcing its value in guiding the sustainable design of future biorefineries.

#### CRedit authorship contribution statement

**Andrea Penedo:** Writing – original draft, Data curation, Conceptualization, Writing – review & editing, Formal analysis. **Jeppie Yndgaard:** Writing – original draft, Data curation, Conceptualization. **Lucas Van der Hauwaert:** Writing – original draft, Software, Conceptualization. **Miguel Mauricio-Iglesias:** Writing – review & editing, Supervision, Funding acquisition. **Almudena Hospido:** Writing – review & editing, Supervision. **Massimiliano Errico:** Writing – review & editing, Writing – original draft, Data curation, Conceptualization.

#### 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.

#### Acknowledgements

This project (AGRILOOP) has received funding from the European Union's Horizon Europe research and innovation programme under the grant agreement No. 101081776, the UK Research and Innovation (UKRI) fund under the UK government's Horizon Europe funding guarantee, the Swiss State Secretariat for Education, Research and Innovation (SERI) and from the National Key Research and Development Program supported by the Ministry of Science and Technology of the People's Republic of China (No. 2023YFE0104900). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of neither of the aforementioned Funding authorities. None of the cited funding authorities can be held responsible for them: <https://agriloop-project.eu/>.

A. Penedo, L. Van der Hauwaert, M. Mauricio-Iglesias, and A. Hospido authors belong to the Galician Competitive Research Group (GRC ED431C 2025/19) and to the Cross-disciplinary Research in Environmental Technologies (CRETUS Research Center, ED431G 2023/12).

#### Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.wasman.2026.115558>.

#### Data availability

The datasets and code generated and/or analyzed during the study are available in the GitHub repository [Penedo \(2025\)](#).

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