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Environmental benefits of large-scale second-generation bioethanol production in the EU

An integrated supply chain network optimization and life cycle assessment approach

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Abstract

The use of agricultural residues for the generation of bioethanol has the potential to substitute fuels such as petrol or first-generation bioethanol and thereby generate environmental benefits. Scientific research in this field typically confines the environmental dimension to global warming, disregarding other environmental impact and damage categories. By multi-criteria mixed-integer linear programming, this work examines environmental benefits and economic viability of optimal second-generation bioethanol production network configurations to substitute petrol and/or first-generation bioethanol in the EU. The results comprise environmentally optimal decisions for 18 impact and 3 damage categories, as well as economically optimal solutions for different excise and carbon tax scenarios. The impact categories global warming potential, particulate matter, and land use are affected the most. Optimal network decisions for different environmental objectives can be clustered into three groups of mutual congruencies, but opportunity costs between the different groups can be very high, indicating conflicting decisions. The decision to substitute petrol or first-generation ethanol has the greatest influence. The results of the multi-dimensional analysis suggest that the damage categories human health and ecosystem quality are suitable to unveil tradeoffs between conflicting environmental impacts, for example, global warming and land use. Taking human health and ecosystem quality as environmental decision criteria, second-generation bioethanol should be used to concurrently substitute first-generation bioethanol and petrol (100% and 18% of today's demand in the EU, respectively). However, economic optimization shows that with current taxation, bioethanol is hardly competitive with petrol, and that excise tax abatement or carbon taxes are needed to achieve these volumes. This article met the requirements for a gold-gold JIE data openness badge described at <http://jie.click/badges>.



KEYWORDS

bioeconomy, environmental benefits, industrial ecology, multi-objective optimization, network planning, second-generation bioethanol

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1 | INTRODUCTION

The promotion of pilot scale technologies to industrial scale has characterized the field of second-generation bioproducts in recent years. After decades of research and repeated setbacks, lignocellulosic bioethanol is on the verge of commercialization (Clariant, 2020; Hauschild et al., 2018). A successful large-scale production of second-generation bioethanol as substitute for liquid fuels and base chemicals has the potential to reduce environmental pressure significantly (Morales, Quintero, Conejeros, & Aroca, 2015). Several studies investigate economic, environmental, or social aspects of lignocellulose biorefineries; however, these dimensions have mostly been assessed independently (Cherubini & Strømman, 2011; Morales et al., 2015; Patel, Zhang, & Kumar, 2016). Existing studies can be clustered into techno-economic evaluations (Hamelinck, Van Hooijdonk, & Faaij, 2005; Lauven, Karschin, & Geldermann, 2018), life cycle assessments (LCA) to compare different production pathways (Bright & Strømman, 2009; Watanabe et al., 2016), LCAs to compare the environmental performance of different feedstocks (Kim & Dale, 2005; Muñoz et al., 2014) and network optimization models (Dunnett, Adjiman, & Shah, 2008; Leduc et al., 2010).

In existing multi-dimensional approaches in the field of advanced biofuels, environmental considerations are often limited to greenhouse gas (GHG) emissions (Budzinski, Cavalett, Nitzsche, & Strømman, 2019; You, Tao, Graziano, & Snyder, 2012; Zamboni, Shah, & Bezzo, 2009) or are represented by an aggregated score like the eco-indicator 99 (Babazadeh, Razmi, Pishvae, & Rabbani, 2017; Santibañez-Aguilar, González-Campos, Ponce-Ortega, Serna-González, & El-Halwagi, 2014). Although climate change is considered one of the most urgent global challenges, the limitation to global warming bears the risk of neglecting other environmental impacts (Cherubini & Ulgiati, 2010; Hauschild et al., 2018). The politically intended implementation of first-generation biofuels in the EU demonstrated the complex interconnection in the “food, energy, and environment trilemma” (Lewandowski, 2015, p. 37) and the problem of a fixation to the single goal *climate change mitigation*. LCAs that cover a wide range of impact and damage categories do not allow a clear statement about the advantageousness of bioproducts compared to their conventional counterparts (Borrion, McManus, & Hammond, 2012), especially in categories such as *eutrophication*, *stratospheric ozone depletion*, *acidification*, and *human and terrestrial toxicity*. In order to avoid problem shifting, it is essential to include all relevant impact categories in decision-making processes (Hauschild et al., 2018). Environmental “single scores” might address societal interests better than a single impact category; however, without full data documentation and intermediate results, these scores lack the necessary transparency (Goedkoop, Hofstetter, Müller-Wenk, & Spriemsma, 2001; Rosenbaum et al., 2018). Understanding competing economic, environmental, and social aspects in regional biomass provision is the central aspect in the optimization of bioeconomic value chains (Lewandowski, 2015).

Agricultural residues as feedstock for biorefineries neither compete directly with food production nor indirectly through land competition, and thus avoid the “food and energy” dilemma. Other studies have shown the environmental advantageousness of agricultural residues compared to feedstocks cultivated particularly for energy use (Morales et al., 2015; Muñoz et al., 2014). For the production of fuels and base chemicals, these considerations render agricultural residues superior to other feedstock and fuels. Nevertheless, the utilization of agricultural residues entails environmental impacts that need to be addressed. The low density and economic value of lignocellulose render feedstock transportation challenging in the planning of production networks. In contrast to large fossil refineries, the disproportionately increasing feedstock transportation cost for large biorefineries may offset economies of scale of refineries, which is why biorefinery production networks tend to be more decentralized with smaller individual refineries (Lauven, 2014). Most existing approaches are based on process analysis with fixed parameters; however, especially in the bioeconomy, environmental repercussions are particularly dependent on regional characteristics of the value chain, such as the feedstock availability (Budzinski et al., 2019).

The specific challenges in the assessment of biofuels require models that are capable of weighing economic and environmental criteria against each other and, at the same time, take regional value chain aspects into account. Decisions have to be made as to whether feedstock is sourced from a certain region, whether biorefineries have to be built and with which capacity, and whether it is worthwhile to transport the final product to sales markets; an echelon of decisions for which multi-objective mixed-integer linear programming is a proven tool in Operations Research (Govindan, Soleimani, & Kannan, 2015). This work develops a multi-objective production network optimization model, where second-generation bioethanol is produced to substitute first-generation bioethanol and fossil petrol in the EU. The environmental dimension is addressed by optimization of a broad range of impact and damage categories, considering regionalized life cycle inventories of different steps in the value chains. The consideration of endpoints and midpoints alike and the regionalization of environmental aspects is novel in the field of strategic network design (Messmann, Helbig, Thorenz, & Tuma, 2019). Economically, the price of fossil fuels does not represent the accruing societal cost of fossil fuels (World Bank, 2019), and advanced biofuels still lack competitiveness vis-à-vis conventional fuels. However, if profitability increases, advanced biofuels like ethanol could be an important element in tackling greenhouse gas reduction targets and other environmental problems related to fossil fuel consumption (Giuntoli, 2018). Therefore, the economic dimension is addressed by profit maximization, considering different excise and carbon tax scenarios, which reflect possible policy instruments to support alternative fuels. This work contributes to existing literature on advanced biofuels by the application region (the EU), by the distinction between substitution of petrol and first-generation ethanol, by the large number of environmental objectives and economic scenarios, and the model's regionalized character. This broad spectrum of perspectives allows to derive insights into the various environmental and economic consequences of different advanced biofuel strategies, which could be of interest for European policy-makers and companies. This work sets out to answer the following research questions:

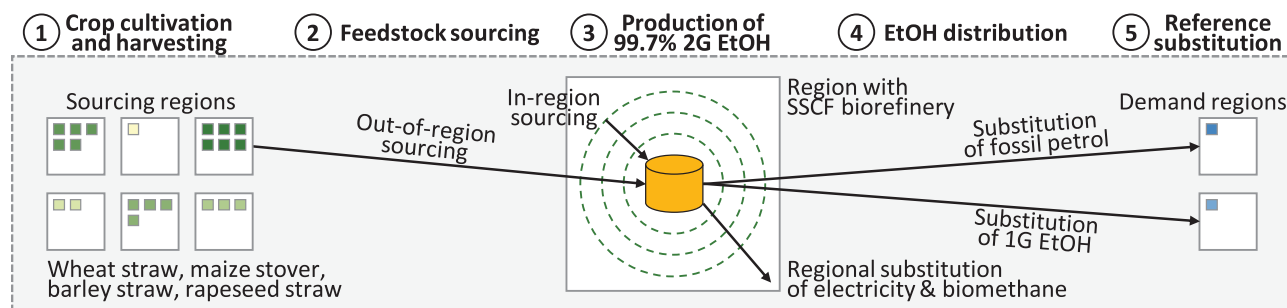


FIGURE 1 Simplified illustration of the value chain structure

- ❖ **RQ1:** What are the benefits of optimal second-generation ethanol production network configurations to substitute petrol and first-generation ethanol, considering different environmental and economic aspects?
- ❖ **RQ2:** Which environmental objectives are congruent, and which are conflicting (considering LCIA midpoints and endpoints)?
- ❖ **RQ3:** Which taxation scenario supports the scale-up of a second-generation ethanol production network in the EU?

In Section 2, key parts of the optimization model and the life cycle assessment are introduced. The results section shows the optimal design of large-scale bioethanol production in the EU, based on economic and different environmental objectives, as well as Pareto-efficient tradeoffs between different objective functions. In the last section, we discuss the implications of the results for policy-makers, the benefits of the applied methodology, and also limitations in the tangibility of the results.

2 | METHODS

This section includes a detailed description of the considered value chain for the production of second-generation bioethanol, the assumptions made regarding feedstock supply and bioethanol demand, as well as brief presentations of the LCA carried out for the parameterization of the optimization model, the multi-objective optimization model, and the experiment design.

2.1 | Value chain

The value chain includes 1) feedstock cultivation and harvesting, 2) feedstock sourcing, 3) the bioethanol production process, 4) ethanol distribution to demand regions, where 5) second-generation bioethanol (2G EtOH) substitutes fossil petrol or first-generation bioethanol (1G EtOH) (see Figure 1). To obtain meaningful results at the regional level, a high level of regional disaggregation is desirable. Since the complexity of the model increases disproportionately with regional granularity, the 98 NUTS-1 regions of the EU, which correspond to the major socio-economic areas, are used as spatial resolution. Every region represents a potential supply, production, and demand region. In the first step of the value chain, the harvested agricultural residues are baled to facilitate storage and transportation. At the biorefinery, the feedstock is converted in several process steps to bioethanol and the by-products electricity and biomethane.

The bioethanol production process is state-of-the-art and can be described as steam explosion pre-treatment and simultaneous saccharification and co-fermentation (SSCF) with integrated enzyme production (Supporting Information S1). Pre-treatment includes mechanical shredding and (acid-free) hydrothermal cracking to separate cellulose and hemicellulose from lignin (Gupta & Verma, 2015). An enzyme mixture produced in an integrated production step hydrolyzes cellulose and hemicellulose chains into sugar monomers (hexoses and pentoses). During fermentation, the hexose and pentose are fermented to ethanol and finally distilled to purified ethanol (>99%) by micro-sieves. Separated lignin is used to generate electricity and process heat by cogeneration, and excess electricity is fed into regional grid. The distillation residue stillage is valorized to biomethane via anaerobic digestion. Distribution of purified ethanol to the regional markets and substitution are the last considered operation.

2.2 | Feedstock availability and bioethanol demand

Lignocellulose typically consists of 30–45% cellulose, 15–30% hemicellulose, and 15–30% lignin; therefore, all lignocellulose biomass can generally be used for bioethanol production (Balat, 2011). A high degree of flexibility with regard to the feedstock is desirable for a biorefinery; however, especially pre-treatment needs a certain focus on a biomass class (Gupta & Verma, 2015; Taherzadeh & Karimi, 2008). This work focuses on the

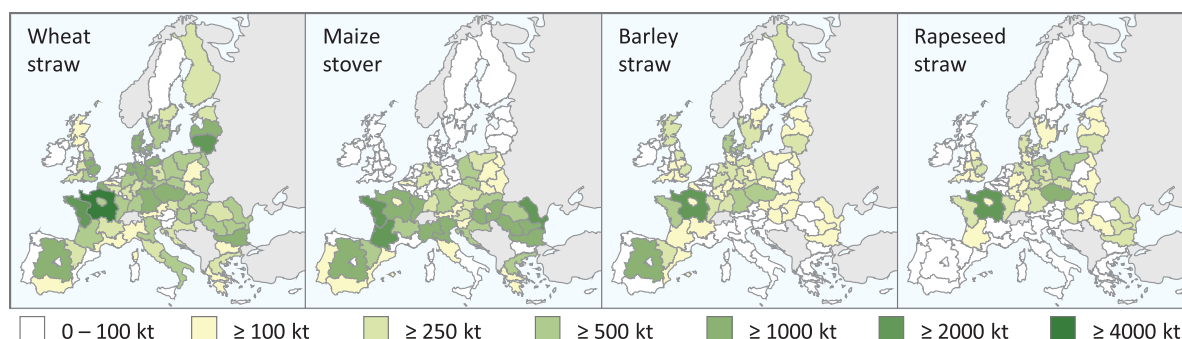


FIGURE 2 Bioeconomic feedstock availability (in metric kilotons) of wheat straw, maize stover, barley straw, and rapeseed straw on NUTS-1 level in 2018 (based on Wietschel et al., 2019). For the four overseas regions (ES7, FR9, PT2, PT3) among the 98 NUTS-1 regions, feedstock potentials and demands are zeroed. Underlying data used to create this figure can be found in Supporting Information S2

main agricultural crop residues (in terms of volume) in the EU, wheat straw, maize stover, barley straw, and rape straw. Estimates on the theoretical energy content of agricultural residues in the EU range from 3673 to 6389 PJ (Scarlat, Fahl, Lugato, Monforti-Ferrario, & Dallemand, 2019), of which only certain shares are available. The bioeconomic potential takes into account a large array of accessibility limitations, such as technical limitations, sustainable removal rates to sustain soil organic carbon, and privileged local biomass demands by applications such as animal bedding, it therefore can be considered as conservative scenario (Thorenz, Wietschel, Stindt, & Tuma, 2018). Data on the *bioeconomic potential* primarily comes from Wietschel, Thorenz, and Tuma (2019) with 2018 as reference. Where necessary, the database is amended by data from the S2BIOM project, who assume slightly higher potentials (Dees et al., 2017).

Figure 2 shows the absolute bioeconomic potential in 2018 for the four considered feedstocks, with wheat straw being the most widespread across EU regions. Maize stover potentials are rather found in the southern temperate zone and northern subtropical zone. Barley and rapeseed straw potentials are almost exclusively found in the temperate zone.

Second-generation bioethanol can substitute fuels in the transportation sector (both fossil petrol and first-generation bioethanol) and industrial ethanol in the chemical sector. As fuel, 2G EtOH can substitute petrol either entirely (E100) in specifically designed spark ignition engines, or partly in a blend, which is currently the common practice (Thangavelu, Ahmed, & Ani, 2016). In 2018, the fuel ethanol consumption of the transportation sector in the EU was 4.33 Mt (million metric tons), and 0.47 Mt in the industrial sector, which was covered almost entirely by first-generation sources (ePure, 2018). The consumption of petrol amounts to 75 Mt in 2018, which is equivalent to about 120 Mt of EtOH (Eurostat, 2019). While substitution between 1G and 2G EtOH is possible without further technical adjustments, the use of E100 in vehicles would require engine adjustments, the implications of which are not further considered in this paper.

2.3 | Life cycle assessment

The main objective of the model is the maximization of environmental benefits in the EU by upscaling second-generation ethanol production and the respective substitution of petrol and first-generation bioethanol. The assessment of environmental benefits is carried out on the basis of life cycle assessment. The life cycle inventory (LCI), that is, the inputs and emissions associated with the environmental parameters, is modeled in SimaPro 9, assessing the ecoinvent database Version 3.5 (Wernet et al., 2016). The life cycle impact assessment (LCIA), that is, the characterization of the inventory in terms of impact and damage categories, is carried out using ReCiPe 2016 (H) v1.1 (Huijbregts et al., 2017). This section provides a brief overview of the assumptions taken for the LCA (assumptions in Supporting Information S1, LCI in Supporting Information S2¹).

The system boundary of the work at hand is depicted in Figure 3 and can be described as cradle-to-tank. It includes feedstock cultivation and transportation, the production process, and the final distribution to the demand region. The functional unit of the model is the **producible volume of second-generation bioethanol per year** (in metric tons, the references are adjusted by energy equivalence) in the resulting production network. The model optimizes the substitution of the **same function** (i.e., the same energy) of the two reference products petrol and first-generation bioethanol. To facilitate a fair comparison between fossil-based and bio-based fuels, biogenic carbon stored in the bio-based fuel is modeled negatively in the carbon balance (Supporting Information S1).

The environmental dimension comprises the 18 midpoints and three endpoints of the LCIA method ReCiPe 2016. Midpoints describe environmental impacts, which can optionally be normalized and aggregated toward endpoints. Endpoints provide information on the damages to the

¹ To support transparency, accessibility, and reusability of data, all input data are openly available. More detailed descriptions, including the mathematical modeling and process descriptions can be found in Supporting Information S1 (PDF document), all numerical data can be found in Supporting Information S2 (MS excel spreadsheet). Supporting Information S2 associated with this article is linked to Zenodo in the online version under 10.5281/zenodo.3941996.

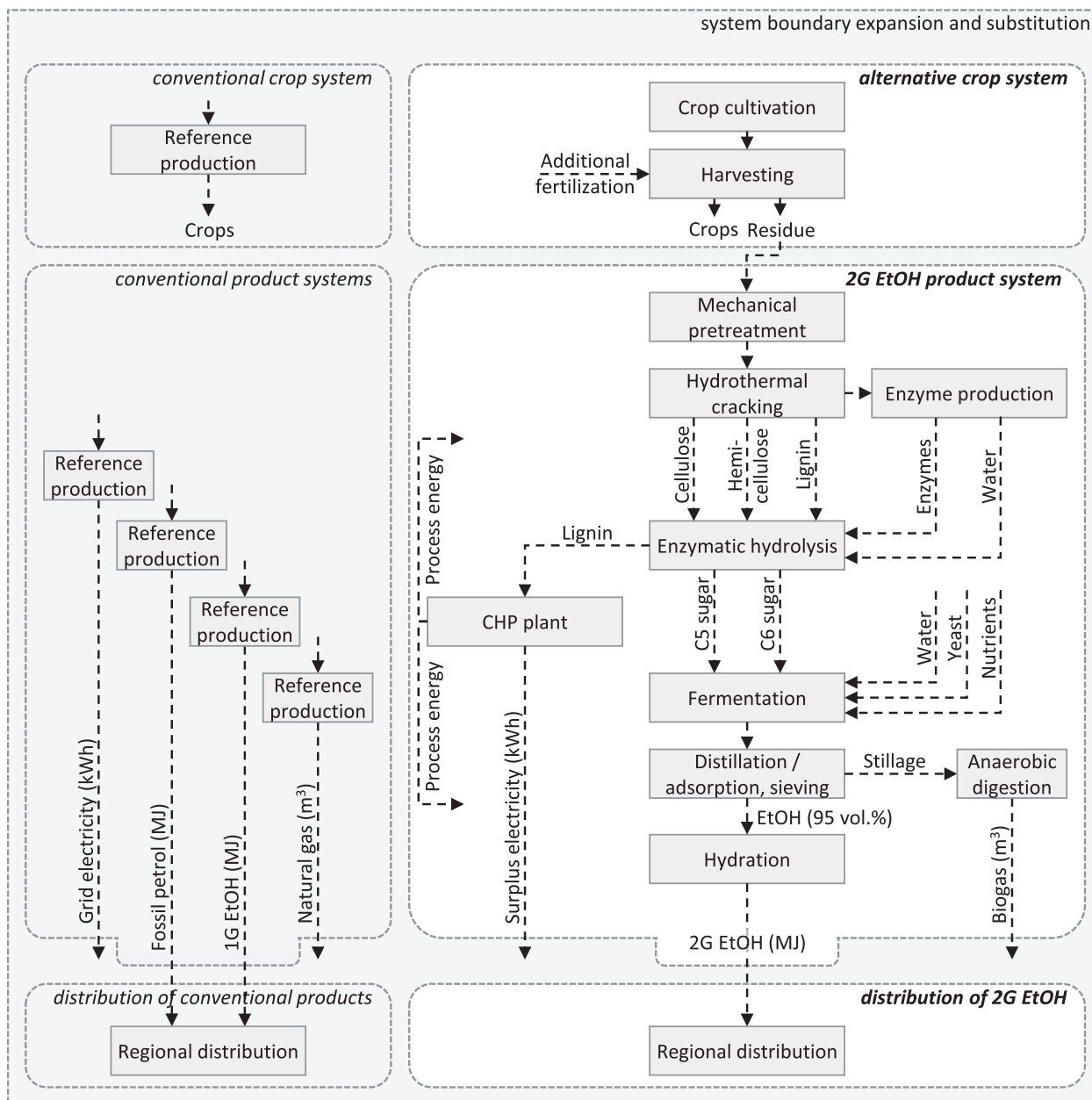


FIGURE 3 System boundaries and simplified flow diagram

respective areas of protection, and can thus be considered more meaningful to the society in decision-making processes. A short description of the considered midpoints and endpoints, their units, and midpoint-to-endpoint aggregation is provided in Tables S1–S5 in Supporting Information S1. By providing both midpoints and endpoints, consequences of decisions become visible and support the interpretation of results (Rosenbaum et al., 2018). The environmental benefits of the production network are assessed by system boundary expansion and substitution (see Figure 3). The feedstock system as well as the biorefinery process is multi-functional processes, which requires an allocation of their environmental implications. The conventional counterpart needs to be selected carefully, as it is a critical step in the system boundary expansion and substitution approach (Heijungs & Guinée, 2007). For the conventional agricultural system, we assume a complete incorporation of straw into the soil. In the alternative system, additional N-P-K fertilization is assumed, based on Cherubini and Ulgiati (2010), to compensate for the nutrient loss through straw evacuation. The co-products biomethane and electricity are expected to be fed into the regional gas and electricity grids, respectively, and thereby substituting natural gas and the regional electricity mix (referring to the same function). For the multiple biorefinery outputs, this approach assumes a direct substitution of reference products that are currently on the market with a given environmental burden, wherefore this model can be considered as consequential LCA (Majeau-Bettez et al., 2018). Equation (1) illustrates that the total environmental benefit calculates as the difference

between avoided burdens of all products and the total production impacts.

$$\text{environmental benefit}^{\text{LCIA}} = \sum_{\text{product}} \text{avoided burden}^{\text{LCIA}}_{\text{product}} - \text{production impact}^{\text{LCIA}} \quad (1)$$

Where possible, environmental impacts are regionalized in their inventory to account for regional characteristics (e.g., electricity mix or water use).

2.4 | Multi-objective model and experiment design

Table 1 lists the key elements of the optimization model (index sets, decision variables, and objective functions). The complete mathematical formulation with all parameters, functions, and constraints is provided in Supporting Information S1. The first set of decisions represents the choice of locations and capacity levels of biorefineries. Biorefineries can be supplied with four feedstock types, which are converted to the main product 2G EtOH and two by-products. Feedstock can either be sourced from another region and transported to the region of a refinery. Alternatively, it can be sourced from within the region of a biorefinery. In the latter case, larger plant capacities require larger sourcing areas, which lead to nonlinear transportation costs (Lauven et al., 2018). To account for the nonlinearity, transportation costs are linearized stepwise in sourcing annuli. The produced 2G EtOH is then shipped from refineries and substitutes either 1G EtOH or fossil petrol demand. The transport of both feedstock and EtOH can be carried out with different transportation modes. The optimization model is implemented as a multi-objective mixed-integer linear program (MILP) and either maximizes the profit ($\max O^{\text{econ}}$), or one of 21 LCIA midpoints and endpoints ($\max O^{\text{env}}_I, \forall I \in L$). Originally, nonlinear scale-dependent parameters (capacity-dependent investment costs and impacts, and sourcing costs and impacts) are stepwise linearized (Supporting Information S1).

As part of the economic assessment, this work examines in five scenarios which taxation policy can promote the role-out of large-scale 2G EtOH production (Table 1). Tax scenario T1 represents the current taxation for petrol and bioethanol, where excise tax abatements for bioethanol exist in some countries, while others raise taxes for all three considered products equally (European Commission, 2020). Tax scenarios T2 and T3 assume a uniform excise tax abatement of 50% and 100%, respectively, in every country. Scenarios T4 and T5 assume additional carbon taxes of €50 (moderate taxation) and €375 (high taxation), respectively, per emitted metric ton of CO₂ eq. T4 corresponds to the minimum price needed in 2020 to be consistent with achieving the temperature target of the Paris agreement of “well below 2°C” (World Bank, 2019). T5 is based on Ricke, Drouet, Caldeira, and Tavoni (2018), who estimated the median social cost of carbon emission at about €375. Tax scenarios T2–T5 improve the competitiveness of second-generation bioethanol compared to petrol. The carbon taxation of scenarios T4 and T5 additionally increases transport costs.

The single-objective optimization is followed by a multi-dimensional consideration on the basis of the equidistant ε -constraint method with the calculation of Pareto-optimal frontiers. This method allows the simultaneous consideration of different objectives in order to gain insights into their interrelationships. Between the economic and an environmental category, the Pareto-optimal frontier presents marginal economic costs to achieve environmental benefits transparently. The environmental dimension is characterized by a plethora of impacts with complex cause-effect chains, which makes it particularly important to point out tradeoffs between the different conflicting environmental objectives.

3 | RESULTS

The first subsection discusses the results of economic optimization and the second subsection discusses the environmental results with focus on the relevance of, and congruencies, and conflicts between the 21 environmental objective functions. In the last subsection, Pareto optimization is carried out between different environmental and economic objectives.

3.1 | Economic network planning

Figure 4 presents optimal network configurations in all five tax scenarios, including the information on the substituted references first-generation bioethanol and fossil petrol, the total amount and location of sourced feedstock, and the number and total capacity of biorefineries. The production networks are rather central, with a concentration of production capacities in countries with lower labor and feedstock costs.

Revenues in scenario T1 are only slightly higher than the costs, which is why the profit margin of €130 million is small compared to the total costs (€2.65 billion). About 10.4% of the available feedstock is used and 2.3% of the total petrol demand is substituted, but only in Sweden, where revenues are competitive due to excise tax abatement. Economic optimization in T1 leads to environmental benefits of up to 10% of the maximum achievable environmental values (e.g., GHG benefits of 4.8 Mt CO₂ eq). Scenario T2 yields the same results as T1, as competitive revenues remain

TABLE 1 Index sets, decision variables, verbal descriptions of objective functions, and scenario definitions

Indices		
Set	Definition	Description
$R = \{1 \dots 98\}$	Regions	NUTS-1 level regions in 28 EU member states
$C = \{1 \dots 37\}$	Capacity levels	25,000, ..., 3,000,000 metric tons (output) ^a
$F = \{1 \dots 4\}$	Feedstock	Wheat straw, maize stover, barley straw, rapeseed straw
$P = \{1 \dots 2\}$	By-products	Surplus energy, biomethane
$M = \{1 \dots 100\}$	Sourcing annulus	5 km, ..., 500 km
$T = \{1 \dots 3\}$	Transport modes	Farm tractor, truck, rail
$L = \{1 \dots 21\}$	LCIA categories	ReCiPe 2016 endpoints (E1-3) and midpoints (M4-21), see Table S5
Decision variables		
Variable	Domain	Definition
$B_{r,c}$	$\in \{0, 1\}$	Construction of a biorefinery in region $r \in R$ with capacity level $c \in C$
$F_{r,m,t}^{in}$	$\in \mathbb{Q}_0^+$	Transported amount of feedstock $f \in F$ within region $r \in R$ from sourcing sector $m \in M$ to biorefinery with transport mode $t \in T$
$F_{r,s,t}^{out}$	$\in \mathbb{Q}_0^+$	Transported amount of feedstock $f \in F$ from region $r \in R$ to biorefinery in region $s \in R$ with transport mode $t \in T$
$p_{r,s,t}^{1G}$	$\in \mathbb{Q}_0^+$	Transported amount of 2G bioethanol from biorefinery in region $r \in R$ to demand in region $s \in R$ with mode $t \in T$, substituting 1G bioethanol
$p_{r,s,t}^{FF}$	$\in \mathbb{Q}_0^+$	Transported amount of 2G bioethanol from biorefinery in region $r \in R$ to demand in region $s \in R$ with mode $t \in T$, substituting petrol (fossil fuel, FF)
Objective functions		
Economic objective: $\max O^{econ}$		Environmental objectives: $\max O_I^{env}, \forall I \in L$
= Revenues (substituted 1G EtOH)		= Benefits (substituted 1G EtOH)
+ Revenues (substituted fossil fuel)		+ Benefits (substituted fossil fuel)
+ Revenues (substituted by-products)		+ Benefits (substituted by-products)
– Refinery costs installation		+ Benefits (carbon storage)
– Refinery costs personnel & others		– Refinery impacts installation
– Refinery costs processes		– Refinery impacts processes
– Feedstock costs		– Feedstock impacts
– Collection costs fixed		– Collection impacts fixed
– Collection costs variable		– Collection impacts variable
– Distribution costs fixed		– Distribution impacts fixed
– Distribution costs variable		– Distribution impacts variable
Scenarios		
#	Verbal definition	Manipulated parameters
Tax scenario T1	Current tax situation per country	α_r^{FF}
Tax scenario T2	Half (50%) excise tax abatement in every country	α_r^{FF}
Tax scenario T3	Full (100%) excise tax abatement in every country	α_r^{FF}
Tax scenario T4	Carbon tax of €50 per metric ton of CO ₂ eq.	$\alpha_r^{FF}, \varepsilon_t^{var}, \eta_t^{var}$
Tax scenario T5	Carbon tax of €375 per metric ton of CO ₂ eq.	$\alpha_r^{FF}, \varepsilon_t^{var}, \eta_t^{var}$

^a The step-width of capacity levels C strongly affects the model's run time. To adequately address the run time and solution accuracy tradeoff, the step-width is 25,000 t for small capacities (25,000–300,000 t), 50,000 t for medium capacities (300,000–1,000,000 t), 100,000 t for high capacities (1,000,000–1,500,000 t), and 250,000 t to account for outliers of maximum optimal capacity (1,500,000–3,000,000 t). The smallest capacity level matches the capacity of an existing pilot plant (Clariant, 2018), and the maximum capacity of 3 Mt corresponds to twice the optimal biorefinery capacity found by other studies (Lauven et al., 2018).

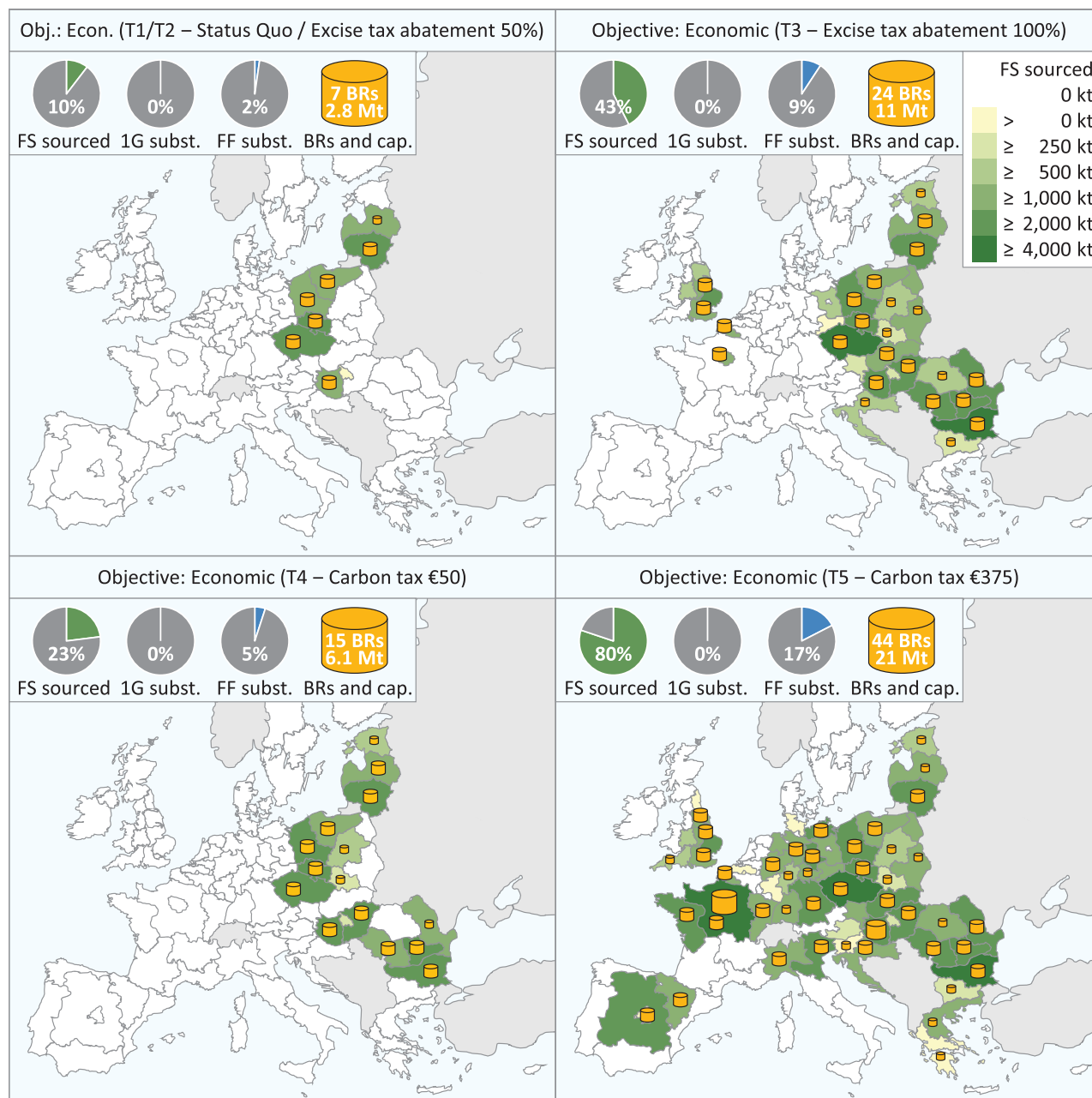


FIGURE 4 Optimal biorefinery locations and capacities (the size of cylinders corresponds to the capacity) and regional amounts of feedstock sourced (green shades) for economic objectives in five tax scenarios (with identical networks for T1 and T2) (in metric kilotons). The legend also includes respective percentages of total feedstock collected (*FS sourced*), 1G demand substituted, and fossil petrol demand substituted (*subst. 1G* and *subst. FF*, pie charts), as well as total number and total capacity of biorefineries (*BRs and cap.*). Underlying data used to create this figure can be found in Supporting Information S2

insufficient with 50% tax abatement. An excise tax abatement of 100% (T3) has significant effects on production volumes (quadrupled to 12.9 Mt, approximately 300 PJ) and collection quotas (42.5% of all feedstock). Increasing production volumes are realized by larger production quantities in Central and Eastern EU countries, and by biorefineries in feedstock rich regions of England and France. The objective value of €1.10 billion is about nine times higher than for T1 and leads to positive environmental benefits in all three damage categories and some impact categories.

A carbon tax of €50 (T4) doubles the produced volumes compared to the status quo (T1). With 23% feedstock collection, the network is rather small, and the production takes place in Central and Eastern EU countries. Although the network is smaller compared to T3, the economic objective value is slightly higher with €1.27 billion. A carbon tax of €375 (T5) leads to a feedstock collection of 80% and a substitution of about 17.4% of the current petrol demand. The production volumes increase eight-fold between scenarios T1 and T5 and the biorefinery network is dispersed across

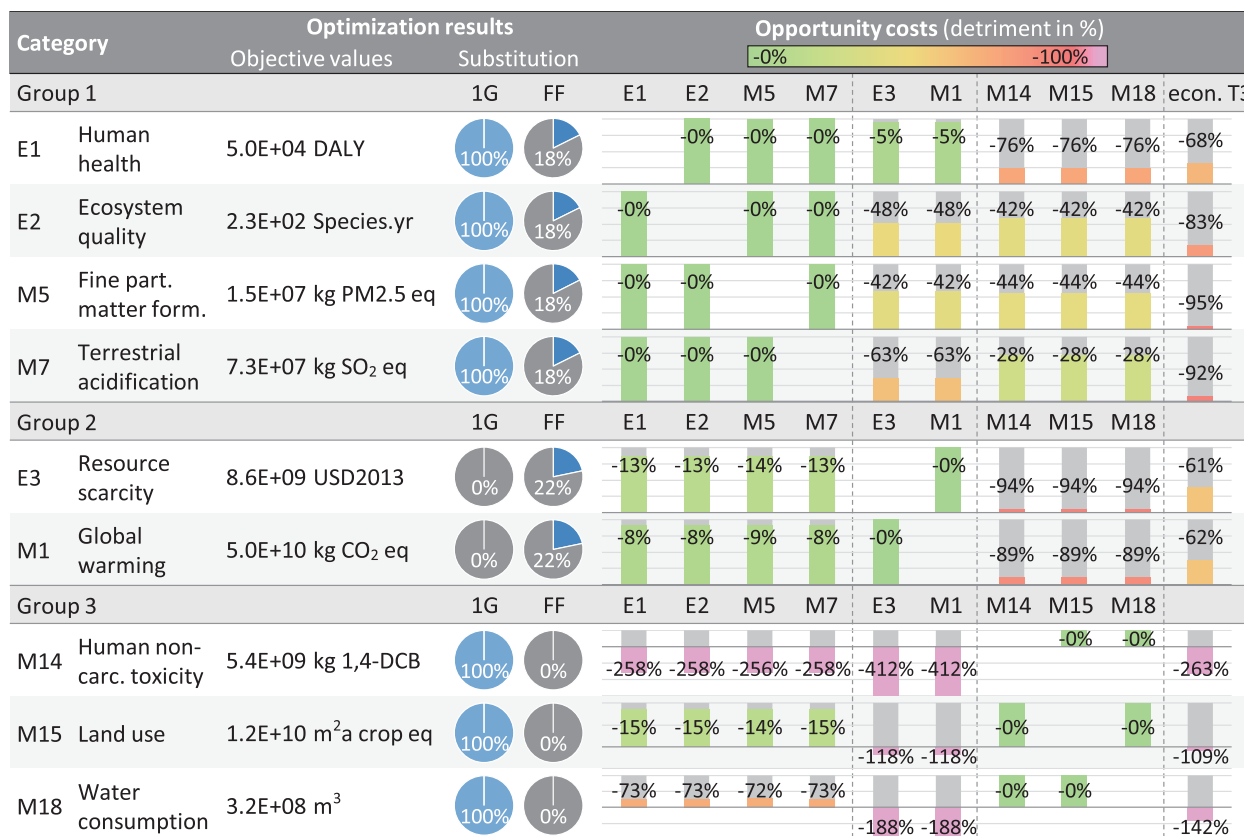


FIGURE 5 Endpoints and relevant midpoints with their objective values and units, clustered in groups of mutual congruencies (i.e., with similar substitution decisions, in percent of the total demand for 1G/FF). The figure also includes opportunity costs in each category for the optimization of the other environmental categories. For example, the objective value of human health (E1) is diminished by 76% when land use (M15) is optimized. Categories of one group have little or no opportunity costs to each other (further information are found in Supporting Information S1). The last column shows the environmental opportunity cost for economic optimization in tax scenario 3. Fossil resource scarcity (M17) is not listed separately, as it constitutes the endpoint resource scarcity (E3) by almost 100%. Underlying data used to create this figure can be found in Supporting Information S2

the EU. Unlike in T1, economic optimization in T5 leads to coincident environmental benefits of up to 79% of the maximum achievable environmental values. In all economic scenarios, petrol is substituted exclusively as the tax abatements also apply to first-generation biofuels.

The economic dimension is sensitive for parameter variations, as the difference between revenues and cumulative magnitude of all cost elements is small (\triangle return on sales of 4.7% in T1). Feedstock costs, biorefinery depreciation, and feedstock transportation are the most relevant elements of the economic objective functions. The sensitivity analysis is thoroughly described in Supporting Information S1.

3.2 | Environmental network planning

Depending on the objective, different impact categories contribute to the respective damage categories differently. These contributions are influenced by the ReCiPe 2016 midpoint-to-endpoint aggregation, but also by the decision taken and parameters used in this specific case. This work focuses on those impact categories that, throughout all optimization runs, contribute the most to their respective damage categories. These are most notably *global warming* (M1), *particulate matter formation* (M5), *land use* (M15), and *fossil resource scarcity* (M17), and to a lesser degree *terrestrial acidification* (M7), *human non-carcinogenic toxicity* (M14), and *water consumption* (M18) (see Section 5.1 in Supporting Information S1).

Figure 5 presents all endpoints and relevant midpoints with their respective optimal objective value. It further displays the substitution decision and the environmental “opportunity cost,” which refers to the percentual deterioration of the optimal objective value when optimizing another objective. Equation (2) displays the calculation of the opportunity cost between two categories l and k ($l, k \in L$), with O_l^{env} being the optimal objective value of l , and $V_{l,k}^{env}$ being the value for l when optimizing k (Supporting Information S1).

$$\text{opportunity costs}_{l,k} = \left(V_{l,k}^{env} - O_l^{env} \right) / O_l^{env} \quad l, k \in L \quad (2)$$

Moreover, it clusters the endpoints and midpoints in groups of mutual congruencies, within which an optimization of another objective function entails no or only small opportunity costs. This does not necessitate that all decisions are entirely equal for all categories within the same group, or that all midpoints of the same group behave identically toward a third category. Figures S1–S4 in Supporting Information S1 is analogous to Figure 5 and shows the detriments in environmental optimal values when optimizing the economic objective function.

Group 1 is characterized by a simultaneous substitution of 1G ethanol and petrol, due to net environmental advantageousness of 2G bioethanol over both reference products. The opportunity costs of Group 1 categories range from –5% to –63% when optimizing Group 2 categories, and from –28% to –76% when optimizing Group 3, which, despite the relative detriments, implies positive absolute benefits for Group 1 regardless of selected objective. For instance, the optimal objective value of *human health* (E1) achieves benefits of $5.0\text{E}+4$ DALY. With only –5%, the opportunity costs of *human health* are small compared to Group 2 categories, which can be explained by a high midpoint-to-endpoint characterization factor of GWP to *human health*. The opportunity costs of *human health* for Group 3 categories are with –76% substantially higher, which is due to much smaller networks with no substitution of petrol in optimal Group 3 solutions. Optimization toward *ecosystem quality* (E2) yields a maximum benefit of $2.3\text{E}+2$ species-years. Compared to E1, the opportunity costs for Group 3 objective functions are lower, as especially land use contributes significantly to the damage category ecosystem quality. For Group 2 categories, the detriment is higher for E2, due to a lower midpoint-to-endpoint factor of GWP to ecosystem quality.

Group 2 is characterized by an exclusive substitution of petrol. The correlation to Group 1 categories is high, which is why optimization of Group 1 categories implies low opportunity costs (–8% to –14%) for Group 2 categories. The enormous opportunity cost when optimizing Group 3 categories indicate that objective functions of Group 3 are mostly conflicting with Groups 1 and 2, resulting in different network decisions.

Group 3 optimization favors small production networks with exclusive substitution of first-generation bioethanol, as substitution of petrol by second-generation bioethanol is not desirable due to associated negative environmental benefits. The opportunity cost when optimizing Group 2 categories are particularly high with –118% to –412%. Since the optimal value is deteriorated by more than 100%, optimization of Group 2 objectives leads to an absolute deterioration of these categories. The opportunity costs vis-à-vis Groups 1 optimization are somewhat ambiguous with a range of –15% to –258%. The consistently high opportunity costs of human non-carcinogenic toxicity can be explained by the additional fertilization. Land use has only low opportunity costs vis-à-vis Group 1 categories, which can be attributed to the substitution of 1G ethanol in Group 1. The finding that petrol can outperform second-generation ethanol in certain environmental categories is mostly consistent with existing LCA studies. Particularly, freshwater eutrophication, marine eutrophication, terrestrial acidification, fine particulate matter, land use, and water consumption may be worse compared to petrol (Borrión et al., 2012; Cherubini & Ulgiati, 2010). For freshwater and marine eutrophication, and land and water use, those findings are supported by the results of study at hand. The underlying technology is assumed to be based on acid-free pretreatment (most existing studies base their assessment on hydrolysis reactions, which are catalyzed by dilute sulfuric acid). This technological progress leads to environmental improvements in terrestrial acidification and fine particulate matter formation and thereby to benefits compared to petrol.

The last column of Figure 5 shows the environmental opportunity costs for economic optimization in scenario T3. Since significantly less petrol and 1G ethanol is substituted in the economically optimal solutions (11 Mt in T3 compared to 27 Mt in Group 1 and 2 categories), the environmental benefits from 2G ethanol cannot be fully exploited, which is the principal cause for the detriment in Groups 1 and 2. For Group 3 categories, economically optimal results even lead to a net deterioration due to contrary substitution decisions.

Figure 6 presents optimal production networks of one representative objective per group, and the economic T3 result. Environmental objectives result in disaggregated and spatially spread production networks in all categories, as transportation (feedstock collection and ethanol distribution) is the dominating impact. Optimizations of Groups 1 and 2 lead to the collection of 100% of the available feedstock. While Group 1 objectives substitute 1G EtOH completely, and then the maximum remaining possible volume of petrol, Group 2 solely replaces petrol. Optimization of Group 2 objectives leads to a substitution of 22% of the currently existing petrol demand, implying inter alia avoided GHG emissions of $50.4\text{ Mt CO}_2\text{ eq.}$ annually. Production networks of Group 3 objectives consist of many dispersed biorefineries with small capacities, which is due to the fact that only 1G EtOH is substituted. 19% of the available feedstock is used to substitute 100% of the 1G EtOH demand, which has, in terms of land use, positive benefits of 12 billion m^2 annual crop land eq. However, optimization of Group 3 objectives entails high opportunity costs for all damage and most impact categories (up to 94%, see Figure 5), which means conflicting goals.

The environmental results are much more robust to alteration of parameter values than the economic ones, as the total benefits are much higher compared to the cumulative magnitude of all impact elements. The most sensitive parameters are the environmental impacts of the reference products first-generation ethanol and petrol (Supporting Information S1).

3.3 | Pareto optimization

To ease finding tradeoffs in between the three environmental congruency groups, and with the economic objective, Pareto-optimal frontiers are calculated with the equidistant ε -constraint method. Between the optimal objective value of the first objective (optimum) and its value when optimizing the second objective (nadir point), 19 equidistant points (steps of 5%) are defined. These are then successively used as lower bounds

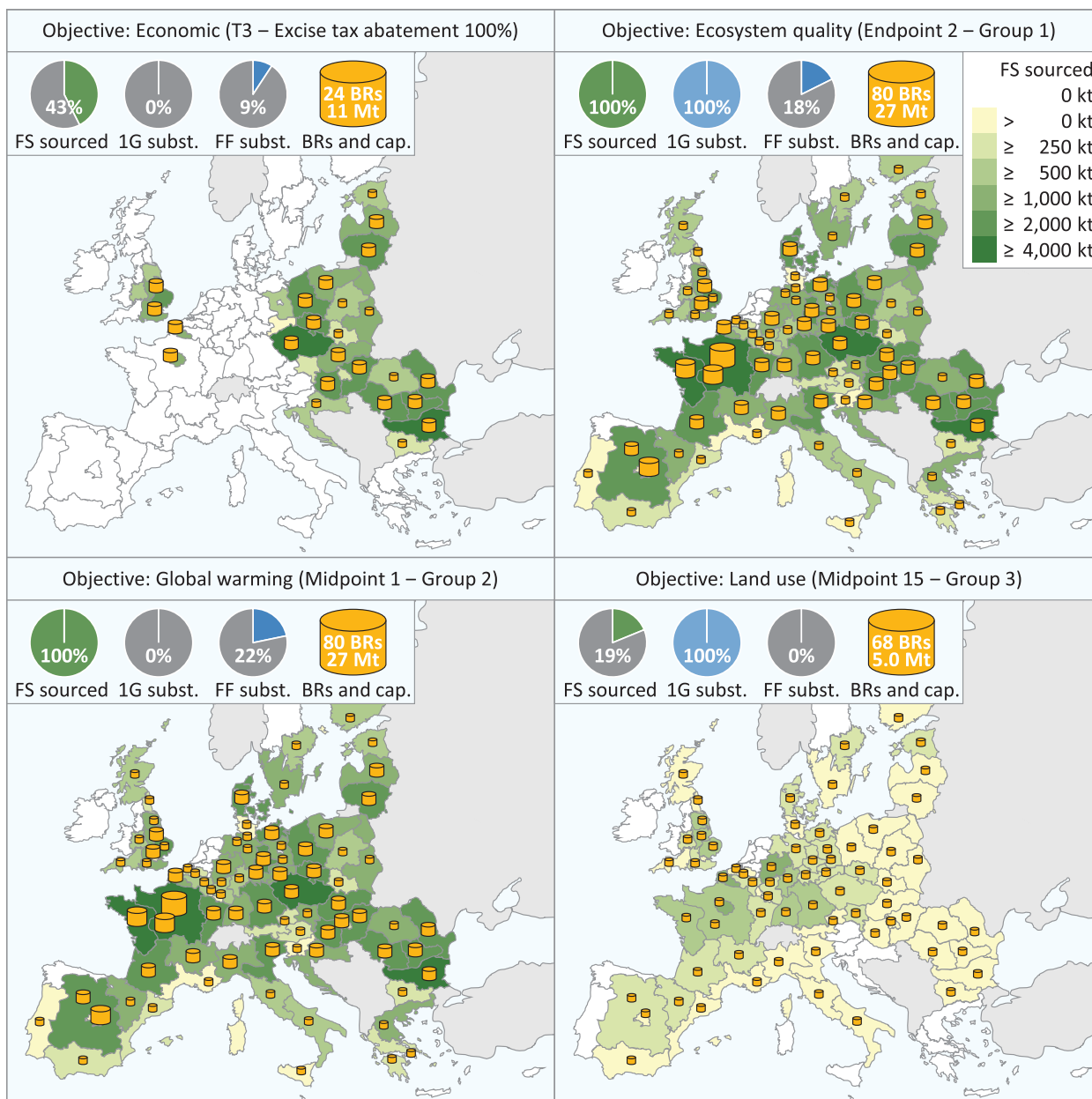


FIGURE 6 Optimal biorefinery locations and capacities (the size of cylinders corresponds to the capacity) and regional amounts of feedstock sourced (green shades) for economic objective (tax scenario 3) and three environmental objectives (in metric kilotons). The legend also includes respective percentages of total feedstock collected (*FS sourced*), 1G demand substituted, and fossil petrol demand substituted (*subst. 1G* and *subst. FF*, pie charts), as well as total number and total capacity of biorefineries (*BRs and cap.*). Underlying data used to create this figure can be found in Supporting Information S2

of the second objective function. This is done for optimization of both objectives, resulting in 40 Pareto-efficient points, where the solution of one objective cannot be improved without deterioration of the other's. From this set, a decision-maker can choose a preferential solution (Kenneth & Zammit-Mangion, 2013). For tax scenarios T1, T2, and T4, a reasonable tradeoff between the economic and an environmental criterion is intricate, as every environmental objective leads to a negative economic value. For T5, the network is almost always beneficial for economic and environmental objectives alike. Since scenario T3 (100% tax abatement) arguably provides the most interesting economic-environmental tradeoffs, only T3 is shown in Figure 7.

Figure 7 includes six Pareto-optimal frontiers, one for each combination of Groups, and the economic dimension. The first and the last Pareto points correspond to the respective optimum when only one objective is optimized. Figure 7a shows that with increasing preference on ecosystem quality, profitability declines moderately and eventually leaves the profitable zone. With increasing preference for ecosystem quality (E2), 1G EtOH is increasingly substituted at the expense of petrol substitution. The frontier for economic (T3) vs. global warming optimization (Figure 7b) behaves similarly; however, the network remains profitable even for high GWP benefits due to low marginal costs (~€10 per metric ton CO₂ eq.), and petrol

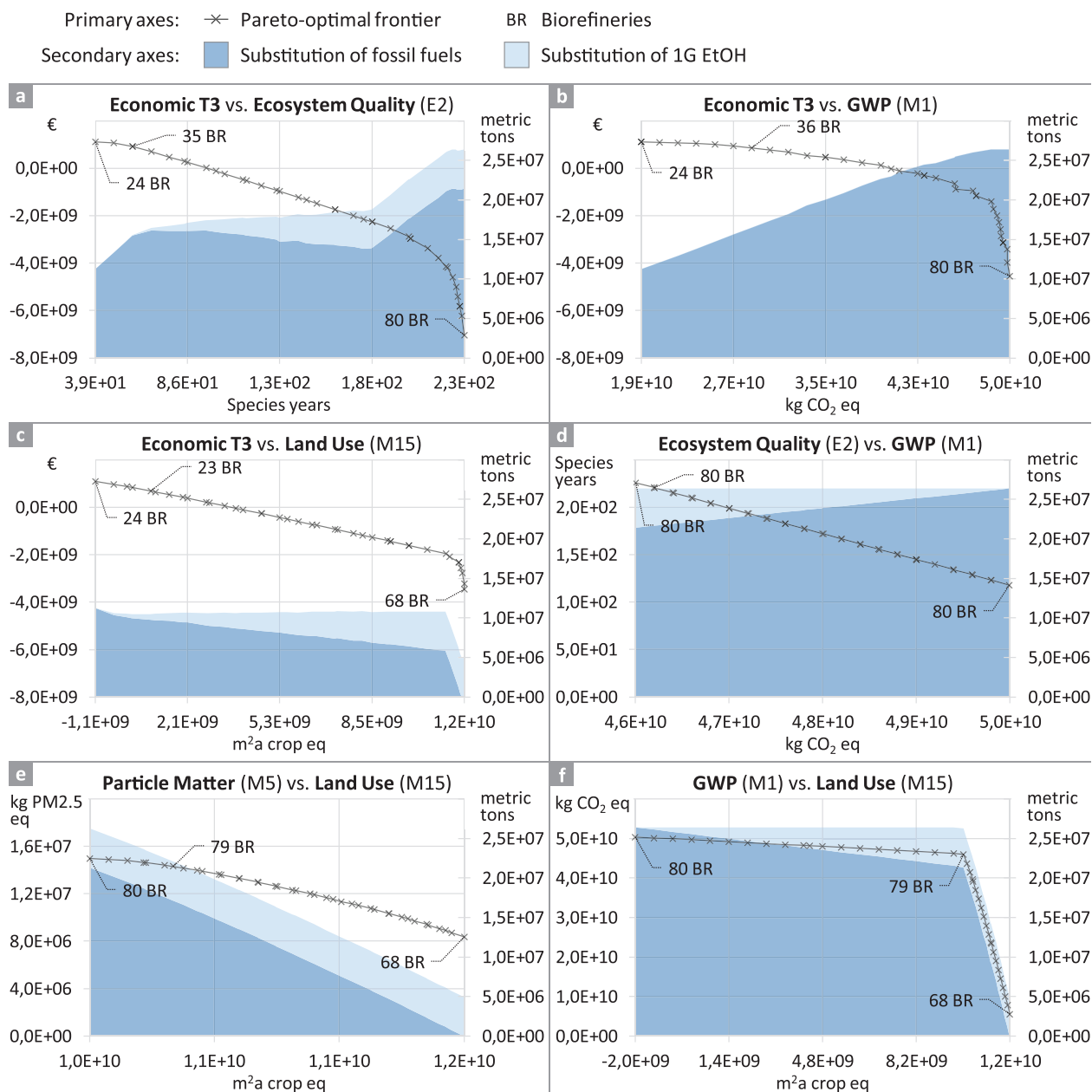


FIGURE 7 Selected Pareto curves between economic and environmental objectives. (a)–(c) shows economic (in T3) versus environmental (one representative per group) Pareto-efficient frontiers. (d)–(f) shows frontiers between these three environmental objectives. The figure additionally includes the substituted volumes of first-generation bioethanol and petrol as stacked area plots, as well as the number of biorefineries at the two respective optima, and at the point of the shortest relative Euclidean distance to both optimum values (Section 5.5 in Supporting Information S1). Underlying data used to create this figure can be found in Supporting Information S2

is replaced exclusively. The end of the curve is characterized by a strong decline, translating to high marginal costs for increased global warming benefits (~€1,500 per metric ton CO₂ eq.), which is attributable to the much larger number of biorefineries.

Figure 7c shows that with increasing preference for land use, 1G bioethanol is substituted instead of petrol. The total amount of produced second-generation bioethanol is constant for most Pareto points, with a sudden drop of production volumes close to the optimal solution for land use, where produced volumes decrease while the number of biorefineries doubles. In Figure 7a–c, it becomes clear that for economically optimal networks, the average biorefinery capacity is larger than for environmentally optimal solutions, translating to more centralized supply chains.

Figure 7d reveals an almost linear frontier between Group 1 and Group 2 (depicted for E2 and M1) as the total feedstock is used to substitute either petrol only (Group 2), or both petrol and 1G ethanol (Group 1). The production volumes, and subsequently the environmental benefits, are only limited by the limited feedstock base. Pareto curves between Group 1 and Group 3 (Figure 7e) show that, with increasing preference on Group

3, the demand for 1G EtOH is the limiting factor, rather than the feedstock supply. As noted above, only 1G EtOH substitution is beneficial for Group 3 categories.

The Pareto frontier between GWP and land use (Figure 7f) is next to linear at both ends with high marginal costs for the less preferred objective. The Pareto frontier has a strong gradient change at the point at which additional land use benefits can only be achieved by reducing 2G ethanol production. Interestingly, the Pareto-optimal solution at this point is almost identical with the optimal solution for the endpoints human health and ecosystem quality. This shows that the endpoint-inherent normalization and weighting between different impact categories is a meaningful aggregator in environmental decision-making processes.

4 | DISCUSSION AND CONCLUSION

The results of this work indicate positive environmental benefits of substituting petrol and 1G bioethanol by 2G bioethanol in most impact and damage categories. Nonetheless, the different environmental categories are not unanimously congruent. We found conflicts between some environmental goals, leading to opposing optimal production networks and substitution decisions. Hence, the general assumption that GHG emissions fully reflect the environmental dimension falls short. Second-generation bioethanol indeed has the potential to avoid GHG emissions, and the maximum achievable benefit of about 50 Mt CO₂ eq. corresponds to the total emissions of a country like Denmark and to 1.15% of the EU's total emissions in 2018 (Eurostat, 2020). However, impact categories like terrestrial acidification, particulate matter formation, human non-carcinogenic toxicity, land use, and water consumption show high opportunity costs for optimization of global warming. This implies that, from a societal perspective, global warming is not sufficient as exclusive objective, as it is not entirely congruent with the areas of protection (health, ecosystems, and resources). While global warming optimization advises the exclusive substitution of petrol, optimization of the two endpoints human health and ecosystem quality indicates the advantageousness of a concurrent substitution of first-generation bioethanol and petrol. The feedstock production for 1G bioethanol in the EU (mainly maize, wheat, and sugar beet) requires substantial agricultural land, which compromises biodiversity. A complete substitution of 1G ethanol would yield about 1.2 million hectares land, which could be used for additional food production (about +5% wheat EU-wide) or as compensation areas to mitigate biodiversity loss. Additionally, substitution of first-generation by second-generation ethanol would significantly reduce particulate matter emissions due to reduced ammonium application and use of agricultural machinery and thereby contribute to human health protection.

While a large-scale production of second-generation bioethanol is advantageous from an environmental point of view, it is hardly conceivable from an economic perspective. With today's oil prices and taxation, the production of second-generation bioethanol is barely competitive vis-à-vis fossil petrol. At best, 0.76 €/l of second-generation bioethanol (production and distribution costs without excise taxes and other duties) is achieved, and for environmentally optimal networks, the price can be as high as 0.93 €/l (Section 5.3 in Supporting Information S1). Currently, the combination of a production in countries with low wages, feedstock, and transportation costs, as well as consumption in countries with excise tax abatement (e.g., Sweden, Croatia, or Austria) is only just or close to being profitable (also reflected in the high sensitivity of the economic model, cf. Section 5.4 in Supporting Information S1). Should EU countries decide to implement advanced biofuels as part of climate change measures, political guidance would be needed. Our results show that already a carbon tax of €50 could double the volume of profitably produced 2G ethanol to 6.1 Mt, which corresponds roughly to today's total 1G ethanol consumption in the EU in 2018. An excise tax abatement of 100% for advanced biofuels could further increase economically profitable production to 11 Mt.

The Pareto optimization shows that additional environmental benefits can be realized with only small economic opportunity cost for many categories. Figure 7b exemplifies that 80% of the maximum GWP benefits can be achieved in tax scenario 3 with a positive profit. Beyond a certain point on the Pareto frontier, the costs of additional environmental benefits increase disproportionately. This implies that an exclusive focus on environmental categories would render any network unprofitable. For a larger degree in congruency between economic and environmental objectives, the five tax scenarios show that significant changes in economic preconditions are required. Pareto optimization between two environmental objectives (Figure 7d–f) demonstrates the meaningfulness of endpoints in environmental decision-making processes in this application case. For example, the strongest gradient change on the Pareto-frontier between the two impacts GWP and land use seems to be a reasonable tradeoff between the two (Figure 7f). A sacrifice of 9% of the optimal GWP value permits to achieve 85% of the optimal land use value, and >99% of the optimal values for human health and ecosystem quality, which proves the endpoint-inherent normalization and weighting of different impact categories. Stefansdottir et al. (2018) propose different methods to reduce objectives in a multi-objective optimization problem, inter alia the δ -error method or using an LCIA-inherent weighting scheme. In the article at hand, the anticipated results of a δ -error method are somewhat preempted by the grouping of objectives into the three congruency groups with similar substitution decisions and low opportunity costs. Furthermore, Pareto optimization shows that the three ReCiPe endpoints are suitable aggregators of the 18 midpoints in this application case. Goal Programming is another possible approach to find a compromise solution between a number of objectives by minimizing the total Euclidean distance between the objectives and their single-optimization optima. Considering that a single environmental impact category hardly covers the whole environmental dimension, we suggest future works on multi-criteria decision-making to base decisions on damage categories rather than impact categories. However, a transparent presentation of all impacts and knowledge about the categories' contributions remains indispensable to reveal possible negative consequences.

Bioethanol could play an important role in the transportation sector in the medium term (~2030); however, BEVs and hydrogen-based propulsion are likely to gain major shares in this sector. For heavy-duty vehicles, international navigation, and aviation, alternative environmentally friendly solutions are rare, and hydrocarbon-based fuels may remain the only viable option in the next decades. Our results show that sustainably available agricultural residues are sufficient to substitute up to 17.2 Mt petrol, which equals 22% of the EU's demand in 2018 (or the entire first-generation ethanol and 18% petrol demand). In T3, 13.3 Mt petrol could profitably be substituted. This work focuses on the most abundant residues, and an expansion of the feedstock base has the potential to further increase producible volumes. The project S2BIOM estimated about 20% higher agricultural residue potentials than this study; additionally, forestry residues could further serve as feedstock for bioethanol production (Dees et al., 2017). However, agricultural residues are increasingly sought-after by bio-based applications, and policy makers should carefully consider how to guide the utilization of this limited resource.

This approach of integrating different methods allows the simultaneous consideration of different research goals. By considering a broad set of environmental categories and a regionalization of the different value chain aspects, this work extends existing models for environmental decision-making in multi-objective network models. Furthermore, the model considers the nonlinear relationship between feedstock collection costs (agricultural residues are distributed in area) and refinery size (economies-of-scale) by step-wise linearization, which is a common approach in Operations Research literature (Lin, Carlsson, Ge, Shi, & Tsai, 2013), but has been neglected by most previous studies in the field of biorefinery configuration (Budzinski et al., 2019; Lauven et al., 2018).

The endpoint human health and the midpoint land use implicitly cover social aspects in the context of advanced biofuels (food-to-energy conflicts, Čuček, Klemeš, & Kravanja, 2012). In particular, with regard to regional development, the additional explicit consideration of a social dimension is a desirable next step toward a holistic sustainability assessment in strategic network design. In addition, different research efforts indicate that the underlying biorefinery technology could improve in efficiency in the future. A high added value valorization of residual lignin in bio-based products could further improve the environmental performance (Ghaffar & Fan, 2014), and environmental benefits could be augmented by a carbon capture and storage/use system for the fermentation emissions. Such technological development would significantly impact the carbon balance of second-generation bioethanol, and even a negative carbon balance of large-scale production, environmentally and technically, within the realms of possibility. Future works should also consider a wider range of consequential aspects of the implementation of second-generation bioethanol, such as abated land use, or in which way a large-scale second-generation EtOH production would alter the overall market situation.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of the article.

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